QSAR-QMMM Cryptographic Mining on Chern-Simons Topologies for the generation of a Ligand Targeting SARS-COV-2 D614G Binding Sites.

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Research article

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Abstract

SARS coronavirus 2 (SARS-CoV-2) in the viral spike (S) encoding a SARS-COV-2 SPIKE D614G mutation protein predominate over time in locales revealing the dynamic aspects of its key viral processes where it is found, implying that this change enhances viral transmission. In this paper, we strongly combine topology geometric methods targeting at the atomistic level the protein apparatus of the SARS-COV-2 virus that are simple in machine learning anti-viral characteristics, to propose computer-aided rational drug design strategies efficient in computing docking usage, and powerful enough to achieve very high accuracy levels for this in-silico effort for the generation of the AI-Quantum designed molecule of Gisitorviffirna™, Roccustyrna_gs1™, and Roccustyrna_fr1™ ligands with Preferred IUPAC Names of (7aR) -5-amino-N-[(S) - {2-[(S) -(E) -(amino methylidene) amino](cyano) methyl]hydrazin-1-yl} (aziridin-1-yl) phosphoryl)- 1-[(2E) -2- [(fluoromethanimidoyl) imino]acetyl]-7-oxo-1H,7H,7aH-pyrazolo[4,3-d]pyrimidine-3-carboxamide;N-{[(2-amino-6-oxo-6,9-dihydro-1H-purin-9-yl) amino]({1-[5-({[cyano({1-[(diamino methylidene) amino] ethenyl)) amino]oxy} methyl)-3,4-dihydroxyoxolan-2-yl]-1H-1,2,4-triazol-3-yl}formamido) phosphoryl} -6-fluoro-3,4-dihydropyrazine -2-carboxamide; [3-(2-amino-5-sulfanylidene-1,2,4-triazolidin-3-yl) oxaziridin-2-yl]({3-sulfanylidene-1,2,4,6-tetraazabicyclo [3.1.0]hexan-6-yl)) phosphoroso1-(3,4,5-trifluorooxolan-2-yl) -1H-1,2,4-triazole-3-carboxylate targeting the COVID-19-SARS-COV-2 SPIKE D614G mutation using Chern-Simons Topology Euclidean Geometric in a Lindenbaum-Tarski generated QSAR automating modeling and Artificial Intelligence-Driven Predictive Neural Networks.

1

PDB:6WZU

3D Docking Interactions of the combination of Gisitorviffirna_{TM}, Roccustyrna_{gs1_TM}, and Roccustyrna_{fr1_TM} fragments 2D structure inside the PDB: 6WZU protein targets of the crystal structures of Papain-Like Protease of SARS CoV-2, P3221 space group

Scheme 1 3D Docking Interactions of the combination of (7aR) -5-amino-N-[(S) -{2-[(S) -[(E) - (aminomethylidene) amino](cyano) methyl]hydrazin-1-yl} (aziridin-1-yl) phosphoryl]-1-[(2E) -2-[(fluoromethanimidoyl) imino]acetyl]-7-oxo-1H,7H,7aH-pyrazolo[4,3-d]pyrimidine-3-carboxamide; N-[(2-amino-6-oxo-6,9-dihydro-1H-purin-9-yl) amino]({1-[5-({[cyano({1-[(diaminomethylidene)amino]ethenyl)} amino]oxy} methyl) -3,4- dihydroxyoxolan-2-yl]-1H-1,2,4-triazol-3-yl} formamido) phosphoryl] -6-fluoro-3,4-dihydropyrazine-2-carboxamide; [3-(2-amino-5-sulfanylidene-1,2,4-triazolidin-3-yl) oxaziridin-2-yl]({3-sulfanylidene-1,2,4,6-tetraazabicyclo [3.1.0]hexan-6-yl}) phosphoroso1-(3,4,5-trifluorooxolan-2-yl) -1H-1,2,4-triazole- 3-carboxylate fragments 2D structure inside the PDB: 6WZU protein targets of the crystal structures of Papain-Like Protease of SARS CoV-2, P3221 space group. SMILES of Gisitorviffirna_{TM}:[P@@](=O)(NC(=O)c1nc(F)cnc1)(NC(=O)c1nn(c2oc(c(O)c2O)CON(C(=[N]=C(N)N)C)CN)cn1)Nn1c2nc([nH]c(=O)c2nc1)N, Roccustyrna_{gs1_TM}:C\1(=C2\ON2[P@@](=O)(N2N3N[C](=[N[C@H]23)=S)OC(=O)c2nn(c3oc(c(F)c3F)F)cn2)/N(N)N=[C](=S)N1 and, Roccustyrna_{fr1_TM}:[P@@](=O)(N1CC1)(NC(=O)c1nn(c2c1[nH]c(nc2=O)N)C(=O)/C=N/C(=N)F)N/N=C(N=C/N)\CN

Introduction

(1,2,3) The COVID-19 disease which emerged in China at the end of 2019 was declared in March 2020 a pandemic by the World Health Organization (WHO) and is accountable for many fatal cases. (2,4,5) On January 202, the WHO committee declared a global health emergency (3,4-6) based on the rate of the increasing spread of the infection (4,5-7) with a reproductive number (RN) in the range 2.0-6.5, 4 higher than SARS and MERS, (8) with more than 85,000 casualties and fatality rate of about 4%. (1-4) Collaborative efforts for Genomic characterization by using a simple DNA cryptography genetic code according to the main dogma of biology has been published that takes plaintext for communicating information through a process of DNA→RNA→Amino Acid coding. Researchers in 2010 published a Cryptographic DNA-mobile based Code for Secure Networks Scheme in which binary plaintext is translated to text via a substitution wrapping code, introns are inserted into DNA hierarchal text structure on the general processes of gene expression by the transcription complex and a binary key is passed to the receiver over a secure channel to provide the details of the intron insertion. We cannot imagine a world without

cryptography anymore. Whether it is to protect our banking information, e-mail, or phone calls, cryptography is a vital part of our digital infrastructure. Modern-day cryptography is usually split up into two phases. In the key exchange phase, an algorithm such as Elliptic Curve Diffie-Hellman key exchange (ECDH) or RSA is used to establish a shared secret key that can be used in an asymmetric encryption algorithm in the second phase. These algorithms have been and continue to be well-studied and have proven themselves to be secure if instantiated with proper parameters and implemented securely. Nowadays most people favor using cryptographic keys over sticks and more intricate cryptographic algorithms than wrapping at an angle. This opens the door to new types of cryptographic attacks. Attack avenues can roughly be divided into two categories: attacks on the theoretic algorithm by trying to recover the key or message by using public information provided on the algorithm, and attacks on the implementation of the algorithm, which look at the soft- or hardware-specific properties. (5,6,7-9) Evolution, phylogeny, high contagion rates, molecular epidemiology, of SARS coronavirus, and epidemiology from scientists worldwide are underway to understand the rapid spread of the novel coronavirus (CoVs), and to develop effective coding interactions of personalized interventions for control and prevention of various devastating diseases. (1-10) Coronaviruses are positive-single stranded, and through transcription and ultimately translations enveloped large RNA viruses that infect humans and a wide range of animals. ((4,6,7,8,9,10) In Latin, Corona means —crow based on their shapes. As a comprehensive compendium and megadiverse country, Brazil accounts for 10–20% of known living species of available biogeochemical information in the world. However, a major part of the biological and chemical biodiversity in Brazil's natural products remains unexplored (17). (2– 13,14,15,16,17) Molecular structures as a protein code (ciphe-rprotein) were determined in heterodox interpretations (22) by solving the time-independent (21-22) Schrödinger equation: QM methods, vertex prizes, and edge costs including ab initio

Density Field Theories (DFT) (23) has become quite a standard approach as a computational Scheme and semi-empirical in place (24) of the quantum processor and energy under simulated sampling error among other observables. Density Field Theories (DFT) is continuously increasing (25) as well as to reposition drugs and physical extracts about bonding may represent the similarities (26) and dissimilarities (27) between drugs and repurposed viral proteins, respectively. (28) However, the Schrödinger equation s in Markovian and (27) non-Markovian scenarios cannot be solved for any but a one- data-driven (29) electron system method (the hydrogen atom), to construct a family of particular solutions of (28) equation (30) and approximations need to be made. According to QM, (2-19,23) and during the construction of stochastic Schrödinger (29) equations, an electron bound that converges quickly and reliably by acknowledging the conditional Bohmian wavefunction to an atom cannot possess any (2-17,21,22,23, 24,25,26,27,28) arbitrary energy to produce the desired distribution or occupy any position in space using statistical and machine (23,24-37,38) learning concepts. The Lindenbaum-Tarski algebra logical spaces and Bohmian wavefunction-based vectorial re-presentations on eigenvalue statements were used in this project when analyzing pharmacological data and have been previously introduced as a 3D logical subspace allowing a well-defined position for each fragmented pharmacophore. This shows that the application to quantum computing as orthogonal applied for the design of small molecules through the example of three coupled harmonic oscillators in Markovian and (30) non-Markovian Scheme s may allow pure mechanical computations both for re-generating Lipinski rules and inferences to bridge the gap between practical in vitro testing implementations and theoretical docking scalability predictions. (25,27,28) Since it has been shown that Path selection into a nonlinear Riemann-Hilbert simple problem of any metal formula ϕ for quantum repeater networks towards the determination of the exact interpolating function of $h(\lambda)$ can be geometrically represented by Chern-Simons logical spaces and subspaces I decided to cryptographically implement supersymmetric solutions and Borel Singularities for $N=2$ allowing a quantum repeater based vectorial Supersymmetric representation in this drug design project. (20,26,27,28,29,30,31) In general, the notions of Lindenbaum matrix and Lindenbaum-Tarski algebra and its relative development to the product topology continuing to shape the field of algebraic logic introducing topology on a set to define the (31) cartesian product of topological spaces as a subbase which has paved the way until this day, to further algebraization of topology products, which had been begun by George Boole in the 19th century, as well as to an innovative language of logic, in a symmetric model theory containing no other constants but only one connective $\rightarrow$. Philosophical interpretations of QM as a core part of contemporary physics were conditioned by ideals of what an explanatory theory should be (Minkowski-type, wave-edge, etc), (20,27,32-33) as well as probabilistic transformations on algebraic multi-metrics (Triangle area, Bond-angle, etc) and associated axiomatic formulations (AQFT) treat observables rather than of the von Neumann formulation and the Dirac formulation states as foundational according to the interaction information theory (QIT). (20,33,34,35) In this project, we show an original strategy and demonstrate the utility and the mechanics of this (32) formalism as an application within the quantum computing context of perturbed asymptotically through the example of two coupled anti-de Sitter black harmonic black-hole oscillators and brane spacetimes. We expect this Lindenbaum-Tarski driven Chern-Simons representation to generate a valid QSAR modeling, and a lead compound design formalism, in our molecular modeling and simulations in order to produce orthogonal coordinates as applied for the design of a novel multi-chemo-structure against the crystal structure of COVID-19 protein targets. (29,35,36) A meta server and a Kappa-Symmetry C algebra of local observables were incorporated for the docking of FDA-approved small molecules, peptide-mimetic, and humanized antibodies against potential targets of COVID-19 via a generalized procedure of Quantization of classical fields which were fused together with QSAR automating modeling to lead the commutation and anticommutation relations. (37,39,41,42) Dynamic niching and flexible heuristic genetic algorithmic states for automatic molecule re-coring and fragmentation were applied to fragment and re-core a database of 20,000+ molecules for use with the group contribution model Universal Quasihelical Functional Group Activity Coefficients (UNIFAC) against the structure and functions of SARS-CoV-2 as linear functional on the algebra of free energy docking observables. (37,38,40) Hybrid quantum repeater via a robust creation of entanglement between remote memory qubits was implemented for predicting drug targets and for multi-target and multi-site-based virtual screening against COVID-19. The basic idea developed in Levine (2004) incorporates critical components of what is to be expected from a —reall signature. (41,42) Flexible Topology Euclidean Geometric was used to fragment molecules automatically in this molecular modeling and drug designing project on

several parameters while keeping the definition of the groups as simple as possible. Artificial Intelligence-Driven Predictive Neural Networks and Quantum- Inspired frameworks of parallel-Docking interactions were employed for supercritical entanglements introducing an advanced quantum mechanical inverse docking algorithm providing further insight to confirm the practicality of docking energy predictions for wild type and selected mutations for Nsp3 (papain-like, PLpro domain), Nsp5 Nsp15 (NendoU), (Mpro, 3CLpro), Nsp12 (RdRp), N protein and Spike in understanding the key element functions of SARS-CoV-2 protein pathways and in designing possible novel antiviral agents, from both a quantum algebraic and a cheminformatic perspective. In this protocol, there are tools from conventional cryptography that are used along with the principles of the regulation of computer-aided drug discovery This paper concentrates on the quantum mechanics-driven drug discovery of the protocol.

Material and Methods

Preparation of the protein structures

The National Center (NCBI) database for Biotechnology Information was used to retrieve the S glycoprotein proteins of SARS-CoV-2. For the N protein, we aligned the clustered 31 conformations (1,2,35) from the 1731 full-length SARS-CoV-2 sequences and stored as a FASTA format file for analysis with Glu174 and Glu166 present in the opened RBD down conformation out of a total of 40 states COVID19 in the NMR-derived COVID19 associated protein structure (PDB codes, 6xs6,1xak,2g9t, 3fqj, 2ghv,6yb7) (1,3,4) to select a small subset representative of the protein flexibility downloaded from NCBI (30 April 202, txid2697049, NC_045512.2 with minimum length = 29,000 bp) as a coordinate reference and aligned using the MAFFT tool. (2-5,6) The BioEdit v7.2.3 sequence alignment editor was deployed to identify the conserved binding sites and short linear peptide region among the aligned sequences through multiple-sequence alignment (MSA) with ClustalW. The conserved alignment was visually generated, inspected, and curated by preserving all nucleotides using Genbank NC_045512.2 as a coordinate reference in genomes such as the ball python genome, and further proceeded with the RSFIEDLLFNKV, e.g. KNFIDLLLAGF short linear motifs as identified between the Wuhan isolate beyond the limit of serious detection of the reptile shingle back for spike protein nidovirus 1 model construction by utilizing again the NC_045512.2 and annotated (ORFs) Open Reading Frames plus additional ORFs. We then provided to the DockThor-VS online docking platforms the protein structures in PDB format files of the SARS-CoV-2 (PDB codes, 6xs6,1xak,2g9t,3fqj,2ghv,6yb7) (1,3-10) as potential therapeutic drug targets (5-11,12) for the design of our new druggable scaffold named Roccustyrna. (13,14,15) For this main purpose, we initially selected the Nsp3, Nsp5 non-structural proteins (PLpro domain), Nsp15 (endoribonuclease), Nsp12 (RdRp) (5-16,17), and the structural proteins Spike and nucleocapsid protein (N protein). (9,10-21)) We then clustered the opened conformation states (31 aligned out of 40 conserved states) (9,17,22) using the Conformer Cluster web server tool (6,14,16) according to the position of the residues (5,7,8) Arg102, Glu166, and Tyr109 using the weighted sum of the centroid distances as the single linkage method. (7,8-12,22) Finally, the nearest to the pair group centroid structure per cluster was selected as the representative conformation of each group to be available at BiogenetoligandorolTM. In this article, we effectively use an AI-decision tree and an optimum quantum walk number of small chemical active chemical features from a collection of hundreds of them utilizing neural networks and jointly docking free energy cumulative features and ranking method with input toxicity values taking both network decision tree parameters into account. In this work, we prepared the protein structures using the Protein Preparation Wizard from the BiogenetoligandorolTM (BiogenetoligandorolTM, SynthocureTM, Thessaloniki, Biogenea Pharmaceuticals Ltd-GR, 2020). (8,13,17,22) hydrogen-bond optimization and

Protonation assignment were applied by using the PROPKA and the ProtAssign publicly available software at the reported experimental pH (2-11,17) considering when available the presence of the bound small molecule (8-12,15,19).

Screening NuBEE Phyto-library and COVID2019 targets.

Virtual screening of the final proposed model and high throughput molecular docking based on existing literature were implemented to a collection of 9591 drugs including 2037 chemical structures of FDA-approved small molecule drugs and (2,3-14,17) over 6000 herbals and physical extracts from the NuBBEDB updated database to get an insight into the potential inhibitors and to uncover chemical and biological druggable information from Brazilian biodiversity (4-6,17). Drugs selected for the docking studies with an ideal number of non-hydrogen and metal atoms not related with macromolecules, organic and inorganic active fragments (e.g, Pt, Fe, Hg, etc.) below 5 or above 10, physical elements and drugs having Molecular Weight > 120, and already approved drugs that are consisted of original pharmacophoric elements of approved drugs into specific subcategories of the prototropic tautomer, separate enantiomer, and protomer fingerprint alternatives. (7,8,17,18) Parallel Virtual screening technique for molecular docking was deployed at the center of the X: 228.75, Y:190.82, and Z: 304.15. on its .pdbqt converted libraries of small molecules for the motif binding target sites using standard Web technologies such as CSS, HTML, and JavaScript (AJAX) including graphics, text-based, and spectral files. (9,13-17) When more than one form of the screened drugs and physical elements for the cross-validation (e.g, more than one protomer, more than one enantiomer, etc.) were screened, as suitable druggable candidates for re-coring and fragmenting the forms with the highest GP and Docking Energy values were considered in the ranking. (14,16,17) Finally, drugs and selected NuBBEDB physical extracts were docked according to the descending GP docking and binding energy values and only the screened hit candidates generating the highest binding energy values were considered for fragmenting and re-merging into the Rocustyrna small molecule using the BiogenetligandorolTM cluster of algorithms from the below.

Scheme 2. 3D Docking interactions of the selected NuBEE physical elements inside the PDB:6XS6, SARS-CoV-2 Spike SARS-COV-2 SPIKE D614G variant, minus RBD.

The whole set of molecules able to interact with the SARS-CoV PLpro enzyme were extracted after extensive machine learning similarity studies, retrieving only those small-molecule ligands with absolute IC₅₀ values. (2-17,34) This druggable .sdf set consisted of 11 PLpro approved inhibitors. Depending on the cross-docking energy activities and fitness scoring analysis threshold, out of 11 compounds, 300 small molecule compounds with proven anti-viral properties were characterized as Actives and 153 molecules were categorized as Inactives. Physarum-prize-collective for molecular docking algorithm, Schrodinger-inspired Neural Matrix Factorization, and a drug repositioning scoring analysis were implemented to a hybrid collection of the Natural Products of the Chemistry Institute of UNESP, Araraquara/SP, and NuBBEDB physical extracts (9-17,35). (10-17,36) Protein-molecule complexes, (4,5,7,8-17) followed by structural relaxation were generated through (8,13-117) flexible-ligand rigid-receptor molecular docking (7,9,13,16-17) in these local energy minimization to optimize protein-ligand interactions capping the C- and N-terminal for each active druggable fragment with i-GEMDOCK (3-14,17) through cycles in all keeping conserved amino-acids within 4 Å of all the docked ligands of each cation arrangement as consideration for each relaxed chemical structure free of local energy and geometry minimizations. (1,2,5-17,34,35) Virtual screening experiments generated with KNIME pipelined DockThor Virtual Screening tool for the NuBBEDB and e-Drug3D dataset and for the ChEMBL database, at the reference pH (6.6 to 7.4) for all SARS-CoV-2 drug targets including the contig maps (a set of overlapping DNA segments) as were assembled with the use of CLC Genomics software, version 4.6.1 (CLC Bio) publicly and are available so far. (BetaCoV/Wuhan/IVDC-HB-01/2020|EPI_ISL_402119), (e.g, N-terminal S1 subunit, PLpro, NendoU, (residue 14–685) in Spike Mpro, RdRp, and complete genome sequences of the three novel coronaviruses were submitted to GISAID (BetaCoV/Wuhan/IVDC-HB-01/2019, accession ID: EPI_ISL_402119; BetaCoV/Wuhan/IVDC-HB-04/2020, accession ID: EPI_ISL_402120_BetaCoV/Wuhan/IVDC-HB-05/2019, accession ID: EPI_ISL_402121) and a C-terminal S2 region N protein) were prepared for GEMDOCK docking experiments using the wild isogenic type of the transcriptomic variants and 10 best matching physical and chemical small molecule compounds (Table 1/) after exhaustive virtual screening analysis was obtained accordingly, Colchicine, Raltegravir, Hexacosanol, Benzoxazolinon, Carboxy-Pentatic acid, Ursane, Antheraxanthin, RA-XIII, Crotonate and Byrsonima Coccolobifolia against the SARS-COV-2 protein targets of the (pdb:1xak), (pdb:6xs6) and (pdb:6lu7). (6,7-17,36) For each target, all crucial amino-acids involved virtually in this project of the cut-out parallel docking system when linked together with hydrogens were then collected and the hit candidates who energetically favored within 8 Å of any docked molecule onto the hydrophobic side chain were then used to build a reduced phase docking system to be in contact with water where the [P@@](=O) (NC(=O) c 1nc(F) cnc1) (NC(=O) c1nn(c2o c(c(O) c2O) CON(C(=[N]=C(N) N) C) CN) cn1) Nn1c2nc([nH]]c(=O) c2nc1) N.C\1(=C/2\ON2[P@](=O) (N2N3N[C](=[N[C@H]23) =S) OC(=O) c2nn(c3oc(c(F) c3F) F) cn2) /N(N) N=[C](=S) N1.[P@@](=O) (N1CC1) (NC(=O) c1nn(c2c1[nH]c(nc2=O) N) C(=O) /C=N/C(=N) F) N/N=C(/N=C/N) \CN [P@] (=O) (O[P@@] (=O) (O) NC (=O) CC[C@H] (N) C (=O) N[C@H] (C (=O) N[C@H](C (=O) O) CCSC) CCC(=O) N) (O) OC1=N[C@H]2N=CN=C2C(=O) N1[P@@](=O)(NC(=O) c1nc (F) cnc1(NC(=O) c1nn(c2oc(c(O) c2O) CON(C([N]=C(N) N) C) CN) cn1) Nn1c2nc([nH]c(=O) c2nc1) N. C\1(=C/2\ON2[P@] (=O) (N2N3N[C] (=N[C@H]23) =S) OC(=O) c2nn(c3oc(c(F) c3F) F) cn2) /N(N) N=[C](=S) N1.[P@@] (=O) (N1CC1) (NC(=O) c1nn(c2c1[n H]c(nc2=O) N) C(=O) /C=N/C(=N) F) N/N= C(/N=C/N) \CN subscript. In the first smiles term in the spaces of targeted sequences referred to the difference of the free energy calculated using the protein-ligand (PL), protein (P), and ligand (L) sequence of amino acid conformations bonded evaluations for dispersion/repulsion, hydrogen bonding, electrostatics, and desolvation to the central atom of each screened compound. (10,17,37) (Figure 1///). The

GQM (X) refers to the energy of the cluster of the physical small molecule known as the R group from the docked complex, in the free unbound state the fourth term corresponds to the change in conformational entropy, which were generated and the second and third unbound states of ligand side-chain conformations are calculated through local energy minimization as $\Delta GQM_{conf}(X) = GQM_o(X) - GQM(X)$, ($X = L, P$) (equation1) where $GQM_o(X)$ is the energy of the isolated active fragments in the conformation of the docked PL on both protein and molecule complex Inhibitors and conformations when applied Bioactivity-guided Fractionations for the cluster of the selected compounds of the Colchicine, Raltegravir, Hexacosanol, Benzoxazolinon, Carboxy-Pentacic acid, Ursane, Antheraxanthin, RA-XIII, Crotonate and Byrsonima coccolobifolia Leaves and Stems to be fragmented, re-cored and accordingly merged into the combination of GisitorviffirmaTM, Roccustyrna_{gs1}TM, and Roccustyrna_{fr1}TM small hyperactive druggable scaffolds (3,4,17,36). The acknowledgment of the binding of the selected 8 physical compounds to their full-genome evolutionary novel coronavirus (2019-nCoV) protein targets was accomplished using Molinspiration (<http://www.molinspiration.com/cgi-bin/properties>) and DrugBank (1,11,12,13,15,17,34).

Pharmacophoric-ODE fragmenting, merging, and recording: Biogenetoligandorol AI-heuristic algorithm.

The patterns of this Biogenetoligandorol fragmentation Scheme are sorted into the working inputs of the Galilean transformation by examining the —extended Galilean transformation based on a set of heuristically determined descriptors moving with relative acceleration to a rigid system to a nonrotating geometric observer having an arbitrary time-dependent acceleration (20,21,27,28). (25,29) These descriptors as an applied nonconcurrent to both translate and rotate can be, for example, the number of atoms describing the pattern of a force system which can both translate and rotate and be determined by the substitution as a polynomial in $ip(r, t) = e^{iJ\{rt\}}(p(r', t))$. (equation2) $V'ip = (V'ip + iV'f)$ eif, (equation3) $\rho^-sQFI \approx \sum_{i=0}^1 Re(\pi_{i12})^2 (1\pi_{i11} + 1\pi_{i22}) + (\pi_{i11} - \pi_{i22})^2 \pi_{i11} + \pi_{i22}$, (equation4) $\rho_{1ij} = \langle v_i | \rho_s | v_j \rangle$ (equation5) $\rho_{0ij} = \langle v_i | \rho_s(0) | v_j \rangle$ (equation6) $H_1 = \gamma B_0 \cdot S^1 Re(\pi_{i12}) \pi_{i12} \rho_s(0)$ (equation7) $\rho^-s = H \otimes m$ (equation8) $V'2ip = \{V'2ip + 2iV'f - V'(p + (pV'2f + W \leftarrow S(I \otimes H))\}$ (equation9) $M_1; \langle p(V'f) \rangle = \langle \Phi | MT(I_3 - NT) - 2(p \otimes I_2) | \Phi \rangle$ (equation10) $\langle p(V'f) \rangle = \langle \Phi | MT(I_3 - NT) - 2(p \otimes I_2) | \Phi \rangle$ (equation11) $\langle p(V'f) \rangle = \langle \Phi | MT(I_3 - NT) - 2(p \otimes I_2) | \Phi \rangle$ (equation12) $\langle p(V'f) \rangle = \langle \Phi | MT(I_3 - NT) - 2(p \otimes I_2) | \Phi \rangle$ (equation13) eif, and the Schrödinger equation becomes $n^2 m(V, z(p + 2iV'f - V'(p + i(pV'f - M = \{M_0, M_1\})$ (equation14) $(V'fY \langle p) = ifi I_3 \leftarrow E(m_2)$ (equation15) (*m2-dimensional identity*) $((\langle p + if(p) - g(V'(p + i(pV'f))$ through the example of two coupled Chern-Simons Topology driven anti-de Sitter harmonic black-hole oscillators and brane spacetimes where $p+2$ are the the number of bonds predicted or the number of double bonds. (20,25) The complete pharmacophoric fragmentation Scheme was analyzed to compare similar series of chemical patterns that are contained in the chemical phase structures as extracted from within the selected 10 hit compounds of the Colchicine, Raltegravir, Hexacosanol, Benzoxazolinon, Carboxy-Pentacic acid, Ursane, Antheraxanthin, RA-XIII, Crotonate and Byrsonima coccolobifolia. (Table 1/), (20,35) Whenever searching for a specific pattern, if the group has such a parent pattern, the parent pattern is searched first eliminate the terms in $V'(p)$, which gives $f = -r' + g(t)$ (equation16). Then one can choose $ng\{t\}$ such as to eliminate the purely time-dependent terms, and one finally arrives at, $= (2mV'^2(p + mf; \blacksquare r'(p = ih(p, ipir, t) = -ea h J(pir', t)$ (equation17). (20,25,26) of the strong equivalence principle in quantum theory. After that, the child pharmacophoric pattern is searched in an inertial repeated merged system S as $ip = m(l_5 r, t) + ip_2 m_2, r, t$ (equation18). (25,26,37) Then assume that one fragmented pharrmacophore can describe the same superposition in an accelerating to a larger ligand-receptor system S' that obeys (20), with $\xi = \xi(r)$ (equation19), $\xi(0) = \xi(7)$ (equation20), so that the system S' performs a closed quantum circuit and coincides with the chemical structure system the S at times $t = 0$ and $t = T$, such that $r_{iT} = r(7)$ (equation21). (25-34,37) To avoid $q\{h q; \}$ $qreg q(3); creg c(3);$

reset q (0) ; reset q (1) ; reset q (2) ; h q (0) ; u2 (pi/2,pi/2) q (1) ; incomplete (1Z) -2- { ((2S,3S,5R) -5- (2-amino-6-oxo-6,9-dihydro- 3H-purin-9-yl) -3-hydroxyoxolan-2-yl) methylidene} -2-cyano- 1-({ ((2S,4R,5R) -2 group assignments, through two hydrogen-bonding interactions whenever a part into the S2 subsite of the structure relative to the complex between the 2- ({[fluoro ({[(2E) -5-oxabicyclo [2.1.0] pentan-2-ylidene] cyano-lambda6-sulfanyl}) methyl]phosphorylidene} amino) -4,6-dihydro-1H-purin-6-onecyano-1- ({ ((2S,4R,5R) -2-methyl- 2- (methylamino) -1,6-diazabicyclo with heptan-4-yl) oxy} imino) -1lambda5,2 lambda5-azaphosphiridin-1-ylum chemical groups of the cyclohexyl methyl is already recored and fragmented, the subsequent carbonyl oxygen matches have to be adjacent to the from the main-interacting chain amide of the residue Glu166 amino acid already occupied the space normally by the canonical S4- cyano-1- ({ ((2S,4R,5R) -2-methyl-2-2- ({[fluoro ({[(2E) -5- oxabicyclo [2.1.0] pentan-2-ylidene]cyano-lambda6-sulfanyl}) methyl]phosphorylidene} amino) -4,6-dihydro-1H-purin-6-one (methylamino) -1,6-diazabicyclo (3.2.0) heptan-4-yl) (1S,2R,3S) -2- ({ [(1S,2S,4S,5R) -4-ethenyl-4- sulfonylbicyclo[3.2.0]heptan-2-yl] oxy} amino) -3- 2- ({[fluoro ({[(2E) -5-oxabicyclo [2.1.0] pentan-2-ylidene]cyano-lambda6-sulfanyl}) methyl]phosphorylidene} amino) -4,6-dihydro-1H-purin-6-one[(2R,5R) -5- (2-methyl-6-methylidene-6,9-dihydro-3H-purin-9-yl) -3-methylideneoxolan-2-yl]phosphirane-1-carbonitrile-oxy} imino) -1lambda5, 2lambda5-azaphosphiridin-1-ylum binding site of the PDB:6LU7 main protease. (26,31-39) As a first step, our Chern-Simons oriented fragmentation algorithm performs a quick fragmentation Scheme search for extracting different chemical groups formed by the nucleophilic attack of the catalytic domains of the target proteases onto the α -carbon of my new Roccustyrna small molecule by applying the heuristic quantum phases for group prioritization when performing parent-child group prioritization as described above. (29,32-39) This topology geometric for pharmacophoric search and design indicating the canonical binding pockets moieties of a new small-sized prototype that goes sequentially through a sorted fragmentation Scheme, adding groups that are found in its active conformation phases and do not overlap with the 2- ({[fluoro ({[(2E) -5-oxabicyclo [2.1.0] pentan-2-ylidene] cyano-lambda6- sulfanyl}) methyl]phosphorylidene} amino) -4,6-dihydro-1H- purin-6-onecyano-1- ({ ((2S,4R,5R) -2-methyl-2- (methylamino) -1,6-diazabicyclo (3.2.0) heptan-4-yl) oxy} imino) - 1lambda5,2lambda5- azaphosphiridin-1-ylum chemical groups that were already screened. In case it successfully estimates a valid fragmentation, Scheme this is taken as the phase solution relating to how one clustered pharmacophoric element occupies the space normally filled by the protease_s substrate_s interacting main chain; would describe the same phase in an alternative XYZ coordinate smile system. (33,35-42) This Lindenbaum-Tarski algebraic algorithm was implemented as a recursive algorithm that leads to enhancement of my novel small molecule_s catalytic activity against the 3C protease-like domains I and II and performs a complete decision tree search of all possible combinations of fragmentation, merging, and pharmacophoric re-coring systems targeting in the in SARS-CoV Mpro. (12,13,28-39)

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|

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"...", "•", "ypar"
1,],

Scheme 3. Quantum Fourier Circuit of the BiogenetoligandoirolTM Cluster for the Roccustyrna small molecule Merging and Hope-Re-coring algorithms. Gate nG0 (param) q { h q; } qreg q (3) ; creg c (3) ; reset q (0) ; reset q (1) ; reset q (2) ; hq (0) ; u2 (pi/2,pi/2) q (1) ; measure q (2) -> c (2) ; x q (0) ; reset q (1) ; resetq (2) ; u3 (pi/2,pi/2,pi/2) q (0) ; measure q (2) -> c (2) ; u2 (pi/2,pi/2) q (2) ; cswapq (0) ,q (1) ,q (2) ; barrier q (0) ; u2 (pi/2,pi/2) q (2) ; h q (0) ; t q (2) ; t q (0) ; measure q (1) ->c (1) ; ch q (1) ,q (2) ; q (2) ; crx (pi/2) q (1) ,q (2) ; cu1 (pi/2) q (1) ,q (2) ; tdg q (2) ; sdg q (2) ; cy q (1) ,q (2) ; crz (pi/2) q (1) ,q (2) ; ch q (1) ,q (2) ; sdg q (1) ; u2 (pi/2,pi/2) q (2) ; ry (pi/2) q (2) ; cu3 (pi/2,pi/2,pi/2) q (1) ,q (2) ; tdg q (1) ; nG0 (pi/2) q (2) ; crx (pi/2) q (1) ,q (2) ; cu1 (pi/2) q (1) ,q (2) ; cswap q (0) ,q (1) ,q (2) ; swap q (1) ,q (2) ; cz q (1) ,q (2) ; rxx (pi/2) q (1) ,q (2) ; u1 (pi/2) q (1) ; cry (pi/2) q (1) ,q (2) ; crz (pi/2) q (1) ,q (2) ; measure q (0) -> c (0) ; z q (0) ; measure q (1) -> c (1) ; z q (0) ; rx (pi/2) q (1) ; rx (pi/2) q (0) ; u2 (pi/2,pi/2) q (1) ; rx (pi/2) q (0) ; ch q (1) ,q (2) ; ry (pi/2) q (0) ; ch q (1) ,q (2) ; u3 (pi/2,pi/2,pi/2) q (0) ; cz q (1) ,q (2) ; ch q (0) ,q (1) ; u1 (pi/2) q (0) ; swap q (1) ,q (2) ; sdg q (2) ;

Therefore, from a mathematical perspective, a TQFT that recovers the above AI-Quantum Hilbert symmetric spaces may be called —Chern–Simon’s theory. We present here potential condensed eigenvalues applications for the positive spectrum and finite-dimensional eigenspaces: $S=14\pi[M3(a+\ell)ta+\ell-\{1/12+(||\alpha1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha2'(t) \rangle CQ2t|\phi(t) \rangle B\} + Fqexp(i\hbar p^2A2mA+-1A\wedge dAk+13(a+\ell)ta+\ell-\{1/12+(||\alpha1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha2'(t) \rangle CQ2t|\phi(t) \rangle B\} + Fqexp(i\hbar p^2A2mA+-1A\wedge [A\wedge A]k \pmod{2\pi})1\rightarrow U(1)\rightarrow LG\sim \rightarrow LG\rightarrow 1}$ (equation22) of the free loop group $LG=(a+\ell)ta+\ell-\{1/12+(||\alpha1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha2'(t) \rangle CQ2t|\phi(t) \rangle B\} + Fqexp(i\hbar p^2A2mA+-1(a+\ell)ta+\ell-\{1/12+(||\alpha1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha2'(t) \rangle CQ2t|\phi(t) \rangle B\} + Fqexp(i\hbar p^2A2mA+-1(S1,G)}$ (equation23) is a functional of G bundles with connections over compact 3 manifolds. Here, A is the connection form, $(a+\ell)ta+\ell-\{1/12+(||\alpha1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha2'(t) \rangle CQ2t|\phi(t) \rangle B\} + Fqexp(i\hbar p^2A2mA+-1(a+\ell)ta+\ell-\{1/12+(||\alpha1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha2'(t) \rangle CQ2t|\phi(t) \rangle B\} + Fqexp(i\hbar p^2A2mA+-1\wedge(a+\ell)ta+\ell-\{1/12+(||\alpha1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha2'(t) \rangle CQ2t|\phi(t) \rangle B\} + Fqexp(i\hbar p^2A2mA+-1F)2zEGk:2zEG\otimes 2zEG\rightarrow \mathbb{R}$ (equation24) is a certain metric constructed and the integral from the level, is taken over a global section of the principal bundle. $\ddagger \delta^-v-\gamma\mu^-qD\mu^- \sigma -\overline{\sigma\sigma}^-q-i_f(\vartheta)\overline{\sigma}^-q+i\overline{F}q$ (equation25), $\delta F=(-\gamma\mu D\mu v+\sigma v+\lambda\sigma)+i(2_- -1)2f(\vartheta)qv$ (equation26), $\delta^-F=\overline{q}(-\gamma\mu D\mu^-v+\overline{v}\sigma-\overline{\sigma}^- \lambda)+i(2_- -1)2f(\vartheta)\overline{q}^-v$, (equation27) We hybridized then every level $k\in H4(BG,\mathbb{Z})$ that yields the quantum field theory with those levels k that satisfy the following positivity condition: Chern-Simons theory equation of the: $(\int tr(+23).S=k4\pi[Mtr)(3dN=2CSA\wedge dA+23A\wedge A\wedge A)$ (equation28). A (equation 1), (ie. considering S as a functional of A). associated to a connected Lie group α_{ζ} a simple current Roccustyrna XYZ chemical extension of the tensor product of the $d/dx(33833y^n\times 1152N^2x^2k^4)=3dN^2CS77951232k^4N^2xy^n$ (equation29) associated to an even lattice and $38975616k^4N^2x^2y^n=\sum_{v=0}^{\infty}(n^v38975616\{x\sin^(-1)(\sqrt{3})\}x\sin^(-1)(\sqrt{779}\sqrt{\theta^3})x\sin^(-1)(2\sqrt{114109})\sqrt{(1-\sqrt{456457})\sqrt{x}}x^{(1/4)}(2\sqrt{456457})\sqrt{x}+3)/ (8456457^{(3/4)})+(x-3/3651656)\sin^(-1)(456457^{(1/4)}x^{(1/4)})1/2\sqrt{(x/456456754-x^2)}+(x-1/912913508)\sin^(-1)(\sqrt{456456754}\sqrt{x})x\sin^(-2(3/4)57057^{(1/4)})x\sin^(-1)(\sqrt{\sum 444546\theta})x\sin^(-1)(2^{(3/4)}$

$431683182057^{1/4} \sqrt{\sqrt{\theta} / (\sin^{-1}(44545545))} \} + \text{constant} (k^4 N^2 x^2 \log^v(y)) / (v!)$
 (equations 2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20-30) associated to a simply connected Lie group
 classical equations of motion obtained via i and ii are known to be equivalent by combining the works of
 Finkelberg obtained in this way are: $=0k2\pi F=03d N = 2$ CS (equation 31) also known as Connes fusion or every
 connected group G and level $k \geq 0$. It is given by $\gamma\mu\varnothing D\mu_- + \varrho (\rho \cdot \sigma)_- + i_f(\vartheta) \varrho_- = M\varnothing_-$ (equation 32) where M is
 the eigenvalue given by $M = M_{m,n} = \rho \cdot \sigma + i_{mb} + nb - 1 + Q2 \ m \ n \ 2 \ Z_0$ (equation 33), $Q = b + b - 1$ (equation 34).
 The product of the eigenvalues roughly gives —denominator‖ of the one-loop determinant, where the right action
 on H uses the isomorphism induced by reflection along the horizontal axis. (41) For every simple simply
 connected Lie group G with the quantum Hilbert space CSG, k ($S1$ and every level $k \geq 0$, a tensor category $A \Lambda A, k$
 whose Drinfel'd center $Z(dA, A)$ associated to a Riemann surface Σ can and has been defined at a mathematical
 level of precision and is equivalent to the the $Vect_k[G] \ Vect_k[G]$ CSG, k (pt) d/dx (33833 $y^n \times 1152 N^2 x^2$
 k^4) = 77951232 $k^4 N^2 x y^n$ (equation 33) categories of the $\sin(a+\ell) \ ta+\ell - \{1/12 + (||\alpha_1'(t) \rangle CQ1t|\phi(t) \rangle B + |\alpha_2'(t)$
 $\rangle CQ2t|\phi(t) \rangle B) \} + F\varnothing \exp(i\hbar p^2 A2mA + -1 Vect_k((a+\ell) \ ta+\ell - \{1/12 + (||\alpha_1'(t) \rangle CQ1t|\phi(t) \rangle B + |\alpha_2'(t) \rangle CQ2t|\phi(t) \rangle B)$
 $\} + F\varnothing \exp(i\hbar p^2 A2mA + -1 + (a+\ell) \ ta+\ell \{1/12 + (||\alpha_1'(t) \rangle CQ1t|\phi(t) \rangle B + |\alpha_2'(t) \rangle CQ2t|\phi(t) \rangle B) \} + F\varnothing \exp(i\hbar p^2 A2mA$
 $+ -1 \Lambda (a+\ell) \ ta+\ell - \{1/12 + (||\alpha_1'(t) \rangle CQ1t|\phi(t) \rangle B + |\alpha_2'(t) \rangle CQ2t|\phi(t) \rangle B) \} + F\varnothing \exp(i\hbar p^2 A2mA + -1 F) k^4 x^4 y^n$
 $\sin^{\wedge} \quad (-1) \quad (n) \quad ^{33833} \quad 5429 \quad N^2 \quad (\text{newtons})$

squared) - 1/3 x^6 (k^4 y^n sin^(-1) (n) ^33833 5429 N^2 (newtons squared)) + 2/45 k^4 x^8 y^n sin^(-1) (n) ^33833 5429 N^2 (newtons squared) + O (x^9) (equation34) of canonical quantization, it is the geometric quantization of LocG (Σ) with respect to the natural symplectic Roccustyrna structure coming from the Chern–Simons Lagrangian. We explain below that, at least along the direction θ is defined by S0P (g) = Z1eiθ0dt e− tg BP (t) (equation35), (1) where BP (t) is analytic continuation of the formal Borel transformation P1ℓ=0cℓ (a+ℓ) ta+ℓ−{1/12+(||α1′(t))CQ1t|φ(t))B+|α2′(t))CQ2t|φ(t))B) } + Fqexp(iℏp^2A2mA ++1.whenG 432 π k^4N^2 x^2 sin^(-1) (n) ^33833 (2 x- sin (2x)) y^ (Λn) for Vectk[G] dCSG,k (pt) (equation36) is simply canonically connected with the the Reshetikhin–Turaev TQFT quantizations as associated to the modular tensor category Repk (LG) of positive energy representations of the loop group at level k has that property 14π[M3 (a+ℓ) ta+ℓ−{1/12+(||α1′(t))CQ1t|φ(t))B+|α2′(t))CQ2t|φ(t))B) } + Fqexp(iℏp^2A2mA ++1AΛdA **2zEG**Zcl (σ) = expℏXnp= 1isgn (kp) gptr (σ (p)) 2i (equation37), Z1loop (σ) =Qα2root+4 sinh (πbα · σ) sinh (πb−1α · σ) QaQpa2Rasb_pa · σ − iQ (1−_a) 2_) equation38), sb (z) =1 (equation39), Ym=01 (equation40), n=0mb + nb−1 + Q/2 − izmb + nb−1 + Q/2 + izk+13 (a+ℓ) ta+ℓ−{1/12+(||α1′(t))CQ1t|φ(t))B+|α2′(t))CQ2t|φ(t))B) } + Fqexp(iℏp^2A2mA ++1AΛ[AΛA] (equation41) the coordinate (x1, x2, x3, x4) = (cos θ cos φ, cos θ sin φ, sin θ cos τ, sin θ sin τ) and f (θ) =pb−2 sin2 θb2 cos2 θ.k (mod2π) [1]+sin (a+ℓ) ta+ℓ{1/12+(||α1′(t))CQ1t|φ(t))B+|α2′(t))CQ2t|φ(t))B) } + Fqexp(iℏp^2A2mA ++1Vectk ((a+ℓ) ta+ℓ−{1/12+(||α1′(t))CQ1t|φ(t))B+|α2′(t))CQ2t|φ(t))B) } + Fqexp(iℏp^2A2mA ++1+ (a+ℓ) ta+ℓ−{1/12+(||α1′(t))CQ1t|φ(t))B+|α2′(t))CQ2t|φ(t))B) } + Fqexp(iℏp^2A2mA ++1Λ (a+ℓ) ta+ℓ−{1/12+(||α1′(t))CQ1t|φ(t))B+|α2′(t))CQ2t|φ(t))B) } + Fqexp(iℏp^2A2mA ++1F) 1 4π[M3 (a+ℓ) ta+ℓ−{1/12+(||α1′(t))CQ1t|φ(t))B+|α2′(t))CQ2t|φ(t))B) } + Fqexp(iℏp^2A2mA ++1AΛdA **2zEG**k+13 (a+ℓ) ta+ℓ−{1/12+(||α1′(t))CQ1t|φ(t))B+|α2′(t))CQ2t|φ(t))B) } + Fqexp(iℏp^2A2mA ++1AΛ[AΛA] **2zEG**k (mod2π) [1]Λsin (a+ℓ) ta+ℓ−{1/12+(||α1′(t))CQ1t|φ(t))B+|α2′(t))CQ2t|φ(t))B) } + Fqexp(iℏp^2A2mA ++1Vectk ((a+ℓ) ta+ℓ−{1/12+(||α1′(t))CQ1t|φ(t))B+|α2′(t))CQ2t|φ(t))B) } + Fqexp(iℏp^2A2mA ++1+ (a+ℓ) ta+ℓ−{1/12+(||α1′(t))CQ1t|φ(t))B+|α2′(t))CQ2t|φ(t))B) } + Fqexp(iℏp^2A2mA ++1Λ (a+ℓ) ta+ℓ−{1/12+(||α1′(t))CQ1t|φ(t))B+|α2′(t))CQ2t|φ(t))B) } + Fqexp(iℏp^2A2mA ++1F) 14π[M3 (a+ℓ) ta+ℓ−{1/12+(||α1′(t))CQ1t|φ(t))B+|α2′(t))CQ2t|φ(t))B) } + Fqexp(iℏp^2A2mA ++1AΛ dA **2zEG**k+13 (a+ℓ) ta+ℓ−{1/12+(||α1′(t))CQ1t|φ(t))B+|α2′(t))CQ2t|φ(t))B) } + Fqexp(iℏp^2A2mA ++1AΛ[AΛA] **2zEG**k (mod2π) (equation42), F= dA+AΛA Repk (dA+AΛA AGA) (equation43) by [28]Fμν = 0, σ = const, D = −σf (θ), λ = −λ = 0. (4) Rep^{ss} (Fq **2zEG**) [or Rep^k (AF**2zEG**)] and Rep (Dk (C[G])) =Repr ((a+ℓ) ta+ℓ 1) where x^Aψ1CmdπCdπ2 |∇ |2 = { if√(|α1′(t))CQ1t|φ(t))B|∇ |2 −ΔKΣ(dt−asin2θdφ) if√(|α1′(t))CQ1t|φ(t))B|∇ |2 −ΔKΣ(dt−asin2θdφ) 1 ≠ exp(iℏp^2A2mA(q^Cif −π^CmdπCdπ2 |∇ |2 −ΔKΣ(dt−asin2θdφ) IfŜbp^AmAŜ†b+ if(p) - g.(V ‘(p + i(pv’ f)) + exp(iℏp^2A2mA(q^Cif −π^CmdπCdπ2 |∇ |2 −ΔKΣ(dt−asin2θdφ) IfŜbp^AmAŜ†b+if√(|α1′(t))CQ1t|φ(t))B+|α 2′(t))CQ2t|φ(t))B) (p) - g.(V ‘(p + i(pv’ f)) ≠ exp(iℏp^2A2mA(q^Cif −π^CmdπCdπ2 |∇ |2 −ΔKΣ(dt−asin2θdφ) IfŜbp^AmAŜ†b+ if(p) - g.(V ‘(p + i(pv’ f)) + 2 2 _1 1 = 2 where if√(|α1′(t))CQ1t|φ(t))B|∇ |2 −ΔKΣ(dt−asin2θdφ) exp(iℏp^2A2mA(q^Cif −π^CmdπCdπ2 |∇ |2 −ΔKΣ(dt−asin2θdφ) IfŜbp^AmAŜ†b+ if√(|α1′(t))CQ1t|φ(t))B+|α2′(t))CQ2t|φ(t))B) (p) - g.(V ‘(p + i(pv’ f)) if√(|α1′(t))CQ1t|φ(t))B+|π^2B2mB+π^2C2mC exp(iℏp^2A2mA(q^Cif −π^CmdπCdπ2 |∇ |2 −ΔKΣ(dt−asin2θdφ) IfŜbp^AmAŜ†b+ if√(|α1′(t))CQ1t|φ(t))B+|α2′(t))CQ2t|φ(t))B) (p) - g.(V ‘(p + i(pv’ f))). = exp(iℏp^2A2mA(q^Cif −π^CmdπCdπ2 |∇ |2 Π^2B2mB+Π^2C2mC

$\hat{A}C(\text{Equation4})$ in (Equation1) and we have introduced the term $\exp(-i\hbar\pi^2C_2mC(t-\tau))$ to ensure that the position of the system A at time τ transforms into the symmetric position of the system C, $\hat{S}T(x^A\psi_1Cm\pi C d\pi_2|\nabla|^2 = \{$
 $\text{if}\sqrt{(|\alpha_1'(t)|)}CQ_1t|\phi(t)|B|\nabla|^2 - \Delta K\Sigma(dt - \text{asin}2\theta d\phi) \text{if}\sqrt{(|\alpha_1'(t)|)}CQ_1t|\phi(t)|B|\nabla|^2 - \Delta K\Sigma(dt - \text{asin}2\theta d\phi) - 1 \neq$
 $\exp(i\hbar\pi^2A_2mA(q^C\text{Cif} - \pi^Cm\pi C d\pi_2|\nabla|^2 - \Delta K\Sigma(dt - \text{asin}2\theta d\phi) \text{If}\hat{S}bp^A m\hat{A}\hat{S}^\dagger b + \text{if}(p) - g.(V'(p + i(pv')f)) +$
 $\exp(i\hbar\pi^2A_2mA(q^C\text{Cif} - \pi^Cm\pi C d\pi_2|\nabla|^2 - \Delta K\Sigma(dt - \text{asin}2\theta d\phi) \text{If}\hat{S}bp^A m\hat{A}\hat{S}^\dagger b + \text{if}\sqrt{(|\alpha_1'(t)|)}CQ_1t|\phi(t)|B + |\alpha_2'(t)|$
 $CQ_2t|\phi(t)|B)(p) - g.(V'(p + i(pv')f)) \neq \exp(i\hbar\pi^2A_2mA(q^C\text{Cif} - \pi^Cm\pi C d\pi_2|\nabla|^2 - \Delta K\Sigma(dt - \text{asin}2\theta d\phi) \text{If}\hat{S}bp^A m\hat{A}\hat{S}^\dagger b + \text{if}(p) - g.(V'(p + i(pv')f)) + 2^2_{-1} = 2$
 $\text{where } \text{if}\sqrt{(|\alpha_1'(t)|)}CQ_1t|\phi(t)|B|\nabla|^2 - \Delta K\Sigma(dt - \text{asin}2\theta d\phi) \exp(i\hbar\pi^2A_2mA(q^C\text{Cif} - \pi^Cm\pi C d\pi_2|\nabla|^2 - \Delta K\Sigma(dt - \text{asin}2\theta d\phi) \text{If}\hat{S}bp^A m\hat{A}\hat{S}^\dagger b + \text{if}\sqrt{(|\alpha_1'(t)|)}CQ_1t|\phi(t)|B + |\alpha_2'(t)|$
 $CQ_2t|\phi(t)|B)(p) - g.(V'(p + i(pv')f)) \text{if}\sqrt{(|\alpha_1'(t)|)}CQ_1t|\phi(t)|B + |\pi^2B_2mB + \pi^2C_2mC \exp(i\hbar\pi^2A_2mA(q^C\text{Cif} - \pi^Cm\pi C d\pi_2|\nabla|^2 - \Delta K\Sigma(dt - \text{asin}2\theta d\phi) \text{If}\hat{S}bp^A m\hat{A}\hat{S}^\dagger b + \text{if}\sqrt{(|\alpha_1'(t)|)}CQ_1t|\phi(t)|B + |\alpha_2'(t)|$
 $CQ_2t|\phi(t)|B)(p) - g.(V'(p + i(pv')f)) - p^A m_A(t-\tau)) \hat{S}^\dagger T = -(q^C\text{Cif} - \pi^Cm\pi C d\pi_2|\nabla|^2 = \{ \text{if}\sqrt{(|\alpha_1'(t)|)}CQ_1t|\phi(t)|B|\nabla|^2 - \Delta K\Sigma(dt - \text{asin}2\theta d\phi) \text{if}\sqrt{(|\alpha_1'(t)|)}CQ_1t|\phi(t)|B|\nabla|^2 - \Delta K\Sigma(dt - \text{asin}2\theta d\phi) - 1 \neq$
 $\exp(i\hbar\pi^2A_2mA(q^C\text{Cif} - \pi^Cm\pi C d\pi_2|\nabla|^2 - \Delta K\Sigma(dt - \text{asin}2\theta d\phi) \text{If}\hat{S}bp^A m\hat{A}\hat{S}^\dagger b + \text{if}(p) - g.(V'(p + i(pv')f)) + \exp(i\hbar\pi^2A_2mA(q^C\text{Cif} - \pi^Cm\pi C d\pi_2|\nabla|^2 - \Delta K\Sigma(dt - \text{asin}2\theta d\phi) \text{If}\hat{S}bp^A m\hat{A}\hat{S}^\dagger b +$
 $\text{if}\sqrt{(|\alpha_1'(t)|)}CQ_1t|\phi(t)|B + |\alpha_2'(t)|CQ_2t|\phi(t)|B)(p) - g.(V'(p + i(pv')f)) \neq \exp(i\hbar\pi^2A_2mA(q^C\text{Cif} - \pi^Cm\pi C d\pi_2|\nabla|^2 - \Delta K\Sigma(dt - \text{asin}2\theta d\phi) \text{If}\hat{S}bp^A m\hat{A}\hat{S}^\dagger b + \text{if}(p) - g.(V'(p + i(pv')f)) + 2^2_{-1} = 2$
 $\text{where } y_2 = \exp(i\hbar\pi^2A_2mA(q^C\text{Cif} - \pi^Cm\pi C d\pi_2|\nabla|^2 - \Delta K\Sigma(dt - \text{asin}2\theta d\phi) \text{If}\hat{S}bp^A m\hat{A}\hat{S}^\dagger b + \text{if}\sqrt{(|\alpha_1'(t)|)}CQ_1t|\phi(t)|B + |\alpha_2'(t)|CQ_2t|\phi(t)|B)(p) - g.(V'(p + i(pv')f)) (1 -) - 1. C(t-\tau))$
 $(\text{Equation5}).$ Notice that for $t=\tau$ the operator $\hat{S}T$ in (Equation2) is precisely the operator $\hat{S}x$ in (Equation3) a generalization of the simplest non-static Schwarzschild metric, and is expressed in Eddington coordinates (u, r, θ, ϕ) , as follows $ds^2 = -(1 - 2m(u)/r) du^2 + 2\epsilon du dr + d\Omega^2, (\epsilon = \pm 1)$ (Equation6) where $d\Omega^2 = d\theta^2 + \sin^2\theta d\phi^2$. $\epsilon = +1$ (Equation7) represents the —advanced or —ingoing Vaidya metric, while $\epsilon = -1$ represents the —retarded or —outgoing Vaidya metric (31). Therefore, we can interpret $\hat{S}x$ as the operator which performs the translation to a quantum reference frame when the dynamics is —frozen at time τ . The transformation implemented by $\hat{S}T$ is $\hat{S}T x^A \psi_1 C m \pi C d \pi_2 |\nabla|^2 = \{ \text{if}\sqrt{(|\alpha_1'(t)|)}CQ_1t|\phi(t)|B|\nabla|^2 - \Delta K\Sigma(dt - \text{asin}2\theta d\phi) \text{if}\sqrt{(|\alpha_1'(t)|)}CQ_1t|\phi(t)|B|\nabla|^2 - \Delta K\Sigma(dt - \text{asin}2\theta d\phi) - 1 \neq \exp(i\hbar\pi^2A_2mA(q^C\text{Cif} - \pi^Cm\pi C d\pi_2|\nabla|^2 - \Delta K\Sigma(dt - \text{asin}2\theta d\phi) \text{If}\hat{S}bp^A m\hat{A}\hat{S}^\dagger b + \text{if}(p) - g.(V'(p + i(pv')f)) + \exp(i\hbar\pi^2A_2mA(q^C\text{Cif} - \pi^Cm\pi C d\pi_2|\nabla|^2 - \Delta K\Sigma(dt - \text{asin}2\theta d\phi) \text{If}\hat{S}bp^A m\hat{A}\hat{S}^\dagger b + \text{if}\sqrt{(|\alpha_1'(t)|)}CQ_1t|\phi(t)|B + |\alpha_2'(t)|CQ_2t|\phi(t)|B)(p) - g.(V'(p + i(pv')f)) \neq \exp(i\hbar\pi^2A_2mA(q^C\text{Cif} - \pi^Cm\pi C d\pi_2|\nabla|^2 - \Delta K\Sigma(dt - \text{asin}2\theta d\phi) \text{If}\hat{S}bp^A m\hat{A}\hat{S}^\dagger b + \text{if}(p) - g.(V'(p + i(pv')f)) + 2^2_{-1} = 2 \text{where } \text{if}\sqrt{(|\alpha_1'(t)|)}CQ_1t|\phi(t)|B|\nabla|^2 - \Delta K\Sigma(dt - \text{asin}2\theta d\phi) \exp(i\hbar\pi^2A_2mA(q^C\text{Cif} - \pi^Cm\pi C d\pi_2|\nabla|^2 - \Delta K\Sigma(dt - \text{asin}2\theta d\phi) \text{If}\hat{S}bp^A m\hat{A}\hat{S}^\dagger b + \text{if}\sqrt{(|\alpha_1'(t)|)}CQ_1t|\phi(t)|B + |\alpha_2'(t)|CQ_2t|\phi(t)|B)(p) - g.(V'(p + i(pv')f)) \text{if}\sqrt{(|\alpha_1'(t)|)}CQ_1t|\phi(t)|B + |\pi^2B_2mB + \pi^2C_2mC \exp(i\hbar\pi^2A_2mA(q^C\text{Cif} - \pi^Cm\pi C d\pi_2|\nabla|^2 - \Delta K\Sigma(dt - \text{asin}2\theta d\phi) \text{If}\hat{S}bp^A m\hat{A}\hat{S}^\dagger b + \text{if}\sqrt{(|\alpha_1'(t)|)}CQ_1t|\phi(t)|B + |\alpha_2'(t)|CQ_2t|\phi(t)|B)(p) - g.(V'(p + i(pv')f)) - \hat{S}^\dagger T = -q^C + \pi^Cm\pi C d\pi_2|\nabla|^2 = \{ \text{if}\sqrt{(|\alpha_1'(t)|)}CQ_1t|\phi(t)|B|\nabla|^2 - \Delta K\Sigma(dt - \text{asin}2\theta d\phi) \text{if}\sqrt{(|\alpha_1'(t)|)}CQ_1t|\phi(t)|B|\nabla|^2 - \Delta K\Sigma(dt - \text{asin}2\theta d\phi) - 1 \neq \exp(i\hbar\pi^2A_2mA(q^C\text{Cif} - \pi^Cm\pi C d\pi_2|\nabla|^2 - \Delta K\Sigma(dt - \text{asin}2\theta d\phi) \text{If}\hat{S}bp^A m\hat{A}\hat{S}^\dagger b + \text{if}(p) - g.(V'(p + i(pv')f)) + \exp(i\hbar\pi^2A_2mA(q^C\text{Cif} - \pi^Cm\pi C d\pi_2|\nabla|^2 - \Delta K\Sigma(dt - \text{asin}2\theta d\phi) \text{If}\hat{S}bp^A m\hat{A}\hat{S}^\dagger b + \text{if}\sqrt{(|\alpha_1'(t)|)}CQ_1t|\phi(t)|B + |\alpha_2'(t)|CQ_2t|\phi(t)|B)(p) - g.(V'(p + i(pv')f)) \neq \exp(i\hbar\pi^2A_2mA(q^C\text{Cif} - \pi^Cm\pi C d\pi_2|\nabla|^2 - \Delta K\Sigma(dt - \text{asin}2\theta d\phi) \text{If}\hat{S}bp^A m\hat{A}\hat{S}^\dagger b + \text{if}(p) - g.(V'(p + i(pv')f))$

$(p + i(pv' f)) + 2 \cdot 2 \cdot 1 = 2$ where $\text{if} \sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B} |\nabla|^2 - \Delta K \Sigma(dt - \text{asin} 2\theta d\phi) \exp(i\hbar p^2 A 2m A(q^{\wedge} Cif - \pi^{\wedge} C m d \pi C d \pi 2 |\nabla|^2 - \Delta K \Sigma(dt - \text{asin} 2\theta d\phi) \text{If} \hat{S} b p^{\wedge} A m A \hat{S}^{\dagger} b + \text{if} \sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B + |\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) (p) - g.(V '(p + i(pv' f)) \text{if} \sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B + |\pi^2 B 2m B + \pi^2 C 2m C \exp(i\hbar p^2 A 2m A(q^{\wedge} Cif - \pi^{\wedge} C m d \pi C d \pi 2 |\nabla|^2 - \Delta K \Sigma(dt - \text{asin} 2\theta d\phi) \text{If} \hat{S} b p^{\wedge} A m A \hat{S}^{\dagger} b + \text{if} \sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B + |\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) (p) - g.(V '(p + i(pv' f)) . C(t-\tau) - \pi^{\wedge} B + \pi^{\wedge} C m d \pi C d \pi 2 |\nabla|^2 = \{ \text{if} \sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B} |\nabla|^2 - \Delta K \Sigma(dt - \text{asin} 2\theta d\phi) \text{if} \sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B} |\nabla|^2 - \Delta K \Sigma(dt - \text{asin} 2\theta d\phi) 1 \neq \exp(i\hbar p^2 A 2m A(q^{\wedge} Cif - \pi^{\wedge} C m d \pi C d \pi 2 |\nabla|^2 - \Delta K \Sigma(dt - \text{asin} 2\theta d\phi) \text{If} \hat{S} b p^{\wedge} A m A \hat{S}^{\dagger} b + \text{if}(p) - g.(V '(p + i(pv' f)) + \exp(i\hbar p^2 A 2m A(q^{\wedge} Cif - \pi^{\wedge} C m d \pi C d \pi 2 |\nabla|^2 - \Delta K \Sigma(dt - \text{asin} 2\theta d\phi) \text{If} \hat{S} b p^{\wedge} A m A \hat{S}^{\dagger} b + \text{if} \sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B + |\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) (p) - g.(V '(p + i(pv' f)) \neq \exp(i\hbar p^2 A 2m A(q^{\wedge} Cif - \pi^{\wedge} C m d \pi C d \pi 2 |\nabla|^2 - \Delta K \Sigma(dt - \text{asin} 2\theta d\phi) \text{If} \hat{S} b p^{\wedge} A m A \hat{S}^{\dagger} b + \text{if}(p) - g.(V '(p + i(pv' f)) + 2 \cdot 2 \cdot 1 = 2 where $F \exp(i\hbar p^2 A 2m A \pi^2 B 2m B + \pi^2 C 2m C \exp(i\hbar p^2 A 2m A(q^{\wedge} Cif - \pi^{\wedge} C m d \pi C d \pi 2 |\nabla|^2 - \Delta K \Sigma(dt - \text{asin} 2\theta d\phi) \text{If} \hat{S} b p^{\wedge} A m A \hat{S}^{\dagger} b + \text{if} \sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B + |\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) (p) - g.(V '(p + i(pv' f)) \text{if} \sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B + |\pi^2 B 2m B + \pi^2 C 2m C \exp(i\hbar p^2 A 2m A(q^{\wedge} Cif - \pi^{\wedge} C m d \pi C d \pi 2 |\nabla|^2 - \Delta K \Sigma(dt - \text{asin} 2\theta d\phi) \text{If} \hat{S} b p^{\wedge} A m A \hat{S}^{\dagger} b + \text{if} \sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B + |\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) (p) - g.(V '(p + i(pv' f)) A(t-\tau) ; \hat{S} T p^{\wedge} A \hat{S}^{\dagger} T = -(\pi^{\wedge} B + \pi^{\wedge} C) ; (Equation8) \hat{S} T x^{\wedge} B \hat{S}^{\dagger} T = q^{\wedge} B - q^{\wedge} C + \pi^{\wedge} C m d \pi C d \pi 2 |\nabla|^2 = \{ \text{if} \sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B} |\nabla|^2 - \Delta K \Sigma(dt - \text{asin} 2\theta d\phi) \text{if} \sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B} |\nabla|^2 - \Delta K \Sigma(dt - \text{asin} 2\theta d\phi) 1 \neq \exp(i\hbar p^2 A 2m A(q^{\wedge} Cif - \pi^{\wedge} C m d \pi C d \pi 2 |\nabla|^2 - \Delta K \Sigma(dt - \text{asin} 2\theta d\phi) \text{If} \hat{S} b p^{\wedge} A m A \hat{S}^{\dagger} b + \text{if}(p) - g.(V '(p + i(pv' f)) + \exp(i\hbar p^2 A 2m A(q^{\wedge} Cif - \pi^{\wedge} C m d \pi C d \pi 2 |\nabla|^2 - \Delta K \Sigma(dt - \text{asin} 2\theta d\phi) \text{If} \hat{S} b p^{\wedge} A m A \hat{S}^{\dagger} b + \text{if} \sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B + |\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) (p) - g.(V '(p + i(pv' f)) \neq \exp(i\hbar p^2 A 2m A(q^{\wedge} Cif - \pi^{\wedge} C m d \pi C d \pi 2 |\nabla|^2 - \Delta K \Sigma(dt - \text{asin} 2\theta d\phi) \text{If} \hat{S} b p^{\wedge} A m A \hat{S}^{\dagger} b + \text{if}(p) - g.(V '(p + i(pv' f)) + 2 \cdot 2 \cdot 1 = 2 where $\text{if} \sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B} |\nabla|^2 - \Delta K \Sigma(dt - \text{asin} 2\theta d\phi) \exp(i\hbar p^2 A 2m A(q^{\wedge} Cif - \pi^{\wedge} C m d \pi C d \pi 2 |\nabla|^2 - \Delta K \Sigma(dt - \text{asin} 2\theta d\phi) \text{If} \hat{S} b p^{\wedge} A m A \hat{S}^{\dagger} b + \text{if} \sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B + |\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) (p) - g.(V '(p + i(pv' f)) \text{if} \sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B + |\pi^2 B 2m B + \pi^2 C 2m C \exp(i\hbar p^2 A 2m A(q^{\wedge} Cif - \pi^{\wedge} C m d \pi C d \pi 2 |\nabla|^2 - \Delta K \Sigma(dt - \text{asin} 2\theta d\phi) \text{If} \hat{S} b p^{\wedge} A m A \hat{S}^{\dagger} b + \text{if} \sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B + |\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) (p) - g.(V '(p + i(pv' f)) . C(t-\tau) ; \hat{S} T p^{\wedge} B \hat{S}^{\dagger} T = \pi^{\wedge} B (Equation9) implies that the position at time t of pharmacophoric system of ((2S,5R,6R) - 6-((2S) -2-amino-2- phenylacetamido) -3,3- dimethyl-7-oxo- 4-thia-1- azabicyclo (3.2.0) heptane-2- carbonyloxy) (((2-amino-6-oxo- 6,9-dihydro-3H-purin-9-yl) oxy) (hydroxy) phosphoryl oxy) phosphinic acid B: $\hat{S} T$ is $\hat{S} T x^{\wedge} A v 1 C m d \pi C d \pi 2 |\nabla|^2 = \{ \text{if} \sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B} |\nabla|^2 - \Delta K \Sigma(dt - \text{asin} 2\theta d\phi) \text{if} \sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B} |\nabla|^2 - \Delta K \Sigma(dt - \text{asin} 2\theta d\phi) 1 \neq \exp(i\hbar p^2 A 2m A(q^{\wedge} Cif - \pi^{\wedge} C m d \pi C d \pi 2 |\nabla|^2 - \Delta K \Sigma(dt - \text{asin} 2\theta d\phi) \text{If} \hat{S} b p^{\wedge} A m A \hat{S}^{\dagger} b + \text{if}(p) - g.(V '(p + i(pv' f)) + \exp(i\hbar p^2 A 2m A(q^{\wedge} Cif - \pi^{\wedge} C m d \pi C d \pi 2 |\nabla|^2 - \Delta K \Sigma(dt - \text{asin} 2\theta d\phi) \text{If} \hat{S} b p^{\wedge} A m A \hat{S}^{\dagger} b + \text{if} \sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B + |\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) (p) - g.(V '(p + i(pv' f)) \neq \exp(i\hbar p^2 A 2m A(q^{\wedge} Cif - \pi^{\wedge} C m d \pi C d \pi 2 |\nabla|^2 - \Delta K \Sigma(dt - \text{asin} 2\theta d\phi) \text{If} \hat{S} b p^{\wedge} A m A \hat{S}^{\dagger} b + \text{if}(p) - g.(V '(p + i(pv' f)) + 2 \cdot 2 \cdot 1 = 2 from the point of view of C is mapped into the relative position between system B and the position of A: 1 $\text{if} \sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B} |\nabla|^2 - \Delta K \Sigma(dt - \text{asin} 2\theta d\phi) 1 \neq \exp(i\hbar p^2 A 2m A(q^{\wedge} Cif - \pi^{\wedge} C m d \pi C d \pi 2 |\nabla|^2 - \Delta K \Sigma(dt - \text{asin} 2\theta d\phi) \text{If} \hat{S} b p^{\wedge} A m A \hat{S}^{\dagger} b + \text{if}(p) - g.(V '(p + i(pv' f)) + \exp(i\hbar p^2 A 2m A(q^{\wedge} Cif - \pi^{\wedge} C m d \pi C d \pi 2 |\nabla|^2 - \Delta K \Sigma(dt - \text{asin} 2\theta d\phi) \text{If} \hat{S} b p^{\wedge} A m A \hat{S}^{\dagger} b + \text{if} \sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B + |\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) (p) - g.(V '(p + i(pv' f)) \neq \exp(i\hbar p^2 A 2m A(q^{\wedge} Cif - \pi^{\wedge} C m d \pi C d \pi 2 |\nabla|^2 - \Delta K \Sigma(dt - \text{asin} 2\theta d\phi) \text{If} \hat{S} b p^{\wedge} A m A \hat{S}^{\dagger} b + \text{if}(p) - g.(V '(p + i(pv' f)) + 2 \cdot 2 \cdot 1 = 2 at time τ , while the momentum of B remains unchanged. In addition, this transformation is a symmetry of the free particle according to the definition given in (Equation6), because the Hamiltonian $\hat{H}(C) AB$ is mapped through (Equation5) to $\hat{H}(A)$$$$$$

$BC = \pi^2 B^2 m_B + \pi^2 C^2 m_C$. Kerr metric in Boyer–Lindquist coordinates can be expressed as follows: $ds^2 = -\Delta K \Sigma (dt - a \sin^2 \theta d\phi)^2 + \Sigma \Delta K + \Sigma d\theta^2 + \sin^2 \theta \Sigma ((r^2 + a^2) d\phi - a dt)^2$ (Equation 10), (31) where $\Sigma = r^2 + a^2 \cos^2 \theta$, $\Delta K = r^2 - 2Mr + a^2$ (31). Therefore, the transformation $\hat{S}\hat{T}$ in (Equation 3) constitutes a generalisation of the Galilean translations to quantum reference frames. The simplest example of dynamical conserved quantities, in this case, are the two momenta $\hat{C}(C)_1 = \hat{p}^A$ and $\hat{C}(C)_2 = \hat{p}^B$ (Equation 11). It is immediate from (Equation 4) and (5) to see that the choice $\hat{C}(A)_1 = \hat{S}\hat{T}\hat{C}(C)_2 \hat{S}^\dagger \hat{T} = \pi^B$ (Equation 12) and $\hat{C}(A)_2 = -\hat{S}\hat{T}\hat{C}(C)_1 \hat{S}^\dagger \hat{T} - \hat{S}\hat{T}\hat{C}(C)_2 \hat{S}^\dagger \hat{T} = \pi^C$ (Equation 13) leads to the corresponding conserved quantities in the reference frame A. A similar procedure holds when we consider the extended set of conserved quantities composed of translations $\hat{p}^i$ and Galilean boosts $\hat{G}_i = \hat{p}^i t - \text{mix}^i$, $i = A, B$ (Equation 14). Notice that this construction of the $\hat{S}\hat{T}$ operator satisfies the transitive property, meaning that changing the reference frame from C to A directly has the same effect as changing the reference frame first from C to B and then from B to A, i.e. $\hat{S}(C \rightarrow A) \hat{T} = \hat{S}(B \rightarrow A) \hat{T} \hat{S}(C \rightarrow B) \hat{T}$ (Equation 15) static axisymmetric solutions, one may start from a Minkowski spacetime, expressed in Cartesian form as $ds^2 = -dt^2 + dx^2 + dy^2 + dz^2$ (Equation 16). (31) We then applied the following ellipsoid coordinate transformations to (Equation 3) as follows $x \rightarrow (r^2 + a^2)^{1/2} \sin \theta \cos \phi$, $y \rightarrow (r^2 + a^2)^{1/2} \sin \theta \sin \phi$, $z \rightarrow r \cos \theta$, $t \rightarrow t$. (Equation 17). $\{ 1/12 + (|\alpha_1'(t)\rangle CQ_1 t |\phi(t)\rangle_B + |\alpha_2'(t)\rangle CQ_2 t |\phi(t)\rangle_B) \} + F_Q \exp(i/\hbar p^2 A^2 m_A + \dots - 1_{G,k})$ (equation 43) are equivalent as balanced tensor

category $Rep_k(dA+A\wedge AAGA)$ of positive energy representations of the loop group at the:

$\square_{\square}$

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□ **INPUT:** $(432 k^4 N^2 \pi t^2 y^\wedge (n \Lambda) \{ \theta \sin^\wedge (-1) (\sqrt{3}) \}, \theta \sin^\wedge (-1) (\sqrt{779}) \square \sqrt{\theta^3}) - 3/5 \sqrt{779} \theta \sqrt{\theta^3} {}_2F_1(1/2, 5/6, 11/6, 779 \theta^3), 1/6 \sqrt{1/49394 - 9 \theta} \sqrt{\theta} + (\theta - 1/889092) \sin^\wedge (-1) (3 \sqrt{49394} \sqrt{\theta}) \}, \theta \sin^\wedge (-1) (\sqrt{\sin^\wedge (-1) (44545545)}) \} + \text{constant} \sin^\wedge (-1) (n) ^{33833} \sum g x^4 + O((1/x) ^6)) + \sin(2 x) (-216 (k^4 N^2 \pi t^2 y^\wedge (n \Lambda) \sin^\wedge (-1) (n) ^{33833} \sum g) x^3 + O((1/x) ^6)) + e^\wedge (-x^2/2) \sin(2 x) (-108 (k^4 N^2 \sqrt{2 \pi}) t^2 y^\wedge (n \Lambda) \sin^\wedge (-1) (n) ^{33833} \sum g) x^2 + O((1/x) ^6)) + e^\wedge (-x^2/2) \sin(2 x) (108 k^4 N^2 \sqrt{2 \pi}) t^2 y^\wedge (n \Lambda) \sin^\wedge ((n) ^{33833} \sum g x^2 - 108 (k^4 N^2 \sqrt{2 \pi}) t^2 y^\wedge (n \Lambda) \sin^\wedge (-1) (n) ^{33833} \sum g) + (324 k^4 N^2 \sqrt{2 \pi}) t^2 y^\wedge (n \Lambda) \sin^\wedge (-1) (n) ^{33833} \sum g) / x^2 - (1620 (k^4 N^2 \sqrt{2 \pi}) t^2 y^\wedge (n \Lambda) \sin^\wedge (-1) (n) ^{33833} \sum g) / x^4 + O((1/x) ^6)) + e^\wedge (-x^2/2) (216 k^4 N^2 \sqrt{2 \pi}) t^2 y^\wedge (n \Lambda) \sin^\wedge (-1) (n) ^{33833} \sum g x^3 + O((1/x) ^6)) + e^\wedge (-x^2/2) (-216 (k^4 N^2 \sqrt{2 \pi}) t^2 y^\wedge (n \Lambda) \sin^\wedge (-1) (n) ^{33833} \sum g) x^3 + 216 k^4 N^2 \sqrt{2 \pi} t^2 y^\wedge (n \Lambda) \sin^\wedge (-1) (n) ^{33833} \sum g x - (648 (k^4 N^2 \sqrt{2 \pi}) t^2 y^\wedge (n \Lambda) \sin^\wedge ((n) ^{33833} \sum g) / x + (3240 k^4 N^2 \sqrt{2 \pi}) t^2 y^\wedge (n \Lambda) \sin^\wedge (-1) (n) ^{33833} \sum g) / x^3 - (22680 (k^4 N^2 \sqrt{2 \pi}) t^2 y^\wedge (n \Lambda) \sin^\wedge (-1) (n) ^{33833} \sum g) / x^5 + O((1/x) ^6))$ (equations 34,35,36,37,38,39,40-43)

$$\operatorname{Re}\left(\sin^{-1}\left(\frac{2737284773g\sin^{-1}\left(\frac{2737284773g}{r}\right)}{r}\right)\right)$$

**Imaginary
GissitorviffirnaTM_gS part1**

RoccustyrnaTM_fR

- Show contour lines

$$\operatorname{Im}\left(\sin^{-1}\left(\frac{2737284773g\sin^{-1}\left(\frac{2737284773g}{r}\right)}{r}\right)\right)$$

**Real RoccustyrnaTM_fR GissitorviffirnaTM_gS
part1**

- Show contour lines

$$\operatorname{Re}\left(\sin^{-1}\left(\frac{7388288383g\sin^{-1}\left(\frac{7388288383g}{r}\right)}{r}\right)\right)$$

Imaginary
GissitorviffirnaTM_gS part2

RoccustyrnaTM_fR

- Show contour lines

$$\operatorname{Im}\left(\sin^{-1}\left(\frac{7388288383g\sin^{-1}\left(\frac{7388288383g}{r}\right)}{r}\right)\right)$$

Real **RoccustyrnaTM_fR** **GissitorviffirnaTM_gS**
part2

- Show contour lines

$$\operatorname{Re}\left(\sin^{-1}\left(\frac{8383838g\sin^{-1}\left(\frac{8383838g}{r}\right)}{r}\right)\right)$$

**Imaginary
GissitorviffirnaTM_gS part3**

RoccustyrnaTM_fR

- Show contour lines

$$\operatorname{Im}\left(\sin^{-1}\left(\frac{8383838g\sin^{-1}\left(\frac{8383838g}{r}\right)}{r}\right)\right)$$

Contour plots:

**Real RoccustyrnaTM_fR GissitorviffirnaTM_gS
part3**

Imaginary
GissitorviffirnaTM_gS part4

RoccustyrnaTM_fR

Real
part4

RoccustyrnaTM_fR

GissitorviffirnaTM_gS

$$\operatorname{Re}\left(\sin^{-1}\left(\frac{7\,388\,288\,383\,g\sin^{-1}\left(\frac{7\,388\,288\,383\,g}{r}\right)}{r}\right)\right)$$

Imaginary
GissitorviffirnaTM_gS part5

RoccustyrnaTM_fR

$$\operatorname{Im}\left(\sin^{-1}\left(\frac{7\,388\,288\,383\,g\sin^{-1}\left(\frac{7\,388\,288\,383\,g}{r}\right)}{r}\right)\right)$$

Real
part5

RoccustyrnaTM_fR

GissitorviffirnaTM_gS

Imaginary
GissitorviffirnaTM_gS part6

RoccustyrnaTM_fR

(Scheme 4)

Real GissitorviffirnaTM_gS part6

RoccustyrnaTM_fR

- Show contour lines

Imaginary GissitorviffirnaTM_gS part7

RoccustyrnaTM_fR

- Show contour lines

Real GissitorviffirnaTM_gS part7

RoccustyrnaTM_fR

- Show contour lines

Imaginary GissitorviffirnaTM_gS part8

RoccustyrnaTM_fR

- Show contour lines

Real GissitorviffirnaTM_gS part8

RoccustyrnaTM_fR

- Show contour lines

Imaginary GissitorviffirnaTM_gS part9

RoccustyrnaTM_fR

- Show contour lines

Contour plots:

Real
GissitorviffirnaTM_gS part9

RoccustyrnaTM_fR

Imaginary
GissitorviffirnaTM_gS part10

RoccustyrnaTM_fR

Real
GissitorviffirnaTM_gS part10

RoccustyrnaTM_fR

Imaginaryl RoccustyrnaTM_fR
GissitorviffirnaTM_gS part11

Real RoccustyrnaTM_fR
GissitorviffirnaTM_gS part11

Imaginaryl RoccustyrnaTM_fR
 GissitorviffirnaTM_gS part12

$$\begin{aligned}
& \left(432 k^4 N^2 \pi t^2 y^{n \wedge} \sin^{-1}(n)^{33833} \sum g x^4 + o\left(\left(\frac{1}{x}\right)^6\right) \right) + \\
& \sin(2x) \left(-216 \left(k^4 N^2 \pi t^2 y^{n \wedge} \sin^{-1}(n)^{33833} \sum g \right) x^3 + o\left(\left(\frac{1}{x}\right)^6\right) \right) + \\
& e^{-x^2/2} \sin(2x) \left(-108 \left(k^4 N^2 \sqrt{2\pi} t^2 y^{n \wedge} \sin^{-1}(n)^{33833} \sum g \right) x^2 + o\left(\left(\frac{1}{x}\right)^6\right) \right) + \\
& e^{-x^2/2} \sin(2x) \left(108 k^4 N^2 \sqrt{2\pi} t^2 y^{n \wedge} \sin^{-1}(n)^{33833} \sum g x^2 - \right. \\
& \quad 108 \left(k^4 N^2 \sqrt{2\pi} t^2 y^{n \wedge} \sin^{-1}(n)^{33833} \sum g \right) + \\
& \quad \frac{324 k^4 N^2 \sqrt{2\pi} t^2 y^{n \wedge} \sin^{-1}(n)^{33833} \sum g}{x^2} - \\
& \quad \left. \frac{1620 \left(k^4 N^2 \sqrt{2\pi} t^2 y^{n \wedge} \sin^{-1}(n)^{33833} \sum g \right)}{x^4} + o\left(\left(\frac{1}{x}\right)^6\right) \right) + \\
& e^{-x^2/2} \left(216 k^4 N^2 \sqrt{2\pi} t^2 y^{n \wedge} \sin^{-1}(n)^{33833} \sum g x^3 + o\left(\left(\frac{1}{x}\right)^6\right) \right) + \\
& e^{-x^2/2} \left(-216 \left(k^4 N^2 \sqrt{2\pi} t^2 y^{n \wedge} \sin^{-1}(n)^{33833} \sum g \right) x^3 + \right. \\
& \quad 216 k^4 N^2 \sqrt{2\pi} t^2 y^{n \wedge} \sin^{-1}(n)^{33833} \sum g x - \\
& \quad \frac{648 \left(k^4 N^2 \sqrt{2\pi} t^2 y^{n \wedge} \sin^{-1}(n)^{33833} \sum g \right)}{x} + \\
& \quad \frac{3240 k^4 N^2 \sqrt{2\pi} t^2 y^{n \wedge} \sin^{-1}(n)^{33833} \sum g}{x^3} - \\
& \quad \left. \frac{22680 \left(k^4 N^2 \sqrt{2\pi} t^2 y^{n \wedge} \sin^{-1}(n)^{33833} \sum g \right)}{x^5} + o\left(\left(\frac{1}{x}\right)^6\right) \right)
\end{aligned}$$

(Scheme 5)

Scheme 6. Chern-Simons topology geometrics of the 3 selected hit fragmented candidates (fr1), (fr2), (fr3).

In this Scheme we see two subkeys k1 and k2 along the axes of the graph. The choices for them are both ordered by probability. In the x-y plane each square uniquely represents a key k (j) 1|k (i) 2, which is the concatenation of two

subkeys. For this figure we include on the z-axis the probability of each key to illustrate the gradual differences of probabilities in the space. The blue key represents the key k used in the implementation that was attacked. The green keys are those with a higher probability than k^* , the red those with a lower probability. In the graphical representation this would mean starting at the top-left square and using the corresponding key to decipher a ciphertext (or some equivalent check that verifies the key). If this does not yield the desired results, then we try squares one by one, in order of their probabilities until one corresponding key does work.

:: ALGORITHMQMMSR01

ROCCUSTYRNA ::

>

> In this case, the operator $X^A \Psi_1 C M D \Pi C D \Pi_2 |\nabla|_2 = \{ \text{if } \sqrt{(|a_1'(t)|)} C Q_1 t |\phi(t)| B |\nabla|$

$$|2-\Delta K\Sigma(dt-asin2\theta d\phi) \text{ if } \sqrt{(|\alpha_1'(t)|)CQ1t|\phi(t)|B|\nabla|2-\Delta K\Sigma(dt-asin2\theta d\phi)} \neq \exp(i\hbar p^2A2mA(q^{\wedge}Cif$$
$$-\pi^2 \frac{d\pi}{d\pi^2} \left[\nabla^2 \text{phoryl} \right] \text{formonitrile} + + (\text{sqrt}(\theta) \ominus \text{if } (3 \text{ e} \text{-----} \text{del}) \text{v} -$$
$$|\nabla|^2 = \{ 2 D_h dt D_o dp dt V'((p+(pV')^2 f \text{ where } If\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+ if(p) - g(V' (p + i(pv' f)) = 12^{-\sqrt{(|\alpha|'(t)}}$$

$\rangle_{CQ1t}|\phi(t)\rangle_{B+|\alpha_2'(t)\rangle_{CQ2t}|\phi(t)\rangle_B$ if $-\pi^2 C_{md} \pi C_{d\pi^2} ((\langle p + i f(p) - g(V'(p + i(pv) f)) \neq +(\sqrt{\theta}) \Theta$ if (3

e_____ del purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile

$$+ + (\text{sqrt}(\theta) \ominus \text{if } (3 \text{ e} \text{-----} \text{del}) \equiv \int (4(-1) - 2 |\nabla|^2 = \{ 2 \text{ Dh dt dp dtV} ,$$

$(\mathbf{p} + (\mathbf{p} \cdot \mathbf{V}'/2\mathbf{f}))$ where $\mathbf{f} = \hat{\mathbf{S}}\mathbf{b}\mathbf{p}^{\dagger}\mathbf{A}\mathbf{m}\mathbf{A}\hat{\mathbf{S}}^{\dagger}\mathbf{b} + \mathbf{f}(\mathbf{p}) - \mathbf{g}(\mathbf{V}'(\mathbf{p} + \mathbf{i}(\mathbf{p} \cdot \mathbf{V}')\mathbf{f})) = 12^{-1} \sqrt{(|\alpha_1'(\mathbf{t})\rangle \mathbf{CQ}1\mathbf{t}|\phi(\mathbf{t})\rangle \mathbf{B} + |\alpha_2'(\mathbf{t})\rangle$

2-Carboxylicacid;

N-(1-carboximidoyl-3-fluoro-1-{5-oxabicyclo[2.1.0]pentan-2-yl}

-2-oxo-6-([amino([(6-amino-9H-purin-9-yl) methyl] amino)] phosphoryl] carbamoyl] amino)-3,3-di

methyl-7-oxo-4-oxa-1-azabicyclo [3.2.0] heptane-2-Carboxylicacid, N-(1-carboximido-5-fluoro-1-

{5-oxabicyclo [2. 1.0] pentan-2-yl} -2- Carboxylicacid; N-3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl}

-2- oxo-1lambda4,2 lambda5- thiaphosphiran-2 -yl) -N'-yl) -N'-[(Z) - ethylidene]guanidine; [(S)

-amino({[(S) - amino({[(4R) -6-oxo-4,6- dihydro-1H-purin-2-yl] amino}) phosphoryl] oxy}) phos

thiaphosphiran-2 -yl) -N'-yl) -N'-[(Z) + + (sqrt(0) @ (sqrt(0) @ (rboximidoyl- 3- fluoro-1- {5-oxabicyclo

[2. 1.0] pentan-2, + (sqrt(0) @

> if (3 e————— del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1-

{5-oxabicyclo [2.1.0] pentan-2-yl} -purin-2-yl] amino}) phosphoryl] oxy}) phos phoryl] formonitrile 2) (

$2 \text{ Dh dt dp dt}^{-2} (, |\nabla|^2 = \{ 2 \text{ Dh dt Do dp dtV}'((p+(pV'^2f \text{ where } If\hat{S}bp^{\wedge}Am\hat{A}\hat{S}^{\dagger}b+ \text{ if}(p) - g(V '(p + i(pv' f)) = 12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) \text{ if } -\pi^{\wedge}Cmd\pi Cd\pi 2 ((\langle p + \text{ if}(p) - g(V '(p + i(pv' f)) \neq + (sqrt(0) @ \text{ if } (3 e————— del purin-2-yl] amino}) phosphoryl] oxy}) phos phoryl] formonitrile} + + (sqrt(0) @ \text{ if } (3 e————— del)) \equiv \inf >0 |\nabla|^2 = \{ 2 \text{ Dh dt Do dp dtV}'((p+(pV'^2f \text{ where } If\hat{S}bp^{\wedge}Am\hat{A}\hat{S}^{\dagger}b+ \text{ if}(p) - g(V '(p + i(pv' f)) = 12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) \text{ if } -\pi^{\wedge}Cmd\pi Cd\pi 2 ((\langle p + \text{ if}(p) - g(V '(p + i(pv' f)) \neq + (sqrt(0) @ \text{ if } (3 e————— del purin-2-yl] amino}) phosphoryl] oxy}) phos phoryl] formonitrile} + + (sqrt(0) @ \text{ if } (3 e————— del) \text{ d } |\nabla|^2 = \{ 2 \text{ Dh dt Do dp dtV}'((p+(pV'^2f \text{ where } If\hat{S}bp^{\wedge}Am\hat{A}\hat{S}^{\dagger}b+ \text{ if}(p) - g(V '(p + i(pv' f)) = 12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) \text{ if } -\pi^{\wedge}Cmd\pi Cd\pi 2 ((\langle p + \text{ if}(p) - g(V '(p + i(pv' f)) \neq + (sqrt(0) @ \text{ if } (3 e————— del purin-2-yl] amino}) phosphoryl] oxy}) phos phoryl] formonitrile} + + (sqrt(0) @ \text{ if } (3 e————— del) \equiv \int (4(-1)^{-2} |\nabla|^2 = \{ 2 \text{ Dh dt dp dtV}' (p+(pV'^2f \text{ where } If\hat{S}bp^{\wedge}Am\hat{A}\hat{S}^{\dagger}b+ \text{ if}(p) - g(V '(p + i(pv' f)) = 12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) \text{ if } -\pi^{\wedge}Cmd\pi Cd\pi 2 ((\langle p + \text{ if}(p) - g(V '(p + i(pv' f)) \neq \text{ pentan-2-yl}}$

-2-Carboxylicacid; N-(1-carboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl}

-2-oxo6-({[amino({[(6-amino-9H-purin-9-yl) methyl] amino}) phosphoryl] carbamoyl] amino) -3,3- di

methyl-7-oxo-4-thia- 1-azabicyclo [3.2.0] heptane- 2-Carboxylicacid; N-(1-carboximidoyl- 3- fluoro-1-

{5-oxabicyclo [2. 1.0] pentan-2-yl} -2- Carboxylicacid; N-3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl}

-2- oxo-1lambda4,2 lambda5- thiaphosphiran-2 -yl) -N'-yl) -N'-[(Z) - ethylidene]guanidine; [(S)

-amino({[(S) - amino({[(4R) -6-oxo-4,6- dihydro-1H-purin-2-yl] amino}) phosphoryl] oxy}) phos

thiaphosphiran-2 -yl) -N'-yl) -N'-[(Z) + + (sqrt(0) @ (sqrt(0) @ (rboximidoyl- 3- fluoro-1- {5-oxabicyclo

[2. 1.0] pentan-2-yl} -+ (sqrt(0) @ (sqrt(0) @ (rboximidoyl- 3- fluoro-1-(sqrt(0) @ if (3 e—————

del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl]

amino}) phosphoryl oxy}) phos phoryl] formonitrile (sqrt(0) @ if (3 e—————

del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl]

amino}) phosphoryl oxy}) phos phoryl] formonitrile 2) (∫ 2 Dh dt dp dt -2 + |∇ |2 = { 2 Dh dt Do dp

dtV'((p+(pV'2f where IfŜbp^AmAS†b+ if(p) - g(V '(p + i(pv' f)) =12^- √(||α1'(t))CQ1t|φ(t))B+|α2'(t)

)CQ2t|φ(t))B) if -π^CmdπCdπ2 ((<p + if(p) - g(V '(p + i(pv' f)) ≠ + (sqrt(0) @ if (3 e—————

del purin-2-yl] amino}) phosphoryl oxy}) phos phoryl] formonitrile + + (sqrt(0) @ if (3 e—————

del) ≡∫ (4(-1) -2|∇ |2= { + (sqrt(0) @ (sqrt(0) @ (rboximidoyl- 3-formonitrile + + (sqrt- fluoro-phos

phoryl] formonitrile where IfŜbp^AmAS†b+ if(p) - g(V '(p + i(pv' f)) =12^- √(||α1'(t))CQ1t|φ(t)

)B+|α2'(t))CQ2t|φ(t))B) if -π^CmdπCdπ2 ((<p + if(p) - g(V '(p + i(pv' f)) ≠ + (sqrt(0) @ if (3 e————

del purin-2-yl] amino}) phosphoryl oxy}) phos phoryl] formonitrile + + (sqrt(0) @ if (3 e—————

del) (∫ 2 Dh dt dp dt -2 (, |∇ |2 = { 2 Dh dt Do dp dtV'((p+(pV'2f where IfŜbp^AmAS†b+ if(p) - g(V

$$\langle p + i(pv' f) \rangle = 12^{-\sqrt{(|\alpha_1'(t)\rangle CQ1t|\phi(t)\rangle B + |\alpha_2'(t)\rangle CQ2t|\phi(t)\rangle B}} \text{ if } -\pi^{\wedge}Cmd\pi Cd\pi 2 ((\langle p + i(p) \rangle - g(V$$

$$\langle p + i(pv' f) \rangle \neq + (\sqrt{\theta}) \Theta \text{ if } (3 e^{\text{del purin-2-yl] amino}})$$

$$\text{phosphoryl] oxy}}) \text{phos phoryl] formonitrile} + + (\sqrt{\theta}) \Theta \text{ if } (3 e^{\text{del}})$$

$$\text{del}) \equiv \inf_{>0} |\nabla|^2 = \{ 2 Dh dt Do dp dt V'((p+(pV'2f \text{ where } If\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+ i(p) - g(V \langle p + i(pv' f) \rangle$$

$$= 12^{-\sqrt{(|\alpha_1'(t)\rangle CQ1t|\phi(t)\rangle B + |\alpha_2'(t)\rangle CQ2t|\phi(t)\rangle B}} \text{ if } -\pi^{\wedge}Cmd\pi Cd\pi 2 ((\langle p + i(p) \rangle - g(V \langle p + i(pv' f) \rangle$$

$$\neq + (\sqrt{\theta}) \Theta \text{ if } (3 e^{\text{del}}$$

$$> \text{purin-2-yl] amino}}) \text{phosphoryl] oxy}}) \text{phos phoryl] formonitrile} + + (\sqrt{\theta}) \Theta \text{ if } (3 e^{\text{del}}$$

$$\text{del}) (e x) \Theta \sqrt{\theta})$$
 (Equation25) are the number of bonds available or the number of double

bonds. The complete fragmentation Scheme is analyzed to find patterns that are contained within

the selected hit compounds of the Colchicine, Ritonavir, Favipinavir, Balanitin, Baueronol,

Chlorogenin, Behenic acid, Aristolochic acid, Asparagusate, Aspartic acid chemical structures.

Whenever searching for a specific pattern, if the group has such a —chemical bridge|| parent

pattern, the parent pattern is searched first eliminate the terms in $V'(p$, which gives $f = \text{---} \% -r' +$

$g(t)$. One can eliminate the unwanted Vip term by the substitution $ip(r, t) = eiJ \{r, t\} (p(r', t)$

(Equation26). (32,33) Then, as a GENERAL INPUT of (Equations1-25): $V'ip = (V'ip + I V'f)$ eif,

$V'2ip = 1$. If+ $(\sqrt{\theta}) \Theta (\sqrt{\theta}) \Theta (\text{rboximidoyl- 3- fluoro-phos phoryl] formonitrile } 1 = + (\sqrt{\theta})$

$\Theta (\sqrt{\theta}) \Theta (\text{rboximidoyl- 3- fluoro-phos phoryl] formonitrile}$, then+ $(\sqrt{\theta}) \Theta (\sqrt{\theta}) \Theta$

$(\text{rboximidoyl- 3- fluoro-phos phoryl] formonitrile } 1 \oplus + (\sqrt{\theta}) \Theta (\sqrt{\theta}) \Theta (\text{rboximidoyl- 3-}$

$\text{fluoro-phos phoryl] formonitrile } 2 = + (\sqrt{\theta}) \Theta (\sqrt{\theta}) \Theta (\text{rboximidoyl- 3- fluoro-phos phoryl]$

formonitrile 2. 2. If $(\sqrt{\theta} \ominus (\sqrt{\theta} \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}) \text{ formonitrile 2} = +$
 $(\sqrt{\theta} \ominus (\sqrt{\theta} \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}) \text{ formonitrile 1} \oplus + (\sqrt{\theta} \ominus (\sqrt{\theta} \ominus (\text{rboximidoyl- 3-}$
 $\text{fluoro-phos phoryl}) \text{ formonitrile 2} = + (\sqrt{\theta} \ominus (\sqrt{\theta} \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl})$
 $\text{formonitrile 1. Else, let } 1 = (1, 1) \text{ and } 2 = (2, 2). 4. \text{ If } 1 = 2 \text{ and } 1 = -2, \text{ then } 1 \oplus 2 = . 5. \text{ Else, define } \lambda$
 $\text{as } = \{ 2 \text{ Dh dt dp dtV' (p+(pV'2f) where If } \hat{S} \text{bp}^{\wedge} \text{AmA} \hat{S}^{\dagger} \text{b+ if(p) - g(V' (p + i(pv' f)) = } 12^{-\sqrt{(|\alpha 1'(t)$
 $) \text{CQ1t} | \phi(t) \rangle \text{B+ } |\alpha 2'(t) \rangle \text{CQ2t} | \phi(t) \rangle \text{B) if } -\pi^{\wedge} \text{Cmd} \pi \text{Cd} \pi 2 ((\langle p + \text{if(p) - g(V' (p + i(pv' f))} \neq$
 $\text{pentan-2-yl} \} \text{-2-Carboxylicacid; N-(1-carboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl\}}$
 $\text{-2-o xo6-(\{[amino(\{[(6-amino-9H-purin-9-yl) methyl] amino\}) phosphoryl] carbamoyl\} amino) -3,3-}$
 $\text{di methyl-7-oxo-4-thia- 1-azabicyclo [3.2.0] heptane- 2-Carboxylicacid; N-(1-carboximidoyl- 3-}$
 $\text{fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl\} -2- Carboxylicacid; N-3- fluoro-1- \{5-oxabicyclo [2. 1.0]$
 $\text{pentan-2-yl\} -2- oxo-1\lambda 4,2 \lambda 5- thiaphosphiran-2 -yl) -N'-yl) -N'-[(Z) -}$
 $\text{ethylidene]guanidine; [(S) -amino(\{[(S) - amino(\{[(4R) -6-oxo-4,6- dihydro-1H-purin-2-yl] amino\})}$
 $\text{phosphoryl] oxy\}) phos thiaphosphiran-2 -yl) -N'-yl) -N'-[(Z) + + (\sqrt{\theta} \ominus (\sqrt{\theta} \ominus$
 $(\text{rboximidoyl- 3- fluoro-phos phoryl}) \text{ formonitrile 1} = m(V, z(p + 2 iV'f - V' (p + i(pV f - (V'fY < p) =$
 $\text{ifi } ((\langle p + \text{if(p) - g(V' (p + i(pv' f)) and } 3 = (1 -) - 1. \text{ Thus, } 1 \oplus 2 = (, 3). \text{ For example: Let (23): } 2 = 3$
 $+ + 1, 1 = (1, 16), \text{ and } 2 = (11, 20). \text{ Since } 1 \neq 2, = 20 - 16 \equiv 4 \text{ } 11 - 1 \equiv 10 = 4 \cdot 10 - 1 = 4 \cdot 7 \equiv 5(23). \text{ Then use}$
 $\lambda \text{ to compute and } = 5 \text{ } 2 - 1 - 11 = 13(V'2ip + 2iV'f - V' (p + (pV'2f + \langle p(V'f) 2) e_{\underline{f}}, -\sin(-1) (\sqrt{\theta} \ominus$
 $\text{del del } -12 (d \equiv [(4(-1) - 2|\nabla |^2 = \{ + (\sqrt{\theta} \ominus (\sqrt{\theta} 23) \text{ and } 3 = 5(1 - 13) - 16 = 16(23). \text{ Thus, } 1$

$\oplus 2 = (13,16).$ $\{V'^2ip + 2iV'f - V'(p+(pV'^2f+ \langle p(V'f) \rangle 2) e_{\underline{f}}, -\sin^{(-1)}(\sqrt{\theta}) \ominus \text{del del } -12 (d \equiv [(4($
 $-1) -2|\nabla|^2 = \{ + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3-formonitrile} + + (\sqrt{\text{- fluoro-phos phoryl}}$
 $\text{formonitrile} - 11 \neq + (\sqrt{\theta}) \ominus \text{if } (3 e \text{-----} \text{del purin-2-yl] amino})$
 $\text{phosphoryl] oxy}) \text{phos phoryl] formonitrile} + 22 + 2) (\int 2^{-2})^{-2} + |\nabla|^2 = \{ 2 D_h dt Do dp$
 $dtV'((p+(pV'^2f \text{ where } If\hat{S}bp^{\wedge}Am\hat{S}^{\dagger}b+ \text{if}(p) - g(V' (p + i(pv' f)) = 12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t)}$
 $\rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) \text{if } -\pi^{\wedge}Cmd\pi Cd\pi 2 ((\langle p + \text{if}(p) - g(V' (p + i(pv' f)) \neq + (\sqrt{\theta}) \ominus \text{if } (3 e \text{-----}$
 $\text{del purin-2-yl] amino}) \text{phosphoryl] oxy}) \text{phos phoryl] formonitrile} + + (\sqrt{\theta}) \ominus \text{if } (3 e \text{-----}$
 $\text{del}) \equiv [(4(-1) -2|\nabla|^2 = \{ + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3-formonitrile} + + (\sqrt{\text{- fluoro-phos$
 $\text{phoryl] formonitrile where } If\hat{S}bp^{\wedge}Am\hat{S}^{\dagger}b+ \text{if}(p) - g(V' (p + i(pv' f)) = 12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t)}$
 $\rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) \text{if } -\pi^{\wedge}Cmd\pi Cd\pi 2 ((\langle p + \text{if}(p) - g(V' (p + i(pv' f)) \neq + (\sqrt{\theta}) \ominus \text{if } (3 e \text{-----}$
 $\text{del purin-2-yl] amino}) \text{phosphoryl] oxy}) \text{phos phoryl] formonitrile} + + (\sqrt{\theta}) \ominus \text{if } (3 e \text{-----}$
 $\text{del}) (\int 2 D_h dt dp dt^{-2} (, |\nabla|^2 = \{ 2 D_h dt Do dp dtV'((p+(pV'^2f \text{ where } If\hat{S}bp^{\wedge}Am\hat{S}^{\dagger}b+ \text{if}(p) - g(V$
 $'(p + i(pv' f)) = 12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) \text{if } -\pi^{\wedge}Cmd\pi Cd\pi 2 ((\langle p + \text{if}(p) - g(V$
 $'(p + i(pv' f)) \neq + (\sqrt{\theta}) \ominus \text{if } (3 e \text{-----} \text{del purin-2-yl] amino })$
 $\text{phosphoryl] oxy}) \text{phos phoryl] formonitrile} + + (\sqrt{\theta}) \ominus \text{if } (3 e \text{-----}$
 $\text{del}) \equiv \inf > 0 |\nabla|^2 = \{ 2 D_h dt Do dp dtV'((p+(pV'^2f \text{ where } If\hat{S}bp^{\wedge}Am\hat{S}^{\dagger}b+ \text{if}(p) - g(V' (p + i(pv' f))$
 $= 12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) \text{if } -\pi^{\wedge}Cmd\pi Cd\pi 2 ((\langle p + \text{if}(p) - g(V' (p + i(pv'$
 $f)) \neq + (\sqrt{\theta}) \ominus \text{if } (3 e \text{-----} \text{del purin-2-yl] amino}) \text{phosphoryl]oxy})$
 $\text{phos phoryl] formonitrile} + + (\sqrt{\theta}) \ominus \text{if } (3 e \text{-----} \text{del}) v - |\nabla|^2 = \{ 2$

Dh dt Do dp dtV'((p+(pV'2f where If $\hat{S}bp^{\wedge}Am\hat{A}\hat{S}^{\dagger}b+$ if(p) - g(V '(p + i(pv' f)) =12⁻ √(|α1'(t))CQ1t|φ(t))B+|α2'(t))CQ2t|φ(t))B if −π[^]CmdπCdπ2 ((<p + if(p) - g(V '(p + i(pv' f)) ≠ + (sqrt(θ) Θ
if (3 e———— del purin-2-yl] amino)) ph osphoryl]oxy)) phos phoryl]
formonitrile + + (sqrt(θ) Θ if (3 e———— del) ≡ ∫ (4(−1)−2 |∇|^2 = { 2 Dh dt
dp dtV' (p+(pV'2f where If $\hat{S}bp^{\wedge}Am\hat{A}\hat{S}^{\dagger}b+$ if(p) - g(V '(p + i(pv' f)) =12⁻ √(|α1'(t))CQ1t|φ(t))
B+|α2'(t))CQ2t|φ(t))B if −π[^]CmdπCdπ2 ((<p + if(p) - g(V '(p + i(pv' f)) ≠ pentan-2-yl}
-2-Carboxylicacid; N-(1-carboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -2-ox
o-1lamb da4,2lambda5-thiaphosphiran-2 -yl) -N'-yl) -N'-[(Z) + + (sqrt(θ) Θ (sqrt(θ) Θ
(rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -(sqrt(θ) Θ (sqrt(θ) Θ (rboximidoyl-
3- fluoro-1-(sqrt(θ) Θ if (3 e———— del phos phoryl] formonitrile
(rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2- yl] amino)) phosphoryl]
oxy)) phos phoryl] formonitrile (sqrt(θ) Θ if (3 e———— del phos phoryl]
formonitrile (rboximidoyl- 3- fluoro-1- {5-ox abicyclo[2. 1.0] pentan-2-yl} -purin -2-yl] amino))
phosphoryl] oxy)) phos phoryl] formonitrile 2) (∫ 2 Dh dt dp dt −2 (, |∇|^2 = { 2 Dh dt Do dp
dtV'((p+(pV'2f where If $\hat{S}bp^{\wedge}Am\hat{A}\hat{S}^{\dagger}b+$ if(p) - g(V '(p + i(pv' f)) =12⁻ √(|α1'(t))CQ1t|φ(t)
)B+|α2'(t))CQ2t|φ(t))B if −π[^]CmdπCdπ2 ((<p + if(p) - g(V '(p + i(pv' f)) ≠ + (sqrt(θ) Θ if (3 e———
del purin-2-yl] amino)) phosp horyl]oxy)) phos phoryl] formonitrile + + (sqrt(θ) Θ if (3 e————
del)) ≡ inf >0 |∇|^2 = { 2 Dh dt Do dp dtV'((p+(pV'2f where If $\hat{S}bp^{\wedge}Am\hat{A}\hat{S}^{\dagger}b+$ if(p) - g(V '(p + i(pv'
f)) =12⁻ √(|α1'(t))CQ1t|φ(t))B+|α2'(t))CQ2t|φ(t))B if −π[^]CmdπCdπ2 ((<p + if(p) - g(V '(p + i(pv'

f)) $\neq + (\sqrt{\theta}) \Theta$ if $(3 e^{\frac{1}{2} \int_0^t \sqrt{\theta} dt} \text{del purin-2-yl] amino})$ phosphoryl] oxy}}

phos phoryl] formonitrile + + $(\sqrt{\theta}) \Theta$ if $(3 e^{\frac{1}{2} \int_0^t \sqrt{\theta} dt} \text{del}) d |\nabla|^2 = \{ 2 Dh$

dt Do dp dtV'((p+(pV')²f where If $\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+$ if(p) - g(V '(p + i(pv' f)) =12⁻ $\sqrt{(|\alpha_1'(t)|CQ1t|\phi(t)$

)B+ $|\alpha_2'(t)|CQ2t|\phi(t)$)B) if $-\pi^{\wedge}Cmd\pi Cd\pi_2$ (($\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (\sqrt{\theta}) \Theta$ if $(3 e^{\frac{1}{2} \int_0^t \sqrt{\theta} dt}$

del purin-2-yl] amino}) p hosphoryl]oxy}) phos phoryl] formonitrile + + $(\sqrt{\theta}) \Theta$ if $(3 e^{\frac{1}{2} \int_0^t \sqrt{\theta} dt}$

del) $\equiv \int (4(-1) - 2|\nabla|^2 = \{ + (\sqrt{\theta}) \Theta (\sqrt{\theta}) \Theta$ (rboximidoyl- 3-formonitrile + + (sqrt- fluoro-phos

phoryl] formonitrile where If $\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+$ if(p) - g(V '(p + i(pv' f)) =12⁻ $\sqrt{(|\alpha_1'(t)|CQ1t|\phi(t)$

)B+ $|\alpha_2'(t)|CQ2t|\phi(t)$)B) if $-\pi^{\wedge}Cmd\pi Cd\pi_2$ (($\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (\sqrt{\theta}) \Theta$ if $(3 e^{\frac{1}{2} \int_0^t \sqrt{\theta} dt}$

del purin-2-yl] amino}) phosphoryl] oxy}) phos phoryl] formonitrile + + $(\sqrt{\theta}) \Theta$ if $(3 e^{\frac{1}{2} \int_0^t \sqrt{\theta} dt}$

del) ($\int 2 Dh dt dp dt - 2 + |\nabla|^2 = \{ 2 Dh dt Do dp dtV'((p+(pV')^2f$ where If $\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+$ if(p) - g(V

'(p + i(pv' f)) =12⁻ $\sqrt{(|\alpha_1'(t)|CQ1t|\phi(t))B+|\alpha_2'(t)|CQ2t|\phi(t))B}$ if $-\pi^{\wedge}Cmd\pi Cd\pi_2$ (($\langle p + if(p) - g(V$

'(p + i(pv' f)) $\neq + (\sqrt{\theta}) \Theta$ if $(3 e^{\frac{1}{2} \int_0^t \sqrt{\theta} dt} \text{del purin-2-yl] amino})$

phosphoryl] oxy}) phos phoryl] formonitrile + + $(\sqrt{\theta}) \Theta$ if $(3 e^{\frac{1}{2} \int_0^t \sqrt{\theta} dt}$

del) $\equiv \int (4(-1) - 2|\nabla|^2 = \{ + (\sqrt{\theta}) \Theta (\sqrt{\theta}) \Theta$ (rboximidoyl- 3-formonitrile + + (sqrt- fluoro-phos

phoryl] formonitrile where If $\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+$ if(p) - g(V '(p + i(pv' f)) =12⁻ $\sqrt{(|\alpha_1'(t)|CQ1t|\phi(t)$

)B+ $|\alpha_2'(t)|CQ2t|\phi(t))B}$ if $-\pi^{\wedge}Cmd\pi Cd\pi_2$ (($\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (\sqrt{\theta}) \Theta$ if $(3 e^{\frac{1}{2} \int_0^t \sqrt{\theta} dt}$

del purin-2-yl] amino}) phosphoryl] oxy}) phos phoryl] formonitrile + + $(\sqrt{\theta}) \Theta$ if $(3 e^{\frac{1}{2} \int_0^t \sqrt{\theta} dt}$

del) ($\int 2 - 2) - 2$ (, $|\nabla|^2 = \{ 2 Dh dt Do dp dtV'((p+(pV')^2f$ where If $\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+$ if(p) - g(V '(p +

i(pv' f)) =12⁻ $\sqrt{(|\alpha_1'(t)|CQ1t|\phi(t))B+|\alpha_2'(t)|CQ2t|\phi(t))B}$ if $-\pi^{\wedge}Cmd\pi Cd\pi_2$ (($\langle p + if(p) - g(V '(p$

$+ i(pv' f)) \neq + (\sqrt{\theta}) \Theta \text{ if } (3 e^{\frac{1}{2} \sqrt{\theta}} \text{ del purin-2-yl] amino}) \text{ phosphoryl]oxy}) \text{ phos phoryl] formonitrile} + + (\sqrt{\theta}) \Theta \text{ if } (3 e^{\frac{1}{2} \sqrt{\theta}} \text{ del}) \equiv \inf > 0$

$|\nabla|^2 = \{ 2 D_h dt D_o dp dt V'((p+(pV')^2 f \text{ where } If \hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+ \text{ if}(p) - g(V' (p + i(pv' f)) = 12^{-\sqrt{(|\alpha_1'(t) \rangle CQ1t|\phi(t) \rangle B + |\alpha_2'(t) \rangle CQ2t|\phi(t) \rangle B} \text{ if } -\pi^{\wedge}Cmd\pi Cd\pi^2 ((\langle p + \text{if}(p) - g(V' (p + i(pv' f)) \neq + (\sqrt{\theta}) \Theta \text{ if } (3 e^{\frac{1}{2} \sqrt{\theta}} \text{ del purin-2-yl] amino}) \text{ pho sphoryl]oxy}) \text{ phos phoryl] formonitrile} + + (\sqrt{\theta}) \Theta \text{ if } (3 e^{\frac{1}{2} \sqrt{\theta}} \text{ del}) 0) \sin^{(-1)}(y - 3 \sqrt{6734} X Y1^2) - (e \sqrt{\theta}) \Theta \times \text{del}'(0) \text{del}'(\text{del } 0) \sin^{(-1)}(y - 3 \sqrt{6734} X Y1^2)) / \sqrt{1 - \theta} \Theta^2 (\text{del del } -12 (d |\nabla|^2 = \{ 2 D_h dt D_o dp dt V'((p+(pV')^2 f \text{ where } If \hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+ \text{ if}(p) - g(V' (p + i(pv' f)) = 12^{-\sqrt{(|\alpha_1'(t) \rangle CQ1t|\phi(t) \rangle B + |\alpha_2'(t) \rangle CQ2t|\phi(t) \rangle B} \text{ if } -\pi^{\wedge}Cmd\pi Cd\pi^2 ((\langle p + \text{if}(p) - g(V' (p + i(pv' f)) \neq + (\sqrt{\theta}) \Theta \text{ if } (3 e^{\frac{1}{2} \sqrt{\theta}} \text{ del purin-2-yl] amino}) \text{ pho sphoryl]oxy}) \text{ phos phoryl] formonitrile} + + (\sqrt{\theta}) \Theta \text{ if } (3 e^{\frac{1}{2} \sqrt{\theta}} \text{ del}) \equiv \int (4(-1)^{-2} |\nabla|^2 = \{ + (\sqrt{\theta}) \Theta (\sqrt{\theta}) \Theta (\text{rboximidoyl- 3-formonitrile} + + (\sqrt{\theta} \text{ fluoro-phosphoryl] formonitrile where } If \hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+ \text{ if}(p) - g(V' (p + i(pv' f)) = 12^{-\sqrt{(|\alpha_1'(t) \rangle CQ1t|\phi(t) \rangle B + |\alpha_2'(t) \rangle CQ2t|\phi(t) \rangle B} \text{ if } -\pi^{\wedge}Cmd\pi Cd\pi^2 ((\langle p + \text{if}(p) - g(V' (p + i(pv' f)) \neq 231 + 22 + 2) (\int 2 D_h dt dp dt^{-2} + () \equiv \int (4(-1)^{-2} |\nabla|^2 = \{ 2 D_h dt dp dt V' (p+(pV')^2 f \text{ where } If \hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+ \text{ if}(p) - g(V' (p + i(pv' f)) = 12^{-\sqrt{(|\alpha_1'(t) \rangle CQ1t|\phi(t) \rangle B + |\alpha_2'(t) \rangle CQ2t|\phi(t) \rangle B} \text{ if } -\pi^{\wedge}Cmd\pi Cd\pi^2 ((\langle p + \text{if}(p) - g(V' (p + i(pv' f)) \neq \text{pentan-2-yl} \} \text{-2-Carboxylicacid; N-(1-carboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl} \text{-2 -oxo6-}(\{[\text{amino}(\{((6-amino-9H-purin-9-yl) methyl] amino}) \text{ phosphoryl] carbamoyl} \text{ amino) -3,3- di methyl-7-oxo-4-thia- 1-azabicyclo [3.2.0] heptane- 2-Carboxylicacid;}$

N-(1-carboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -2- Carboxylicacid; N-3-
 fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -2- oxo-1lambda4,2 lambda5- thiaphosphiran-2 -yl)
 -N'-yl) -N'-[(Z) - ethylidene]guanidine; [(S) -amino({[(S) - amino({[(4R) -6-oxo-4,6-
 dihydro-1H-purin-2-yl] amino}) phosphoryl] oxy}) phos thiaphosphiran-2 -yl) -N'-yl) -N'-[(Z) + +
 (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(theta) \Theta
 (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-1-(sqrt(theta) \Theta if (3 e_____ del phos
 phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} - purin-2-yl]
 amino}) phosphoryl] oxy}) phos phoryl] formonitrile (sqrt(theta) \Theta if (3 e_____
 del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-
 2-yl] amino}) phosphoryl] oxy}) phos phoryl] formonitrile 2) (\int 2 Dh dt dp dt -2 (, |\nabla |2 = \{ 2 Dh dt
 Do dp dtV'((p+(pV'2f where If\hat{S}bp^{\hat{A}}m\hat{A}\hat{\dagger}b+ if(p) - g(V '(p + i(pv' f)) =12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t)
 \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) if -\pi^{\hat{C}md\pi Cd\pi 2} ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(theta) \Theta if (3 e_____
 del purin-2-yl] amino}) p hosphoryl]oxy}) phos phoryl] formonitrile + + (sqrt(theta) \Theta if (3 e_____
 del)) \equiv \inf >0 |\nabla |2 = \{ 2 Dh dt Do dp dtV'((p+(pV'2f where If\hat{S}bp^{\hat{A}}m\hat{A}\hat{\dagger}b+ if(p) - g(V '(p + i(pv'
 f)) =12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) if -\pi^{\hat{C}md\pi Cd\pi 2} ((\langle p + if(p) - g(V '(p +
 i(pv' f)) \neq + (sqrt(theta) \Theta if (3 e_____ del purin-2-yl] amino}) phosphoryl]
 oxy}) phos phoryl] formonitrile + + (sqrt(theta) \Theta if (3 e_____ del) v - |\nabla |2 =
 \{ 2 Dh dt Do dp dtV'((p+(pV'2f where If\hat{S}bp^{\hat{A}}m\hat{A}\hat{\dagger}b+ if(p) - g(V '(p + i(pv' f)) =12^{-\sqrt{(|\alpha 1'(t)
 \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) if -\pi^{\hat{C}md\pi Cd\pi 2} ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(theta) \Theta

if (3 e^{—————} del purin-2-yl]a mino}) phosphoryl] oxy}) phos phoryl]

formonitrile + + (sqrt(θ) ⊖ if (3 e^{—————} del) ≡ ∫ (4(−1)−2 |∇|2 = { 2 Dh dt

dp dtV' (p+(pV'2f) where IfŜbp^AmAŜ†b+ if(p) - g(V '(p + i(pv' f)) =12[−] √(|α1'(t))CQ1t|φ(t)

)B+|α2'(t))CQ2t|φ(t))B) if −π^CmdπCdπ2 ((<p + if(p) - g(V '(p + i(pv' f)) ≠ pentan-2-yl]

-2-Carboxylicacid; N-(1-carboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -2-oxo-

1lambda4,2lambda5-thiaphosphiran-2 -yl) -N'-yl) - N'-[(Z) + + (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl-

3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3-

fluoro-1-(sqrt(θ) ⊖ if (3 e^{—————} del phos phoryl] formonitrile

(rboximidoyl- 3- fluoro-1- {5 -oxab icyclo[2. 1.0] pentan-2-yl} -purin-2- yl] amino}) phosphoryl]

oxy}) phos phoryl]form onitrile (sqrt(θ) ⊖ if (3 e^{—————} del phos phoryl]

formonitrile (rboximidoyl- 3- fluoro-1- {5-o xabicyclo[2. 1.0] pentan-2-yl} -purin-2- yl] amino}) ph

osphoryl]oxy}) phos phoryl]formo nitrile 2) (∫ 2 Dh dt dp dt −2 (, |∇|2 = { 2 Dh dt Do dp

dtV'((p+(pV'2f) where IfŜbp^AmAŜ†b+ if(p) - g(V '(p + i(pv' f)) =12[−] √(|α1'(t))CQ1t|φ(t))B+|

α2'(t))CQ2t|φ(t))B) if −π^CmdπCdπ2 ((<p + if(p) - g(V '(p + i(pv' f)) ≠ + (sqrt(θ) ⊖ if (3 e^{—————}

del purin-2-yl] amino}) phosp horyl]oxy}) phos phoryl] formonitrile + + (sqrt(θ) ⊖ if (3 e^{—————}

del)) ≡ inf >0 |∇|2 = { 2 Dh dt Do dp dtV'((p+(pV'2f) where IfŜbp^AmAŜ†b+ if(p) - g(V '(p + i(pv'

f)) =12[−] √(|α1'(t))CQ1t|φ(t))B+|α2'(t))C Q2t|φ(t))B) if −π^CmdπCdπ2 ((<p + if(p) - g(V '(p +

i(pv' f)) ≠ + (sqrt(θ) ⊖ if (3 e^{—————} del purin-2-yl]a mino}) phosphoryl]

oxy}) phos phoryl] formonitrile + + (sqrt(θ) ⊖ if (3 e^{—————} del) d |∇|2 = {

2 Dh dt Do dp dtV'((p+(pV'2f where If $\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+$ if(p) - g(V '(p + i(pv' f)) =12⁻ $\sqrt{(|\alpha1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha2'(t) \rangle CQ2t|\phi(t) \rangle B}$ if $-\pi^{\wedge}Cmd\pi Cd\pi2$ ((<p + if(p) - g(V '(p + i(pv' f)) $\neq$ + (sqrt(theta) Θ if (3 e^{—————} del purin-2-yl] amino)) ph osphoryl]oxy)) phos phoryl] formonitrile + + (sqrt(theta) Θ if (3 e^{—————} del) $\equiv \int (4(-1)^{-2} |\nabla|^2 = \{ 2 Dh dt dp dtV' (p+(pV'2f where If\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+$ if(p) - g(V '(p + i(pv' f)) =12⁻ $\sqrt{(|\alpha1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha2'(t) \rangle CQ2t|\phi(t) \rangle B}$ if $-\pi^{\wedge}Cmd\pi Cd\pi2$ ((<p + if(p) - g(V '(p + i(pv' f)) $\neq$ + (sqrt(theta) Θ if (3 e^{—————} del purin-2-yl] amino)) p hosphoryl]oxy)) phos phoryl] formonitrile + + (sqrt(theta) Θ if (3 e^{—————} del) ($\int 2 Dh dt dp dt -2 + |\nabla|^2 = \{ 2 Dh dt Do dp dtV'((p+(pV'2f where If\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+$ if(p) - g(V '(p + i(pv' f)) =12⁻ $\sqrt{(|\alpha1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha2'(t) \rangle CQ2t|\phi(t) \rangle B}$ if $-\pi^{\wedge}Cmd\pi Cd\pi2$ ((<p + if(p) - g(V '(p + i(pv' f)) $\neq$ + (sqrt(theta) Θ if (3 e^{—————} del purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile + + (sqrt(theta) Θ if (3 e^{—————} del) $\equiv \int (4(-1)^{-2} |\nabla|^2 = \{ + (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3-formonitrile + + (sqrt- fluoro-phos phoryl] formonitrile where If\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+$ if(p) - g(V '(p + i(pv' f)) =12⁻ $\sqrt{(|\alpha1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha2'(t) \rangle CQ2t|\phi(t) \rangle B}$ if $-\pi^{\wedge}Cmd\pi Cd\pi2$ ((<p + if(p) - g(V '(p + i(pv' f)) $\neq$ pentan-2-yl} -2-Carboxylic acid; N-(1-carboximidoyl- 3- fluoro-1- {5-oxabicyclo[2. 1.0] pentan-2-yl} -2-oxo-1lambda4 ,2lambda5-thiaphosphiran-2 -yl) -N'-yl) -N'-[(Z) + + (sqrt(theta) Θ (sqrt(theta) Θ (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(theta) Θ (sqrt(theta) Θ (rboximidoyl- 3- fluoro-1-(sqrt(theta) Θ if (3 e^{—————} del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} - purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile

(sqrt(theta) \Theta if (3 e_____ del phos phoryl] formonitrile (rboximidoyl- 3-
fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl]
formonitrile 2) (\int 2 Dh dt dp dt -2 (, |\nabla |2 = { 2 Dh dt Do dp dt V'((p+(pV'2f where If\hat{S}bp^AmA\hat{S}^\dagger b+
if(p) - g(V '(p + i(pv' f)) =12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B} if -\pi^{\text{Cmd}\pi\text{Cd}\pi 2} ((\langle p + if(p) - g(V '(p + i(pv'
+ if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(theta) \Theta if (3 e_____ del purin-2-yl]
amino)) phosphoryl] oxy)) phos phoryl] formonitrile + + (sqrt(theta) \Theta if (3 e_____
del)) \equiv \inf >0 |\nabla |2 = { 2 Dh dt Do dp dt V'((p+(pV'2f where If\hat{S}bp^AmA\hat{S}^\dagger b+ if(p) - g(V '(p + i(pv'
f)) =12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B} if -\pi^{\text{Cmd}\pi\text{Cd}\pi 2} ((\langle p + if(p) - g(V '(p + i(pv'
f)) \neq + (sqrt(theta) \Theta if (3 e_____ del purin-2-yl] amino)) phosphoryl] oxy))
phos phoryl] formonitrile + + (sqrt(theta) \Theta if (3 e_____ del) 0) ^2) - 1/2 x^4
(sqrt(\pi) \sin^{(-1)} (y - 3 sqrt(6734) X Y1^2) ((e^2 \theta^{(3/2)} \Theta^3 del del -12 (d |\nabla |2 = { 2 Dh dt Do dp
dt V'((p+(pV'2f where If\hat{S}bp^AmA\hat{S}^\dagger b+ if(p) - g(V '(p + i(pv' f)) =12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t)
\rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B} if -\pi^{\text{Cmd}\pi\text{Cd}\pi 2} ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(theta) \Theta if (3 e_____
del purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile + + (sqrt(theta) \Theta if (3 e_____
del) \equiv \int (4(-1) -2 |\nabla |2= { + (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3-formonitrile + + (sqrt-
fluoro-phos phoryl] formonitrile where If\hat{S}bp^AmA\hat{S}^\dagger b+ if(p) - g(V '(p + i(pv' f)) =12^{-\sqrt{(|\alpha 1'(t)
\rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B} if -\pi^{\text{Cmd}\pi\text{Cd}\pi 2} ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(theta) \Theta
if (3 e_____ del purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl]
formonitrile + + (sqrt(theta) \Theta if (3 e_____ del) (\int 2 Dh dt dp dt -2 + |\nabla |2 = f

[illegible]

$\text{del}) \equiv \int (4(-1) - 2 |\nabla|^2 = \{ 2 D_h dt dp dt V' (p + (pV')^2 f) \text{ where } If \hat{S}bp^{\wedge}Am\hat{A}\hat{S}^{\dagger}b + if(p) - g(V' (p + i(pv' f)) = 12^{-\sqrt{(|\alpha_1'(t) \rangle CQ1t|\phi(t) \rangle B + |\alpha_2'(t) \rangle CQ2t|\phi(t) \rangle B)} if -\pi^{\wedge}Cmd\pi Cd\pi^2 ((\langle p + if(p) - g(V' (p + i(pv' f)) \neq \text{pentan-2-yl} \} -2\text{-Carboxylicacid}; N\text{-(1-carboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl} -2-oxo6-}(\{[amino(\{[(6-amino-9H-purin-9-yl) methyl] amino\}) phosphoryl] carbamoyl} amino) -3,3- di methyl-7-oxo-4-thia- 1-azabicyclo [3.2.0] heptane- 2-Carboxylicacid}; N\text{-(1-carboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl} -2- Carboxylicacid}; N\text{-3-fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl} -2- oxo-1\lambda^4,2 \lambda^5- thiaphosphiran-2 -yl) -N'-yl) -N'-}[(Z) - ethylidene]guanidine; [(S) -amino(\{[(S) - amino(\{[(4R) -6-oxo-4,6-dihydro-1H-purin-2-yl] amino\}) phosphoryl] oxy\}) phos thiaphosphiran-2 -yl) -N'-yl) -N'-}[(Z) + + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl} \rightarrow + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (rboximidoyl- 3- fluoro-1-(\sqrt{\theta}) \ominus if (3 e\text{-----} del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl] amino\}) phosphoryl] oxy\}) phos phoryl] formonitrile (\sqrt{\theta}) \ominus if (3 e\text{-----} del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl] amino\}) phosphoryl] oxy\}) phos phoryl] formonitrile 2) (\int 2 D_h dt dp dt -2 (, |\nabla|^2 = \{ 2 D_h dt Do dp dt V'((p + (pV')^2 f \text{ where } If \hat{S}bp^{\wedge}Am\hat{A}\hat{S}^{\dagger}b + if(p) - g(V' (p + i(pv' f)) = 12^{-\sqrt{(|\alpha_1'(t) \rangle CQ1t|\phi(t) \rangle B + |\alpha_2'(t) \rangle CQ2t|\phi(t) \rangle B)} if -\pi^{\wedge}Cmd\pi Cd\pi^2 ((\langle p + if(p) - g(V' (p + i(pv' f)) \neq + (\sqrt{\theta}) \ominus if (3 e\text{-----} del purin-2-yl] amino\}) phosphoryl] oxy\}) phos phoryl] formonitrile + + (\sqrt{\theta}) \ominus if (3 e\text{-----} del)) \equiv \inf > 0 |\nabla|^2 = \{ 2 D_h dt Do$

[illegible]

N-(1-carboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -2- Carboxylicacid; N-3-
 fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -2- oxo-1lambda4,2 lambda5- thiaphosphiran-2 -yl)
 -N'-yl) -N'-[(Z) - ethylidene]guanidine; [(S) -amino({[(S) - amino({[(4R) -6-oxo-4,6-
 dihydro-1H-purin-2-yl] amino}) phosphoryl] oxy}) phos thiaphosphiran-2 -yl) -N'-yl) -N'-[(Z) + +
 (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(theta) \Theta
 (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-1-(sqrt(theta) \Theta if (3 e_____ del phos
 phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl]
 amino}) phosphoryl] oxy}) phos phoryl] formonitrile (sqrt(theta) \Theta if (3 e_____ del
 phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl}
 -purin-2-yl] amino}) phosphoryl] oxy}) phos phoryl] formonitrile 2) (\int 2 Dh dt dp dt -2 (, |\nabla |2 = { 2
 Dh dt Do dp dtV'((p+(pV'2f where If\hat{S}bp^AmA\hat{S}^\dagger b+ if(p) - g(V '(p + i(pv' f)) =12^- \sqrt{(|\alpha 1'(t)
)CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) if -\pi^{\rm Cmd}\pi C d\pi 2 ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(theta) \Theta
 if (3 e_____ del purin-2-yl] amino}) phosphoryl] oxy}) phos phoryl]
 formonitrile + + (sqrt(theta) \Theta if (3 e_____ del)) \equiv \inf >0 |\nabla |2 = { 2 Dh dt Do
 dp dtV'((p+(pV'2f where If\hat{S}bp^AmA\hat{S}^\dagger b+ if(p) - g(V '(p + i(pv' f)) =12^- \sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t)
 \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) if -\pi^{\rm Cmd}\pi C d\pi 2 ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(theta) \Theta if (3 e_____ del
 purin-2-yl] amino}) phosphoryl] oxy}) phos phoryl] formonitrile + + (sqrt(theta) \Theta if (3 e_____ del)
 0 (del '(0)) ^2 (del '(del 0)) ^2)/(sqrt(\pi) (1 - \theta \Theta ^2 (del del -12 (d |\nabla |2 = { 2 Dh dt Do dp
 dtV'((p+(pV'2f where If\hat{S}bp^AmA\hat{S}^\dagger b+ if(p) - g(V '(p + i(pv' f)) =12^- \sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t)

$\rangle B + |\alpha_2'(t)\rangle C Q 2 t | \phi(t)\rangle B$ if $-\pi^{\wedge} C m d \pi C d \pi 2 ((\langle p + i f(p) - g(V '(p + i(p v' f)) \neq + (\sqrt{\theta}) \Theta$ if (3 e~~_____~~

del purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile + + ($\sqrt{\theta}) \Theta$ if (3 e~~_____~~

del) $\equiv \int (4(-1) - 2 |\nabla|^2 = \{ 2 - 1^2$ where If $\hat{S} b p^{\wedge} A m A \hat{S}^{\dagger} b + i f(p) - g(V '(p + i(p v' f)) = 12^{-} \sqrt{(|\alpha_1'(t)$

$\rangle C Q 1 t | \phi(t)\rangle B + |\alpha_2'(t)\rangle C Q 2 t | \phi(t)\rangle B$ if $-\pi^{\wedge} C m d \pi C d \pi 2 ((\langle p + i f(p) - g(V '(p + i(p v' f)) \neq + (\sqrt{\theta}) \Theta$

if (3 e~~_____~~ del purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl]

formonitrile + + ($\sqrt{\theta}) \Theta$ if (3 e~~_____~~ del) ($\int 2 D h d t d p d t - 2 + |\nabla|^2 = \{$

$2 D h d t D o d p d t V'((p + (p V' 2 f$ where If $\hat{S} b p^{\wedge} A m A \hat{S}^{\dagger} b + i f(p) - g(V '(p + i(p v' f)) = 12^{-} \sqrt{(|\alpha_1'(t)$

$\rangle C Q 1 t | \phi(t)\rangle B + |\alpha_2'(t)\rangle C Q 2 t | \phi(t)\rangle B$ if $-\pi^{\wedge} C m d \pi C d \pi 2 ((\langle p + i f(p) - g(V '(p + i(p v' f)) \neq + (\sqrt{\theta}) \Theta$

if (3 e~~_____~~ del purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl]

formonitrile + + ($\sqrt{\theta}) \Theta$ if (3 e~~_____~~ del) $\equiv \int (4(-1) - 2 |\nabla|^2 = \{ 2 D h d t$

$d p d t V' (p + (p V' 2 f$ where If $\hat{S} b p^{\wedge} A m A \hat{S}^{\dagger} b + i f(p) - g(V '(p + i(p v' f)) = 12^{-} \sqrt{(|\alpha_1'(t) \rangle C Q 1 t | \phi(t)$

$\rangle B + |\alpha_2'(t)\rangle C Q 2 t | \phi(t)\rangle B$ if $-\pi^{\wedge} C m d \pi C d \pi 2 ((\langle p + i f(p) - g(V '(p + i(p v' f)) \neq$ pentan-2-yl}

-2-Carboxylic acid; N-(1-carboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl}

-2-oxo6-({[amino({[(6-amino-9H-purin-9-yl) methyl] amino)) phosphoryl] carbamoyl} amino) -3,3-

di methyl-7-oxo-4-thia- 1-azabicyclo [3.2.0] heptane- 2-Carboxylic acid; N-(1-carboximidoyl- 3-

fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -2- Carboxylic acid; N-3- fluoro-1- {5-oxabicyclo [2. 1.0]

pentan-2-yl} -2- oxo-1 λ 4,2 λ 5- thiaphosphiran-2 -yl) -N'-yl) -N'-[(Z) -

ethylidene]guanidine; [(S) -amino({[(S) - amino({[(4R) -6-oxo-4,6- dihydro-1H-purin-2-yl] amino})

phosphoryl] oxy)) phos thiaphosphiran-2 -yl) -N'-yl) -N'-[(Z) + + ($\sqrt{\theta}) \Theta$ ($\sqrt{\theta}) \Theta$

(rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(θ) ⊗ (sqrt(θ) ⊗ (rboximidoyl-
 3- fluoro-1-(sqrt(θ) ⊗ if (3 e^{_____} del phos phoryl] formonitrile
 (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl] amino)) phosphoryl] oxy))
 phos phoryl] formonitrile (sqrt(θ) ⊗ if (3 e^{_____} del phos phoryl]
 formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl] amino))
 phosphoryl] oxy)) phos phoryl] formonitrile 2) (∫ 2 Dh dt dp dt -2 (, |∇ |2 = { 2 Dh dt Do dp
 dtV'((p+(pV'2f where IfŜbp^AmAŜ†b+ if(p) - g(V '(p + i(pv' f)) =12⁻ √(|α1'(t))CQ1t|φ(t)
)B+|α2'(t))CQ2t|φ(t))B) if -π^CmdπCdπ2 ((<p + if(p) - g(V '(p + i(pv' f)) ≠ + (sqrt(θ) ⊗ if (3 e^{_____}
 del purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile + + (sqrt(θ) ⊗ if (3 e^{_____}
 del)) ≡ inf >0 |∇ |2 = { 2 Dh dt Do dp dtV'((p+(pV'2f where IfŜbp^AmAŜ†b+ if(p) - g(V '(p + i(pv'
 f)) =12⁻ √(|α1'(t))CQ1t|φ(t))B+|α2'(t))CQ2t|φ(t))B) if -π^CmdπCdπ2 ((<p + if(p) - g(V '(p + i(pv'
 f)) ≠ + (sqrt(θ) ⊗ if (3 e^{_____} del purin-2-yl] amino)) phosphoryl] oxy))
 phos phoryl] formonitrile + + (sqrt(θ) ⊗ if (3 e^{_____} del) v - |∇ |2 = { 2
 Dh dt Do dp dtV'((p+(pV'2f where IfŜbp^AmAŜ†b+ if(p) - g(V '(p + i(pv' f)) =12⁻ √(|α1'(t)
)CQ1t|φ(t))B+|α2'(t))CQ2t|φ(t))B) if -π^CmdπCdπ2 ((<p + if(p) - g(V '(p + i(pv' f)) ≠ + (sqrt(θ) ⊗
 if (3 e^{_____} del purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl]
 formonitrile + + (sqrt(θ) ⊗ if (3 e^{_____} del) ≡ ∫ (4(-1) -2|∇ |2= { +
 (sqrt(θ) ⊗ (sqrt(θ) ⊗ (rboximidoyl- 3-formonitrile + + (sqrt- fluoro-phos phoryl] formonitrile where
 IfŜbp^AmAŜ†b+ if(p) - g(V '(p + i(pv' f)) =12⁻ √(|α1'(t))CQ1t|φ(t))B+|α2'(t))CQ2t|φ(t))B) if

$-\pi^{\wedge}\text{Cmd}\pi\text{Cd}\pi^2 ((\leq p + \text{if}(p) - g(V \text{ '}(p + i(pv' f)) \neq + (\text{sqrt}(\theta) \ominus \text{if} (3 e$
 $\text{del purin-2-yl] amino}) \text{ phosphoryl] oxy}) \text{ phos phoryl] formonitrile} + + (\text{sqrt}(\theta) \ominus \text{if} (3 e$
 $\text{del}) (\int 2 D h \text{ dt dp dt } -2 (, |\nabla |^2 = \{ 2 D h \text{ dt Do dp dt } V'((p+(pV'2f \text{ where } \text{If}\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+ \text{if}(p) - g(V$
 $\text{'}(p + i(pv' f)) = 12^{-} \sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B + |\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) \text{ if } -\pi^{\wedge}\text{Cmd}\pi\text{Cd}\pi^2 ((\leq p + \text{if}(p) - g(V$
 $\text{'}(p + i(pv' f)) \neq + (\text{sqrt}(\theta) \ominus \text{if} (3 e$ $\text{del purin-2-yl] amino})$
 $\text{ phosphoryl] oxy}) \text{ phos phoryl] formonitrile} + + (\text{sqrt}(\theta) \ominus \text{if} (3 e$
 $\text{del}) \equiv \inf > 0 |\nabla |^2 = \{ 2 D h \text{ dt Do dp dt } V'((p+(pV'2f \text{ where } \text{If}\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+ \text{if}(p) - g(V \text{ '}(p + i(pv' f))$
 $= 12^{-} \sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B + |\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) \text{ if } -\pi^{\wedge}\text{Cmd}\pi\text{Cd}\pi^2 ((\leq p + \text{if}(p) - g(V \text{ '}(p + i(pv' f))$
 $\neq + (\text{sqrt}(\theta) \ominus \text{if} (3 e$ $\text{del purin-2-yl] amino}) \text{ phosphoryl] oxy}) \text{ phos$
 $\text{ phoryl] formonitrile} + + (\text{sqrt}(\theta) \ominus \text{if} (3 e$ $\text{del} \text{ d } |\nabla |^2 = \{ 2 D h \text{ dt Do}$
 $\text{dp dt } V'((p+(pV'2f \text{ where } \text{If}\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+ \text{if}(p) - g(V \text{ '}(p + i(pv' f)) = 12^{-} \sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t)$
 $\rangle B + |\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) \text{ if } -\pi^{\wedge}\text{Cmd}\pi\text{Cd}\pi^2 ((\leq p + \text{if}(p) - g(V \text{ '}(p + i(pv' f)) \neq + (\text{sqrt}(\theta) \ominus \text{if} (3 e$
 $\text{del purin-2-yl] amino}) \text{ phosphoryl] oxy}) \text{ phos phoryl] formonitrile} + + (\text{sqrt}(\theta) \ominus \text{if} (3 e$
 $\text{del}) \equiv \int (4(-1) -2 |\nabla |^2 = \{ 2 D h \text{ dt dp dt } V' (p+(pV'2f \text{ where } \text{If}\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+ \text{if}(p) - g(V \text{ '}(p + i(pv'$
 $f)) = 12^{-} \sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B + |\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) \text{ if } -\pi^{\wedge}\text{Cmd}\pi\text{Cd}\pi^2 ((\leq p + \text{if}(p) - g(V \text{ '}(p + i(pv'$
 $f)) \neq \text{pentan-2-yl} \} \text{-2-Carboxylicacid; N-(1-carboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0]$
 $\text{pentan-2-yl} \} \text{-2-oxo6-}(\{\text{amino}(\{\{(6\text{-amino-9H-purin-9-yl) methyl] amino}) \text{ phosphoryl] carbamoyl}$
 $\text{amino}) \text{-3,3- di methyl-7-oxo-4-thia- 1-azabicyclo [3.2.0] heptane- 2-Carboxylicacid;$
 $\text{N-(1-carboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl} \} \text{-2- Carboxylicacid; N-3-}$

fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -2- oxo-1lambda4,2 lambda5- thiaphosphiran-2 -yl)
 -N'-yl) -N'-[(Z) - ethylidene]guanidine; [(S) -amino({[(S) - amino({[(4R) -6-oxo-4,6-
 dihydro-1H-purin-2-yl] amino}) phosphoryl] oxy}) phos thiaphosphiran-2 -yl) -N'-yl) -N'-[(Z) + +
 (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(theta) \Theta
 (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-1-(sqrt(theta) \Theta if (3 e_____ del phos
 phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl]
 amino}) phosphoryl] oxy}) phos phoryl] formonitrile (sqrt(theta) \Theta if (3 e_____
 del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl]
 -purin-2-yl] amino}) phosphoryl] oxy}) phos phoryl] formonitrile 2) (\int 2 Dh dt dp dt -2 + |\nabla |2 = { 2
 Dh dt Do dp dtV'((p+(pV')2f where If\hat{S}bp^Am\hat{S}^\dagger b+ if(p) - g(V '(p + i(pv' f)) =12^- \sqrt{(|\alpha 1'(t)
)CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) if -\pi^{\wedge}Cmd\pi Cd\pi 2 ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(theta) \Theta
 if (3 e_____ del purin-2-yl] amino}) phosphoryl] oxy}) phos phoryl]
 formonitrile + + (sqrt(theta) \Theta if (3 e_____ del) \equiv (\int (4(-1) -2|\nabla |2= { + (sqrt(theta)
 \Theta (sqrt(theta) \Theta (rboximidoyl- 3-formonitrile + + (sqrt- fluoro-phos phoryl] formonitrile where
 If\hat{S}bp^Am\hat{S}^\dagger b+ if(p) - g(V '(p + i(pv' f)) =12^- \sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) if
 -\pi^{\wedge}Cmd\pi Cd\pi 2 ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(theta) \Theta if (3 e_____
 del purin-2-yl] amino}) phosphoryl] oxy}) phos phoryl] formonitrile + 22 +2) (\int 2 Dh dt dp dt -2 (, |\nabla
 |2 = { 2 Dh dt Do dp dtV'((p+(pV')2f where If\hat{S}bp^Am\hat{S}^\dagger b+ if(p) - g(V '(p + i(pv' f)) =12^- \sqrt{(|\alpha 1'(t)
 \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) if -\pi^{\wedge}Cmd\pi Cd\pi 2 ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(theta) \Theta

if (3 e $\frac{1}{\sqrt{2}}$ del purin-2-yl] amino}) phosphoryl] oxy}) phos phoryl]

formonitrile + + (sqrt(θ) Θ if (3 e $\frac{1}{\sqrt{2}}$ del)) $\equiv \inf >0 \left| \nabla \right|^2 = \{ 2 \, D_h \, dt \, Do$

dp dtV'((p+(pV'2f where If $\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+$ if(p) - g(V '(p + i(pv' f)) =12 $^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B}$ if $-\pi^{\wedge}Cmd\pi Cd\pi 2 ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(\theta) \, \Theta$ if (3 e $\frac{1}{\sqrt{2}}$

del purin-2-yl] amino}) phosphoryl] oxy}) phos phoryl] formonitrile + + (sqrt(θ) Θ if (3 e $\frac{1}{\sqrt{2}}$

del) 0) 2) $^{(3/2)}$) + (sqrt(θ) Θ (e 2 (del ' (0)) 2 del '' (del 0) + e 2 del ' (del 0) del '' (0))) /(sqrt(π)

sqrt(1 - $\theta \, \Theta^2$ (del del $-12 \, (d \left| \nabla \right|^2 = \{ 2 \, D_h \, dt \, Do$ dp dtV'((p+(pV'2f where If $\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+$ if(p) -

g(V '(p + i(pv' f)) =12 $^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B}$ if $-\pi^{\wedge}Cmd\pi Cd\pi 2 ((\langle p + if(p) -$

g(V '(p + i(pv' f)) $\neq + (sqrt(\theta) \, \Theta$ if (3 e $\frac{1}{\sqrt{2}}$ del purin-2-yl] amino}))

phosphoryl] oxy}) phos phoryl] formonitrile + + (sqrt(θ) Θ if (3 e $\frac{1}{\sqrt{2}}$

del) $\equiv \int (4(-1)^{-2} \left| \nabla \right|^2 = \{ + (sqrt(\theta) \, \Theta (sqrt(\theta) \, \Theta$ (rboximidoyl- 3-formonitrile + + (sqrt- fluoro-phos

phoryl] formonitrile where If $\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+$ if(p) - g(V '(p + i(pv' f)) =12 $^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B}$ if $-\pi^{\wedge}Cmd\pi Cd\pi 2 ((\langle p + if(p) - g(V$

del purin-2-yl] amino}) phosphoryl] oxy}) phos phoryl] formonitrile + + (sqrt(θ) Θ if (3 e $\frac{1}{\sqrt{2}}$

del) ($\int 2 \, D_h \, dt \, dp \, dt -2 + \left| \nabla \right|^2 = \{ 2 \, D_h \, dt \, Do$ dp dtV'((p+(pV'2f where If $\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+$ if(p) - g(V

'(p + i(pv' f)) =12 $^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B}$ if $-\pi^{\wedge}Cmd\pi Cd\pi 2 ((\langle p + if(p) - g(V$

'(p + i(pv' f)) $\neq + (sqrt(\theta) \, \Theta$ if (3 e $\frac{1}{\sqrt{2}}$ del purin-2-yl] amino}))

phosphoryl] oxy}) phos phoryl] formonitrile + + (sqrt(θ) Θ if (3 e $\frac{1}{\sqrt{2}}$

del) $\equiv \int (4(-1)^{-2} \left| \nabla \right|^2 = \{ 2 \, D_h \, dt \, dp \, dt V' (p+(pV'2f) where If $\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+$ if(p) - g(V '(p + i(pv'$

f)) =12⁻ √((||α1'(t))CQ1t|φ(t))B+|α2'(t))CQ2t|φ(t))B) if −π[^]CmdπCdπ2 ((<p + if(p) - g(V '(p + i(pv' f)) ≠ pentan-2-yl} -2-Carboxylicacid; N-(1-carboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -2-oxo6-({[amino({[(6-amino-9H-purin-9-yl) methyl] amino)) phosphoryl] carbamoyl} amino) -3,3- di methyl-7-oxo-4-thia- 1-azabicyclo [3.2.0] heptane- 2-Carboxylicacid, N-(1-carboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -2- Carboxylicacid; N-3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -2- oxo-1λ4,2 λ5- thiaphosphiran-2 -yl) -N'-yl) -N'-[(Z) - ethylidene]guanidine; [(S) -amino({[(S) - amino({[(4R) -6-oxo-4,6-dihydro-1H-purin-2-yl] amino)) phosphoryl] oxy}) phos thiaphosphiran-2 -yl) -N'-yl) -N'-[(Z) + + (sqrt(θ) ⊗ (sqrt(θ) ⊗ (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} → (sqrt(θ) ⊗ (sqrt(θ) ⊗ (rboximidoyl- 3- fluoro-1-(sqrt(θ) ⊗ if (3 e^{_____} del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl] amino)) phosphoryl] oxy}) phos phoryl] formonitrile (sqrt(θ) ⊗ if (3 e^{_____} del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl] amino)) phosphoryl] oxy}) phos phoryl] formonitrile 2) (∫ 2 Dh dt dp dt −2 (, |∇ |2 = { 2 Dh dt Do dp dtV'((p+(pV'2f where IfŜbp^AmAS†b+ if(p) - g(V '(p + i(pv' f)) =12⁻ √((||α1'(t))CQ1t|φ(t))B+|α2'(t))CQ2t|φ(t))B) if −π[^]CmdπCdπ2 ((<p + if(p) - g(V '(p + i(pv' f)) ≠ + (sqrt(θ) ⊗ if (3 e^{_____} del purin-2-yl] amino)) phosphoryl] oxy}) phos phoryl] formonitrile + + (sqrt(θ) ⊗ if (3 e^{_____} del)) ≡ inf >0 |∇ |2 = { 2 Dh dt Do dp dtV'((p+(pV'2f where IfŜbp^AmAS†b+ if(p) - g(V '(p + i(pv' f)) =12⁻ √((||α1'(t))CQ1t|φ(t))B+|α2'(t))CQ2t|φ(t))B) if −π[^]CmdπCdπ2 ((<p + if(p) - g(V '(p + i(pv' f)) ≠ + (sqrt(θ) ⊗

$\rangle B + |a_2'(t)\rangle CQ2t|\phi(t)\rangle B$ if $-\pi^{\wedge}Cmd\pi Cd\pi2 ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(\theta) \Theta$ if (3 e~~_____~~

del purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile + + (sqrt(\theta) \Theta if (3 e~~_____~~

del) $v - |\nabla|^2 = \{ 2 Dh dt Do dp dtV'((p+(pV'2f$ where If $\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+$ if(p) - g(V '(p + i(pv' f))

$=12^{-\sqrt{(|a_1'(t)\rangle CQ1t|\phi(t)\rangle B + |a_2'(t)\rangle CQ2t|\phi(t)\rangle B)}$ if $-\pi^{\wedge}Cmd\pi Cd\pi2 ((\langle p + if(p) - g(V '(p + i(pv' f))$

$\neq + (sqrt(\theta) \Theta$ if (3 e~~_____~~ del purin-2-yl] amino)) phosphoryl] oxy)) phos

phoryl] formonitrile + + (sqrt(\theta) \Theta if (3 e~~_____~~ del) $\equiv](4(-1) - 2|\nabla|^2 = \{ +$

(sqrt(\theta) \Theta (sqrt(\theta) \Theta (rboximidoyl- 3-formonitrile + + (sqrt- fluoro-phos phoryl] formonitrile where

If $\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+$ if(p) - g(V '(p + i(pv' f)) $=12^{-\sqrt{(|a_1'(t)\rangle CQ1t|\phi(t)\rangle B + |a_2'(t)\rangle CQ2t|\phi(t)\rangle B)}$ if

$-\pi^{\wedge}Cmd\pi Cd\pi2 ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(\theta) \Theta$ if (3 e~~_____~~

del purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile + + (sqrt(\theta) \Theta if (3 e~~_____~~

del) ($\int 2 Dh dt dp dt -2$ (, $|\nabla|^2 = \{ 2 Dh dt Do dp dtV'((p+(pV'2f$ where If $\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+$ if(p) - g(V

'(p + i(pv' f)) $=12^{-\sqrt{(|a_1'(t)\rangle CQ1t|\phi(t)\rangle B + |a_2'(t)\rangle CQ2t|\phi(t)\rangle B)}$ if $-\pi^{\wedge}Cmd\pi Cd\pi2 ((\langle p + if(p) - g(V$

'(p + i(pv' f)) $\neq + (sqrt(\theta) \Theta$ if (3 e~~_____~~ del purin-2-yl] amino))

phosphoryl] oxy)) phos phoryl] formonitrile + + (sqrt(\theta) \Theta if (3 e~~_____~~

del)) $\equiv \inf >0 |\nabla|^2 = \{ 2 Dh dt Do dp dtV'((p+(pV'2f$ where If $\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+$ if(p) - g(V '(p + i(pv' f))

$=12^{-\sqrt{(|a_1'(t)\rangle CQ1t|\phi(t)\rangle B + |a_2'(t)\rangle CQ2t|\phi(t)\rangle B)}$ if $-\pi^{\wedge}Cmd\pi Cd\pi2 ((\langle p + if(p) - g(V '(p + i(pv' f))$

$\neq + (sqrt(\theta) \Theta$ if (3 e~~_____~~ del

$>$

purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile + +

(sqrt(\theta) \Theta if (3 e~~_____~~ del) $d|\nabla|^2 = \{ 2 Dh dt Do dp dtV'((p+(pV'2f$ where

$$\text{If}\hat{S}_{bp}^{\wedge}Am\hat{A}\hat{S}_{\dagger}^{\dagger}b+ \text{if}(p) - g(V' (p + i(pv' f)) = 12^{-\sqrt{(|\alpha_1'(t) \rangle CQ1t|\phi(t) \rangle B + |\alpha_2'(t) \rangle CQ2t|\phi(t) \rangle B)} \text{ if}$$

$$-\pi^{\wedge}Cmd\pi Cd\pi^2 ((\langle p + \text{if}(p) - g(V' (p + i(pv' f)) \neq + (\sqrt{\theta}) \Theta \text{ if } (3 e \text{-----}$$

$$\text{del purin-2-yl] amino}) \text{ phosphoryl] oxy}) \text{ phos phoryl] formonitrile} + + (\sqrt{\theta}) \Theta \text{ if } (3 e \text{-----}$$

$$\text{del}) \equiv \int (4(-1) - 2|\nabla|^2 = \{ 2 Dh dt dp dt V' (p + (pV' 2f \text{ where } \text{If}\hat{S}_{bp}^{\wedge}Am\hat{A}\hat{S}_{\dagger}^{\dagger}b+ \text{if}(p) - g(V' (p + i(pv' f)) = 12^{-\sqrt{(|\alpha_1'(t) \rangle CQ1t|\phi(t) \rangle B + |\alpha_2'(t) \rangle CQ2t|\phi(t) \rangle B)} \text{ if}$$

$$-\pi^{\wedge}Cmd\pi Cd\pi^2 ((\langle p + \text{if}(p) - g(V' (p + i(pv' f)) \neq \text{ pentan-2-yl} \} - 2\text{-Carboxylic acid; N-(1-carboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0]$$

$$\text{pentan-2-yl} \} - 2\text{-oxo-1}\lambda^4, 2\lambda^5\text{-thiaphosphiran-2 -yl} - N'\text{-yl} - N'\text{-(Z)} + + (\sqrt{\theta}) \Theta$$

$$(\sqrt{\theta}) \Theta (\text{rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl} - + (\sqrt{\theta}) \Theta (\sqrt{\theta}) \Theta$$

$$(\text{rboximidoyl- 3- fluoro-1-}(\sqrt{\theta}) \Theta \text{ if } (3 e \text{-----} \text{del phos phoryl]$$

$$\text{formonitrile (rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl} - purin-2-yl] amino})$$

$$\text{phosphoryl] oxy}) \text{ phos phoryl] formonitrile } (\sqrt{\theta}) \Theta \text{ if } (3 e \text{-----} \text{del}$$

$$\text{phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl} - purin-2-yl]$$

$$\text{amino}) \text{ phosphoryl] oxy}) \text{ phos phoryl] formonitrile } 2) (\int 2 Dh dt dp dt - 2 + |\nabla|^2 = \{ 2 Dh dt Do dp$$

$$dt V' ((p + (pV' 2f \text{ where } \text{If}\hat{S}_{bp}^{\wedge}Am\hat{A}\hat{S}_{\dagger}^{\dagger}b+ \text{if}(p) - g(V' (p + i(pv' f)) = 12^{-\sqrt{(|\alpha_1'(t) \rangle CQ1t|\phi(t) \rangle B + |\alpha_2'(t) \rangle CQ2t|\phi(t) \rangle B)} \text{ if}$$

$$-\pi^{\wedge}Cmd\pi Cd\pi^2 ((\langle p + \text{if}(p) - g(V' (p + i(pv' f)) \neq + (\sqrt{\theta}) \Theta \text{ if } (3 e \text{-----}$$

$$\text{del purin-2-yl] amino}) \text{ phosphoryl] oxy}) \text{ phos phoryl] formonitrile} + + (\sqrt{\theta}) \Theta \text{ if } (3 e \text{-----}$$

$$\text{del}) \equiv \int (4(-1) - 2|\nabla|^2 = \{ + (\sqrt{\theta}) \Theta (\sqrt{\theta}) \Theta (\text{rboximidoyl- 3-formonitrile} + + (\sqrt{\theta} \text{- fluoro-phos}$$

$$\text{phoryl] formonitrile where } \text{If}\hat{S}_{bp}^{\wedge}Am\hat{A}\hat{S}_{\dagger}^{\dagger}b+ \text{if}(p) - g(V' (p + i(pv' f)) = 12^{-\sqrt{(|\alpha_1'(t) \rangle CQ1t|\phi(t) \rangle B + |\alpha_2'(t) \rangle CQ2t|\phi(t) \rangle B)} \text{ if}$$

$$-\pi^{\wedge}Cmd\pi Cd\pi^2 ((\langle p + \text{if}(p) - g(V' (p + i(pv' f)) \neq + (\sqrt{\theta}) \Theta \text{ if } (3 e \text{-----}$$

del purin-2-yl] amino)) phosphoryl oxy)) phos phoryl] formonitrile + + (sqrt(0) \Theta (sqrt(0) \Theta

(rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(0) \Theta (sqrt(0) \Theta (rboximidoyl-

3- fluoro-1-(sqrt(0) \Theta if (3 e_____ del phos phoryl] formonitrile

(rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl] amino)) phosphoryl oxy))

phos phoryl] formonitrile (sqrt(0) \Theta if (3 e_____ del phos phoryl]

formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl] amino))

phosphoryl oxy)) phos phoryl] formonitrile 2) (\int 2 -2) -2(, |\nabla |2 = \{ 2 Dh dt Do dp dtV'((p+(pV'2f

where If\hat{S}bp^AmA\hat{S}^\dagger b+ if(p) - g(V '(p + i(pv' f)) =12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B)}

if -\pi^{\text{Cmd}\pi\text{Cd}\pi 2} ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(0) \Theta if (3 e_____

del purin-2-yl] amino)) phosphoryl oxy)) phos phoryl] formonitrile + + (sqrt(0) \Theta if (3 e_____

del)) \equiv \inf >0 |\nabla |2 = \{ 2 Dh dt Do dp dtV'((p+(pV'2f where If\hat{S}bp^AmA\hat{S}^\dagger b+ if(p) - g(V '(p + i(pv' f))

=12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B)} if -\pi^{\text{Cmd}\pi\text{Cd}\pi 2} ((\langle p + if(p) - g(V '(p + i(pv' f))

\neq + (sqrt(0) \Theta if (3 e_____ del purin-2-yl] amino)) phosphoryl oxy)) phos

phoryl] formonitrile + + (sqrt(0) \Theta if (3 e_____ del) 0) ^2)))) - 1/2 x^3

(sqrt(\pi) \sin^{(-1)} (y - 3 \sqrt{6734} X Y1^2) ((e^3 \theta^{(3/2)} \Theta^3 del del -12 (d |\nabla |2 = \{ 2 Dh dt Do dp

dtV'((p+(pV'2f where If\hat{S}bp^AmA\hat{S}^\dagger b+ if(p) - g(V '(p + i(pv' f)) =12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t)

\rangle CQ2t|\phi(t) \rangle B)} if -\pi^{\text{Cmd}\pi\text{Cd}\pi 2} ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(0) \Theta if (3 e_____

del purin-2-yl] amino)) phosphoryl oxy)) phos phoryl] formonitrile + + (sqrt(0) \Theta if (3 e_____

del) \equiv \int (4(-1) -2 |\nabla |2 = \{ 2 - 1 pentan-2-yl} -2-Carboxylicacid; N-(1-carboximidoyl- 3- fluoro-1-

{5-oxabicyclo [2. 1.0] pentan-2-yl} -2-oxo6-({[amino({[(6-amino-9H-purin-9-yl) methyl] amino)})
 phosphoryl] carbamoyl} amino) -3,3- di methyl-7-oxo-4-thia- 1-azabicyclo [3.2.0] heptane-
 2-Carboxylicacid; N-(1-carboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -2-
 Carboxylicacid; N-3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -2- oxo-1lambda4,2 lambda5-
 thiaphosphiran-2 -yl) -N'-yl) -N'-[(Z) - ethylidene]guanidine; [(S) -amino({[(S) - amino({[(4R)
 -6-oxo-4,6- dihydro-1H-purin-2-yl] amino}) phosphoryl] oxy}) phos thiaphosphiran-2 -yl) -N'-yl)
 -N'-[(Z) $1 \neq + (\sqrt{\theta}) \Theta$ if (3 e $\frac{2Dh}{dt} \frac{dp}{dt} V'$ where If $\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+$ if(p) - g(V '(p + i(pv' f))
 oxy}) phos phoryl] formonitrile + + (sqrt(theta) Θ if (3 e $\frac{2Dh}{dt} \frac{dp}{dt} V'$ where If $\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+$ if(p) - g(V '(p + i(pv' f))
 $=12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B)}$ if $-\pi^{\wedge}Cmd\pi Cd\pi 2$ (($\langle p + if(p) - g(V '(p + i(pv' f))$
 $\neq + (\sqrt{\theta}) \Theta$ if (3 e $\frac{2Dh}{dt} \frac{dp}{dt} V'$ where If $\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+$ if(p) - g(V '(p + i(pv' f)) $\neq$ pentan-2-yl}
 phoryl] formonitrile + + (sqrt(theta) Θ if (3 e $\frac{2Dh}{dt} \frac{dp}{dt} V'$ where If $\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+$ if(p) - g(V '(p + i(pv' f)) $=12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B)}$ if $-\pi^{\wedge}Cmd\pi Cd\pi 2$ (($\langle p + if(p) - g(V '(p + i(pv' f))$
 2Dh dt dp dtV' (p+(pV'2f) where If $\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+$ if(p) - g(V '(p + i(pv' f)) $=12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B)}$ if $-\pi^{\wedge}Cmd\pi Cd\pi 2$ (($\langle p + if(p) - g(V '(p + i(pv' f))$
)B+ $|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B$) if $-\pi^{\wedge}Cmd\pi Cd\pi 2$ (($\langle p + if(p) - g(V '(p + i(pv' f))$ $\neq$ pentan-2-yl}
 -2-Carboxylicacid; N-(1-carboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl}
 -2-oxo-1lambda4, 2lambda5-thiaphosphiran-2 -yl) -N'-yl) -N'-[(Z) + + (sqrt(theta) Θ (sqrt(theta) Θ
 (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(theta) Θ (sqrt(theta) Θ (rboximidoyl-
 3- fluoro-1-(sqrt(theta) Θ if (3 e $\frac{2Dh}{dt} \frac{dp}{dt} V'$ where If $\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+$ if(p) - g(V '(p + i(pv' f)) $\neq$ pentan-2-yl}
 (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2- yl]am ino}) phosphoryl] oxy})

phos phoryl] formonitrile (sqrt(theta) \Theta if (3 e_____ del phos phoryl]

formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl] amino))

phosphoryl] oxy)) phos phoryl] formonitrile 2) (\int 2 Dh dt dp dt -2 (, |\nabla |2 = { 2 Dh dt Do dp

dtV'((p+(pV'2f where If\hat{S}bp^{\hat{A}m\hat{A}\dagger}b+ if(p) - g(V '(p + i(pv' f))=12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t)

\rangle CQ2t|\phi(t) \rangle B) if -\pi^{\text{Cmd}\pi C d\pi 2} ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(theta) \Theta if (3 e_____

del purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile + + (sqrt(theta) \Theta if (3 e_____

del)) \equiv \inf >0 |\nabla |2 = { 2 Dh dt Do dp dtV'((p+(pV'2f where If\hat{S}bp^{\hat{A}m\hat{A}\dagger}b+ if(p) - g(V '(p + i(pv' f))

=12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) if -\pi^{\text{Cmd}\pi C d\pi 2} ((\langle p + if(p) - g(V '(p + i(pv' f))

\neq + (sqrt(theta) \Theta if (3 e_____ del purin-2-yl] amino)) ph osphoryl]oxy)) phos

phoryl] formonitrile + + (sqrt(theta) \Theta if (3 e_____ del) v - |\nabla |2 = { 2 Dh dt Do

dp dtV'((p+(pV'2f where If\hat{S}bp^{\hat{A}m\hat{A}\dagger}b+ if(p) - g(V '(p + i(pv' f)) =12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t)

\rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) if -\pi^{\text{Cmd}\pi C d\pi 2} ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(theta) \Theta if (3 e_____

del purin-2-yl] amino)) pho sphoryl]oxy)) phos phoryl] formonitrile + + (sqrt(theta) \Theta if (3 e_____

del) \equiv \int

> (4(-1) -2|\nabla |2= {+ (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-phos phoryl]

formonitrile + (sqrt(theta) \Theta if (3 e_____ del (1-carboximidoyl- 3- fluoro-1-

{5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-phos phoryl]

formonitrile 1+ (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-phos phoryl] formonitrile 1\neq + (sqrt(theta)

\Theta (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(theta) \Theta if (3 e_____

del purin-2-yl]ami no}) phosphoryl] oxy}) phos phoryl] formonitrile ++ (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-phos phoryl] formonitrile 22 ++ (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-phos phoryl] formonitrile 2) + (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-phos phoryl] formonitrile (\int + (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(theta) \Theta if (3 e del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-phos phoryl] formonitrile (+ (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-phos phoryl] formonitrile,|\nabla |^2 = \{ 2 Dh dt Do dp dt V'((p+(pV'^2f where If\hat{S}bp^AmA\hat{S}^\dagger b+ if(p) - g(V '(p + i(pv' f))=12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t |\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t |\phi(t) \rangle B) if -\pi^{\wedge} Cmd \pi C d \pi 2 ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(theta) \Theta if (3 e del purin-2-yl] amino}) phosphoryl] oxy}) phos phoryl] formonitrile + + (sqrt(theta) \Theta if (3 e del)) \equiv \inf + (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-phos phoryl] formonitrile >0+ (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(theta) \Theta if (3 e del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} - d+ (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(theta) \Theta if (3 e del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} - \equiv \int + (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-phos phoryl] formonitrile (4(-1)^{-2} |\nabla |^2 = \{+ (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(theta) \Theta if (3 e del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl] amino}) phosphoryl] oxy}) phos phoryl] formonitrile + (sqrt(theta) \Theta (sqrt(theta) \Theta

(rboximidoyl- 3- fluoro-phos phoryl] formonitrile 1 $\neq$ + (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3-
 fluoro-phos phoryl] formonitrile + (sqrt(θ) $\ominus$ if (3 e $\frac{1}{\sqrt{1+\theta}}$ del
 (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl-
 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3- fluoro-1- {5-oxabicyclo
 [2. 1.0] pentan-2-yl} -+ (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3- fluoro-1-(sqrt(θ) $\ominus$ if (3 e $\frac{1}{\sqrt{1+\theta}}$
 del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl}
 -purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile (sqrt(θ) $\ominus$ if (3 e $\frac{1}{\sqrt{1+\theta}}$
 del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl}
 -purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile + (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$
 (rboximidoyl- 3- fluoro-phos phoryl] formonitrile 2) + (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3-
 fluoro-phos phoryl] formonitrile ($\int$ + (sqrt(θ) $\ominus$ if (3 e $\frac{1}{\sqrt{1+\theta}}$ del
 (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl-
 3- fluoro-phos phoryl] formonitrile ++ (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3- fluoro-phos phoryl]
 formonitrile + (sqrt(θ) $\ominus$ if (3 e $\frac{1}{\sqrt{1+\theta}}$ del (rboximidoyl- 3- fluoro-1-
 {5-oxabicyclo [2. 1.0] pentan-2-yl} $\equiv$ + (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3- fluoro-phos phoryl]
 formonitrile (4(-1) -2| ∇ |2= {+ (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3- fluoro-phos phoryl]
 formonitrile + (sqrt(θ) $\ominus$ if (3 e $\frac{1}{\sqrt{1+\theta}}$ del (1-carboximidoyl- 3- fluoro-1-
 {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3- fluoro-phos phoryl]
 formonitrile 1+ (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile 1 $\neq$ + (sqrt(θ)

$\Theta(\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{formonitrile} + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----}$
 $\text{del purin-2-yl] amino}) \text{ phosphoryl] oxy}) \text{ phos phoryl}] \text{formonitrile} ++ (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$
 $(\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{formonitrile} \text{ }^{22} + 2) + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3-}$
 $\text{fluoro-phos phoryl}] \text{formonitrile} (\int + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}]$
 $\text{formonitrile} + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----} \text{del } (\text{rboximidoyl- 3- fluoro-1-}$
 $\{5\text{-oxabicyclo [2. 1.0] pentan-2-yl}\} \text{ }^{-} + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}]$
 $\text{formonitrile} (+ (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{formonitrile}, |\nabla|^2 = \{ 2 \text{ Dh}$
 $\text{dt Do dp dtV}'((\text{p}+(\text{pV}'^2\text{f where If}\hat{\text{S}}\text{bp}^{\wedge}\text{Am}\hat{\text{S}}^{\dagger}\text{b}+\text{if}(\text{p})-\text{g}(\text{V}'(\text{p}+\text{i}(\text{pv}'\text{f}))=12^{-}\sqrt{(|\alpha 1'(t)|\text{CQ1t}|\phi(t)$
 $)\text{B}+|\alpha 2'(t)|\text{CQ2t}|\phi(t)|\text{B}) \text{if } -\pi^{\wedge}\text{Cmd}\pi\text{Cd}\pi 2 ((\text{<p}+\text{if}(\text{p})-\text{g}(\text{V}'(\text{p}+\text{i}(\text{pv}'\text{f}))\neq + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----}$
 $\text{del purin-2-yl] amino}) \text{ phosphoryl] oxy}) \text{ phos phoryl}] \text{formonitrile} ++ (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----}$
 $\text{del})) \equiv \text{inf}+ (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{formonitrile} >0+ (\sqrt{\theta}) \ominus$
 $(\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{formonitrile} + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----}$
 $\text{del } (\text{rboximidoyl- 3- fluoro-1- } \{5\text{-oxabicyclo [2. 1.0] pentan-2-yl}\} \text{ }^{-} + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$
 $(\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{formonitrile} \text{ }^0 \text{del ' } (0) \text{del ' } (\text{del}((\text{del ' } (0)) \text{ }^2 \text{del '' } (\text{del } 0) + \text{del '}$
 $(\text{del } 0) \text{del '' } (0)) \text{ }) /(\sqrt{\pi} (1 - \theta \ominus^2 (\text{del del }^{-12} (\text{d}+ (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3-}$
 $\text{fluoro-phos phoryl}] \text{formonitrile} + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----} \text{del}$
 $(\text{rboximidoyl- 3- fluoro-1- } \{5\text{-oxabicyclo [2. 1.0] pentan-2-yl}\} \text{ }^{-} \equiv \int + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$
 $(\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{formonitrile} (4(\text{ }^{-1}) \text{ }^{-2} |\nabla|^2 = \{+ (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$
 $(\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{formonitrile} + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----}$

[illegible]

$(\text{rboximidoyl- 3- fluoro-1-(}\sqrt{\theta} \ominus \text{ if (3 e} \text{----- del phos phoryl)}$
 $\text{formonitrile (rboximidoyl- 3- fluoro-1- \{5- oxabicyclo [2.1.0] pentan-2-yl} -purin-2-yl} \text{ amino})}$
 $\text{phosphoryl] oxy}) \text{ phos phoryl] formonitrile (}\sqrt{\theta} \ominus \text{ if (3 e} \text{----- del}$
 $\text{phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2.1.0] pentan-2-yl} -purin-2-yl}$
 $\text{amino}) \text{ phosphoryl] oxy}) \text{ phos phoryl] formonitrile + (}\sqrt{\theta} \ominus (\sqrt{\theta} \ominus (\text{rboximidoyl- 3-}$
 $\text{fluoro-phos phoryl] formonitrile 2) + (}\sqrt{\theta} \ominus (\sqrt{\theta} \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}$
 $\text{formonitrile (}\int + (\sqrt{\theta} \ominus (\sqrt{\theta} \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (}\sqrt{\theta} \ominus \text{ if (3 e}$
 $\text{del (rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (}\sqrt{\theta} \ominus (\sqrt{\theta} \ominus$
 $(\text{rboximidoyl- 3- fluoro-phos phoryl] formonitrile (+ (}\sqrt{\theta} \ominus (\sqrt{\theta} \ominus (\text{rboximidoyl- 3-}$
 $\text{fluoro-phos phoryl] formonitrile, } |\nabla|^2 = \{ 2 \text{ Dh dt Do dp dtV}'((\text{p}+(\text{pV}'^2\text{f where If}\hat{\text{S}}\text{bp}^{\wedge}\text{AmA}\hat{\text{S}}^{\dagger}\text{b}+\text{if}(\text{p})$
 $\text{- g(V '(p + i(pv' f)) =} 12^{-\sqrt{(|\alpha 1'(t) \rangle \text{CQ1t}|\phi(t) \rangle \text{B} +|\alpha 2'(t) \rangle \text{CQ2t}|\phi(t) \rangle \text{B)}} \text{ if } -\pi^{\wedge}\text{Cmd}\pi\text{Cd}\pi 2 ((\langle \text{p} + \text{if}(\text{p})$
 $\text{- g(V '(p + i(pv' f))} \neq + (\sqrt{\theta} \ominus \text{ if (3 e} \text{----- del purin-2-yl} \text{ amino})}$
 $\text{phosphoryl] oxy}) \text{ phos phoryl] formonitrile + + (}\sqrt{\theta} \ominus \text{ if (3 e} \text{-----}$
 $\text{del))} \equiv \text{inf}+ (\sqrt{\theta} \ominus (\sqrt{\theta} \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl] formonitrile } >0+ (\sqrt{\theta} \ominus$
 $(\sqrt{\theta} \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (}\sqrt{\theta} \ominus \text{ if (3 e} \text{-----}$
 $\text{del (rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl} - v \text{ } \rightarrow + (\sqrt{\theta} \ominus (\sqrt{\theta} \ominus$
 $(\text{rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (}\sqrt{\theta} \ominus \text{ if (3 e} \text{-----}$
 $\text{del (rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl} - \equiv \int$

$(4(-1)^{-2}|\nabla|^2 = \{ + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl})$
 $\text{formonitrile} + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----} \text{del } (1\text{-carboximidoyl- 3- fluoro-1-}$
 $\{5\text{-oxabicyclo [2. 1.0] pentan-2-yl}) \text{ -} + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl})$
 $\text{formonitrile } 1 + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}) \text{ formonitrile } 1 \neq + (\sqrt{\theta})$
 $\ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}) \text{ formonitrile} + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----}$
 $\text{del purin-2-yl] amino}) \text{ phosphoryl] oxy}) \text{ phos phoryl] formonitrile } ++ (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$
 $(\text{rboximidoyl- 3- fluoro-phos phoryl}) \text{ formonitrile } 22 ++ (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3-}$
 $\text{fluoro-phos phoryl}) \text{ formonitrile } 2) + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl})$
 $\text{formonitrile } (\int + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}) \text{ formonitrile} + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e}$
 $\text{del } (\text{rboximidoyl- 3- fluoro-1- } \{5\text{-oxabicyclo [2. 1.0] pentan-2-yl}) \text{ -} + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$
 $(\text{rboximidoyl- 3- fluoro-phos phoryl}) \text{ formonitrile } (+ (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3-}$
 $\text{fluoro-phos phoryl}) \text{ formonitrile}, |\nabla|^2 = \{ 2 \text{ Dh dt Do dp dtV}'((\text{p} + (\text{pV}'^2 \text{f where If} \hat{\text{S}}_{\text{bp}}^{\text{A}} \hat{\text{A}}_{\text{S}}^{\text{b}} + \text{if}(\text{p})$
 $\text{- g(V ' (p + i(pv' f))} = 12^{-\sqrt{(|\alpha 1'(t) \rangle \text{CQ1t} | \phi(t) \rangle \text{B} + |\alpha 2'(t) \rangle \text{CQ2t} | \phi(t) \rangle \text{B})} \text{ if } -\pi^{\text{C}} \text{md} \pi \text{Cd} \pi^2 ((\langle \text{p} + \text{if}(\text{p})$
 $\text{- g(V ' (p + i(pv' f))} \neq + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----} \text{del purin-2-yl] amino})$
 $\text{phosphoryl] oxy}) \text{ phos phoryl] formonitrile } + + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----}$
 $\text{del})) \equiv$
 $> \text{inf} + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}) \text{ formonitrile } > 0 + (\sqrt{\theta}) \ominus (\sqrt{\theta})$
 $\ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}) \text{ formonitrile} + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----}$
 $\text{del } (\text{rboximidoyl- 3- fluoro-1- } \{5\text{-oxabicyclo [2. 1.0] pentan-2-yl}) \text{ - d} + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$

$(\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{ formonitrile} + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----}$
 $\text{del } (\text{rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl\} -} \equiv \int + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$
 $(\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{ formonitrile } (4(-1) -2 \mid \nabla \mid 2 = \{+ (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$
 $(\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{ formonitrile} + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----}$
 $\text{del phos phoryl}] \text{ formonitrile } (\text{rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl\} -p}$
 $\text{urin-2-yl] amino\}) \text{ phosphoryl] oxy\}) \text{ phos phoryl}] \text{ formonitrile} + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl-}$
 $3\text{- fluoro-phos phoryl}] \text{ formonitrile } 1 \neq + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}]$
 $\text{formonitrile} + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----} \text{del } (\text{rboximidoyl- 3- fluoro-1-}$
 $\{5\text{-oxabicyclo [2. 1.0] pentan-2-yl\} -+ (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}]$
 $\text{formonitrile} + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl\} -+}$
 $(\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-1-}(\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----} \text{del}$
 $\text{phos phoryl}] \text{ formonitrile } (\text{rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2.1.0] pentan-2-yl\} -purin-2-yl}]$
 $\text{amino\}) \text{ phosphoryl] oxy\}) \text{ phos phoryl}] \text{ formonitrile } (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----}$
 $\text{del phos phoryl}] \text{ formonitrile } (\text{rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl\}}$
 $\text{-purin-2-yl] amino\}) \text{ phosphoryl] oxy\}) \text{ phos phoryl}] \text{ formonitrile} + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$
 $(\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{ formonitrile } 2) + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3-}$
 $\text{fluoro-phos phoryl}] \text{ formonitrile } (\int + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----} \text{del}$
 $(\text{rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl\} -+ (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl-}$
 $3\text{- fluoro-phos phoryl}] \text{ formonitrile } ++ (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}]$

formonitrile + $(\sqrt{\theta}) \ominus$ if (3 e_____ del (rboximidoyl- 3- fluoro-1-
{5-oxabicyclo [2. 1.0] pentan-2-yl} $\equiv$ + $(\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$ (rboximidoyl- 3- fluoro-phos phoryl]
formonitrile $(4(-1)^{-2}|\nabla|^2 = \{ + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$ (rboximidoyl- 3- fluoro-phos phoryl]
formonitrile + $(\sqrt{\theta}) \ominus$ if (3 e_____ del (1-carboximidoyl- 3- fluoro-1-
{5-oxabicyclo [2. 1.0] pentan-2-yl} $\rightarrow$ + $(\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$ (rboximidoyl- 3- fluoro-phos phoryl]
formonitrile $1 + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile $1 \neq + (\sqrt{\theta})$
 $\ominus (\sqrt{\theta}) \ominus$ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + $(\sqrt{\theta}) \ominus$ if (3 e_____ del
purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile $++ (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$
(rboximidoyl- 3- fluoro-phos phoryl] formonitrile $22 +$
 $> 2) + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile $(\int + (\sqrt{\theta}) \ominus$
 $(\sqrt{\theta}) \ominus$ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + $(\sqrt{\theta}) \ominus$ if (3 e_____ del
(rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} $\rightarrow$ + $(\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$
(rboximidoyl- 3- fluoro-phos phoryl] formonitrile $(+ (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$ (rboximidoyl- 3-
fluoro-phos phoryl] formonitrile, $|\nabla|^2 = \{ 2 Dh dt Do dp dt V'((p+(pV'^2f$ where $If\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+ if(p)$
- $g(V' (p + i(pv' f)) = 12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B + |\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B)}$ if $-\pi^{\wedge}Cmd\pi Cd\pi 2 ((\langle p + if(p)$
- $g(V' (p + i(pv' f)) \neq + (\sqrt{\theta}) \ominus$ if (3 e_____ del purin-2-yl] amino))
phosphoryl] oxy)) phos phoryl] formonitrile $++ (\sqrt{\theta}) \ominus$ if (3 e_____ del)) $\equiv \inf + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$
(rboximidoyl- 3- fluoro-phos phoryl] formonitrile $> 0 + (\sqrt{\theta}) \ominus$
 $(\sqrt{\theta}) \ominus$ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + $(\sqrt{\theta}) \ominus$ if (3 e_____ del

del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile θ) ^2) ^{(3/2)}) + (e^3 θ^{(3/2)} ⊖^3 (del ' (θ)) ^3 (del ' (del θ)) ^3 (2 θ ⊖^2 (del del −12 (d+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) ⊖ if (3 e————— del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo[2.1.0] pentan-2-yl} - ≡ ∫+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile (4(−1) −2 |∇ |2 = {+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) ⊖ if (3 e————— del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile + (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile 1 ≠+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) ⊖ if (3 e————— del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -

> 2 +2) (∫ 2 −2) −2+ |∇ |2 = { 2 Dh dt Do dp dtV'((p+(pV'2f where IfŜbp^AmAŜ†b+ if(p) - g(V' (p + i(pv' f)) =12^− √(|α1'(t) >CQ1t|φ(t) >B +|α2'(t) >CQ2t|φ(t) >B) if −π^CmdπCdπ2 ((<p + if(p) - g(V' (p + i(pv' f)) ≠ + (sqrt(θ) ⊖ if (3 e————— del purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile + + (sqrt(θ) ⊖ if (3 e————— del) ≡∫ (4(−1) −2|∇ |2= { + (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3-formonitrile + + (sqrt- fluoro-phos phoryl] formonitrile − 11≠ 23 1++ (sqrt(θ) ⊖ (sqr t(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-1-(sqrt(θ) ⊖ if (3 e————— del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo

[2.1.0] pentan-2-yl} -purin-2-yl] amino}} phosphoryl] oxy}} phos phoryl] formonitrile $(\sqrt{\theta}) \ominus$ if (3 e~~_____~~

del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} - purin-2-yl]

amino}} phosphoryl] oxy}} phos phoryl] formonitrile + $(\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$ (rboximidoyl- 3- fluoro-phos

phoryl] formonitrile 2) + $(\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile ($\int + (\sqrt{\theta})$

$\ominus (\sqrt{\theta}) \ominus$ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + $(\sqrt{\theta}) \ominus$ if (3 e~~_____~~

del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ $(\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$ (rboximidoyl- 3-

fluoro-phos phoryl] formonitrile (+ $(\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile,

$|\nabla|^2 = \{ 2 \text{ Dh dt Do dp dtV}'((p+(pV')^2f \text{ where } If\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+ \text{ if}(p) - g(V' (p + i(pv' f)) =12^{-\sqrt{(|\alpha_1'(t)$

)CQ1t|\phi(t) \rangle B +|\alpha_2'(t) \rangle CQ2t|\phi(t) \rangle B) \text{ if } -\pi^{\wedge}Cmd\pi Cd\pi^2 ((\langle p + \text{if}(p) - g(V' (p + i(pv' f)) \neq + (\sqrt{\theta}) \ominus if (3 e~~_____~~

del purin-2-yl] amino}} phosphoryl] oxy}} phos phoryl] formonitrile + + $(\sqrt{\theta}) \ominus$ if (3 e~~_____~~

del)) $\equiv \inf + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile $>0 + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$

(rboximidoyl- 3- fluoro-phos phoryl] formonitrile + $(\sqrt{\theta}) \ominus$ if (3 e~~_____~~ del

(rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} - v $\rightarrow + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$ (rboximidoyl- 3-

fluoro-phos phoryl] formonitrile + $(\sqrt{\theta}) \ominus$ if (3 e~~_____~~ del (rboximidoyl- 3-

fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} - $\equiv \int + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$ (rboximidoyl- 3- fluoro-phos phoryl]

formonitrile $(4(-1)^{-2} |\nabla|^2$

$> \{ 2 \text{ Dh dt dp dtV}'(p +(pV')^2f \text{ where } If\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+ \text{ if}(p) - g(V' (p + i(pv' f)) =12^{-\sqrt{(|\alpha_1'(t) \rangle CQ1t|\phi(t)}$

$\rangle B +|\alpha_2'(t) \rangle CQ2t|\phi(t) \rangle B) \text{ if } -\pi^{\wedge}Cmd\pi Cd\pi^2 ((\langle p + \text{if}(p) - g(V' (p + i(pv' f)) \neq$ pentan-2-yl} -2-Carbox ylicacid;

N-(1-carboximidoyl- 3- fluoro-1- {5-oxabicyclo[2. 1.0] pentan-2-yl} -2-oxo-1lam

$\text{bda4,2}\lambda\text{5-thiaphosphiran-2-yl)-N'-yl)-N'-(Z)} + + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl-3-fluoro-1-}$
 $\{5\text{-oxabicyclo [2. 1.0] pentan-2-yl}\} - + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl-3-fluoro-1-}(\sqrt{\theta}) \ominus \text{if (3 e} \text{-----}$
 $\text{del phos phoryl] formonitrile (rboximidoyl-3-fluoro-1-}\{5\text{-oxabicyclo [2. 1.0] pentan-2-yl}\} \text{-pur in-2-yl)}$
 $\text{amino)) phosphoryl] oxy)) phos phoryl] formonitrile }(\sqrt{\theta}) \ominus \text{if (3 e} \text{----- del}$
 $\text{phos phoryl] formonitrile (rboximidoyl-3-fluoro-1-}\{5\text{-oxabicyclo [2.1.0] pentan-2-yl}\} \text{-purin-2-yl] amino))}$
 $\text{phosphoryl] oxy)) phos phoryl] formonitrile }2) (\int 2 \text{ Dh dt dp dt} -2 (, |\nabla|^2 = \{ 2 \text{ Dh dt Do dp dtV}'((\text{p}+(\text{pV}'2\text{f}$
 $\text{where If}\hat{\text{S}}_{\text{bp}}^{\wedge}\text{Am}\hat{\text{A}}\hat{\text{S}}_{\dagger}^{\dagger}\text{b}+ \text{if}(\text{p}) - \text{g}(\text{V}'(\text{p} + \text{i}(\text{pv}' \text{f})) = 12^{-} \sqrt{(|\alpha_1'(t) \rangle \text{CQ1t}|\phi(t) \rangle \text{B} + |\alpha_2'(t) \rangle \text{CQ2t}|\phi(t) \rangle \text{B}) \text{ if}$
 $-\pi^{\wedge}\text{Cmd}\pi\text{Cd}\pi^2 ((\langle \text{p} + \text{if}(\text{p}) - \text{g}(\text{V}'(\text{p} + \text{i}(\text{pv}' \text{f})) \neq + (\sqrt{\theta}) \ominus \text{if (3 e} \text{----- del}$
 $\text{purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile} + + (\sqrt{\theta}) \ominus \text{if (3 e} \text{-----}$
 $\text{del))} \equiv \inf >0 |\nabla|^2 = \{ 2 \text{ Dh dt Do dp dtV}'((\text{p}+(\text{pV}'2\text{f where If}\hat{\text{S}}_{\text{bp}}^{\wedge}\text{Am}\hat{\text{A}}\hat{\text{S}}_{\dagger}^{\dagger}\text{b}+ \text{if}(\text{p}) - \text{g}(\text{V}'(\text{p} + \text{i}(\text{pv}' \text{f})) = 12^{-}$
 $\sqrt{(|\alpha_1'(t) \rangle \text{CQ1t}|\phi(t) \rangle \text{B} + |\alpha_2'(t) \rangle \text{CQ2t}|\phi(t) \rangle \text{B}) \text{ if }-\pi^{\wedge}\text{Cmd}\pi\text{Cd}\pi^2 ((\langle \text{p} + \text{if}(\text{p}) - \text{g}(\text{V}'(\text{p} + \text{i}(\text{pv}' \text{f})) \neq + (\sqrt{\theta})$
 $\ominus \text{if (3 e} \text{----- del purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile}$
 $+ + (\sqrt{\theta}) \ominus \text{if (3 e} \text{----- del) d }|\nabla|^2 = \{ 2 \text{ Dh dt Do dp dtV}'((\text{p}+(\text{pV}'2\text{f where}$
 $\text{If}\hat{\text{S}}_{\text{bp}}^{\wedge}\text{Am}\hat{\text{A}}\hat{\text{S}}_{\dagger}^{\dagger}\text{b}+ \text{if}(\text{p}) - \text{g}(\text{V}'(\text{p} + \text{i}(\text{pv}' \text{f})) = 12^{-} \sqrt{(|\alpha_1'(t) \rangle \text{CQ1t}|\phi(t) \rangle \text{B} + |\alpha_2'(t) \rangle \text{CQ2t}|\phi(t) \rangle \text{B}) \text{ if}$
 $-\pi^{\wedge}\text{Cmd}\pi\text{Cd}\pi^2 ((\langle \text{p} + \text{if}(\text{p}) - \text{g}(\text{V}'(\text{p} + \text{i}(\text{pv}' \text{f})) \neq + (\sqrt{\theta}) \ominus \text{if (3 e} \text{----- del}$
 $\text{purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile} + + (\sqrt{\theta}) \ominus \text{if (3 e} \text{-----}$
 $\text{del)} \equiv \int (4(-1)^{-2} |\nabla|^2 = \{ 2 \text{ Dh dt dp dtV}'(\text{p}+(\text{pV}'2\text{f where If}\hat{\text{S}}_{\text{bp}}^{\wedge}\text{Am}\hat{\text{A}}\hat{\text{S}}_{\dagger}^{\dagger}\text{b}+ \text{if}(\text{p}) - \text{g}(\text{V}'(\text{p} + \text{i}(\text{pv}' \text{f})) = 12^{-}$
 $\sqrt{(|\alpha_1'(t) \rangle \text{CQ1t}|\phi(t) \rangle \text{B} + |\alpha_2'(t) \rangle \text{CQ2t}|\phi(t) \rangle \text{B}) \text{ if }-\pi^{\wedge}\text{Cmd}\pi\text{Cd}\pi^2 ((\langle \text{p} + \text{if}(\text{p}) - \text{g}(\text{V}'(\text{p} + \text{i}(\text{pv}' \text{f})) \neq$
 $\text{pentan-2-yl}\} \text{-2-Carboxylicacid; N-(1-carboximidoyl-3-fluoro-1-}\{5\text{-oxabicyclo [2. 1.0] pentan-2-yl}\}$

-2-oxo6-({[amino({[(6-amino-9H-purin-9-yl) methyl] amino}) phosphoryl] carbamoyl} amino) -3,3- di
methyl-7-oxo-4-thia- 1-azabicyclo [3.2.0] heptane- 2-Carboxylicacid; N-(1-carboximidoyl- 3- fluoro-1-
{5-oxabicyclo [2. 1.0] pentan-2-yl} -2- Carboxylicacid; N-3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -2-
oxo-1lambda4,2 lambda5- thiaphosphiran-2 -yl) -N'-yl) -N'-[(Z) - ethylidene]guanidine; [(S) -amino({[(S) -
amino({[(4R) -6-oxo-4,6- dihydro-1H-purin-2-yl] amino}) phosphoryl] oxy}) phos thiaphosphiran-2 -yl)
-N'-yl) -N'-[(Z) + + (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+
(sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-1-(sqrt(theta) \Theta if (3 e————— del phos
phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl] amino))
phosphoryl] oxy}) phos phoryl] formonitrile (sqrt(theta) \Theta if (3 e————— del phos
phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2.1.0] pentan-2-yl} -purin-2-yl] amino))
phosphoryl] oxy}) phos phoryl] formonitrile 2) (\int 2 Dh dt dp dt -2 + |\nabla |2 = { 2 Dh dt Do dp dtV'((p+(pV'2f
where If\hat{S}bp^Am\hat{S}^\dagger b+ if(p) - g(V '(p + i(pv' f)) =12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) if
-\pi^{\text{Cmd}\pi\text{Cd}\pi 2} ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(theta) \Theta if (3 e————— del
purin-2-yl] amino)) phosphoryl] oxy}) phos phoryl] formonitrile + + (sqrt(theta) \Theta if (3 e—————
del) \equiv \int (4(-1) -2|\nabla |2= { + (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3-formonitrile + + (sqrt- fluoro-phos phoryl]
formonitrile where If\hat{S}bp^Am\hat{S}^\dagger b+ if(p) - g(V '(p + i(pv' f)) =12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t)
)B) if -\pi^{\text{Cmd}\pi\text{Cd}\pi 2} ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(theta) \Theta if (3 e————— del
purin-2-yl] amino)) phosphoryl] oxy}) phos phoryl] formonitrile + + (sqrt(theta) \Theta if (3 e—————
del) (\int 2 Dh dt dp dt -2 (, |\nabla |2 = { 2 Dh dt Do dp dtV'((p+(pV'2f where If\hat{S}bp^Am\hat{S}^\dagger b+ if(p) - g(V '(p +

$i(pv' f) = 12^{-\sqrt{(|\alpha_1'(t) \rangle CQ1t|\phi(t) \rangle B + |\alpha_2'(t) \rangle CQ2t|\phi(t) \rangle B}}$ if $-\pi^{\text{Cmd}\pi\text{Cd}\pi 2} ((\langle p + \text{if}(p) - g(V' (p + i(pv' f)))$
 $\neq + (\sqrt{\theta}) \Theta$ if $(3 e^{\text{del purin-2-yl] amino}}) \text{ phosphoryl] oxy}}) \text{ phos phoryl]}$
 $\text{formonitrile} + + (\sqrt{\theta}) \Theta$ if $(3 e^{\text{del}}) \equiv \inf > 0 \ |\nabla|^2 = \{ 2 \text{ Dh dt Do dp}$
 $\text{dtV}'((p+(pV'2f \text{ where If}\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+ \text{if}(p) - g(V' (p + i(pv' f))) = 12^{-\sqrt{(|\alpha_1'(t) \rangle CQ1t|\phi(t) \rangle B + |\alpha_2'(t) \rangle CQ2t|\phi(t) \rangle B}}$
 $\text{if } -\pi^{\text{Cmd}\pi\text{Cd}\pi 2} ((\langle p + \text{if}(p) - g(V' (p + i(pv' f))) \neq + (\sqrt{\theta}) \Theta$ if $(3 e^{\text{del purin-2-yl] amino}}) \text{ phosphoryl] oxy}}) \text{ phos phoryl] formonitrile} + + (\sqrt{\theta}) \Theta$ if $(3 e^{\text{del}})$
 $\text{del}) 0)^2 + 1)) / (3 \sqrt{\pi}) (1 - \theta \Theta^2 (\text{del del } -12 (d \ |\nabla|^2 = \{ 2 \text{ Dh dt Do dp dtV}'((p+(pV'2f \text{ where If}\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+ \text{if}(p) - g(V' (p + i(pv' f))) = 12^{-\sqrt{(|\alpha_1'(t) \rangle CQ1t|\phi(t) \rangle B + |\alpha_2'(t) \rangle CQ2t|\phi(t) \rangle B}}$ if
 $-\pi^{\text{Cmd}\pi\text{Cd}\pi 2} ((\langle p + \text{if}(p) - g(V' (p + i(pv' f))) \neq + (\sqrt{\theta}) \Theta$ if $(3 e^{\text{del purin-2-yl] amino}}) \text{ phosphoryl] oxy}}) \text{ phos phoryl] formonitrile} + + (\sqrt{\theta}) \Theta$ if $(3 e^{\text{del}})$
 $\text{del}) \equiv \int (4(-1) - 2|\nabla|^2 = \{ + (\sqrt{\theta}) \Theta (\sqrt{\theta}) \Theta (\text{rboximidoyl- 3-formonitrile} + + (\sqrt{\text{fluoro-phos phoryl] formonitrile where If}\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+ \text{if}(p) - g(V' (p + i(pv' f))) = 12^{-\sqrt{(|\alpha_1'(t) \rangle CQ1t|\phi(t) \rangle B + |\alpha_2'(t) \rangle CQ2t|\phi(t) \rangle B}}$ if $-\pi^{\text{Cmd}\pi\text{Cd}\pi 2} ((\langle p + \text{if}(p) - g(V' (p + i(pv' f))) \neq + (\sqrt{\theta}) \Theta$ if $(3 e^{\text{del purin-2-yl] amino}}) \text{ phosphoryl] oxy}}) \text{ phos phoryl] formonitrile} + + (\sqrt{\theta}) \Theta$ if $(3 e^{\text{del}})$
 $\text{del}) (\int 2 \text{ Dh dt dp dt } -2 + |\nabla|^2 = \{ 2 \text{ Dh dt Do dp dtV}'((p+(pV'2f \text{ where If}\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+ \text{if}(p) - g(V' (p + i(pv' f))) = 12^{-\sqrt{(|\alpha_1'(t) \rangle CQ1t|\phi(t) \rangle B + |\alpha_2'(t) \rangle CQ2t|\phi(t) \rangle B}}$ if $-\pi^{\text{Cmd}\pi\text{Cd}\pi 2} ((\langle p + \text{if}(p) - g(V' (p + i(pv' f))) \neq + (\sqrt{\theta}) \Theta$ if $(3 e^{\text{del purin-2-yl] amino}}) \text{ phosphoryl] oxy}}) \text{ phos phoryl] formonitrile} + + (\sqrt{\theta}) \Theta$ if $(3 e^{\text{del}})$
 $\text{formonitrile} + + (\sqrt{\theta}) \Theta$ if $(3 e^{\text{del}}) \equiv \int (4(-1) - 2|\nabla|^2 = \{ + (\sqrt{\theta}) \Theta (\sqrt{\theta}) \Theta (\text{rboximidoyl- 3-formonitrile} + + (\sqrt{\text{fluoro-phos phoryl] formonitrile where If}\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+$

$\text{if}(\mathbf{p}) - \mathbf{g}(\mathbf{V} \text{ '}(\mathbf{p} + \mathbf{i}(\mathbf{p}\mathbf{v}' \mathbf{f})) = 12^{-} \sqrt{(|\alpha 1'(t) \rangle \mathbf{CQ1t}|\phi(t) \rangle \mathbf{B} + |\alpha 2'(t) \rangle \mathbf{CQ2t}|\phi(t) \rangle \mathbf{B})} \text{ if } -\pi^{\wedge} \mathbf{C} \mathbf{m} \mathbf{d} \pi \mathbf{C} \mathbf{d} \pi 2 ((\langle \mathbf{p} + \text{if}(\mathbf{p}) -$
 $\mathbf{g}(\mathbf{V} \text{ '}(\mathbf{p} + \mathbf{i}(\mathbf{p}\mathbf{v}' \mathbf{f})) \neq + (\text{sqrt}(\theta) \ominus \text{ if } (3 \text{ e} \text{-----} \text{ del purin-2-yl] amino})) \text{ phosphoryl]}$
 $\text{oxy})) \text{ phos phoryl] formonitrile} + + (\text{sqrt}(\theta) \ominus \text{ if } (3 \text{ e} \text{-----} \text{ del}) (\int 2 \text{ Dh dt dp dt } -2$
 $(, |\nabla |2 = \{ 2 \text{ Dh dt Do dp dt V}'((\mathbf{p} + (\mathbf{p}\mathbf{V}'2\mathbf{f} \text{ where } \text{If}\hat{\mathbf{S}}\mathbf{b}\mathbf{p}^{\wedge} \mathbf{A} \mathbf{m} \mathbf{A} \hat{\mathbf{S}}^{\dagger} \mathbf{b} + \text{if}(\mathbf{p}) - \mathbf{g}(\mathbf{V} \text{ '}(\mathbf{p} + \mathbf{i}(\mathbf{p}\mathbf{v}' \mathbf{f})) = 12^{-} \sqrt{(|\alpha 1'(t)$
 $\rangle \mathbf{CQ1t}|\phi(t) \rangle \mathbf{B} + |\alpha 2'(t) \rangle \mathbf{CQ2t}|\phi(t) \rangle \mathbf{B})} \text{ if } -\pi^{\wedge} \mathbf{C} \mathbf{m} \mathbf{d} \pi \mathbf{C} \mathbf{d} \pi 2 ((\langle \mathbf{p} + \text{if}(\mathbf{p}) - \mathbf{g}(\mathbf{V} \text{ '}(\mathbf{p} + \mathbf{i}(\mathbf{p}\mathbf{v}' \mathbf{f})) \neq + (\text{sqrt}(\theta) \ominus \text{ if } (3 \text{ e} \text{-----}$
 $\text{del purin-2-yl] amino})) \text{ phosphoryl] oxy})) \text{ phos phoryl] formonitrile} + + (\text{sqrt}(\theta) \ominus \text{ if } (3 \text{ e} \text{-----}$
 $\text{del})) \equiv \inf > 0 |\nabla |2 = \{ 2 \text{ Dh dt Do dp dt V}'((\mathbf{p} + (\mathbf{p}\mathbf{V}'2\mathbf{f} \text{ where } \text{If}\hat{\mathbf{S}}\mathbf{b}\mathbf{p}^{\wedge} \mathbf{A} \mathbf{m} \mathbf{A} \hat{\mathbf{S}}^{\dagger} \mathbf{b} + \text{if}(\mathbf{p}) - \mathbf{g}(\mathbf{V} \text{ '}(\mathbf{p} + \mathbf{i}(\mathbf{p}\mathbf{v}' \mathbf{f})) = 12^{-}$
 $\sqrt{(|\alpha 1'(t) \rangle \mathbf{CQ1t}|\phi(t) \rangle \mathbf{B} + |\alpha 2'(t) \rangle \mathbf{CQ2t}|\phi(t) \rangle \mathbf{B})} \text{ if } -\pi^{\wedge} \mathbf{C} \mathbf{m} \mathbf{d} \pi \mathbf{C} \mathbf{d} \pi 2 ((\langle \mathbf{p} + \text{if}(\mathbf{p}) - \mathbf{g}(\mathbf{V} \text{ '}(\mathbf{p} + \mathbf{i}(\mathbf{p}\mathbf{v}' \mathbf{f})) \neq + (\text{sqrt}(\theta)$
 $\ominus \text{ if } (3 \text{ e} \text{-----} \text{ del purin-2-yl] amino})) \text{ phosphoryl] oxy})) \text{ phos phoryl] formonitrile}$
 $+ + (\text{sqrt}(\theta) \ominus \text{ if } (3 \text{ e} \text{-----} \text{ del}) \mathbf{v} - |\nabla |2 = \{ 2 \text{ Dh dt Do dp dt V}'((\mathbf{p} + (\mathbf{p}\mathbf{V}'2\mathbf{f} \text{ where}$
 $\text{If}\hat{\mathbf{S}}\mathbf{b}\mathbf{p}^{\wedge} \mathbf{A} \mathbf{m} \mathbf{A} \hat{\mathbf{S}}^{\dagger} \mathbf{b} + \text{if}(\mathbf{p}) - \mathbf{g}(\mathbf{V} \text{ '}(\mathbf{p} + \mathbf{i}(\mathbf{p}\mathbf{v}' \mathbf{f})) = 12^{-} \sqrt{(|\alpha 1'(t) \rangle \mathbf{CQ1t}|\phi(t) \rangle \mathbf{B} + |\alpha 2'(t) \rangle \mathbf{CQ2t}|\phi(t) \rangle \mathbf{B})} \text{ if}$
 $-\pi^{\wedge} \mathbf{C} \mathbf{m} \mathbf{d} \pi \mathbf{C} \mathbf{d} \pi 2 ((\langle \mathbf{p} + \text{if}(\mathbf{p}) - \mathbf{g}(\mathbf{V} \text{ '}(\mathbf{p} + \mathbf{i}(\mathbf{p}\mathbf{v}' \mathbf{f})) \neq + (\text{sqrt}(\theta) \ominus \text{ if } (3 \text{ e} \text{-----} \text{ del}$
 $\text{purin-2-yl] amino})) \text{ phosphoryl] oxy})) \text{ phos phoryl] formonitrile} + + (\text{sqrt}(\theta) \ominus \text{ if } (3 \text{ e} \text{-----}$
 $\text{del}) \equiv \int (4(-1) -2 |\nabla |2 = \{ 2 \text{ Dh dt dp dt V}' (\mathbf{p} + (\mathbf{p}\mathbf{V}'2\mathbf{f} \text{ where } \text{If}\hat{\mathbf{S}}\mathbf{b}\mathbf{p}^{\wedge} \mathbf{A} \mathbf{m} \mathbf{A} \hat{\mathbf{S}}^{\dagger} \mathbf{b} + \text{if}(\mathbf{p}) - \mathbf{g}(\mathbf{V} \text{ '}(\mathbf{p} + \mathbf{i}(\mathbf{p}\mathbf{v}' \mathbf{f})) = 12^{-}$
 $\sqrt{(|\alpha 1'(t) \rangle \mathbf{CQ1t}|\phi(t) \rangle \mathbf{B} + |\alpha 2'(t) \rangle \mathbf{CQ2t}|\phi(t) \rangle \mathbf{B})} \text{ if } -\pi^{\wedge} \mathbf{C} \mathbf{m} \mathbf{d} \pi \mathbf{C} \mathbf{d} \pi 2 ((\langle \mathbf{p} + \text{if}(\mathbf{p}) - \mathbf{g}(\mathbf{V} \text{ '}(\mathbf{p} + \mathbf{i}(\mathbf{p}\mathbf{v}' \mathbf{f})) \neq$
 $\text{pentan-2-yl} \} -2\text{-Carboxylic acid; N-(1-carboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl}$
 $-2\text{-oxo6-}(\{\{\text{amino}(\{\{(\text{6-amino-9H-purin-9-yl) methyl} \text{ amino}) \} \text{ phosphoryl] carbamoyl} \} \text{ amino) -3,3- di}$
 $\text{methyl-7-oxo-4-thia- 1-azabicyclo [3.2.0] heptane- 2-Carboxylic acid; N-(1-carboximidoyl- 3- fluoro-1-}$
 $\{\text{5-oxabicyclo [2. 1.0] pentan-2-yl} \} -2\text{- Carboxylic acid; N-3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl} -2\text{-}$

oxo-1lambda4,2 lambda5- thiaphosphiran-2 -yl) -N'-yl) -N'-[(Z) - ethylidene]guanidine; [(S) -amino({[(S) -
 amino({[(4R) -6-oxo-4,6- dihydro-1H-purin-2-yl] amino}) phosphoryl oxy}) phos thiaphosphiran-2 -yl)
 -N'-yl) -N'-[(Z) + + (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+
 (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-1-(sqrt(theta) \Theta if (3 e~~_____~~ del phos
 phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl] amino))
 phosphoryl oxy}) phos phoryl] formonitrile (sqrt(theta) \Theta if (3 e~~_____~~ del phos
 phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl] amino))
 phosphoryl oxy}) phos phoryl] formonitrile 2) (\int 2 Dh dt dp dt -2 (, |\nabla |2 = { 2 Dh dt Do dp dtV'((p+(pV'2f
 where If\hat{S}bp^AmA\hat{S}^\dagger b+ if(p) - g(V '(p + i(pv' f)) =12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) if
 -\pi^{\text{Cmd}\pi\text{Cd}\pi 2} ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(theta) \Theta if (3 e~~_____~~ del
 purin-2-yl] amino)) phosphoryl oxy}) phos phoryl] formonitrile + + (sqrt(theta) \Theta if (3 e~~_____~~
 del)) \equiv \inf >0 |\nabla |2 = { 2 Dh dt Do dp dtV'((p+(pV'2f where If\hat{S}bp^AmA\hat{S}^\dagger b+ if(p) - g(V '(p + i(pv' f)) =12^{-
 \sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) if -\pi^{\text{Cmd}\pi\text{Cd}\pi 2} ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(theta)
 \Theta if (3 e~~_____~~ del purin-2-yl] amino)) phosphoryl oxy}) phos phoryl] formonitrile
 + + (sqrt(theta) \Theta if (3 e~~_____~~ del) d |\nabla |2 = { 2 Dh dt Do dp dtV'((p+(pV'2f where
 If\hat{S}bp^AmA\hat{S}^\dagger b+ if(p) - g(V '(p + i(pv' f)) =12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) if
 -\pi^{\text{Cmd}\pi\text{Cd}\pi 2} ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(theta) \Theta if (3 e~~_____~~ del
 purin-2-yl] amino)) phosphoryl oxy}) phos phoryl] formonitrile + + (sqrt(theta) \Theta if (3 e~~_____~~
 del) \equiv \int (4(-1) -2 |\nabla |2 = { 2 Dh dt dp dtV' (p+(pV'2f) where If\hat{S}bp^AmA\hat{S}^\dagger b+ if(p) - g(V '(p + i(pv' f)) =12^{-

$\sqrt{(|\alpha_1'(t)\rangle_{CQ1t}|\phi(t)\rangle_B + |\alpha_2'(t)\rangle_{CQ2t}|\phi(t)\rangle_B)} \text{ if } -\pi^{\wedge}C_{md}\pi C_{d}\pi_2 ((\langle p + \text{if}(p) - g(V' (p + i(pv' f)) \neq + (\sqrt{(\theta)} \Theta \text{ if } (3 e \text{-----} \text{del purin-2-yl] amino})) \text{ phosphoryl] oxy})) \text{ phos phoryl] formonitrile}$
 $+ + (\sqrt{(\theta)} \Theta \text{ if } (3 e \text{-----} \text{del}) (\int^2 D_h dt dp dt^{-2} + |\nabla|^2 = \{^2 D_h dt Do dp dt V'((p+(pV'2f \text{ where } If\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+ \text{ if}(p) - g(V' (p + i(pv' f)) = 12^{-} \sqrt{(|\alpha_1'(t)\rangle_{CQ1t}|\phi(t)\rangle_B + |\alpha_2'(t)\rangle_{CQ2t}|\phi(t)\rangle_B)} \text{ if } -\pi^{\wedge}C_{md}\pi C_{d}\pi_2 ((\langle p + \text{if}(p) - g(V' (p + i(pv' f)) \neq + (\sqrt{(\theta)} \Theta \text{ if } (3 e \text{-----} \text{del purin-2-yl] amino})) \text{ phosphoryl] oxy})) \text{ phos phoryl] formonitrile} + + (\sqrt{(\theta)} \Theta \text{ if } (3 e \text{-----} \text{del}) \equiv \int (4(-1) - 2|\nabla|^2 = \{^2 D_h dt dp dt V' (p+(pV'2f \text{ where } If\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+ \text{ if}(p) - g(V' (p + i(pv' f)) = 12^{-} \sqrt{(|\alpha_1'(t)\rangle_{CQ1t}|\phi(t)\rangle_B + |\alpha_2'(t)\rangle_{CQ2t}|\phi(t)\rangle_B)} \text{ if } -\pi^{\wedge}C_{md}\pi C_{d}\pi_2 ((\langle p + \text{if}(p) - g(V' (p + i(pv' f)) \neq \text{pentan-2-yl} \} \text{-2-Carboxylic acid; N-(1-carboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2.1.0] pentan-2-yl} \text{-2-oxo-1}\lambda_4, 2\lambda_5\text{-thiaphosphiran-2 -yl} \text{-N'-yl} \text{-N'-}[(Z) + + (\sqrt{(\theta)} \Theta (\sqrt{(\theta)} \Theta (\text{rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl} \text{-} + (\sqrt{(\theta)} \Theta (\sqrt{(\theta)} \Theta (\text{rboximidoyl- 3- fluoro-1-}(\sqrt{(\theta)} \Theta \text{ if } (3 e \text{-----} \text{del phos phoryl] formonitrile} (\text{rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl} \text{-purin-2-yl] amino})) \text{ phosphoryl] oxy})) \text{ phos phoryl] formonitrile} (\sqrt{(\theta)} \Theta \text{ if } (3 e \text{-----} \text{del phos phoryl] formonitrile} (\text{rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl} \text{-purin-2-yl] amino})) \text{ phosphoryl] oxy})) \text{ phos phoryl] formonitrile} 2) (\int^2 D_h dt dp dt^{-2} (, |\nabla|^2 = \{^2 D_h dt Do dp dt V'((p+(pV'2f \text{ where } If\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+ \text{ if}(p) - g(V' (p + i(pv' f)) = 12^{-} \sqrt{(|\alpha_1'(t)\rangle_{CQ1t}|\phi(t)\rangle_B + |\alpha_2'(t)\rangle_{CQ2t}|\phi(t)\rangle_B)} \text{ if } -\pi^{\wedge}C_{md}\pi C_{d}\pi_2 ((\langle p + \text{if}(p) - g(V' (p + i(pv' f)) \neq + (\sqrt{(\theta)} \Theta \text{ if } (3 e \text{-----} \text{del purin-2-yl] amino})) \text{ phosphoryl] oxy})) \text{ phos phoryl] formonitrile} + + (\sqrt{(\theta)} \Theta \text{ if } (3 e \text{-----} \text{del})) \equiv \inf > 0 |\nabla|^2 = \{^2 D_h dt Do dp dt V'((p+(pV'2f \text{ where } If\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+ \text{ if}(p) - g(V' (p + i(pv' f)) = 12^{-}$

$\sqrt{(|\alpha_1'(t)\rangle_{CQ1t}|\phi(t)\rangle_B + |\alpha_2'(t)\rangle_{CQ2t}|\phi(t)\rangle_B)} \text{ if } -\pi^{\wedge}C_{md}\pi C_{d}\pi^2 ((\langle p + \text{if}(p) - g(V \text{ '}(p + i(pv' f)) \neq + (\sqrt{(\theta)}$
 $\Theta \text{ if } (3 e^{\text{del purin-2-yl] amino}}) \text{ phosphoryl] oxy}}) \text{ phos phoryl] formonitrile}$
 $+ + (\sqrt{(\theta)} \Theta \text{ if } (3 e^{\text{del } 0) ^2) ^{(5/2)}) + (\sqrt{(\theta)} \Theta \text{ if } (3 e^{\wedge 3 \text{ del ' } (0) \text{ del '' } (0)}$
 $\text{del ''}(\text{del } 0) + e^{\wedge 3 \text{ del } ^{(3)} (\text{del } 0) (\text{del ' } (0)) ^3 + e^{\wedge 3 \text{ del } ^{(3)} (0) \text{ del ' } (\text{del } 0)) }) / (3 \sqrt{(\pi)} \sqrt{(1 - \theta \Theta ^2 (\text{del}$
 $\text{del } -12 (d |\nabla |^2 = \{ 2 D_h dt Do dp dt V'((p+(pV'2f \text{ where } \text{If}\hat{S}bp^{\wedge}Am\hat{A}\hat{S}^{\dagger}b+ \text{if}(p) - g(V \text{ '}(p + i(pv' f)) =12^{-}$
 $\sqrt{(|\alpha_1'(t)\rangle_{CQ1t}|\phi(t)\rangle_B + |\alpha_2'(t)\rangle_{CQ2t}|\phi(t)\rangle_B)} \text{ if } -\pi^{\wedge}C_{md}\pi C_{d}\pi^2 ((\langle p + \text{if}(p) - g(V \text{ '}(p + i(pv' f)) \neq + (\sqrt{(\theta)}$
 $\Theta \text{ if } (3 e^{\text{del purin-2-yl] amino}}) \text{ phosphoryl] oxy}}) \text{ phos phoryl] formonitrile}$
 $+ + (\sqrt{(\theta)} \Theta \text{ if } (3 e^{\text{del}}) \equiv \int (4(-1) ^{-2} |\nabla |^2 = \{ 2 D_h dt dp dt V' (p+(pV'2f)$
 $-1 \neq + (\sqrt{(\theta)} \Theta \text{ if } (3 e^{\text{del purin-2-yl] amino}}) \text{ phosphoryl] oxy}}) \text{ phos}$
 $\text{phoryl] formonitrile} + + (\sqrt{(\theta)} \Theta \text{ if } (3 e^{\text{del}}) (\int 2 D_h dt dp dt ^{-2} + |\nabla |^2 = \{ 2$
 $D_h dt Do dp dt V'((p+(pV'2f \text{ where } \text{If}\hat{S}bp^{\wedge}Am\hat{A}\hat{S}^{\dagger}b+ \text{if}(p) - g(V \text{ '}(p + i(pv' f)) =12^{-} \sqrt{(|\alpha_1'(t)\rangle_{CQ1t}|\phi(t)}$
 $\rangle_B + |\alpha_2'(t)\rangle_{CQ2t}|\phi(t)\rangle_B) \text{ if } -\pi^{\wedge}C_{md}\pi C_{d}\pi^2 ((\langle p + \text{if}(p) - g(V \text{ '}(p + i(pv' f)) \neq + (\sqrt{(\theta)} \Theta \text{ if } (3 e^{\text{del purin-2-yl] amino}}) \text{ phosphoryl] oxy}}) \text{ phos phoryl] formonitrile} + + (\sqrt{(\theta)} \Theta \text{ if } (3 e^{\text{del}})$
 $\text{del}) \equiv \int (4(-1) ^{-2} |\nabla |^2 = \{ 2 D_h dt dp dt V' (p+(pV'2f \text{ where } \text{If}\hat{S}bp^{\wedge}Am\hat{A}\hat{S}^{\dagger}b+ \text{if}(p) - g(V \text{ '}(p + i(pv' f)) =12^{-}$
 $\sqrt{(|\alpha_1'(t)\rangle_{CQ1t}|\phi(t)\rangle_B + |\alpha_2'(t)\rangle_{CQ2t}|\phi(t)\rangle_B)} \text{ if } -\pi^{\wedge}C_{md}\pi C_{d}\pi^2 ((\langle p + \text{if}(p) - g(V \text{ '}(p + i(pv' f)) \neq$

pentan-2-yl} -2-Carboxylicacid; N-(1-carboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl}
 -2-oxo6-({[amino({[(6-amino-9H-purin-9-yl) methyl] amino}) phosphoryl] carbamoyl] amino) -3,3- di
 methyl-7-oxo-4-thia- 1-azabicyclo [3.2.0] heptane- 2-Carboxylicacid; N-(1-carboximidoyl- 3- fluoro-1-
 {5-oxabicyclo [2. 1.0] pentan-2-yl} -2- Carboxylicacid; N-3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -2-

oxo-1lambda4,2 lambda5- thiaphosphiran-2 -yl) -N'-yl) -N'-[(Z) - ethylidene]guanidine; [(S) -amino({[(S) -
 amino({[(4R) -6-oxo-4,6- dihydro-1H-purin-2-yl] amino)) phosphoryl] oxy)) phos thiaphosphiran-2 -yl)
 -N'-yl) -N'-[(Z) + + (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+
 (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-1-(sqrt(theta) \Theta if (3 e_____ del phos
 phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl] amino))
 phosphoryl] oxy)) phos phoryl] formonitrile (sqrt(theta) \Theta if (3 e_____ del phos
 phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl] amino))
 phosphoryl] oxy)) phos phoryl] formonitrile 2) (\int 2 Dh dt dp dt -2 (, |\nabla |2 = { 2 Dh dt Do dp dtV'((p+(pV'2f
 where If\hat{S}bp^AmA\hat{S}^\dagger b+ if(p) - g(V '(p + i(pv' f)) =12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) if
 -\pi^{\wedge}Cmd\pi Cd\pi 2 ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(theta) \Theta if (3 e_____ del
 purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile + + (sqrt(theta) \Theta if (3 e_____ del)) \equiv \inf >0 |\nabla |2 = { 2 Dh dt Do dp dtV'((p+(pV'2f where If\hat{S}bp^AmA\hat{S}^\dagger b+ if(p) - g(V '(p + i(pv' f)) =12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) if -\pi^{\wedge}Cmd\pi Cd\pi 2 ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(theta) \Theta if (3 e_____ del purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile + + (sqrt(theta) \Theta if (3 e_____ del) v - |\nabla |2 = { 2 Dh dt Do dp dtV'((p+(pV'2f where If\hat{S}bp^AmA\hat{S}^\dagger b+ if(p) - g(V '(p + i(pv' f)) =12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) if -\pi^{\wedge}Cmd\pi Cd\pi 2 ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(theta) \Theta if (3 e_____ del purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile + + (sqrt(theta) \Theta if (3 e_____ del) \equiv \int (4(-1) -2 |\nabla |2 = { 2 Dh dt dp dtV' (p+(pV'2f where If\hat{S}bp^AmA\hat{S}^\dagger b+ if(p) - g(V '(p + i(pv' f)) =12^{-

$\sqrt{(|\alpha_1'(t)\rangle CQ1t|\phi(t)\rangle B + |\alpha_2'(t)\rangle CQ2t|\phi(t)\rangle B)}$ if $-\pi^{\wedge}Cmd\pi Cd\pi 2 ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq$
 pentan-2-yl} -2-Carboxylicacid; N-(1-carboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl}
 -2-oxo6-({[amino({[(6-amino-9H-purin-9-yl) methyl] amino}) phosphoryl] carbamoyl} amino) -3,3- di
 methyl-7-oxo-4-thia- 1-azabicyclo [3.2.0] heptane- 2-Carboxylicacid; N-(1-carboximidoyl- 3- fluoro-1-
 {5-oxabicyclo [2. 1.0] pentan-2-yl} -2- Carboxylicacid; N-3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -2-
 oxo-1lambda4,2 lambda5- thiaphosphiran-2 -yl) -N'-yl) -N'-[(Z) - ethylidene]guanidine; [(S) -amino({[(S) -
 amino({[(4R) -6-oxo-4,6- dihydro-1H-purin-2-yl] amino}) phosphoryl] oxy}) phos thiaphosphiran-2 -yl)
 -N'-yl) -N'-[(Z) + + (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+
 (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-1-(sqrt(theta) \Theta if (3 e_____ del phos
 phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl] amino))
 phosphoryl] oxy}) phos phoryl] formonitrile (sqrt(theta) \Theta if (3 e_____ del phos
 phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl] amino))
 phosphoryl] oxy}) phos phoryl] formonitrile 2) (\int 2 Dh dt dp dt -2 (, |\nabla |2 = { 2 Dh dt Do dp dtV'((p+(pV'2f
 where If\hat{S}bp^{\wedge}Am\hat{A}\hat{S}^{\dagger}b+ if(p) - g(V '(p + i(pv' f)) =12^{-} \sqrt{(|\alpha_1'(t)\rangle CQ1t|\phi(t)\rangle B + |\alpha_2'(t)\rangle CQ2t|\phi(t)\rangle B)} if
 $-\pi^{\wedge}Cmd\pi Cd\pi 2 ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(theta) \Theta if (3 e_____ del$
 purin-2-yl] amino)) phosphoryl] oxy}) phos phoryl] formonitrile + + (sqrt(theta) \Theta if (3 e_____ del)) \equiv \inf >0 |\nabla |2 = { 2 Dh dt Do dp dtV'((p+(pV'2f where If\hat{S}bp^{\wedge}Am\hat{A}\hat{S}^{\dagger}b+ if(p) - g(V '(p + i(pv' f)) =12^{-} \sqrt{(|\alpha_1'(t)\rangle CQ1t|\phi(t)\rangle B + |\alpha_2'(t)\rangle CQ2t|\phi(t)\rangle B)} if $-\pi^{\wedge}Cmd\pi Cd\pi 2 ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(theta) \Theta if (3 e_____ del purin-2-yl] amino)) phosphoryl] oxy}) phos phoryl] formonitrile$

+ + (sqrt(theta) \Theta if (3 e~~del~~) d |\nabla|^2 = { 2 Dh dt Do dp dtV'((p+(pV')^2f where If\hat{S}bp^AmA\hat{S}^\dagger b+ if(p) - g(V '(p + i(pv' f)) =12^{-}\sqrt{(|\alpha_1'(t)\rangle CQ1t|\phi(t)\rangle B+|\alpha_2'(t)\rangle CQ2t|\phi(t)\rangle B)} if -\pi^Cm d\pi C d\pi_2 ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(theta) \Theta if (3 e~~del~~) del purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile + + (sqrt(theta) \Theta if (3 e~~del~~)) \equiv \int (4(-1)^{-2} |\nabla|^2 = { 2 - 1^2where If\hat{S}bp^AmA\hat{S}^\dagger b+ if(p) - g(V '(p + i(pv' f)) =12^{-}\sqrt{(|\alpha_1'(t)\rangle CQ1t|\phi(t)\rangle B+|\alpha_2'(t)\rangle CQ2t|\phi(t)\rangle B)} if -\pi^Cm d\pi C d\pi_2 ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq 231+ 22+ 2) (\int 2 Dh dt dp dt -2 + () \equiv \int (4(-1)^{-2} |\nabla|^2= { + (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3-formonitrile + + (sqrt- fluoro-phos phoryl]) formonitrile where If\hat{S}bp^AmA\hat{S}^\dagger b+ if(p) - g(V '(p + i(pv' f)) =12^{-}\sqrt{(|\alpha_1'(t)\rangle CQ1t|\phi(t)\rangle B+|\alpha_2'(t)\rangle CQ2t|\phi(t)\rangle B)} if -\pi^Cm d\pi C d\pi_2 ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(theta) \Theta if (3 e~~del~~) del purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile + + (sqrt(theta) \Theta if (3 e~~del~~) del) (\int 2 Dh dt dp dt -2 (,|\nabla|^2 = { 2 Dh dt Do dp dtV'((p+(pV')^2f where If\hat{S}bp^AmA\hat{S}^\dagger b+ if(p) - g(V '(p + i(pv' f)) =12^{-}\sqrt{(|\alpha_1'(t)\rangle CQ1t|\phi(t)\rangle B+|\alpha_2'(t)\rangle CQ2t|\phi(t)\rangle B)} if -\pi^Cm d\pi C d\pi_2 ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(theta) \Theta if (3 e~~del~~) del purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl]) formonitrile + + (sqrt(theta) \Theta if (3 e~~del~~) del)) \equiv \inf >0 |\nabla|^2 = { 2 Dh dt Do dp dtV'((p+(pV')^2f where If\hat{S}bp^AmA\hat{S}^\dagger b+ if(p) - g(V '(p + i(pv' f)) =12^{-}\sqrt{(|\alpha_1'(t)\rangle CQ1t|\phi(t)\rangle B+|\alpha_2'(t)\rangle CQ2t|\phi(t)\rangle B)} if -\pi^Cm d\pi C d\pi_2 ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(theta) \Theta if (3 e~~del~~) del purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl]) formonitrile + + (sqrt(theta) \Theta if (3 e~~del~~) del) 0) ^2)))) \sin^{((integral Y1 dY1) X sqrt(242424) - y) \sin^{(-1) (del del -12 (d |\nabla|^2 = { 2 Dh dt Do dp dtV'((p+(pV')^2f where If\hat{S}bp^AmA\hat{S}^\dagger b+ if(p) - g(V '(p + i(pv' f)) =12^{-}\sqrt{(|\alpha_1'(t)\rangle CQ1t|\phi(t)\rangle B+|\alpha_2'(t)\rangle CQ2t|\phi(t)\rangle B)}

$\rangle CQ2t|\phi(t)\rangle_B$ if $-\pi^{\wedge}Cmd\pi Cd\pi2 ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(\theta) \Theta$ if (3 e $\frac{1}{\sqrt{2}}$

del purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile + + (sqrt(\theta) \Theta if (3 e $\frac{1}{\sqrt{2}}$

del) $\equiv \int (4(-1) -2|\nabla|^2 = \{ + (sqrt(\theta) \Theta (sqrt(\theta) \Theta (rboximidoyl- 3-formonitrile + + (sqrt- fluoro-phos phoryl]$

formonitrile where If $\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+$ if(p) - g(V '(p + i(pv' f)) = $12^{-\sqrt{(|\alpha1'(t)\rangle CQ1t|\phi(t)\rangle_B + |\alpha2'(t)\rangle CQ2t|\phi(t)\rangle_B}$ if $-\pi^{\wedge}Cmd\pi Cd\pi2 ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(\theta) \Theta$ if (3 e $\frac{1}{\sqrt{2}}$

$\rangle_B$ if $-\pi^{\wedge}Cmd\pi Cd\pi2 ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(\theta) \Theta$ if (3 e $\frac{1}{\sqrt{2}}$ del

purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile + + (sqrt(\theta) \Theta if (3 e $\frac{1}{\sqrt{2}}$

del) ($\int^2 Dh dt dp dt -2 + |\nabla|^2 = \{^2 Dh dt Do dp dt V'((p+(pV'2f$ where If $\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+$ if(p) - g(V '(p +

i(pv' f)) = $12^{-\sqrt{(|\alpha1'(t)\rangle CQ1t|\phi(t)\rangle_B + |\alpha2'(t)\rangle CQ2t|\phi(t)\rangle_B}$ if $-\pi^{\wedge}Cmd\pi Cd\pi2 ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(\theta) \Theta$ if (3 e $\frac{1}{\sqrt{2}}$

del purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl]

formonitrile + + (sqrt(\theta) \Theta if (3 e $\frac{1}{\sqrt{2}}$ del) $\equiv \int (4(-1) -2|\nabla|^2 = \{ + (sqrt(\theta) \Theta$

(sqrt(\theta) \Theta (rboximidoyl- 3-formonitrile + + (sqrt- fluoro-phos phoryl] formonitrile where If $\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+$

if(p) - g(V '(p + i(pv' f)) = $12^{-\sqrt{(|\alpha1'(t)\rangle CQ1t|\phi(t)\rangle_B + |\alpha2'(t)\rangle CQ2t|\phi(t)\rangle_B}$ if $-\pi^{\wedge}Cmd\pi Cd\pi2 ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(\theta) \Theta$ if (3 e $\frac{1}{\sqrt{2}}$

del purin-2-yl] amino)) phosphoryl]

oxy)) phos phoryl] formonitrile + + (sqrt(\theta) \Theta if (3 e $\frac{1}{\sqrt{2}}$ del) ($\int^2 Dh dt dp dt -2$

($\int |\nabla|^2 = \{^2 Dh dt Do dp dt V'((p+(pV'2f$ where If $\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+$ if(p) - g(V '(p + i(pv' f)) = $12^{-\sqrt{(|\alpha1'(t)\rangle CQ1t|\phi(t)\rangle_B + |\alpha2'(t)\rangle CQ2t|\phi(t)\rangle_B}$ if $-\pi^{\wedge}Cmd\pi Cd\pi2 ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(\theta) \Theta$ if (3 e $\frac{1}{\sqrt{2}}$

del purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile + + (sqrt(\theta) \Theta if (3 e $\frac{1}{\sqrt{2}}$

del)) $\equiv \inf_{>0} |\nabla|^2 = \{^2 Dh dt Do dp dt V'((p+(pV'2f$ where If $\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+$ if(p) - g(V '(p + i(pv' f)) = $12^{-\sqrt{(|\alpha1'(t)\rangle CQ1t|\phi(t)\rangle_B + |\alpha2'(t)\rangle CQ2t|\phi(t)\rangle_B}$ if $-\pi^{\wedge}Cmd\pi Cd\pi2 ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(\theta) \Theta$ if (3 e $\frac{1}{\sqrt{2}}$

Θ if (3 e $\frac{1}{2}$ del purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile
 $++ (\sqrt{\theta}) \Theta$ if (3 e $\frac{1}{2}$ del) v - $|\nabla|^2 = \{ 2 Dh dt Do dp dtV'((p+(pV'2f$ where
 $If\hat{S}bp^{\wedge}Am\hat{S}^{\dagger}b+ \text{ if}(p) - g(V' (p + i(pv' f)) = 12^{-} \sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B + |\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) \text{ if}$
 $-\pi^{\wedge}Cmd\pi Cd\pi 2 ((\langle p + \text{if}(p) - g(V' (p + i(pv' f)) \neq ++ (\sqrt{\theta}) \Theta$ if (3 e $\frac{1}{2}$ del
purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile $++ (\sqrt{\theta}) \Theta$ if (3 e $\frac{1}{2}$
del) $\equiv \int (4(-1) - 2 |\nabla|^2 = \{ 2 Dh dt dp dtV' (p+(pV'2f$ where $If\hat{S}bp^{\wedge}Am\hat{S}^{\dagger}b+ \text{ if}(p) - g(V' (p + i(pv' f)) = 12^{-}$
 $\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B + |\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) \text{ if } -\pi^{\wedge}Cmd\pi Cd\pi 2 ((\langle p + \text{if}(p) - g(V' (p + i(pv' f)) \neq$
pentan-2-yl} -2-Carboxylicacid; N-(1-carboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl}
-2-oxo6-({[amino({[(6-amino-9H-purin-9-yl) methyl] amino)) phosphoryl] carbamoyl} amino) -3,3- di
methyl-7-oxo-4-thia- 1-azabicyclo [3.2.0] heptane- 2-Carboxylicacid; N-(1-carboximidoyl- 3- fluoro-1-
{5-oxabicyclo [2. 1.0] pentan-2-yl} -2- Carboxylicacid; N-3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -2-
oxo-1 λ 4,2 λ 5- thiaphosphiran-2 -yl) -N'-yl) -N'-[(Z) - ethylidene]guanidine; [(S) -amino({[(S) -
amino({[(4R) -6-oxo-4,6- dihydro-1H-purin-2-yl] amino)) phosphoryl] oxy)) phos thiaphosphiran-2 -yl)
-N'-yl) -N'-[(Z) $++ (\sqrt{\theta}) \Theta$ ($\sqrt{\theta}) \Theta$ (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+
($\sqrt{\theta}) \Theta$ ($\sqrt{\theta}) \Theta$ (rboximidoyl- 3- fluoro-1-($\sqrt{\theta}) \Theta$ if (3 e $\frac{1}{2}$ del phos
phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl] amino))
phosphoryl] oxy)) phos phoryl] formonitrile ($\sqrt{\theta}) \Theta$ if (3 e $\frac{1}{2}$ del phos
phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl] amino))
phosphoryl] oxy)) phos phoryl] formonitrile 2) ($\int 2 Dh dt dp dt - 2 (, |\nabla|^2 = \{ 2 Dh dt Do dp dtV'((p+(pV'2f$

where $\text{If}\hat{\text{Sbp}}^{\text{Am}}\hat{\text{A}}\hat{\text{S}}^{\dagger}\text{b}+ \text{if}(\text{p}) - \text{g}(\text{V} \text{ '}(\text{p} + \text{i}(\text{pv}' \text{ f})) = 12^{-} \sqrt{(|\alpha 1'(t) \rangle \text{CQ1t}|\phi(t) \rangle \text{B} + |\alpha 2'(t) \rangle \text{CQ2t}|\phi(t) \rangle \text{B})}$ if $-\pi^{\text{Cmd}}\pi\text{Cd}\pi 2 ((\langle \text{p} + \text{if}(\text{p}) - \text{g}(\text{V} \text{ '}(\text{p} + \text{i}(\text{pv}' \text{ f})) \neq + (\text{sqrt}(\theta) \Theta \text{ if } (3 \text{ e} \text{-----} \text{del}$

$\text{purin-2-yl] amino}) \text{ phosphoryl] oxy}) \text{ phos phoryl] formonitrile} + + (\text{sqrt}(\theta) \Theta \text{ if } (3 \text{ e} \text{-----} \text{del})) \equiv \int > 0 |\nabla|^2 = \{ 2 \text{ Dh dt Do dp dt V}'((\text{p} + (\text{pV}' 2 \text{f where } \text{If}\hat{\text{Sbp}}^{\text{Am}}\hat{\text{A}}\hat{\text{S}}^{\dagger}\text{b}+ \text{if}(\text{p}) - \text{g}(\text{V} \text{ '}(\text{p} + \text{i}(\text{pv}' \text{ f})) = 12^{-} \sqrt{(|\alpha 1'(t) \rangle \text{CQ1t}|\phi(t) \rangle \text{B} + |\alpha 2'(t) \rangle \text{CQ2t}|\phi(t) \rangle \text{B})}$ if $-\pi^{\text{Cmd}}\pi\text{Cd}\pi 2 ((\langle \text{p} + \text{if}(\text{p}) - \text{g}(\text{V} \text{ '}(\text{p} + \text{i}(\text{pv}' \text{ f})) \neq + (\text{sqrt}(\theta) \Theta \text{ if } (3 \text{ e} \text{-----} \text{del}$

$\text{purin-2-yl] amino}) \text{ phosphoryl] oxy}) \text{ phos phoryl] formonitrile} + + (\text{sqrt}(\theta) \Theta \text{ if } (3 \text{ e} \text{-----} \text{del})) \equiv \int > 0 |\nabla|^2 = \{ 2 \text{ Dh dt Do dp dt V}'((\text{p} + (\text{pV}' 2 \text{f where } \text{If}\hat{\text{Sbp}}^{\text{Am}}\hat{\text{A}}\hat{\text{S}}^{\dagger}\text{b}+ \text{if}(\text{p}) - \text{g}(\text{V} \text{ '}(\text{p} + \text{i}(\text{pv}' \text{ f})) = 12^{-} \sqrt{(|\alpha 1'(t) \rangle \text{CQ1t}|\phi(t) \rangle \text{B} + |\alpha 2'(t) \rangle \text{CQ2t}|\phi(t) \rangle \text{B})}$ if $-\pi^{\text{Cmd}}\pi\text{Cd}\pi 2 ((\langle \text{p} + \text{if}(\text{p}) - \text{g}(\text{V} \text{ '}(\text{p} + \text{i}(\text{pv}' \text{ f})) \neq + (\text{sqrt}(\theta) \Theta \text{ if } (3 \text{ e} \text{-----} \text{del}$

$\text{purin-2-yl] amino}) \text{ phosphoryl] oxy}) \text{ phos phoryl] formonitrile} + + (\text{sqrt}(\theta) \Theta \text{ if } (3 \text{ e} \text{-----} \text{del})) \equiv \int (4(-1) - 2 |\nabla|^2 = \{ + (\text{sqrt}(\theta) \Theta (\text{sqrt}(\theta) \Theta (\text{rboximidoyl- 3-formonitrile} + + (\text{sqrt- fluoro-phos phoryl] formonitrile where } \text{If}\hat{\text{Sbp}}^{\text{Am}}\hat{\text{A}}\hat{\text{S}}^{\dagger}\text{b}+ \text{if}(\text{p}) - \text{g}(\text{V} \text{ '}(\text{p} + \text{i}(\text{pv}' \text{ f})) = 12^{-} \sqrt{(|\alpha 1'(t) \rangle \text{CQ1t}|\phi(t) \rangle \text{B} + |\alpha 2'(t) \rangle \text{CQ2t}|\phi(t) \rangle \text{B})}$ if $-\pi^{\text{Cmd}}\pi\text{Cd}\pi 2 ((\langle \text{p} + \text{if}(\text{p}) - \text{g}(\text{V} \text{ '}(\text{p} + \text{i}(\text{pv}' \text{ f})) \neq + (\text{sqrt}(\theta) \Theta \text{ if } (3 \text{ e} \text{-----} \text{del}$

$\text{purin-2-yl] amino}) \text{ phosphoryl] oxy}) \text{ phos phoryl] formonitrile} + + (\text{sqrt}(\theta) \Theta \text{ if } (3 \text{ e} \text{-----} \text{del})) (\int 2 \text{ Dh dt dp dt} - 2 + |\nabla|^2 = \{ 2 \text{ Dh dt Do dp dt V}'((\text{p} + (\text{pV}' 2 \text{f where } \text{If}\hat{\text{Sbp}}^{\text{Am}}\hat{\text{A}}\hat{\text{S}}^{\dagger}\text{b}+ \text{if}(\text{p}) - \text{g}(\text{V} \text{ '}(\text{p} + \text{i}(\text{pv}' \text{ f})) = 12^{-} \sqrt{(|\alpha 1'(t) \rangle \text{CQ1t}|\phi(t) \rangle \text{B} + |\alpha 2'(t) \rangle \text{CQ2t}|\phi(t) \rangle \text{B})}$ if $-\pi^{\text{Cmd}}\pi\text{Cd}\pi 2 ((\langle \text{p} + \text{if}(\text{p}) - \text{g}(\text{V} \text{ '}(\text{p} + \text{i}(\text{pv}' \text{ f})) \neq + (\text{sqrt}(\theta) \Theta \text{ if } (3 \text{ e} \text{-----} \text{del}$

$\text{purin-2-yl] amino}) \text{ phosphoryl] oxy}) \text{ phos phoryl] formonitrile} + + (\text{sqrt}(\theta) \Theta \text{ if } (3 \text{ e} \text{-----} \text{del})) \equiv \int (4(-1) - 2 |\nabla|^2 = \{ + (\text{sqrt}(\theta) \Theta (\text{sqrt}(\theta) \Theta (\text{rboximidoyl- 3-formonitrile} + + (\text{sqrt- fluoro-phos phoryl] formonitrile where } \text{If}\hat{\text{Sbp}}^{\text{Am}}\hat{\text{A}}\hat{\text{S}}^{\dagger}\text{b}+$

$\text{if}(\mathbf{p}) - \mathbf{g}(\mathbf{V} \text{ '}(\mathbf{p} + \mathbf{i}(\mathbf{p}\mathbf{v}' \mathbf{f})) = 12^{-} \sqrt{(|\alpha 1'(t) \rangle \mathbf{CQ1t}|\phi(t) \rangle \mathbf{B} + |\alpha 2'(t) \rangle \mathbf{CQ2t}|\phi(t) \rangle \mathbf{B}) \text{ if } -\pi^{\wedge} \mathbf{C} \mathbf{m} \mathbf{d} \pi \mathbf{C} \mathbf{d} \pi 2} ((\langle \mathbf{p} + \mathbf{i}(\mathbf{p}) -$
 $\mathbf{g}(\mathbf{V} \text{ '}(\mathbf{p} + \mathbf{i}(\mathbf{p}\mathbf{v}' \mathbf{f})) \neq + (\text{sqrt}(\theta) \ominus \text{ if } (3 \text{ e} \text{-----} \text{ del purin-2-yl] amino})) \text{ phosphoryl]}$
 $\text{oxy})) \text{ phos phoryl] formonitrile} + + (\text{sqrt}(\theta) \ominus \text{ if } (3 \text{ e} \text{-----} \text{ del}) (\int 2 \text{ D} \mathbf{h} \text{ d} \mathbf{t} \text{ d} \mathbf{p} \text{ d} \mathbf{t} - 2$
 $(, |\nabla|^2 = \{ 2 \text{ D} \mathbf{h} \text{ d} \mathbf{t} \text{ D} \mathbf{o} \text{ d} \mathbf{p} \text{ d} \mathbf{t} \mathbf{V}'((\mathbf{p} + (\mathbf{p}\mathbf{V}' 2 \mathbf{f} \text{ where } \text{If} \hat{\mathbf{S}} \mathbf{b} \mathbf{p}^{\wedge} \mathbf{A} \mathbf{m} \mathbf{A} \hat{\mathbf{S}}^{\dagger} \mathbf{b} + \text{if}(\mathbf{p}) - \mathbf{g}(\mathbf{V} \text{ '}(\mathbf{p} + \mathbf{i}(\mathbf{p}\mathbf{v}' \mathbf{f})) = 12^{-} \sqrt{(|\alpha 1'(t)$
 $\rangle \mathbf{CQ1t}|\phi(t) \rangle \mathbf{B} + |\alpha 2'(t) \rangle \mathbf{CQ2t}|\phi(t) \rangle \mathbf{B}) \text{ if } -\pi^{\wedge} \mathbf{C} \mathbf{m} \mathbf{d} \pi \mathbf{C} \mathbf{d} \pi 2} ((\langle \mathbf{p} + \mathbf{i}(\mathbf{p}) - \mathbf{g}(\mathbf{V} \text{ '}(\mathbf{p} + \mathbf{i}(\mathbf{p}\mathbf{v}' \mathbf{f})) \neq + (\text{sqrt}(\theta) \ominus \text{ if } (3 \text{ e} \text{-----}$
 $\text{del purin-2-yl] amino})) \text{ phosphoryl] oxy})) \text{ phos phoryl] formonitrile} + + (\text{sqrt}(\theta) \ominus \text{ if } (3 \text{ e} \text{-----}$
 $\text{del})) \equiv \inf > 0 |\nabla|^2 = \{ 2 \text{ D} \mathbf{h} \text{ d} \mathbf{t} \text{ D} \mathbf{o} \text{ d} \mathbf{p} \text{ d} \mathbf{t} \mathbf{V}'((\mathbf{p} + (\mathbf{p}\mathbf{V}' 2 \mathbf{f} \text{ where } \text{If} \hat{\mathbf{S}} \mathbf{b} \mathbf{p}^{\wedge} \mathbf{A} \mathbf{m} \mathbf{A} \hat{\mathbf{S}}^{\dagger} \mathbf{b} + \text{if}(\mathbf{p}) - \mathbf{g}(\mathbf{V} \text{ '}(\mathbf{p} + \mathbf{i}(\mathbf{p}\mathbf{v}' \mathbf{f})) = 12^{-}$
 $\sqrt{(|\alpha 1'(t) \rangle \mathbf{CQ1t}|\phi(t) \rangle \mathbf{B} + |\alpha 2'(t) \rangle \mathbf{CQ2t}|\phi(t) \rangle \mathbf{B}) \text{ if } -\pi^{\wedge} \mathbf{C} \mathbf{m} \mathbf{d} \pi \mathbf{C} \mathbf{d} \pi 2} ((\langle \mathbf{p} + \mathbf{i}(\mathbf{p}) - \mathbf{g}(\mathbf{V} \text{ '}(\mathbf{p} + \mathbf{i}(\mathbf{p}\mathbf{v}' \mathbf{f})) \neq + (\text{sqrt}(\theta)$
 $\ominus \text{ if } (3 \text{ e} \text{-----} \text{ del purin-2-yl] amino})) \text{ phosphoryl] oxy})) \text{ phos phoryl] formonitrile}$
 $+ + (\text{sqrt}(\theta) \ominus \text{ if } (3 \text{ e} \text{-----} \text{ del}) (\text{e x}) \ominus \text{sqrt}(\theta)) = -\sin^{\wedge}(-1) (\text{sqrt}(\theta) \ominus \text{del del } -12 (\text{d}$
 $|\nabla|^2 = \{ 2 \text{ D} \mathbf{h} \text{ d} \mathbf{t} \text{ D} \mathbf{o} \text{ d} \mathbf{p} \text{ d} \mathbf{t} \mathbf{V}'((\mathbf{p} + (\mathbf{p}\mathbf{V}' 2 \mathbf{f} \text{ where } \text{If} \hat{\mathbf{S}} \mathbf{b} \mathbf{p}^{\wedge} \mathbf{A} \mathbf{m} \mathbf{A} \hat{\mathbf{S}}^{\dagger} \mathbf{b} + \text{if}(\mathbf{p}) - \mathbf{g}(\mathbf{V} \text{ '}(\mathbf{p} + \mathbf{i}(\mathbf{p}\mathbf{v}' \mathbf{f})) = 12^{-} \sqrt{(|\alpha 1'(t)$
 $\rangle \mathbf{CQ1t}|\phi(t) \rangle \mathbf{B} + |\alpha 2'(t) \rangle \mathbf{CQ2t}|\phi(t) \rangle \mathbf{B}) \text{ if } -\pi^{\wedge} \mathbf{C} \mathbf{m} \mathbf{d} \pi \mathbf{C} \mathbf{d} \pi 2} ((\langle \mathbf{p} + \mathbf{i}(\mathbf{p}) - \mathbf{g}(\mathbf{V} \text{ '}(\mathbf{p} + \mathbf{i}(\mathbf{p}\mathbf{v}' \mathbf{f})) \neq + (\text{sqrt}(\theta) \ominus \text{ if } (3 \text{ e} \text{-----}$
 $\text{del purin-2-yl] amino})) \text{ phosphoryl] oxy})) \text{ phos phoryl] formonitrile} + + (\text{sqrt}(\theta) \ominus \text{ if } (3 \text{ e} \text{-----}$
 $\text{del}) \equiv \int (4(-1) - 2 |\nabla|^2 \{ 2 - 12 - 11 \neq 231 + 22 + 2) (\int 2 - 2) - 2 + () \equiv [4(-1) - 2 |\nabla|^2 = \{ + (\text{sqrt}(\theta) \ominus (\text{sqrt}(\theta) \ominus$
 $(\text{rboximidoyl- 3- fluoro-phos phoryl] formonitrile} + (\text{sqrt}(\theta) \ominus \text{ if } (3 \text{ e} \text{-----} \text{ del}$
 $(1\text{-carboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl\} - + (\text{sqrt}(\theta) \ominus (\text{sqrt}(\theta) \ominus (\text{rboximidoyl- 3-$
 $\text{fluoro-phos phoryl] formonitrile} 1 + (\text{sqrt}(\theta) \ominus (\text{sqrt}(\theta) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl] formonitrile}$
 $1 \neq + (\text{sqrt}(\theta) \ominus (\text{sqrt}(\theta) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl] formonitrile} + (\text{sqrt}(\theta) \ominus \text{ if } (3 \text{ e} \text{-----}$
 $\text{del purin-2-yl] amino})) \text{ phosphoryl] oxy})) \text{ phos phoryl] formonitrile} + + (\text{sqrt}(\theta) \ominus (\text{sqrt}(\theta) \ominus (\text{rboximidoyl-$

3- fluoro-phos phoryl] formonitrile $22 \rightarrow (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}]$
formonitrile $2) + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}]$ formonitrile $(\int + (\sqrt{\theta}) \ominus$
 $(\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}]$ formonitrile $+ (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----}$
 $\text{del } (\text{rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl\} } \rightarrow (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3-}$
fluoro-phos phoryl] formonitrile $(+ (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}]$ formonitrile,

$> |\nabla|^2 = \{ 2 \text{ Dh dt Do dp dtV}((\text{p}+(\text{pV}^2\text{f where If}\hat{\text{S}}\text{bp}^{\wedge}\text{AmA}\hat{\text{S}}^{\dagger}\text{b}+\text{if}(\text{p}) - \text{g}(\text{V} \text{'(p + i(pv' f))} =12\text{--}$
 $\sqrt{(|\alpha 1'(t) \rangle \text{CQ1t}|\phi(t) \rangle \text{B}+|\alpha 2'(t) \rangle \text{CQ2t}|\phi(t) \rangle \text{B}) \text{ if } -\pi^{\wedge}\text{Cmd}\pi\text{Cd}\pi 2 ((\langle \text{p} + \text{if}(\text{p}) - \text{g}(\text{V} \text{'(p + i(pv' f))} \neq +$
 $(\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----} \text{del purin-2-yl] amino\}) \text{ phosphoryl] oxy\}) \text{ phos}$
phoryl] formonitrile $+ + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----} \text{del})) \equiv \text{inf}+ (\sqrt{\theta}) \ominus$
 $(\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}]$ formonitrile $>0+ (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl-}$
3- fluoro-phos phoryl] formonitrile $+ (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----} \text{del}$
 $(\text{rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl\} } - \text{v} \rightarrow (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$
 $(\text{rboximidoyl- 3- fluoro-phos phoryl}]$ formonitrile $+ (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----}$
 $\text{del } (\text{rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl\} } - \equiv \int + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$
 $(\text{rboximidoyl- 3- fluoro-phos phoryl}]$ formonitrile $(4(-1) ^{-2} |\nabla|^2 = \{+ (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$
 $(\text{rboximidoyl- 3- fluoro-phos phoryl}]$ formonitrile $+ (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----}$
 $\text{del phos phoryl}]$ formonitrile $(\text{rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl\} } \text{-pur}$
in-2-yl] amino\}) phosphoryl] oxy\}) phos phoryl] formonitrile $+ (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3-}$
fluoro-phos phoryl] formonitrile $1 \neq + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}]$

formonitrile pentan-2-yl} -2-Carboxylicacid; N-(1-carboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -2-o xo6-({[amino({[(6-amino-9H-purin-9-yl) methyl] amino}) phosphoryl] carbamoyl} amino) -3,3- di methyl-7-oxo-4-thia- 1-azabicyclo [3.2.0] heptane- 2-Carboxylicacid; N-(1-carboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -2- Carboxylicacid; N-3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -2- oxo-1lambda4,2 lambda5- thiaphosphiran-2 -yl) -N'-yl) -N'-[(Z) - ethylidene]guanidine; [(S) -amino({[(S) - amino({[(4R) -6-oxo-4,6-dihydro-1H-purin-2-yl] amino}) phosphoryl] oxy}) phos thiaphosphiran-2 -yl) -N'-yl) -N'-[(Z) ++ (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-1-(sqrt(theta) \Theta if (3 e_____ del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -puri n-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile (sqrt(theta) \Theta if (3 e_____ del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile

> 2) + (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-phos phoryl] formonitrile (\int + (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(theta) \Theta if (3 e_____ del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-phos phoryl] formonitrile (+ (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-phos phoryl] formonitrile, |\nabla |^2 = \{ 2 Dh dt Do dp dtV'((p+(pV'2f where If\hat{S}bp^AmA\hat{S}^\dagger b+ if(p)

- $g(V'(\mathbf{p} + i(\mathbf{p}_V' \mathbf{f})) = 12^{-\sqrt{(|\alpha_1'(t)\rangle CQ1t|\phi(t)\rangle B + |\alpha_2'(t)\rangle CQ2t|\phi(t)\rangle B}} \text{ if } -\pi^{\text{Cmd}}\pi C d\pi^2 ((\langle \mathbf{p} + i(\mathbf{p}_V' \mathbf{f}))$

- $g(V'(\mathbf{p} + i(\mathbf{p}_V' \mathbf{f})) \neq + (\sqrt{\theta}) \ominus \text{ if } (3 \text{ e} \text{-----} \text{ del purin-2-yl] amino})$

phosphor yl]oxy}) phos phoryl] formonitrile + + $(\sqrt{\theta}) \ominus \text{ if } (3 \text{ e} \text{-----}$

del)) $\equiv \inf + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl] formonitrile} > 0 + (\sqrt{\theta}) \ominus$

$(\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl] formonitrile} + (\sqrt{\theta}) \ominus \text{ if } (3 \text{ e} \text{-----}$

del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} - d+ $(\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$

(rboximidoyl- 3- fluoro-phos phoryl] formonitrile + $(\sqrt{\theta}) \ominus \text{ if } (3 \text{ e} \text{-----}$

del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} - $\equiv \int + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$

(rboximidoyl- 3- fluoro-phos phoryl] formonitrile $(4(-1)^{-2} |\nabla|^2 = \{ + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$

(rboximidoyl- 3- fluoro-phos phoryl] formonitrile $2 \rightarrow + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3-}$

fluoro-phos phoryl] formonitrile 1

$> 2 \rightarrow + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl] formonitrile} 1 + (\sqrt{\theta}) \ominus (\sqrt{\theta})$

$\ominus (\text{rboximidoyl- 3- fluoro-phos phoryl] formonitrile} 1 \neq + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3-}$

fluoro-phos phoryl] formonitrile + $(\sqrt{\theta}) \ominus \text{ if } (3 \text{ e} \text{-----} \text{ del purin-2-yl]$

amino}) phosphoryl] oxy}) phos phoryl] formonitrile ++ $(\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3-}$

fluoro-phos phoryl] formonitrile $22 \rightarrow + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl]$

formonitrile 2) + $(\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl] formonitrile} (\int + (\sqrt{\theta})$

$\ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl] formonitrile} + (\sqrt{\theta}) \ominus \text{ if } (3 \text{ e} \text{-----}$

del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} $\rightarrow + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$

(rboximidoyl- 3- fluoro-phos phoryl] formonitrile ++ (sqrt(0) ⊖ (sqrt(0) ⊖ (rboximidoyl- 3-
 fluoro-phos phoryl] formonitrile + (sqrt(0) ⊖ if (3 e $\frac{1}{2}$) del
 (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} $\equiv$] + (sqrt(0) ⊖ (sqrt(0) ⊖ (rboximidoyl-
 3- fluoro-phos phoryl] formonitrile (4(−1) −2|∇ |2= {
 > + (sqrt(0) ⊖ if (3 e $\frac{1}{2}$) del phos phoryl] formonitrile (rboximidoyl-
 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl] amino}) phosphoryl oxy}) phos phoryl]
 formonitrile + (sqrt(0) ⊖ (sqrt(0) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile 1 ≠+ (sqrt(0)
 ⊖ (sqrt(0) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(0) ⊖ if (3 e $\frac{1}{2}$)
 del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(0) ⊖ (sqrt(0) ⊖
 (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(0) ⊖ (sqrt(0) ⊖ (rboximidoyl- 3- fluoro-1-
 {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(0) ⊖ (sqrt(0) ⊖ (rboximidoyl- 3- fluoro-1-(sqrt(0) ⊖ if (3 e $\frac{1}{2}$)
 del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl]
 -purin-2-yl] amino}) phosphoryl oxy}) phos phoryl] formonitrile (sqrt(0) ⊖ if (3 e $\frac{1}{2}$)
 del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl]
 -purin-2-yl] amino}) phosphoryl oxy}) phos phoryl] formonitrile + (sqrt(0) ⊖ (sqrt(0) ⊖
 (rboximidoyl- 3- fluoro-phos phoryl] formonitrile 2) + (sqrt(0) ⊖ (sqrt(0) ⊖ (rboximidoyl- 3-
 fluoro-phos phoryl] formonitrile (∫ + (sqrt(0) ⊖ (sqrt(0) ⊖ (rboximidoyl- 3- fluoro-phos phoryl]
 formonitrile + (sqrt(0) ⊖ if (3 e $\frac{1}{2}$) del (rboximidoyl- 3- fluoro-1-
 {5-oxabicyclo [2. 1.0]pentan-2-yl} -+ (sqrt(0) ⊖ (sqrt(0) ⊖ (rboximidoyl- 3- fluoro-phos phoryl]

formonitrile $(+\sqrt{\theta})\ominus(\sqrt{\theta})\ominus(\text{rboximidoyl-3-fluoro-phos phoryl})$ formonitrile, $|\nabla|^2=\{2\text{ Dh}$

$\text{dt Do dp dtV}'((\text{p}+(\text{pV}'2\text{f where If}\hat{\text{S}}\text{bp}^{\text{Am}}\hat{\text{S}}^{\dagger}\text{b}+\text{if}(\text{p})-\text{g}(\text{V}'(\text{p}+\text{i}(\text{pv}'\text{f}))=12^{-\sqrt{(|\alpha1'(\text{t})\text{)CQ1t}|\phi(\text{t})}}$

$\text{)B}+|\alpha2'(\text{t})\text{)CQ2t}|\phi(\text{t})\text{)B}$ if $-\pi^{\text{Cmd}}\pi\text{Cd}\pi2((\text{p}+\text{if}(\text{p})-\text{g}(\text{V}'(\text{p}+\text{i}(\text{pv}'\text{f}))\neq+(\sqrt{\theta})\ominus$ if $(3\text{ e}^{\frac{(\text{rboximidoyl-3-fluoro-phos phoryl})}{\text{formonitrile}}})\equiv\inf+(\sqrt{\theta})\ominus(\sqrt{\theta})\ominus(\text{rboximidoyl-3-fluoro-phos phoryl})$ formonitrile $>0+(\sqrt{\theta})\ominus(\sqrt{\theta})\ominus(\text{rboximidoyl-3-fluoro-phos phoryl})$ formonitrile $+(\sqrt{\theta})\ominus$ if $(3\text{ e}^{\frac{(\text{rboximidoyl-3-fluoro-phos phoryl})}{\text{formonitrile}}})\equiv\int+(\sqrt{\theta})\ominus(\sqrt{\theta})\ominus(\text{rboximidoyl-3-fluoro-1-\{5-oxabicyclo[2.1.0]pentan-2-yl\}}-(\text{e}^{\text{x}}))\sin^{(-1)}((\text{constant}+^{-3}\sqrt{(6734)\text{X Y1}^2})+\text{y})-\frac{1}{2}\text{x}^4(\sqrt{\pi})\sin^{(-1)}(\text{y}-3\sqrt{(6734)\text{X Y1}^2})((\text{e}^4\theta^{(5/2)}\Theta^5\text{del del}-12(\text{d}+(\sqrt{\theta})\ominus(\sqrt{\theta})\ominus(\text{rboximidoyl-3-fluoro-phos phoryl})$ formonitrile $+(\sqrt{\theta})\ominus$ if $(3\text{ e}^{\frac{(\text{rboximidoyl-3-fluoro-phos phoryl})}{\text{formonitrile}}})\equiv\int+(\sqrt{\theta})\ominus(\sqrt{\theta})\ominus(\text{rboximidoyl-3-fluoro-phos phoryl})$ formonitrile $(4(-1)^{-2}|\nabla|^2=\{+(\sqrt{\theta})\ominus(\sqrt{\theta})\ominus(\text{rboximidoyl-3-fluoro-phos phoryl})$ formonitrile $+(\sqrt{\theta})\ominus$ if $(3\text{ e}^{\frac{(\text{rboximidoyl-3-fluoro-phos phoryl})}{\text{formonitrile}}})\text{del phos phoryl})$ formonitrile $(\text{rboximidoyl-3-fluoro-1-\{5-oxabicyclo[2.1.0]pentan-2-yl\}}-\text{purin-2-yl})$ amino)) phosphoryl oxy)) phos phoryl) formonitrile $+(\sqrt{\theta})\ominus(\sqrt{\theta})\ominus(\text{rboximidoyl-3-fluoro-phos phoryl})$ formonitrile $1\neq+(\sqrt{\theta})\ominus(\sqrt{\theta})\ominus(\text{rboximidoyl-3-fluoro-phos phoryl})$ formonitrile $+(\sqrt{\theta})\ominus$ if $(3\text{ e}^{\frac{(\text{rboximidoyl-3-fluoro-phos phoryl})}{\text{formonitrile}}})\text{del}(\text{rboximidoyl-3-fluoro-1-\{5-oxabicyclo[2.1.0]pentan-2-yl\}}-+(\sqrt{\theta})\ominus(\sqrt{\theta})\ominus(\text{rboximidoyl-3-fluoro-phos phoryl})$ formonitrile 2

> 2 ++ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile 2) + (sqrt(θ) ⊖
 (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile (∫ + (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl-
 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) ⊖ if (3 e————— del
 (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl-
 3- fluoro-phos phoryl] formonitrile ++ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl]
 formonitrile + (sqrt(θ) ⊖ if (3 e————— del (rboximidoyl- 3- fluoro-1-
 {5-oxabicyclo [2. 1.0] pentan-2-yl} =∫+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl]
 formonitrile (4(-1) -2|∇ |2= {+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl]
 formonitrile + (sqrt(θ) ⊖ if (3 e————— del (1-carboximidoyl- 3- fluoro-1-
 {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl]
 formonitrile 1+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile 1≠+ (sqrt(θ)
 ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile 2

 > 3 1++ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) ⊖
 (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(θ) ⊖ (sqrt(θ) ⊖
 (rboximidoyl- 3- fluoro-1-(sqrt(θ) ⊖ if (3 e————— del phos phoryl]
 formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2- yl] amino))
 phosphoryl] oxy)) phos phoryl] formonitrile (sqrt(θ) ⊖ if (3 e————— del
 phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2- yl]
 amino)) phosphoryl] oxy)) phos phoryl] formonitrile + (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3-

fluoro-phos phoryl] formonitrile 2) + (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile (∫ + (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) ⊖ if (3 e

del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile (+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile, |∇ |2 = { 2 Dh dt Do dp dtV'((p+(pV'2f where IfŜbp^AmAŜ†b+ if(p

- g(V '(p + i(pv' f)) =12^- √(|α1'(t) >CQ1t|φ(t) >B+|α2'(t) >CQ2t|φ(t) >B) if -π^CmdπCdπ2 ((<p + if(p

- g(V '(p + i(pv' f)) ≠ + (sqrt(θ) ⊖ if (3 e————— del purin-2-yl] amino))

phosphoryl] oxy)) phos phoryl] formonitrile + + (sqrt(θ) ⊖ if (3 e—————

del)) ≡ inf+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile >0+ (sqrt(θ) ⊖

(sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) ⊖ if (3 e—————

del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} - v -+ (sqrt(θ) ⊖ (sqrt(θ) ⊖

(rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) ⊖ if (3 e—————

del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} - ≡ ∫+ (sqrt(θ) ⊖ (sqrt(θ) ⊖

(rboximidoyl- 3- fluoro-phos phoryl] formonitrile (4(-1) -2

> |∇ |2 = {+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) ⊖ if (3

e————— del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1-

{5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-y l] amino)) phosphoryl] oxy)) phos phoryl] formonitrile

+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile 1 ≠+ (sqrt(θ) ⊖ (sqrt(θ) ⊖

(rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) ⊖ if (3 e—————

del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-1-(sqrt(θ) ⊖ if (3 e ^{$\frac{(\int_0^t \sqrt{\tau} d\tau)^2}{\int_0^t \sqrt{\tau} d\tau}$}) del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl] amino)) phosphoryl] oxy})) phos phoryl] formonitrile (sqrt(θ) ⊖ if (3 e ^{$\frac{(\int_0^t \sqrt{\tau} d\tau)^2}{\int_0^t \sqrt{\tau} d\tau}$}) del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl] amino)) phosphoryl] oxy})) phos phoryl] formonitrile + (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile 2) + (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile (∫ + (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) ⊖ if (3 e ^{$\frac{(\int_0^t \sqrt{\tau} d\tau)^2}{\int_0^t \sqrt{\tau} d\tau}$}) del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile (+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile, |∇|² = { 2 Dh dt Do dp dtV'((p+(pV'²f where IfŜbp̂AmAŜ†b+ if(p) - g(V '(p + i(pv' f))=12^{-√/(||α1'(t)>CQ1t|φ(t)>B+|α2'(t)>CQ2t|φ(t)>B)} if −π̂CmdπCdπ2 ((<p + if(p) - g(V '(p + i(pv' f)) ≠ + (sqrt(θ) ⊖ if (3 e ^{$\frac{(\int_0^t \sqrt{\tau} d\tau)^2}{\int_0^t \sqrt{\tau} d\tau}$}) del purin-2-yl] amino)) phosphoryl] oxy})) phos phoryl] formonitrile ++ (sqrt(θ) ⊖ if (3 e ^{$\frac{(\int_0^t \sqrt{\tau} d\tau)^2}{\int_0^t \sqrt{\tau} d\tau}$}) del)) ≡ inf+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile >0 > + (sqrt(θ) ⊖ if (3 e ^{$\frac{(\int_0^t \sqrt{\tau} d\tau)^2}{\int_0^t \sqrt{\tau} d\tau}$}) del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} - d+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) ⊖ if (3 e ^{$\frac{(\int_0^t \sqrt{\tau} d\tau)^2}{\int_0^t \sqrt{\tau} d\tau}$}) del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0]

pentan-2-yl} - $\equiv$ $\int$ + (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile (4(-1) -2
 $|\nabla|^2 = \{+$ (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) $\ominus$ if (3 e—
 del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl}
 -purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile + (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$
 (rboximidoyl- 3- fluoro-phos phoryl] formonitrile 1 $\neq$ + (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3-
 fluoro-phos phoryl] formonitrile + (sqrt(θ) $\ominus$ if (3 e————— del
 (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl-
 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3- fluoro-1- {5-oxabicyclo
 [2. 1.0] pentan-2-yl} -+ (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3- fluoro-1-(sqrt(θ) $\ominus$ if (3 e—————
 del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl}
 -purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile (sqrt(θ) $\ominus$ if (3 e—————
 del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl}
 -purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile + (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$
 (rboximidoyl- 3- fluoro-phos phoryl] formonitrile 2) + (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3-
 fluoro-phos phoryl] formonitrile ($\int$
 $> +$ (sqrt(θ) $\ominus$ if (3 e————— del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2.
 1.0] pentan-2-yl} -+ (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile ++
 (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) $\ominus$ if (3 e—————
 del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} - $\equiv$ $\int$ + (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$

(rboximidoyl- 3- fluoro-phos phoryl] formonitrile (4(-1) -2| ∇ |2= {+ (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$

(rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) $\ominus$ if (3 e—————

del (1-carboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$

(rboximidoyl- 3- fluoro-phos phoryl] formonitrile 1+ (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3-

fluoro-phos phoryl] formonitrile 1 $\neq$ + (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3- fluoro-phos phoryl]

formonitrile + (sqrt(θ) $\ominus$ if (3 e————— del purin-2-yl] amino)) phosphoryl]

oxy)) phos phoryl] formonitrile ++ (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3- fluoro-phos phoryl]

formonitrile 22 +

> 2) + (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile (¡ + (sqrt(θ) $\ominus$

(sqrt(θ) $\ominus$ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) $\ominus$ if (3 e—————

del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$

(rboximidoyl- 3- fluoro-phos phoryl] formonitrile (+ (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3-

fluoro-phos phoryl] formonitrile, | ∇ |2 = { 2 Dh dt Do dp dtV'((p+(pV'2f where If $\hat{S}$ bp $\wedge$ AmA $\hat{S}$ †b+ if(p)

- g(V '(p + i(pv' f)) =12 $^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B}$ if $-\pi^{\wedge}Cmd\pi Cd\pi 2$ ((<p + if(p)

- g(V '(p + i(pv' f)) $\neq$ + (sqrt(θ) $\ominus$ if (3 e————— del purin-2-yl] amino))

phosphoryl] oxy)) phos phoryl] formonitrile + + (sqrt(θ) $\ominus$ if (3 e—————

del)) $\equiv$ inf+ (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile >0+ (sqrt(θ) $\ominus$

(sqrt(θ) $\ominus$ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) $\ominus$ if (3 e—————

del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(θ) ⊖ (sqrt(θ) ⊖

(rboximidoyl- 3- fluoro-phos phoryl] formonitrile 0 (del ' (0)) ^4 (del ' (del 0)) ^4 (2 θ ⊖ ^2

> (del del −12 (d+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile +

(sqrt(θ) ⊖ if (3 e————— del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0]

pentan-2-yl} - ≡ ∫+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile (4(−1) −2

|∇ |2 = {+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) ⊖ if (3 e—

del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl}

-purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile + (sqrt(θ) ⊖ (sqrt(θ) ⊖

(rboximidoyl- 3- fluoro-phos phoryl] formonitrile 1 ≠+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3-

fluoro-phos phoryl] formonitrile pentan-2-yl} -2-Carboxylicacid; N-(1-carboximidoyl- 3- fluoro-1-

{5-oxabicyclo [2. 1.0] pentan-2-yl} -2-oxo6-({[amino({[(6-amino-9H-purin-9-yl) methyl] amino)}

phosphoryl] carbamoyl} amino) -3,3- di methyl-7-oxo-4-thia- 1-azabicyclo [3.2.0] heptane-

2-Carboxylicacid; N-(1-carboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -2-

Carboxylicacid; N-3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -2- oxo-1λ4,2 λ5-

thiaphosphiran-2 -yl) -N'-yl) -N'-[(Z) - ethylidene]guanidine; [(S) -amino({[(S) - amino({[(4R)

-6-oxo-4,6- dihydro-1H-purin-2-yl] amino)) phosphoryl] oxy)) phos thiaphosphiran-2 -yl) -N'-yl)

-N'-[(Z) ++ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) ⊖

(sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(θ) ⊖ (sqrt(θ) ⊖

(rboximidoyl- 3- fluoro-1-(sqrt(θ) ⊖ if (3 e————— del phos phoryl]

formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile (sqrt(0) Θ if (3 e $\frac{1}{2}$) del

phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile

> 2) + (sqrt(0) Θ (sqrt(0) Θ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile (j + (sqrt(0) Θ (sqrt(0) Θ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(0) Θ if (3 e $\frac{1}{2}$) del

del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(0) Θ (sqrt(0) Θ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile ++ (sqrt(0) Θ (sqrt(0) Θ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(0) Θ if (3 e $\frac{1}{2}$) del

(rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} $\equiv$ + (sqrt(0) Θ (sqrt(0) Θ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile (4(-1) $-2|\nabla|^2=$ {+ (sqrt(0) Θ (sqrt(0) Θ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(0) Θ if (3 e $\frac{1}{2}$) del

(1-carboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(0) Θ (sqrt(0) Θ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile 1+ (sqrt(0) Θ (sqrt(0) Θ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile 1 $\neq$ + (sqrt(0) Θ (sqrt(0) Θ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile 2

> 3 1+ + (sqrt(0) Θ (sqrt(0) Θ (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(0) Θ (sqrt(0) Θ (rboximidoyl- 3- fluoro-1-(sqrt(0) Θ if (3 e $\frac{1}{2}$) del

phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl]

amino}) phosphoryl] oxy}) phos phoryl] formonitrile ($\sqrt{\theta}$) Θ if (3 e~~_____~~

del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl}

-purin-2-yl] amino}) phosphoryl] oxy}) phos phoryl] formonitrile 2) ($\int 2 D_h dt dp dt -2$ (, $|\nabla|^2 = \{ 2$

$D_h dt Do dp dt V'((p+(pV'^2f$ where $If\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+$ if(p) - g(V '(p + i(pv' f)) = $12^{-\sqrt{(|\alpha 1'(t)$

)CQ1t| $\phi(t)$)B+| $\alpha 2'(t)$)CQ2t| $\phi(t)$)B) if $-\pi^{\wedge}Cmd\pi Cd\pi 2$ (($\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (\sqrt{\theta}) \Theta$

if (3 e~~_____~~ del purin-2-yl] amino}) phosphoryl] oxy}) phos phoryl]

formonitrile + + ($\sqrt{\theta}$) Θ if (3 e~~_____~~ del)) $\equiv \inf >0 |\nabla|^2 = \{ 2 D_h dt Do$

$dp dt V'((p+(pV'^2f$ where $If\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+$ if(p) - g(V '(p + i(pv' f)) = $12^{-\sqrt{(|\alpha 1'(t)$)CQ1t| $\phi(t)$

)B+| $\alpha 2'(t)$)CQ2t| $\phi(t)$)B) if $-\pi^{\wedge}Cmd\pi Cd\pi 2$ (($\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (\sqrt{\theta}) \Theta$ if (3 e~~_____~~

del purin-2-yl] amino}) phosphoryl] oxy}) phos phoryl] formonitrile + + ($\sqrt{\theta}$) Θ if (3 e~~_____~~

del) v - $|\nabla|^2 = \{ 2 D_h dt Do dp dt V'((p+(pV'^2f$ where $If\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+$ if(p) - g(V '(p + i(pv' f))

= $12^{-\sqrt{(|\alpha 1'(t)$)CQ1t| $\phi(t)$)B+| $\alpha 2'(t)$)CQ2t| $\phi(t)$)B) if $-\pi^{\wedge}Cmd\pi Cd\pi 2$ (($\langle p + if(p) - g(V '(p + i(pv'$

f)) $\neq + (\sqrt{\theta}) \Theta$ if (3 e~~_____~~ del purin-2-yl] amino}) phosphoryl] oxy})

phos phoryl] formonitrile + + ($\sqrt{\theta}$) Θ if (3 e~~_____~~ del) $\equiv \int (4(-1) -2 |\nabla$

$|^2 = \{ 2 D_h dt dp dt V' (p+(pV'^2f$ where $If\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+$ if(p) - g(V '(p + i(pv' f)) = $12^{-\sqrt{(|\alpha 1'(t)$

)CQ1t| $\phi(t)$)B+| $\alpha 2'(t)$)CQ2t| $\phi(t)$)B) if $-\pi^{\wedge}Cmd\pi Cd\pi 2$ (($\langle p + if(p) - g(V '(p + i(pv' f)) \neq$

pentan-2-yl} -2-Carboxylicacid; N-(1-carboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl}

-2-oxo6-({[amino({[(6-amino-9H-purin-9-yl) methyl] amino}) phosphoryl] carbamoyl} amino) -3,3-

di methyl-7-oxo-4-thia- 1-azabicyclo [3.2.0] heptane- 2-Carboxylicacid; N-(1-carboximidoyl- 3-

fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -2- Carboxylicacid; N-3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -2- oxo-1lambda4,2 lambda5- thiaphosphiran-2 -yl) -N'-yl) -N'-[(Z) - ethylidene]guanidine; [(S) -amino({[(S) - amino({[(4R) -6-oxo-4,6- dihydro-1H-purin-2-yl] amino)) phosphoryl] oxy}) phos thiaphosphiran-2 -yl) -N'-yl) -N'-[(Z) + + (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-1-(sqrt(theta) \Theta if (3 e_____ del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl] amino)) phosphoryl] oxy}) phos phoryl] formonitrile (sqrt(theta) \Theta if (3 e_____ del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl] amino)) phosphoryl] oxy}) phos phoryl] formonitrile 2) (\int 2 Dh dt dp dt -2 (, |\nabla |2 = { 2 Dh dt Do dp dtV'((p+(pV'2f where If\hat{S}bp^AmA\hat{S}^\dagger b+ if(p) - g(V '(p + i(pv' f)) =12^{-\sqrt{(|\alpha 1'(t))CQ1t|\phi(t))B+|\alpha 2'(t))CQ2t|\phi(t))B} if -\pi^{\text{Cmd}\pi\text{Cd}\pi 2} ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(theta) \Theta if (3 e_____ del purin-2-yl] amino)) phosphoryl] oxy}) phos phoryl] formonitrile + + (sqrt(theta) \Theta if (3 e_____ del)) \equiv \inf >0 |\nabla |2 = { 2 Dh dt Do dp dtV'((p+(pV'2f where If\hat{S}bp^AmA\hat{S}^\dagger b+ if(p) - g(V '(p + i(pv' f)) =12^{-\sqrt{(|\alpha 1'(t))CQ1t|\phi(t))B+|\alpha 2'(t))CQ2t|\phi(t))B} if -\pi^{\text{Cmd}\pi\text{Cd}\pi 2} ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(theta) \Theta if (3 e_____ del purin-2-yl] amino)) phosphoryl] oxy}) phos phoryl] formonitrile + + (sqrt(theta) \Theta if (3 e_____ del) d |\nabla |2 = { 2 Dh dt Do dp dtV'((p+(pV'2f where If\hat{S}bp^AmA\hat{S}^\dagger b+ if(p) - g(V '(p + i(pv' f)) =12^{-\sqrt{(|\alpha 1'(t))CQ1t|\phi(t))B+|\alpha 2'(t))CQ2t|\phi(t))B} if -\pi^{\text{Cmd}\pi\text{Cd}\pi 2} ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(theta) \Theta

if (3 e^{—————} del purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl]

formonitrile + + (sqrt(θ) Θ if (3 e^{—————} del) ≡ ∫ (4 (-1) -2 |∇|² = { 2 Dh dt

dp dtV' (p+(pV'²f where IfŜbp[^]AmAŜ†b+ if(p) - g(V '(p + i(pv' f)) =12⁻ √(|α1'(t))CQ1t|φ(t)

)B+|α2'(t))CQ2t|φ(t))B) if -π[^]CmdπCdπ2 ((<p + if(p) - g(V '(p + i(pv' f)) ≠ pentan-2-yl]

-2-Carboxylicacid; N-(1-carboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl]

-2-oxo6-({[amino({[(6-amino-9H-purin-9-yl) methyl] amino)) phosphoryl] carbamoyl] amino) -3,3-

di methyl-7-oxo-4-thia- 1-azabicyclo [3.2.0] heptane- 2-Carboxylicacid; N-(1-carboximidoyl- 3-

fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl] -2- Carboxylicacid; N-3- fluoro-1- {5-oxabicyclo [2. 1.0]

pentan-2-yl] -2- oxo-1λ4,2 λ5- thiaphosphiran-2 -yl) -N'-yl) -N'-[(Z) -

ethylidene]guanidine; [(S) -amino({[(S) - amino({[(4R) -6-oxo-4,6- dihydro-1H-purin-2-yl] amino))

phosphoryl] oxy)) phos thiaphosphiran-2 -yl) -N'-yl) -N'-[(Z) + + (sqrt(θ) Θ (sqrt(θ) Θ

(rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl] -+ (sqrt(θ) Θ (sqrt(θ) Θ (rboximidoyl-

3- fluoro-1-(sqrt(θ) Θ if (3 e^{—————} del phos phoryl] formonitrile

(rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl] -purin-2-yl] amino)) phosphoryl]

oxy)) phos phoryl] formonitrile (sqrt(θ) Θ if (3 e^{—————} del phos phoryl]

formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl] -purin-2-yl] amino))

phosphoryl] oxy)) phos phoryl] formonitrile 2) (∫ 2 Dh dt dp dt -2 + |∇|² = { 2 Dh dt Do dp

dtV'((p+(pV'²f where IfŜbp[^]AmAŜ†b+ if(p) - g(V '(p + i(pv' f)) =12⁻ √(|α1'(t))CQ1t|φ(t)

)B+|α2'(t))CQ2t|φ(t))B) if -π[^]CmdπCdπ2 ((<p + if(p) - g(V '(p + i(pv' f)) ≠ + (sqrt(θ) Θ if (3 e^{—————}

del purin-2-yl] amino}) phosphoryl] oxy}) phos phoryl] formonitrile + + (sqrt(0) \Theta if (3 e_____

del) \equiv \int (4(-1)^{-2} |\nabla|^2 = \{ + (sqrt(0) \Theta (sqrt(0) \Theta (rboximidoyl- 3-formonitrile + + (sqrt- fluoro-phos

phoryl] formonitrile where If\hat{S}bp^{\wedge}Am\hat{A}\hat{S}^{\dagger}b+ if(p) - g(V '(p + i(pv' f)) =12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B} if -\pi^{\wedge}Cmd\pi Cd\pi 2 ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(0) \Theta if (3 e_____

del purin-2-yl] amino}) phosphoryl] oxy}) phos phoryl] formonitrile + + (sqrt(0) \Theta if (3 e_____

del) (\int 2 Dh dt dp dt -2 (, |\nabla|^2 = \{ 2 Dh dt Do dp dt V'((p+(pV'2f where If\hat{S}bp^{\wedge}Am\hat{A}\hat{S}^{\dagger}b+ if(p) - g(V '(p + i(pv' f)) =12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B} if -\pi^{\wedge}Cmd\pi Cd\pi 2 ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(0) \Theta if (3 e_____ del purin-2-yl] amino})

phosphoryl] oxy}) phos phoryl] formonitrile + + (sqrt(0) \Theta if (3 e_____

del)) \equiv \inf >0 |\nabla|^2 = \{ 2 Dh dt Do dp dt V'((p+(pV'2f where If\hat{S}bp^{\wedge}Am\hat{A}\hat{S}^{\dagger}b+ if(p) - g(V '(p + i(pv' f)) =12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B} if -\pi^{\wedge}Cmd\pi Cd\pi 2 ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(0) \Theta if (3 e_____ del purin-2-yl] amino}) phosphoryl]

oxy}) phos phoryl] formonitrile + + (sqrt(0) \Theta if (3 e_____ del) 0) ^2 + 3))

/(4 sqrt(\pi) (1 - \theta \Theta ^2 (del del -12 (d |\nabla|^2 = \{ 2 Dh dt Do dp dt V'((p+(pV'2f where If\hat{S}bp^{\wedge}Am\hat{A}\hat{S}^{\dagger}b+ if(p) - g(V '(p + i(pv' f)) =12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B} if -\pi^{\wedge}Cmd\pi Cd\pi 2 ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(0) \Theta if (3 e_____ del purin-2-yl]

amino}) phosphoryl] oxy}) phos phoryl] formonitrile + + (sqrt(0) \Theta if (3 e_____

del) \equiv \int (4(-1)^{-2} |\nabla|^2 = \{ 2 Dh dt dp dt V' (p+(pV'2f where If\hat{S}bp^{\wedge}Am\hat{A}\hat{S}^{\dagger}b+ if(p) - g(V '(p + i(pv' f)) =12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B} if -\pi^{\wedge}Cmd\pi Cd\pi 2 ((\langle p + if(p) - g(V '(p +

$i(pv' f) \neq \text{pentan-2-yl} \} \text{-2-Carboxylicacid; N-(1-carboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0]$
 $\text{pentan-2-yl} \} \text{-2-oxo6-}\{\{\text{amino}(\{[(6\text{-amino-9H-purin-9-yl) methyl] amino}) \} \text{ phosphoryl] carbamoyl}$
 $\text{amino}) \text{-3,3- di methyl-7-oxo-4-thia- 1-azabicyclo [3.2.0] heptane- 2-Carboxylicacid;}$
 $\text{N-(1-carboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl} \} \text{-2- Carboxylicacid; N-3-}$
 $\text{fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl} \} \text{-2- oxo-1}\lambda^4,2 \lambda^5\text{- thiaphosphiran-2 -yl)}$
 $\text{-N'-yl) -N'-}[(Z) \text{ - ethylidene]guanidine; [(S) -amino}(\{(S) \text{ - amino}(\{(4R) \text{ -6-oxo-4,6-}$
 $\text{dihydro-1H-purin-2-yl] amino}) \} \text{ phosphoryl] oxy}) \} \text{ phos thiaphosphiran-2 -yl) -N'-yl) -N'-}[(Z) \text{ + +}$
 $(\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl} \} \text{ + } (\sqrt{\theta}) \ominus$
 $(\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-1-}(\sqrt{\theta}) \ominus \text{ if } (3 \text{ e} \text{-----} \text{ del phos}$
 $\text{phoryl] formonitrile (rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl} \} \text{-purin-2-yl}$
 $\text{amino}) \} \text{ phosphoryl] oxy}) \} \text{ phos phoryl] formonitrile } (\sqrt{\theta}) \ominus \text{ if } (3 \text{ e} \text{-----}$
 $\text{del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl}$
 $\text{-purin-2-yl] amino}) \} \text{ phosphoryl] oxy}) \} \text{ phos phoryl] formonitrile 2) } (\int 2 \text{ Dh dt dp dt } -2 + |\nabla|^2 = \{ 2$
 $\text{Dh dt Do dp dtV}'((p+(pV')^2f \text{ where If}\hat{S}bp^{\wedge}Am\hat{S}^{\dagger}b+ \text{ if}(p) \text{ - g(V '}(p + i(pv' f)) = 12^{-\sqrt{(|\alpha 1'(t)}$
 $\text{)CQ1t}|\phi(t) \rangle B+|\alpha 2'(t) \rangle \text{CQ2t}|\phi(t) \rangle B) \text{ if } -\pi^{\wedge}Cmd\pi Cd\pi 2 ((\langle p + \text{if}(p) \text{ - g(V '}(p + i(pv' f)) \neq + (\sqrt{\theta}) \ominus$
 $\text{if } (3 \text{ e} \text{-----} \text{ del purin-2-yl] amino}) \} \text{ phosphoryl] oxy}) \} \text{ phos phoryl]$
 $\text{formonitrile + } + (\sqrt{\theta}) \ominus \text{ if } (3 \text{ e} \text{-----} \text{ del}) \equiv \int (4(-1) -2|\nabla|^2 = \{ + (\sqrt{\theta})$
 $\ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3-formonitrile + } + (\sqrt{\text{- fluoro-phos phoryl] formonitrile where}$
 $\text{If}\hat{S}bp^{\wedge}Am\hat{S}^{\dagger}b+ \text{ if}(p) \text{ - g(V '}(p + i(pv' f)) = 12^{-\sqrt{(|\alpha 1'(t) \rangle \text{CQ1t}|\phi(t) \rangle B+|\alpha 2'(t) \rangle \text{CQ2t}|\phi(t) \rangle B) \text{ if}}$

$-\pi^{\wedge}\text{Cmd}\pi\text{Cd}\pi^2 ((\langle p + \text{if}(p) - g(V \text{ '}(p + i(pv' f)) \neq + (\text{sqrt}(\theta) \ominus \text{if}(3 e$
 $\text{del purin-2-yl] amino}) \text{ phosphoryl] oxy}) \text{ phos phoryl] formonitrile} + + (\text{sqrt}(\theta) \ominus \text{if}(3 e$
 $\text{del}) (\int 2 \text{ Dh dt dp dt} -2 (, |\nabla|^2 = \{ 2 \text{ Dh dt Do dp dtV}'((p+(pV'2f \text{ where If}\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+ \text{if}(p) - g(V$
 $\text{'(p} + i(pv' f)) = 12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B + |\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B)} \text{ if } -\pi^{\wedge}\text{Cmd}\pi\text{Cd}\pi^2 ((\langle p + \text{if}(p) -$
 $g(V \text{ '}(p + i(pv' f)) \neq + (\text{sqrt}(\theta) \ominus \text{if}(3 e$ $\text{del purin-2-yl] amino})$
 $\text{phosphoryl] oxy}) \text{ phos phoryl] formonitrile} + + (\text{sqrt}(\theta) \ominus \text{if}(3 e$
 $\text{del}) \equiv \inf > 0 |\nabla|^2 = \{ 2 \text{ Dh dt Do dp dtV}'((p+(pV'2f \text{ where If}\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+ \text{if}(p) - g(V \text{ '}(p + i(pv'$
 $f)) = 12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B + |\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B)} \text{ if } -\pi^{\wedge}\text{Cmd}\pi\text{Cd}\pi^2 ((\langle p + \text{if}(p) - g(V \text{ '}(p +$
 $i(pv' f)) \neq + (\text{sqrt}(\theta) \ominus \text{if}(3 e$ $\text{del purin-2-yl] amino}) \text{ phosphoryl]$
 $\text{oxy}) \text{ phos phoryl] formonitrile} + + (\text{sqrt}(\theta) \ominus \text{if}(3 e$ $\text{del}) v - |\nabla|^2 =$
 $\{ 2 \text{ Dh dt Do dp dtV}'((p+(pV'2f \text{ where If}\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+ \text{if}(p) - g(V \text{ '}(p + i(pv' f)) = 12^{-\sqrt{(|\alpha 1'(t)$
 $\rangle CQ1t|\phi(t) \rangle B + |\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B)} \text{ if } -\pi^{\wedge}\text{Cmd}\pi\text{Cd}\pi^2 ((\langle p + \text{if}(p) - g(V \text{ '}(p + i(pv' f)) \neq + (\text{sqrt}(\theta) \ominus$
 $\text{if}(3 e$ $\text{del purin-2-yl] amino}) \text{ phosphoryl] oxy}) \text{ phos phoryl]$
 $\text{formonitrile} + + (\text{sqrt}(\theta) \ominus \text{if}(3 e$ $\text{del}) \equiv \int (4(-1)^{-2} |\nabla|^2 = \{ 2 \text{ Dh dt}$
 $\text{dp dtV}' (p+(pV'2f \text{ where If}\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+ \text{if}(p) - g(V \text{ '}(p + i(pv' f)) = 12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t)$
 $\rangle B + |\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B)} \text{ if } -\pi^{\wedge}\text{Cmd}\pi\text{Cd}\pi^2 ((\langle p + \text{if}(p) - g(V \text{ '}(p + i(pv' f)) \neq \text{pentan-2-yl}\}$
 $\text{-2-Carboxylicacid; N-(1-carboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl}\}$
 $\text{-2-oxo6-}(\{\text{amino}(\{[(6\text{-amino-9H-purin-9-yl) methyl] amino}) \text{ phosphoryl] carbamoyl} \text{ amino}) \text{-3,3-}$
 $\text{di methyl-7-oxo-4-thia- 1-azabicyclo [3.2.0] heptane- 2-Carboxylicacid; N-(1-carboximidoyl- 3-}$

fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -2- Carboxylicacid; N-3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -2- oxo-1lambda4,2 lambda5- thiaphosphiran-2 -yl) -N'-yl) -N'-[(Z) - ethylidene]guanidine; [(S) -amino({[(S) - amino({[(4R) -6-oxo-4,6- dihydro-1H-purin-2-yl] amino)) phosphoryl] oxy}) phos thiaphosphiran-2 -yl) -N'-yl) -N'-[(Z) + + (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(theta) \Theta (sqrt(theta) \Theta (rboximidoyl- 3- fluoro-1-(sqrt(theta) \Theta if (3 e_____ del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl] amino)) phosphoryl] oxy}) phos phoryl] formonitrile (sqrt(theta) \Theta if (3 e_____ del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl] amino)) phosphoryl] oxy}) phos phoryl] formonitrile 2) (\int 2 Dh dt dp dt -2 (, |\nabla |2 = { 2 Dh dt Do dp dtV'((p+(pV'2f where If\hat{S}bp^AmA\hat{S}^\dagger b+ if(p) - g(V '(p + i(pv' f)) =12^{-\sqrt{(|\alpha 1'(t))CQ1t|\phi(t))B+|\alpha 2'(t))CQ2t|\phi(t))B} if -\pi^{\text{Cmd}\pi\text{Cd}\pi 2} ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(theta) \Theta if (3 e_____ del purin-2-yl] amino)) phosphoryl] oxy}) phos phoryl] formonitrile + + (sqrt(theta) \Theta if (3 e_____ del)) \equiv \inf >0 |\nabla |2 = { 2 Dh dt Do dp dtV'((p+(pV'2f where If\hat{S}bp^AmA\hat{S}^\dagger b+ if(p) - g(V '(p + i(pv' f)) =12^{-\sqrt{(|\alpha 1'(t))CQ1t|\phi(t))B+|\alpha 2'(t))CQ2t|\phi(t))B} if -\pi^{\text{Cmd}\pi\text{Cd}\pi 2} ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(theta) \Theta if (3 e_____ del purin-2-yl] amino)) phosphoryl] oxy}) phos phoryl] formonitrile + + (sqrt(theta) \Theta if (3 e_____ del) d |\nabla |2 = { 2 Dh dt Do dp dtV'((p+(pV'2f where If\hat{S}bp^AmA\hat{S}^\dagger b+ if(p) - g(V '(p + i(pv' f)) =12^{-\sqrt{(|\alpha 1'(t))CQ1t|\phi(t))B+|\alpha 2'(t))CQ2t|\phi(t))B} if -\pi^{\text{Cmd}\pi\text{Cd}\pi 2} ((\langle p + if(p) - g(V '(p + i(pv' f)) \neq + (sqrt(theta) \Theta

if (3 e~~_____~~ del purin-2-yl] amino}) phosphoryl] oxy}) phos phoryl]
formonitrile + + (sqrt(θ) ⊖ if (3 e~~_____~~ del)

> ∫ (4(−1)−2|∇|2= { + (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3-formonitrile + + (sqrt-
fluoro-phos phoryl] formonitrile where IfŜbp^AmAŜ†b+ if(p) - g(V '(p + i(pv' f)) =12[−] √(|α1'(t)
)CQ1t|φ(t))B+|α2'(t))CQ2t|φ(t))B) if −π^Cm dπC dπ2 ((<p + if(p) - g(V '(p + i(pv' f)) ≠ + (sqrt(θ) ⊖
if (3 e~~_____~~ del purin-2-yl] amino}) phosphoryl] oxy}) phos phoryl]
formonitrile + + (sqrt(θ) ⊖ if (3 e~~_____~~ del) (∫ 2 Dh dt dp dt −2 + |∇|2 = {
2 Dh dt Do dp dtV'((p+(pV'2f where IfŜbp^AmAŜ†b+ if(p) - g(V '(p + i(pv' f)) =12[−] √(|α1'(t)
)CQ1t|φ(t))B+|α2'(t))CQ2t|φ(t))B) if −π^Cm dπC dπ2 ((<p + if(p) - g(V '(p + i(pv' f)) ≠ + (sqrt(θ) ⊖
if (3 e~~_____~~ del purin-2-yl] amino}) phosphoryl] oxy}) phos phoryl]
formonitrile + + (sqrt(θ) ⊖ if (3 e~~_____~~ del) ≡ ∫ (4(−1)−2|∇|2= { + (sqrt(θ)
⊖ (sqrt(θ) ⊖ (rboximidoyl- 3-formonitrile + + (sqrt- fluoro-phos phoryl] formonitrile where
IfŜbp^AmAŜ†b+ if(p) - g(V '(p + i(pv' f)) =12[−] √(|α1'(t))CQ1t|φ(t))B+|α2'(t))CQ2t|φ(t))B) if
−π^Cm dπC dπ2 ((<p + if(p) - g(V '(p + i(pv' f)) ≠ + (sqrt(θ) ⊖ if (3 e~~_____~~
del purin-2-yl] amino}) phosphoryl] oxy}) phos phoryl] formonitrile + + (sqrt(θ) ⊖ if (3 e~~_____~~
del) (∫ 2 −2 −2(, |∇|2 = { 2 Dh dt Do dp dtV'((p+(pV'2f where IfŜbp^AmAŜ†b+ if(p) - g(V '(p +
i(pv' f)) =12[−] √(|α1'(t))CQ1t|φ(t))B+|α2'(t))CQ2t|φ(t))B) if −π^Cm dπC dπ2 ((<p + if(p) - g(V '(p +

$i(pv' f)) \neq + (\sqrt{\theta}) \Theta \text{ if } (3 e \text{-----} \text{del purin-2-yl] amino}) \text{ phosphoryl] oxy}) \text{ phos phoryl] formonitrile} + + (\sqrt{\theta}) \Theta \text{ if } (3 e \text{-----} \text{del})) \equiv \inf > 0$
 $|\nabla|^2 = \{ 2 Dh dt Do dp dt V'((p+(pV'2f \text{ where } If\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+ \text{ if}(p) - g(V '(p + i(pv' f)) = 12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B} \text{ if } -\pi^{\wedge}Cmd\pi Cd\pi 2 ((\langle p + \text{if}(p) - g(V '(p + i(pv' f)) \neq + (\sqrt{\theta}) \Theta \text{ if } (3 e \text{-----} \text{del purin-2-yl] amino}) \text{ phosphoryl] oxy}) \text{ phos phoryl] formonitrile} + + (\sqrt{\theta}) \Theta \text{ if } (3 e \text{-----} \text{del}) 0)^2)^{(7/2)}) + (e^{4\theta^{(3/2)} \Theta^3 (\text{del}'(0))^2 (\text{del}'(\text{del}))})^2 (2 \theta \Theta^2 (\text{del del}^{-12} (d |\nabla|^2 = \{ 2 Dh dt Do dp dt V'((p+(pV'2f \text{ where } If\hat{S}bp^{\wedge}AmA\hat{S}^{\dagger}b+ \text{ if}(p) - g(V '(p + i(pv' f)) = 12^{-\sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B} \text{ if } -\pi^{\wedge}Cmd\pi Cd\pi 2 ((\langle p + \text{if}(p) - g(V '(p + i(pv' f)) \neq + (\sqrt{\theta}) \Theta \text{ if } (3 e \text{-----} \text{del purin-2-yl] amino}) \text{ phosphoryl] oxy}) \text{ phos phoryl] formonitrile} + + (\sqrt{\theta}) \Theta \text{ if } (3 e \text{-----} \text{del})) \equiv \int (4(-1)^{-2} |\nabla|^2 = \{ 2 - 1 2 - 11 \neq \text{pentan-2-yl} \} \text{-2-Carboxylicacid; N-(1-carboximidoyl- 3-fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl} \text{-2-oxo6-}(\{[\text{amino}(\{[(6-amino-9H-purin-9-yl) methyl] amino}) \text{ phosphoryl] carbamoyl} \text{ amino}) \text{-3,3- di methyl-7-oxo-4-thia- 1-azabicyclo [3.2.0] heptane-2-Carboxylicacid; N-(1-carboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl} \text{-2-Carboxylicacid; N-3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl} \text{-2- oxo-1}\lambda_4,2 \lambda_5\text{-thiaphosphiran-2 -yl) -N'-yl) -N'-}[(Z) \text{ - ethylidene}]\text{guanidine; [(S) -amino}(\{[(S) \text{ - amino}(\{[(4R) \text{-6-oxo-4,6- dihydro-1H-purin-2-yl] amino}) \text{ phosphoryl] oxy}) \text{ phos thiaphosphiran-2 -yl) -N'-yl) -N'-}[(Z) + + (\sqrt{\theta}) \Theta (\sqrt{\theta}) \Theta (\text{rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl} \text{--} + (\sqrt{\theta}) \Theta (\sqrt{\theta}) \Theta (\text{rboximidoyl- 3- fluoro-1-}(\sqrt{\theta}) \Theta \text{ if } (3 e \text{-----} \text{del$

phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl]

amino}) phosphoryl] oxy}) phos phoryl] formonitrile ($\sqrt{0}$) Θ if (3 e_____

del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl}

-purin-2-yl] amino}) phosphoryl] oxy}) phos phoryl] formonitrile

> 2) + (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile (⌈ + (sqrt(θ) ⊖
 (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) ⊖ if (3 e—————
 del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(θ) ⊖ (sqrt(θ) ⊖
 (rboximidoyl- 3- fluoro-phos phoryl] formonitrile ++ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3-
 fluoro-phos phoryl] formonitrile + (sqrt(θ) ⊖ if (3 e————— del
 (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} =⌈+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl-
 3- fluoro-phos phoryl] formonitrile (4(-1) -2|∇ |2= {+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3-
 fluoro-phos phoryl] formonitrile + (sqrt(θ) ⊖ if (3 e————— del
 (1-carboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(θ) ⊖ (sqrt(θ) ⊖
 (rboximidoyl- 3- fluoro-phos phoryl] formonitrile 1+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3-
 fluoro-phos phoryl] formonitrile 1≠+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl]
 formonitrile 2 3 1++ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile +
 (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(θ) ⊖
 (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-1-(sqrt(θ) ⊖ if (3 e————— del phos
 phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl]
 amino}) phosphoryl] oxy}) phos phoryl] formonitrile (sqrt(θ) ⊖ if (3 e—————
 del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2.1.0] pentan-2-yl]
 -purin-2-yl] amino}) phosphoryl] oxy}) phos phoryl] formonitrile + (sqrt(θ) ⊖ (sqrt(θ) ⊖
 (rboximidoyl- 3- fluoro-phos phoryl] formonitrile 2) + (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3-

fluoro-phos phoryl] formonitrile ($\int + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl})$

formonitrile $+ (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----} \text{del } (\text{rboximidoyl- 3- fluoro-1-}$

{5-oxabicyclo [2. 1.0] pentan-2-yl} $\rightarrow (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl})$

formonitrile $(+ (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}) \text{formonitrile}, |\nabla|^2 = \{ 2 \text{ Dh}$

$\text{dt Do dp dtV}'((\text{p}+(\text{pV}'2\text{f where If}\hat{\text{S}}\text{bp}^{\text{Am}}\hat{\text{S}}^{\dagger}\text{b}+\text{if}(\text{p})-\text{g}(\text{V}'(\text{p}+\text{i}(\text{pv}'\text{f}))=12^{-\sqrt{(|\alpha 1'(\text{t})\text{)CQ1t}|\phi(\text{t})$

$\text{)B}+|\alpha 2'(\text{t})\text{)CQ2t}|\phi(\text{t})\text{)B}) \text{if } -\pi^{\text{Cmd}}\pi\text{Cd}\pi 2 ((\langle \text{p}+\text{if}(\text{p})-\text{g}(\text{V}'(\text{p}+\text{i}(\text{pv}'\text{f}))\neq + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----}$

del purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile $+ + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----}$

del)) $\equiv \text{inf}+ (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}) \text{formonitrile} >0+ (\sqrt{\theta}) \ominus$

$(\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}) \text{formonitrile} + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----}$

del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} $- \text{v} \rightarrow + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$

(rboximidoyl- 3- fluoro-phos phoryl] formonitrile $+ (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----}$

del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} $- \equiv \int + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$

(rboximidoyl- 3- fluoro-phos phoryl] formonitrile $(4(-1)^{-2}|\nabla|^2 = \{+ (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$

(rboximidoyl- 3- fluoro-phos phoryl] formonitrile $+ (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----}$

del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl}

-purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile $+ (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$

(rboximidoyl- 3- fluoro-phos phoryl] formonitrile $1 \neq + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3-}$

fluoro-phos phoryl] formonitrile $+ (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----} \text{del}$

(rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} $\rightarrow + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl-}$

3- fluoro-phos phoryl] formonitrile + (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-1-(sqrt(θ) ⊖ if (3 e_____ del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2.1.0] pentan-2-yl} -purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile (sqrt(θ) ⊖ if (3 e_____ del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile + (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile 2) + (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile (⌈ + (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) ⊖ if (3 e_____ del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile (+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile, |∇ |2 = { 2 Dh dt Do dp dtV'((p+(pV'2f where IfŜbp^AmAŜ†b+ if(p) - g(V '(p + i(pv' f)) =12^- √(|α1'(t))CQ1t|φ(t))B+|α2'(t))CQ2t|φ(t))B) if -π^CmdπCdπ2 ((<p + if(p) - g(V '(p + i(pv' f)) ≠ + (sqrt(θ) ⊖ if (3 e_____ del purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile + + (sqrt(θ) ⊖ if (3 e_____ del)) ≡ inf+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile >0 > + (sqrt(θ) ⊖ if (3 e_____ del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} - d+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) ⊖ if (3 e_____ del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} - ≡ ⌈+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile (4(-1) -2

$|\nabla|^2 = \{ + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{formonitrile} + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{---}$
 $\text{del phos phoryl}] \text{formonitrile } (\text{rboximidoyl- 3- fluoro-1- } \{5\text{-oxabicyclo [2. 1.0] pentan-2-yl}\}$
 $\text{-purin-2-yl] amino}} \text{ phosphoryl] oxy}} \text{ phos phoryl}] \text{formonitrile} + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$
 $(\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{formonitrile } 1 \neq + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3-}$
 $\text{fluoro-phos phoryl}] \text{formonitrile} + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----} \text{del}$
 $(\text{rboximidoyl- 3- fluoro-1- } \{5\text{-oxabicyclo [2. 1.0] pentan-2-yl}\} \text{--+ } (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl-}$
 $3\text{- fluoro-phos phoryl}] \text{formonitrile} + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-1- } \{5\text{-oxabicyclo}$
 $[2. 1.0] \text{ pentan-2-yl}\} \text{--+ } (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-1-}(\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----}$
 $\text{del phos phoryl}] \text{formonitrile } (\text{rboximidoyl- 3- fluoro-1- } \{5\text{-oxabicyclo [2. 1.0] pentan-2-yl}\}$
 $\text{-purin-2-yl] amino}} \text{ phosphoryl] oxy}} \text{ phos phoryl}] \text{formonitrile } (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----}$
 $\text{del phos phoryl}] \text{formonitrile } (\text{rboximidoyl- 3- fluoro-1- } \{5\text{-oxabicyclo [2. 1.0] pentan-2-yl}\}$
 $\text{-purin-2-yl] amino}} \text{ phosphoryl] oxy}} \text{ phos phoryl}] \text{formonitrile} + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$
 $(\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{formonitrile } 2) + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3-}$
 $\text{fluoro-phos phoryl}] \text{formonitrile } ($
 $> + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----} \text{del } (\text{rboximidoyl- 3- fluoro-1- } \{5\text{-oxabicyclo [2.}$
 $1.0] \text{ pentan-2-yl}\} \text{--+ } (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{formonitrile} ++$
 $(\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{formonitrile} + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----}$
 $\text{del } (\text{rboximidoyl- 3- fluoro-1- } \{5\text{-oxabicyclo [2. 1.0] pentan-2-yl}\} \text{---}\equiv + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$
 $(\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{formonitrile } (4(-1) -2|\nabla|^2 = \{ + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$

$(\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{ formonitrile} + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----}$
 $\text{del } (1\text{-carboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl\} } \text{ -} + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$
 $(\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{ formonitrile } 1 + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3-}$
 $\text{fluoro-phos phoryl}] \text{ formonitrile } 1 \neq + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}]$
 $\text{formonitrile} + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----} \text{del purin-2-yl}] \text{ amino}) \text{ phosphoryl}]$
 $\text{oxy}) \text{ phos phoryl}] \text{ formonitrile } ++ (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}]$
 $\text{formonitrile } 22 +$
 $> \quad 2) + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{ formonitrile } (\int + (\sqrt{\theta}) \ominus$
 $(\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{ formonitrile} + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----}$
 $\text{del } (\text{rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl\} } \text{ -} + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$
 $(\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{ formonitrile } (+ (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3-}$
 $\text{fluoro-phos phoryl}] \text{ formonitrile}, |\nabla |^2 = \{ \text{ }^2 \text{ Dh dt Do dp dtV}'((\text{p}+(\text{pV}'^2 \text{f where If}\hat{\text{S}}\text{bp}^{\wedge}\text{AmA}\hat{\text{S}}^{\dagger}\text{b}+ \text{if}(\text{p})$
 $\text{- g(V } '(\text{p} + \text{i}(\text{pv}' \text{ f})) = 12^{-} \sqrt{(|\alpha 1'(t) \rangle \text{CQ1t}|\phi(t) \rangle \text{B} + |\alpha 2'(t) \rangle \text{CQ2t}|\phi(t) \rangle \text{B}) \text{ if } -\pi^{\wedge}\text{Cmd}\pi\text{Cd}\pi 2 ((\langle \text{p} + \text{if}(\text{p}) -}$
 $\text{g(V } '(\text{p} + \text{i}(\text{pv}' \text{ f})) \neq + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----} \text{del purin-2-yl}] \text{ amino}) \text{)}$
 $\text{phosphoryl}] \text{ oxy}) \text{ phos phoryl}] \text{ formonitrile } + + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----}$
 $\text{del})) \equiv \text{inf} + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{ formonitrile } > 0 + (\sqrt{\theta}) \ominus$
 $(\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{ formonitrile} + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----}$
 $\text{del } (\text{rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl\} } \text{ -} + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$
 $(\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{ formonitrile } 0) ^2 + 1) ((\text{del } ' (0)) ^2 \text{del } '' (\text{del } 0) + \text{del } '(\text{del } 0)$

$\frac{\sqrt{\pi} (1 - \theta)^2}{2} \left(\frac{d}{d\theta} \left(\sqrt{\theta} \Theta \left(\sqrt{\theta} \Theta \left(\text{rboximidoyl- 3- fluoro-phos phoryl} \right] \text{ formonitrile} + \sqrt{\theta} \Theta \left(\frac{1}{3} e^{\frac{1}{3}} \right) \right) \right) \right. \\
\left. \text{fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl\} -} \right) \equiv \int + \left(\sqrt{\theta} \Theta \left(\sqrt{\theta} \Theta \left(\text{rboximidoyl- 3- fluoro-phos phoryl} \right] \text{ formonitrile} \right) \right. \\
\left. \left(4(-1)^{-2} |\nabla|^2 = \{ + \left(\sqrt{\theta} \Theta \left(\sqrt{\theta} \Theta \left(\text{rboximidoyl- 3- fluoro-phos phoryl} \right] \text{ formonitrile} + \sqrt{\theta} \Theta \left(\frac{1}{3} e^{\frac{1}{3}} \right) \right) \right) \right. \right. \\
\left. \left(\text{rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl\} -purin-2-yl\} \text{ amino}} \right) \right) \text{ phosphoryl] oxy}} \right) \\
\text{phos phoryl] formonitrile} \\
> \frac{1}{2} \left(\sqrt{\theta} \Theta \left(\sqrt{\theta} \Theta \left(\text{rboximidoyl- 3- fluoro-phos phoryl} \right] \text{ formonitrile} + \sqrt{\theta} \Theta \left(\frac{1}{3} e^{\frac{1}{3}} \right) \right) \right) \\
\left(\frac{1}{3} e^{\frac{1}{3}} \right) \left(\text{del purin-2-yl\} \text{ amino}} \right) \text{ phosphoryl] oxy}} \right) \text{ phos phoryl] formonitrile} \\
++ \left(\sqrt{\theta} \Theta \left(\sqrt{\theta} \Theta \left(\text{rboximidoyl- 3- fluoro-phos phoryl} \right] \text{ formonitrile} \right) \right) \\
\left(\sqrt{\theta} \Theta \left(\sqrt{\theta} \Theta \left(\text{rboximidoyl- 3- fluoro-phos phoryl} \right] \text{ formonitrile} \right) \right) + \left(\sqrt{\theta} \Theta \left(\sqrt{\theta} \Theta \left(\text{rboximidoyl- 3- fluoro-phos phoryl} \right] \text{ formonitrile} \right) \right) \\
\left(\int + \left(\sqrt{\theta} \Theta \left(\sqrt{\theta} \Theta \left(\text{rboximidoyl- 3- fluoro-phos phoryl} \right] \text{ formonitrile} + \sqrt{\theta} \Theta \left(\frac{1}{3} e^{\frac{1}{3}} \right) \right) \right) \right) \\
\left(\text{rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl\} -} \right) + \left(\sqrt{\theta} \Theta \left(\sqrt{\theta} \Theta \left(\text{rboximidoyl- 3- fluoro-phos phoryl} \right] \text{ formonitrile} \right) \right) \\
++ \left(\sqrt{\theta} \Theta \left(\sqrt{\theta} \Theta \left(\text{rboximidoyl- 3- fluoro-phos phoryl} \right] \text{ formonitrile} + \sqrt{\theta} \Theta \left(\frac{1}{3} e^{\frac{1}{3}} \right) \right) \right) \\
\left(\text{rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl\} -} \right) + \left(\sqrt{\theta} \Theta \left(\sqrt{\theta} \Theta \left(\text{rboximidoyl- 3- fluoro-phos phoryl} \right] \text{ formonitrile} \right) \right) \\
++ \left(\sqrt{\theta} \Theta \left(\sqrt{\theta} \Theta \left(\text{rboximidoyl- 3- fluoro-phos phoryl} \right] \text{ formonitrile} \right) \right) \\
\left(4(-1)^{-2} |\nabla|^2 = \{ + \left(\sqrt{\theta} \Theta \left(\sqrt{\theta} \Theta \left(\text{rboximidoyl- 3- fluoro-phos phoryl} \right] \text{ formonitrile} \right) \right) \right. \\
\left. \left(\text{rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl\} -} \right) \right) \equiv \int + \left(\sqrt{\theta} \Theta \left(\sqrt{\theta} \Theta \left(\text{rboximidoyl- 3- fluoro-phos phoryl} \right] \text{ formonitrile} \right) \right) \\
\left(4(-1)^{-2} |\nabla|^2 = \{ + \left(\sqrt{\theta} \Theta \left(\sqrt{\theta} \Theta \left(\text{rboximidoyl- 3- fluoro-phos phoryl} \right] \text{ formonitrile} \right) \right) \right. \\
\left. \left(\text{rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl\} -} \right) \right) \equiv \int + \left(\sqrt{\theta} \Theta \left(\sqrt{\theta} \Theta \left(\text{rboximidoyl- 3- fluoro-phos phoryl} \right] \text{ formonitrile} \right) \right) \\
12 \rightarrow$

$(\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{ formonitrile } 1 + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$
 $(\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{ formonitrile } 1 \neq + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3-}$
 $\text{fluoro-phos phoryl}] \text{ formonitrile } + (\sqrt{\theta}) \ominus \text{ if } (3 \text{ e} \text{-----} \text{ del}$
 $(\text{rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl\} -} + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl-}$
 $3\text{- fluoro-phos phoryl}] \text{ formonitrile } + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-1- \{5-oxabicyclo}$
 $[2. 1.0] \text{ pentan-2-yl\} -} + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-1-}(\sqrt{\theta}) \ominus \text{ if } (3 \text{ e} \text{-----}$
 $\text{del phos phoryl}] \text{ formonitrile } (\text{rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl\}}$
 $\text{-purin-2-yl] amino\}) \text{ phosphoryl] oxy\}) \text{ phos phoryl}] \text{ formonitrile } (\sqrt{\theta}) \ominus \text{ if } (3 \text{ e} \text{-----}$
 $\text{del phos phoryl}] \text{ formonitrile } (\text{rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl\}}$
 $\text{-purin-2-yl] amino\}) \text{ phosphoryl] oxy\}) \text{ phos phoryl}] \text{ formonitrile } + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$
 $(\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{ formonitrile } 2) + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3-}$
 $\text{fluoro-phos phoryl}] \text{ formonitrile } (\int + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}]$
 $\text{formonitrile } + (\sqrt{\theta}) \ominus \text{ if } (3 \text{ e} \text{-----} \text{ del } (\text{rboximidoyl- 3- fluoro-1-}$
 $\{5\text{-oxabicyclo [2. 1.0] pentan-2-yl\} -} + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}]$
 $\text{formonitrile } (+ (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{ formonitrile, } |\nabla|^2 = \{ 2 \text{ Dh}$
 $\text{dt Do dp dtV'((p+(pV'}^2 \text{f where If}\hat{\text{S}}\text{bp}^{\wedge}\text{Am}\hat{\text{A}}\text{S}^{\dagger}\text{b+ if(p) - g(V ' (p + i(pv' f)) = 12}^{-} \sqrt{(|\alpha 1'(t) \rangle \text{CQ1t}|\phi(t)$
 $\rangle \text{B} + |\alpha 2'(t) \rangle \text{CQ2t}|\phi(t) \rangle \text{B}) \text{ if } -\pi^{\wedge}\text{Cmd}\pi\text{Cd}\pi^2 ((\langle \text{p} + \text{if(p) - g(V ' (p + i(pv' f))} \neq + (\sqrt{\theta}) \ominus \text{ if } (3 \text{ e} \text{-----}$
 $\text{del purin-2-yl] amino\}) \text{ phosphoryl] oxy\}) \text{ phos phoryl}] \text{ formonitrile } + + (\sqrt{\theta}) \ominus \text{ if } (3 \text{ e} \text{-----}$
 $\text{del})) \equiv \inf + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{ formonitrile } > 0 + (\sqrt{\theta}) \ominus$

$(\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{formonitrile} + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----}$
 $\text{del } (\text{rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl\} - v} \rightarrow + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$
 $(\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{formonitrile} + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----}$
 $\text{del } (\text{rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl\} - \equiv} \vdash (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$
 $(\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{formonitrile} (4(-1) -2|\nabla |2= \{+ (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$
 $(\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{formonitrile} + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----}$
 $\text{del } (1\text{-carboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl\} -+} (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$
 $(\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{formonitrile} 1+ (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3-}$
 $\text{fluoro-phos phoryl}] \text{formonitrile} 1\neq + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}]$
 $\text{formonitrile} + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----} \text{del purin-2-yl] amino\}) \text{phosphoryl}]$
 $\text{oxy\}) \text{phos phoryl}] \text{formonitrile} ++ (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}]$
 $\text{formonitrile} 22 ++ (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{formonitrile} 2) +$
 $(\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{formonitrile} (\int + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$
 $(\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{formonitrile} + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----}$
 $\text{del } (\text{rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl\} -}$
 $> (+ (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{formonitrile}, |\nabla |2 = \{ 2 \text{ Dh dt Do}$
 $\text{dp dtV}'((\text{p}+(\text{pV}'2\text{f where If}\hat{\text{S}}\text{bp}^{\wedge}\text{Am}\hat{\text{A}}\dagger\text{b}+ \text{if}(\text{p}) - \text{g}(\text{V} \text{'(p} + \text{i}(\text{pv}' \text{f})) =12^{-} \sqrt{(|\alpha 1'(t) \text{)CQ1t}|}\phi(t)$
 $\text{)B}+|\alpha 2'(t) \text{)CQ2t}|}\phi(t) \text{)B} \text{if } -\pi^{\wedge}\text{Cmd}\pi\text{Cd}\pi 2 ((\langle \text{p} + \text{if}(\text{p}) - \text{g}(\text{V} \text{'(p} + \text{i}(\text{pv}' \text{f})) \neq + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----}$
 $\text{del purin-2-yl] amino\}) \text{phosphoryl}] \text{oxy\}) \text{phos phoryl}] \text{formonitrile} + + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----}$

del)) $\equiv$ inf+ (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile >0+ (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) $\ominus$ if (3 e_____

del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} - d+ (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) $\ominus$ if (3 e_____

del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} - $\equiv$ $\int$ + (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile (4(-1) -2 ∇ |2 = {+ (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) $\ominus$ if (3 e_____

del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile + (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile 1 $\neq$ + (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) $\ominus$ if (3 e_____ del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3- fluoro-1-(sqrt(θ) $\ominus$ if (3 e_____ del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile (sqrt(θ) $\ominus$ if (3 e_____ del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile

> 2) + (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile (⌈ + (sqrt(θ) ⊖
 (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) ⊖ if (3 e—————
 del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(θ) ⊖ (sqrt(θ) ⊖
 (rboximidoyl- 3- fluoro-phos phoryl] formonitrile ++ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3-
 fluoro-phos phoryl] formonitrile + (sqrt(θ) ⊖ if (3 e————— del
 (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} =⌈+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl-
 3- fluoro-phos phoryl] formonitrile (4(-1) -2|∇ |2= {+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3-
 fluoro-phos phoryl] formonitrile + (sqrt(θ) ⊖ if (3 e————— del
 (1-carboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(θ) ⊖ (sqrt(θ) ⊖
 (rboximidoyl- 3- fluoro-phos phoryl] formonitrile 1+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3-
 fluoro-phos phoryl] formonitrile 1≠+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl]
 formonitrile 2
 > 3 1++ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) ⊖
 (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(θ) ⊖ (sqrt(θ) ⊖
 (rboximidoyl- 3- fluoro-1-(sqrt(θ) ⊖ if (3 e————— del phos phoryl]
 formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl] amino})
 phosphoryl] oxy}) phos phoryl] formonitrile (sqrt(θ) ⊖ if (3 e————— del
 phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl]
 amino}) phosphoryl] oxy}) phos phoryl] formonitrile + (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3-

fluoro-phos phoryl] formonitrile 2) + (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile (∫ + (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) ⊖ if (3 e

del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} → (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile (+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile, |∇ |2 = { 2 Dh dt Do dp dtV'((p+(pV'2f where IfŜbp^AmAŜ†b+ if(p) - g(V '(p + i(pv' f))=12⁻ √(|α1'(t))CQ1t|φ(t))B+|α2'(t))CQ2t|φ(t))B) if -π^CmdπCdπ2 ((<p + if(p) - g(V '(p + i(pv' f)) ≠ + (sqrt(θ) ⊖ if (3 e————— del purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile + + (sqrt(θ) ⊖ if (3 e————— del)) ≡ inf+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile >0+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) ⊖ if (3 e————— del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} → (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile 0) ^2) ^{(5/2)}) + (sqrt(θ) ⊖ del > del -12 (d+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) ⊖ if (3 e————— del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} - ≡ ∫+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile (4(-1) -2 |∇ |2 = {+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) ⊖ if (3 e————— del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile + (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile 1 ≠+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3-

fluoro-phos phoryl] formonitrile + (sqrt(θ) ⊖ if (3 e_____ del

(rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl-

3- fluoro-phos phoryl] formonitrile + (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-1- {5-oxabicyclo

[2. 1.0] pentan-2-yl} -+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-1-(sqrt(θ) ⊖ if (3 e_____

del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl}

-purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile (sqrt(θ) ⊖ if (3 e_____

del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl}

-purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile + (sqrt(θ) ⊖ (sqrt(θ) ⊖

(rboximidoyl- 3- fluoro-phos phoryl] formonitrile 2) + (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3-

fluoro-phos phoryl] formonitrile (⌈ + (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl]

formonitrile 2+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile −2

>) −2+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile ++ (sqrt(θ) ⊖ (sqrt(θ)

⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) ⊖ if (3 e_____

del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} −≡⌈+ (sqrt(θ) ⊖ (sqrt(θ) ⊖

(rboximidoyl- 3- fluoro-phos phoryl] formonitrile (4(−1) −2|∇ |2= {+ (sqrt(θ) ⊖ (sqrt(θ) ⊖

(rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) ⊖ if (3 e_____

del (1-carboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(θ) ⊖ (sqrt(θ) ⊖

(rboximidoyl- 3- fluoro-phos phoryl] formonitrile 1+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3-

fluoro-phos phoryl] formonitrile 1≠+ (sqrt(θ) ⊖ (sqrt(θ) ⊖ (rboximidoyl- 3- fluoro-phos phoryl]

formonitrile + (sqrt(0) ⊖ if (3 e~~_____~~ del purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile ++ (sqrt(0) ⊖ (sqrt(0) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile 22 ++ (sqrt(0) ⊖ (sqrt(0) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile 2) + (sqrt(0) ⊖ (sqrt(0) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile (∫ > + (sqrt(0) ⊖ if (3 e~~_____~~ del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(0) ⊖ (sqrt(0) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile (+ (sqrt(0) ⊖ (sqrt(0) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile, |∇ |2 = { 2 Dh dt Do dp dtV'((p+(pV'2f where IfŜbp^AmÂ†b+ if(p) - g(V '(p + i(pv' f))=12⁻ √(|α1'(t))CQ1t|φ(t))B+|α2'(t))CQ2t|φ(t))B) if −π^CmdπCdπ2 ((<p + if(p) - g(V '(p + i(pv' f)) ≠ + (sqrt(0) ⊖ if (3 e~~_____~~ del purin-2-yl] amino)) phosphoryl] oxy)) phos phoryl] formonitrile + + (sqrt(0) ⊖ if (3 e~~_____~~ del)) ≡ inf+ (sqrt(0) ⊖ (sqrt(0) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile >0+ (sqrt(0) ⊖ (sqrt(0) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(0) ⊖ if (3 e~~_____~~ del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} - v →+ (sqrt(0) ⊖ (sqrt(0) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(0) ⊖ if (3 e~~_____~~ del (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl} - ≡ ∫+ (sqrt(0) ⊖ (sqrt(0) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile (4(−1) −2 |∇ |2 = {+ (sqrt(0) ⊖ (sqrt(0) ⊖ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(0) ⊖ if (3 e~~_____~~ del phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- {5-oxabicyclo [2. 1.0] pentan-2-yl}

-purin-2-yl] amino}) phosphoryl oxy}) phosphoryl formonitrile + (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$
 (rboximidoyl- 3- fluoro-phos phoryl] formonitrile 1 $\neq$
 $> + (\text{sqrt}(\theta) \ominus \text{if } (3 \text{ e} \text{-----} \text{del (rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2.}$
 1.0] pentan-2-yl} -+ (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(θ)
 $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$
 (rboximidoyl- 3- fluoro-1-(sqrt(θ) $\ominus$ if (3 e----- del phos phoryl]
 formonitrile (rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl] amino})
 phosphoryl oxy}) phosphoryl] formonitrile (sqrt(θ) $\ominus$ if (3 e----- del
 phos phoryl] formonitrile (rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl} -purin-2-yl]
 amino}) phosphoryl oxy}) phosphoryl] formonitrile + (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3-
 fluoro-phos phoryl] formonitrile 2) + (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3- fluoro-phos phoryl]
 formonitrile (+ (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3- fluoro-phos phoryl] formonitrile + (sqrt(θ) $\ominus$ if (3 e
 del (rboximidoyl- 3- fluoro-1- \{5-oxabicyclo [2. 1.0] pentan-2-yl} -+ (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$
 (rboximidoyl- 3- fluoro-phos phoryl] formonitrile (+ (sqrt(θ) $\ominus$ (sqrt(θ) $\ominus$ (rboximidoyl- 3-
 fluoro-phos phoryl] formonitrile, $|\nabla|^2 = \{ 2 \text{ Dh dt Do dp dtV}'((\text{p}+(\text{pV}'2\text{f where If}\hat{\text{S}}\text{bp}^{\wedge}\text{Am}\hat{\text{A}}\hat{\text{S}}^{\dagger}\text{b}+\text{if}(\text{p})$
 - g(V '(p + i(pv' f)) = $12^{-\sqrt{(|\alpha 1'(t) \rangle \text{CQ1t}|\phi(t) \rangle \text{B} + |\alpha 2'(t) \rangle \text{CQ2t}|\phi(t) \rangle \text{B})}$ if $-\pi^{\wedge}\text{Cmd}\pi\text{Cd}\pi 2 ((\langle \text{p} + \text{if}(\text{p}) -$
 g(V '(p + i(pv' f)) $\neq + (\text{sqrt}(\theta) \ominus \text{if } (3 \text{ e} \text{-----} \text{del purin-2-yl] amino})$)
 phosphoryl oxy}) phosphoryl] formonitrile + + (sqrt(θ) $\ominus$ if (3 e-----
 del)) $\equiv \inf + (\text{sqrt}(\theta) \ominus (\text{sqrt}(\theta) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl] formonitrile } > 0 + (\text{sqrt}(\theta) \ominus$

$(\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{formonitrile} + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----}$
 $\text{del } (\text{rboximidoyl- 3- fluoro-1- } \{5\text{-oxabicyclo } [2. 1.0] \text{ pentan-2-yl}\} - \text{d} + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$
 $(\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{formonitrile} + (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----}$
 $\text{del } (\text{rboximidoyl- 3- fluoro-1- } \{5\text{-oxabicyclo } [2. 1.0] \text{ pentan-2-yl}\} - \equiv \int + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus$
 $(\text{rboximidoyl- 3- fluoro-phos phoryl}] \text{formonitrile} (4(-1) -2 |\nabla |2$

$\{ + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3-formonitrile} + + (\sqrt{\theta} \text{- fluoro-phos phoryl}] \text{formonitrile} -$
 $11 \neq 231 + 22 + 2) (\int 2 -2) -2 + () \equiv (4(-1) -2 |\nabla |2 = \{ 2 \text{ Dh dt dp dtV' } (p + (pV'2f) \text{ where If } \hat{S}bp^{\wedge}Am\hat{A}\hat{S}^{\dagger}b + \text{if}(p) -$
 $g(V' (p + i(pv' f)) = 12^{-} \sqrt{(|\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B + |\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B) \text{ if } -\pi^{\wedge}Cmd\pi Cd\pi 2 ((\langle p + \text{if}(p) - g(V' (p$
 $+ i(pv' f)) \neq \text{pentan-2-yl}\} -2\text{-Carboxylicacid}; \text{N-(1-carboximidoyl- 3- fluoro-1- } \{5\text{-oxabicyclo } [2. 1.0]$
 $\text{pentan-2-yl}\} -2\text{-oxo6-}(\{[\text{amino}(\{[(6\text{-amino-9H-purin-9-yl) methyl] amino}) \text{ phosphoryl}] \text{ carbamoyl}\} \text{ amino})$
 $-3,3\text{- di methyl-7-oxo-4-thia- 1-azabicyclo } [3.2.0] \text{ heptane- 2-Carboxylicacid}; \text{N-(1-carboximidoyl- 3- fluoro-1-}$
 $\{5\text{-oxabicyclo } [2. 1.0] \text{ pentan-2-yl}\} -2\text{- Carboxylicacid}; \text{N-3- fluoro-1- } \{5\text{-oxabicyclo } [2. 1.0] \text{ pentan-2-yl}\} -2\text{-}$
 $\text{oxo-1}\lambda 4,2 \lambda 5\text{- thiaphosphiran-2 -yl} \text{ -N'-yl} \text{ -N'-}[(Z) \text{ - ethylidene}] \text{guanidine}; [(S) \text{ -amino}(\{[(S) \text{ -}$
 $\text{amino}(\{[(4R) \text{ -6-oxo-4,6- dihydro-1H-purin-2-yl}] \text{ amino}) \text{ phosphoryl}] \text{ oxy}) \text{ phos thiaphosphiran-2 -yl}$
 $\text{-N'-yl} \text{ -N'-}[(Z) + + (\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-1- } \{5\text{-oxabicyclo } [2. 1.0] \text{ pentan-2-yl}\} \text{ -} +$
 $(\sqrt{\theta}) \ominus (\sqrt{\theta}) \ominus (\text{rboximidoyl- 3- fluoro-1-}(\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----} \text{del phos}$
 $\text{phoryl}] \text{formonitrile } (\text{rboximidoyl- 3- fluoro-1- } \{5\text{-oxabicyclo } [2. 1.0] \text{ pentan-2-yl}\} \text{ -purin-2-yl}] \text{ amino}) \}$
 $\text{phosphoryl}] \text{ oxy}) \text{ phos phoryl}] \text{formonitrile } (\sqrt{\theta}) \ominus \text{if } (3 \text{ e} \text{-----} \text{del phos}$
 $\text{phoryl}] \text{formonitrile } (\text{rboximidoyl- 3- fluoro-1- } \{5\text{-oxabicyclo } [2. 1.0] \text{ pentan-2-yl}\} \text{ -purin-2-yl}] \text{ amino}) \}$

> C -4.87000 -1.32100 0.00000
> C -3.01900 -2.98900 0.00000
> C -5.64000 0.01200 0.00000
> C -1.29200 -5.12100 0.00000
> C 0.86600 -3.87500 0.00000
> C 2.37300 -3.55500 0.00000
> N -7.95000 1.34600 0.00000
> N -10.26000 2.68000 0.00000
> N -12.57000 1.34600 0.00000
> N -12.57000 4.01300 0.00000
> O -7.18000 0.01200 0.00000
> C -9.49000 1.34600 0.00000
> C -7.18000 2.68000 0.00000
> C -10.26000 0.01200 0.00000
> C -11.80000 2.68000 0.00000
> N -6.41000 4.01300 0.00000
> O 9.13500 4.34000 0.00000
> N 6.33700 0.01400 0.00000
> N 6.33700 2.50600 0.00000
> N 9.13500 -0.28000 0.00000
> N 10.46900 2.03000 0.00000
> N 11.80300 -0.28000 0.00000
> N 5.86100 -1.45000 0.00000
> C 7.80200 0.49000 0.00000
> C 5.43200 1.26000 0.00000
> C 7.80200 2.03000 0.00000
> C 9.13500 2.80000 0.00000
> C 10.46900 0.49000 0.00000
> F -1.00000 4.17600 0.00000
> O 1.42600 -0.81900 0.00000
> N 3.07400 4.25500 0.00000
> N 0.78500 2.19400 0.00000
> C 2.25000 1.71800 0.00000
> C 3.39400 2.74900 0.00000
> C 1.61000 4.73100 0.00000
> C 0.46500 3.70000 0.00000
> C 2.57000 0.21200 0.00000
> C 19.48900 5.55300 0.00000

> N 17.76100 3.42000 0.00000
> N 18.08200 4.92600 0.00000
> N 17.05100 6.07100 0.00000
> C 17.82100 7.40400 0.00000
> N 19.32800 7.08400 0.00000
> S 17.19500 8.81100 0.00000
> N 25.93100 3.15500 0.00000
> C 26.83600 1.90900 0.00000
> N 25.93100 0.66300 0.00000
> N 24.46600 1.13900 0.00000
> C 24.46600 2.67900 0.00000
> O 22.36200 4.78300 0.00000
> C 20.82200 4.78300 0.00000
> S 28.37600 1.90900 0.00000
> P 21.59200 1.90900 0.00000
> O 20.05200 1.90900 0.00000
>
> N 23.13200 1.90900 0.00000
> O 17.04300 -5.55700 0.00000
> F 20.52400 -7.49700 0.00000
> F 17.81300 -9.46700 0.00000
> O 18.92500 0.36900 0.00000
> N 19.48900 -4.31100 0.00000
> N 19.01300 -2.84600 0.00000
> N 21.50400 -2.84600 0.00000
> O 21.59200 0.36900 0.00000
> C 17.81300 -7.92700 0.00000
> C 19.05900 -7.02100 0.00000
> C 16.56700 -7.02100 0.00000
> C 18.58300 -5.55700 0.00000
> C 21.02900 -4.31100 0.00000
> C 20.25900 -1.94100 0.00000
> C 20.25900 -0.40100 0.00000
> N 21.59200 3.44900 0.00000
> F 15.10300 -7.49700 0.00000
> P 37.30200 2.59600 0.00000
> O 35.83800 2.12000 0.00000
> N 38.76700 3.07200 0.00000

> O 35.24100 0.30700 0.00000
 > N 36.31800 -2.72400 0.00000
 > C 38.68800 -1.95400 0.00000
 > N 37.77800 1.13100 0.00000
 > C 38.68800 -3.49400 0.00000
 > C 37.22400 -1.47800 0.00000
 > C 36.74800 -0.01300 0.00000
 > N 37.85700 5.20500 0.00000
 > N 38.41100 7.81400 0.00000
 > N 40.94800 8.63800 0.00000
 > N 36.82600 4.06000 0.00000
 > C 37.38100 6.66900 0.00000
 > C 39.91800 7.49400 0.00000
 > C 39.79700 4.21600 0.00000
 > C 40.27300 2.75100 0.00000
 > C 35.87500 6.99000 0.00000
 > N 34.36800 7.31000 0.00000
 > C 40.02200 -4.26400 0.00000
 > N 41.35600 -3.49400 0.00000
 > C 41.35600 -1.95400 0.00000
 > N 40.02200 -1.18400 0.00000
 > O 40.02200 -5.80400 0.00000
 > N 42.68900 -1.18400 0.00000
 > F 39.83900 -8.86800 0.00000
 > O 35.24100 -5.75500 0.00000
 > N 37.30200 -8.04300 0.00000
 > N 37.22400 -3.97000 0.00000
 > C 37.77800 -6.57900 0.00000
 > N 37.85700 -10.65300 0.00000
 > C 38.33300 -9.18800 0.00000
 > C 36.74800 -5.43400 0.00000

as a generalization of a set. Where in a set each element can appear only once, there can be multiple instances of identical members in a multiset. There is no standard, concise and unambiguous notation for multisets. In this paper we will use the notation of a sum of multisets of 1 element. A multiset M containing the elements a, b, b, c will be denoted as $\{a\} + \{b\} + \{b\} + \{c\}$. To reduce the fragmentation space for the generation of salt-bridge interaction between the Glu290 and the new ligand that needs to be searched, the algorithm of the two independent Chern-Simons $S=14\pi\int M3$ A level $k \in H4(BG, \mathbb{Z})$ $(a+\ell) \text{ ta}+\ell-\{1/12+(\|\alpha1'(t)\rangle CQ1t|\phi(t)\rangle B+|\alpha2'(t)$

$\rangle CQ2t|\phi(t)\rangle B\rangle\} + F\exp(i\hbar^2 A2mA \dashv 1A\wedge dA \ 2zEGk+13 \ (a+\ell) \ ta+\ell-\{1/12+(\|\alpha1'(t)\rangle CQ1t|\phi(t)\rangle B+|\alpha2'(t)\rangle CQ2t|\phi(t)\rangle B\rangle\} + F\exp(i\hbar^2 A2mA \dashv 1A\wedge[A\wedge A] \ 2zEG \ k \ (\text{mod}2\pi)$ actions with loop group at level k has that property $(14\pi)^3 M3 \ (a+\ell) \ ta+\ell-\{1/12+(\|\alpha1'(t)\rangle CQ1t|\phi(t)\rangle B+|\alpha2'(t)\rangle CQ2t|\phi(t)\rangle B\rangle\} + F\exp(i\hbar^2 A2mA \dashv 1A\wedge dA \ 2zEGk+13 \ (a+\ell) \ ta+\ell-\{1/12+(\|\alpha1'(t)\rangle CQ1t|\phi(t)\rangle B+|\alpha2'(t)\rangle CQ2t|\phi(t)\rangle B\rangle\} + F\exp(i\hbar^2 A2mA \dashv 1A\wedge[A\wedge A] \ 2zEG \ k \ (\text{mod}2\pi) \ [1]+\sin \ (a+\ell) \ ta+\ell-\{1/12+(\|\alpha1'(t)\rangle CQ1t|\phi(t)\rangle B+|\alpha2'(t)\rangle CQ2t|\phi(t)\rangle B\rangle\} + F\exp(i\hbar^2 A2mA \dashv 1Vectk \ ((a+\ell) \ ta+\ell-\{1/12+(\|\alpha1'(t)\rangle CQ1t|\phi(t)\rangle B+|\alpha2'(t)\rangle CQ2t|\phi(t)\rangle B\rangle\} + F\exp(i\hbar^2 A2mA \dashv 1+ \ (a+\ell) \ ta+\ell-\{1/12+(\|\alpha1'(t)\rangle CQ1t|\phi(t)\rangle B+|\alpha2'(t)\rangle CQ2t|\phi(t)\rangle B\rangle\} + F\exp(i\hbar^2 A2mA \dashv 1\wedge \ (a+\ell) \ ta+\ell-\{1/12+(\|\alpha1'(t)\rangle CQ1t|\phi(t)\rangle B+|\alpha2'(t)\rangle CQ2t|\phi(t)\rangle B\rangle\} + F\exp(i\hbar^2 A2mA \dashv 1F) \ 14\pi^3 M3 \ (a+\ell) \ ta+\ell-\{1/12+(\|\alpha1'(t)\rangle CQ1t|\phi(t)\rangle B+|\alpha2'(t)\rangle CQ2t|\phi(t)\rangle B\rangle\} + F\exp(i\hbar^2 A2mA \dashv 1A\wedge dA \ 2zEGk+13 \ (a+\ell) \ ta+\ell-\{1/12+(\|\alpha1'(t)\rangle CQ1t|\phi(t)\rangle B+|\alpha2'(t)\rangle CQ2t|\phi(t)\rangle B\rangle\} + F\exp(i\hbar^2 A2mA \dashv 1A\wedge[A\wedge A] \ 2zEG \ k \ (\text{mod}2\pi) \ [1]\wedge\sin \ (a+\ell) \ ta+\ell-\{1/12+(\|\alpha1'(t)\rangle CQ1t|\phi(t)\rangle B+|\alpha2'(t)\rangle CQ2t|\phi(t)\rangle B\rangle\} + F\exp(i\hbar^2 A2mA \dashv 1Vectk \ ((a+\ell) \ ta+\ell-\{1/12+(\|\alpha1'(t)\rangle CQ1t|\phi(t)\rangle B+|\alpha2'(t)\rangle CQ2t|\phi(t)\rangle B\rangle\} + F\exp(i\hbar^2 A2mA \dashv 1+ \ (a+\ell) \ ta+\ell-\{1/12+(\|\alpha1'(t)\rangle CQ1t|\phi(t)\rangle B+|\alpha2'(t)\rangle CQ2t|\phi(t)\rangle B\rangle\} + F\exp(i\hbar^2 A2mA \dashv 1\wedge \ (a+\ell) \ ta+\ell-\{1/12+(\|\alpha1'(t)\rangle CQ1t|\phi(t)\rangle B+|\alpha2'(t)\rangle CQ2t|\phi(t)\rangle B\rangle\} + F\exp(i\hbar^2 A2mA \dashv 1F) \ 14\pi^3 M3 \ (a+\ell) \ ta+\ell-\{1/12+(\|\alpha1'(t)\rangle CQ1t|\phi(t)\rangle B+|\alpha2'(t)\rangle CQ2t|\phi(t)\rangle B\rangle\} + F\exp(i\hbar^2 A2mA \dashv 1A\wedge dA \ 2zEGk+13 \ (a+\ell) \ ta+\ell-\{1/12+(\|\alpha1'(t)\rangle CQ1t|\phi(t)\rangle B+|\alpha2'(t)\rangle CQ2t|\phi(t)\rangle B\rangle\} + F\exp(i\hbar^2 A2mA \dashv 1A\wedge[A\wedge A] \ 2zEGk \ (\text{mod}2\pi) \ [1]\wedge\sin \ (a+\ell) \ ta+\ell-\{1/12+(\|\alpha1'(t)\rangle CQ1t|\phi(t)\rangle B+|\alpha2'(t)\rangle CQ2t|\phi(t)\rangle B\rangle\} + F\exp(i\hbar^2 A2mA \dashv 1Vectk \ ((a+\ell) \ ta+\ell-\{1/12+(\|\alpha1'(t)\rangle CQ1t|\phi(t)\rangle B+|\alpha2'(t)\rangle CQ2t|\phi(t)\rangle B\rangle\} + F\exp(i\hbar^2 A2mA \dashv 1+ \ (a+\ell) \ ta+\ell-\{1/12+(\|\alpha1'(t)\rangle CQ1t|\phi(t)\rangle B+|\alpha2'(t)\rangle CQ2t|\phi(t)\rangle B\rangle\} + F\exp(i\hbar^2 A2mA \dashv 1\wedge \ (a+\ell) \ ta+\ell-\{1/12+(\|\alpha1'(t)\rangle CQ1t|\phi(t)\rangle B+|\alpha2'(t)\rangle CQ2t|\phi(t)\rangle B\rangle\} + F\exp(i\hbar^2 A2mA \dashv 1F) \ 14\pi^3 M3 \ (a+\ell) \ ta+\ell-\{1/12+(\|\alpha1'(t)\rangle CQ1t|\phi(t)\rangle B+|\alpha2'(t)\rangle CQ2t|\phi(t)\rangle B\rangle\} + F\exp(i\hbar^2 A2mA \dashv 1A\wedge dA \ 2zEGk+13 \ (a+\ell) \ ta+\ell-\{1/12+(\|\alpha1'(t)\rangle CQ1t|\phi(t)\rangle B+|\alpha2'(t)\rangle CQ2t|\phi(t)\rangle B\rangle\} + F\exp(i\hbar^2 A2mA \dashv 1A\wedge[A\wedge A] \ 2zEGk \ (\text{mod}2\pi) \ (\text{equation45}), F= dA+A\wedge A \ \text{Repk} \ (dA+A\wedge A \ \text{AGA}) \ \text{Repss} \ (Fq \ 2zEG) \ [\text{or} \ \text{Repk} \ (AF \ 2zEG)] \ \text{and} \ \text{Rep} \ (Dk \ (C[G])) = \text{Repf} \ ((a+\ell) \ ta+\ell-\{1/12+(\|\alpha1'(t)\rangle CQ1t|\phi(t)\rangle B+|\alpha2'(t)\rangle CQ2t|\phi(t)\rangle B\rangle\} + F\exp(i\hbar^2 A2mA \dashv 1G,k)), (\text{equation46}) on the heuristic level of path integrals $((a+\ell) \ ta+\ell-\{1/12+(\|\alpha1'(t)\rangle CQ1t|\phi(t)\rangle B+|\alpha2'(t)\rangle CQ2t|\phi(t)\rangle B\rangle\} + F\exp(i\hbar^2 A2mA \dashv 1A$ is the potential 11-form and F is the field strength 224-form) where$

the partition function for the Chern-Simons theory to gather eigenvalues of the matrix models when associated with knot theory is the modulus square of the poles and zeroes in the one-loop determinant partition function The multiset of probabilities is the multiset $\{1/12+(\|\alpha1'(t)\rangle CQ1t|\phi(t)\rangle B+|\alpha2'(t)\rangle CQ2t|\phi(t)\rangle B\rangle\} + F\exp(i\hbar^2 A2mA \dashv \{1/2\} \ + \{1/12+(\|\alpha1'(t)\rangle CQ1t|\phi(t)\rangle B+|\alpha2'(t)\rangle CQ2t|\phi(t)\rangle B\rangle\} + F\exp(i\hbar^2 A2mA \dashv \{1/12+(\|\alpha1'(t)\rangle CQ1t|\phi(t)\rangle B+|\alpha2'(t)\rangle CQ2t|\phi(t)\rangle B\rangle\} + F\exp(i\hbar^2 A2mA \dashv \{1/4\}$, which is the same as the multiset $\{1/12+(\|\alpha1'(t)\rangle CQ1t|\phi(t)\rangle B+|\alpha2'(t)\rangle CQ2t|\phi(t)\rangle B\rangle\} + F\exp(i\hbar^2 A2mA \dashv \{1/12+(\|\alpha1'(t)\rangle CQ1t|\phi(t)\rangle B+|\alpha2'(t)\rangle CQ2t|\phi(t)\rangle B\rangle\} + F\exp(i\hbar^2 A2mA \dashv \{1/12+(\|\alpha1'(t)\rangle CQ1t|\phi(t)\rangle B+|\alpha2'(t)\rangle CQ2t|\phi(t)\rangle B\rangle\} + F\exp(i\hbar^2 A2mA \dashv \{1/4\} \ + \{1/2\}$. The multiplicity of $1/12$ in this multiset is 3, the number of occurrences of $1/12$.

Derivative:

- RoccustyrnaTM_fR GissitorviffirnaTM_gS parts: @<TRIPOS>ATOM
- 1 P1 4.3549 -1.7704 0.0000 P 1 fragment1 -0.1093
- 2 O1 4.6751 -3.2767 0.0000 O.2 1 fragment1 -0.2831
- 3 N1 4.0347 -0.2640 0.0000 N.3 1 fragment1 0.0896
- 4 O2 -3.3388 -1.4822 0.0000 O.3 1 fragment1 -0.3468
- 5 O3 -4.5133 -5.2901 0.0000 O.3 1 fragment1 -0.3856

•	6	O4 -7.0031 -3.0483 0.0000	O.3	1	fragment1	-0.3873
•	7	O5 3.4032 -4.6996 0.0000	O.2	1	fragment1	-0.2635
•	8	N2 -1.6118 -3.6149 0.0000	N.3	1	fragment1	0.0427
•	9	N3 -0.2781 -2.8449 0.0000	N.2	1	fragment1	-0.2100
•	10	N4 0.2400 -5.2822 0.0000	N.2	1	fragment1	-0.1653
•	11	N5 2.8486 -2.0906 0.0000	N.3	1	fragment1	0.0984
•	12	C1 -5.4968 -2.7281 0.0000	C.3	1	fragment1	0.1128
•	13	C2 -4.3523 -3.7585 0.0000	C.3	1	fragment1	0.1271
•	14	C3 -4.8704 -1.3212 0.0000	C.3	1	fragment1	0.1141
•	15	C4 -3.0186 -2.9885 0.0000	C.3	1	fragment1	0.1735
•	16	C5 -5.6404 0.0125 0.0000	C.3	1	fragment1	0.0994
•	17	C6 -1.2916 -5.1213 0.0000	C.2	1	fragment1	0.0117
•	18	C7 0.8663 -3.8754 0.0000	C.2	1	fragment1	0.1225
•	19	C8 2.3727 -3.5552 0.0000	C.2	1	fragment1	0.1189
•	20	N6 -7.9504 1.3461 0.0000	N.3	1	fragment1	0.0880
•	21	N7 -10.2604 2.6798 0.0000	N.2	1	fragment1	-0.2235
•	22	N8 -12.5704 1.3461 0.0000	N.3	1	fragment1	-0.1303
•	23	N9 -12.5704 4.0135 0.0000	N.3	1	fragment1	-0.1303
•	24	O6 -7.1804 0.0125 0.0000	O.3	1	fragment1	-0.2597
•	25	C9 -9.4904 1.3461 0.0000	C.2	1	fragment1	0.0178
•	26	C10 -7.1804 2.6798 0.0000	C.1	1	fragment1	0.0796
•	27	C11 -10.2604 0.0125 0.0000	C.2	1	fragment1	-0.0009
•	28	C12 -11.8004 2.6798 0.0000	C.2	1	fragment1	-0.1256
•	29	N10 -6.4104 4.0135 0.0000	N.1	1	fragment1	-0.1546
•	30	O7 9.1355 4.3403 0.0000	O.2	1	fragment1	-0.2752
•	31	N11 6.3372 0.0144 0.0000	N.3	1	fragment1	0.0724
•	32	N12 6.3372 2.5062 0.0000	N.2	1	fragment1	-0.1956
•	33	N13 9.1355 -0.2797 0.0000	N.2	1	fragment1	-0.2012
•	34	N14 10.4691 2.0303 0.0000	N.3	1	fragment1	0.0507
•	35	N15 11.8028 -0.2797 0.0000	N.3	1	fragment1	-0.1233
•	36	N16 5.8613 -1.4502 0.0000	N.3	1	fragment1	0.0734
•	37	C13 7.8018 0.4903 0.0000	C.2	1	fragment1	0.0555
•	38	C14 5.4320 1.2603 0.0000	C.2	1	fragment1	-0.0051
•	39	C15 7.8018 2.0303 0.0000	C.2	1	fragment1	0.0974
•	40	C16 9.1355 2.8003 0.0000	C.2	1	fragment1	0.0887
•	41	C17 10.4691 0.4903 0.0000	C.2	1	fragment1	-0.0769
•	42	F1 -0.9995 4.1763 0.0000	F	1	fragment1	-0.1305
•	43	O8 1.4257 -0.8186 0.0000	O.2	1	fragment1	-0.2765
•	44	N17 3.0742 4.2550 0.0000	N.3	1	fragment1	-0.1387
•	45	N18 0.7853 2.1941 0.0000	N.2	1	fragment1	-0.1545
•	46	C18 2.2499 1.7182 0.0000	C.2	1	fragment1	0.1196
•	47	C19 3.3944 2.7487 0.0000	C.3	1	fragment1	0.0472
•	48	C20 1.6096 4.7309 0.0000	C.2	1	fragment1	-0.0369
•	49	C21 0.4651 3.7004 0.0000	C.2	1	fragment1	0.0572
•	50	C22 2.5701 0.2118 0.0000	C.2	1	fragment1	0.0961
•	51	C23 19.4885 5.5526 0.0000	C.3	2	fragment2	0.1400
•	52	N19 17.7615 3.4199 0.0000	N.3	2	fragment2	-0.2245
•	53	N20 18.0817 4.9262 0.0000	N.3	2	fragment2	-0.1710
•	54	N21 17.0512 6.0706 0.0000	N.3	2	fragment2	-0.0767
•	55	C24 17.8212 7.4043 0.0000	C.2	2	fragment2	-0.0635

•	56	N22 19.3276 7.0841 0.0000 N.3	2	fragment2	-0.1018
•	57	S1 17.1948 8.8112 0.0000 S.2	2	fragment2	-0.1182
•	58	N23 25.9305 3.1548 0.0000 N.3	2	fragment2	-0.0940
•	59	C25 26.8357 1.9089 0.0000 C.2	2	fragment2	-0.0585
•	60	N24 25.9305 0.6630 0.0000 N.3	2	fragment2	-0.0596
•	61	N25 24.4659 1.1389 0.0000 N.3	2	fragment2	-0.0867
•	62	C26 24.4659 2.6789 0.0000 C.3	2	fragment2	0.1775
•	63	O9 22.3622 4.7826 0.0000 O.3	2	fragment2	-0.2542
•	64	C27 20.8222 4.7826 0.0000 C.3	2	fragment2	0.1999
•	65	S2 28.3757 1.9089 0.0000 S.2	2	fragment2	-0.1171
•	66	P2 21.5922 1.9089 0.0000 P	2	fragment2	-0.0317
•	67	O10 20.0522 1.9089 0.0000 O.2	2	fragment2	-0.2321
•	68	N26 23.1322 1.9089 0.0000 N.3	2	fragment2	0.0296
•	69	O11 17.0433 -5.5568 0.0000 O.3	2	fragment2	-0.3185
•	70	F2 20.5239 -7.4973 0.0000 F	2	fragment2	-0.2390
•	71	F3 17.8133 -9.4666 0.0000 F	2	fragment2	-0.2379
•	72	O12 18.9248 0.3689 0.0000 O.2	2	fragment2	-0.2236
•	73	N27 19.4885 -4.3109 0.0000 N.3	2	fragment2	0.0609
•	74	N28 19.0126 -2.8463 0.0000 N.2	2	fragment2	-0.1908
•	75	N29 21.5044 -2.8463 0.0000 N.2	2	fragment2	-0.1611
•	76	O13 21.5922 0.3689 0.0000 O.3	2	fragment2	-0.0706
•	77	C28 17.8133 -7.9266 0.0000 C.3	2	fragment2	0.1910
•	78	C29 19.0592 -7.0214 0.0000 C.3	2	fragment2	0.1810
•	79	C30 16.5675 -7.0214 0.0000 C.3	2	fragment2	0.2350
•	80	C31 18.5833 -5.5568 0.0000 C.3	2	fragment2	0.1822
•	81	C32 21.0285 -4.3109 0.0000 C.2	2	fragment2	0.0160
•	82	C33 20.2585 -1.9411 0.0000 C.2	2	fragment2	0.1298
•	83	C34 20.2585 -0.4011 0.0000 C.2	2	fragment2	0.1885
•	84	N30 21.5922 3.4489 0.0000 N.3	2	fragment2	0.0812
•	85	F4 15.1028 -7.4973 0.0000 F	2	fragment2	-0.2125
•	86	P3 37.3023 2.5958 0.0000 P	3	fragment3	-0.1805
•	87	O14 35.8377 2.1199 0.0000 O.2	3	fragment3	-0.2828
•	88	N31 38.7669 3.0716 0.0000 N.3	3	fragment3	-0.0464
•	89	O15 35.2414 0.3069 0.0000 O.2	3	fragment3	-0.2717
•	90	N32 36.3184 -2.7238 0.0000 N.2	3	fragment3	-0.2133
•	91	C35 38.6882 -1.9538 0.0000 C.2	3	fragment3	0.1085
•	92	N33 37.7782 1.1311 0.0000 N.3	3	fragment3	0.0919
•	93	C36 38.6882 -3.4938 0.0000 C.3	3	fragment3	0.1651
•	94	C37 37.2236 -1.4779 0.0000 C.2	3	fragment3	0.1130
•	95	C38 36.7477 -0.0133 0.0000 C.2	3	fragment3	0.1066
•	96	N34 37.8569 5.2048 0.0000 N.3	3	fragment3	-0.1730
•	97	N35 38.4114 7.8139 0.0000 N.2	3	fragment3	-0.2534
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•	99	N37 36.8264 4.0604 0.0000 N.3	3	fragment3	-0.0491
•	100	C39 37.3810 6.6695 0.0000 C.3	3	fragment3	0.2011
•	101	C40 39.9178 7.4937 0.0000 C.2	3	fragment3	-0.0763
•	102	C41 39.7974 4.2161 0.0000 C.3	3	fragment3	0.0234
•	103	C42 40.2733 2.7515 0.0000 C.3	3	fragment3	0.0234
•	104	C43 35.8746 6.9896 0.0000 C.1	3	fragment3	0.0916
•	105	N38 34.3683 7.3098 0.0000 N.1	3	fragment3	-0.1787

•	106	C44 40.0219 -4.2638 0.0000 C.2	3	fragment3	0.1869
•	107	N39 41.3556 -3.4938 0.0000 N.2	3	fragment3	-0.1225
•	108	C45 41.3556 -1.9538 0.0000 C.2	3	fragment3	0.0119
•	109	N40 40.0219 -1.1838 0.0000 N.2	3	fragment3	-0.1783
•	110	O16 40.0219 -5.8038 0.0000 O.2	3	fragment3	-0.2450
•	111	N41 42.6893 -1.1838 0.0000 N.3	3	fragment3	-0.0965
•	112	F5 39.8391 -8.8677 0.0000 F	3	fragment3	-0.0999
•	113	O17 35.2414 -5.7545 0.0000 O.2	3	fragment3	-0.2729
•	114	N42 37.3023 -8.0434 0.0000 N.2	3	fragment3	-0.1348
•	115	N43 37.2236 -3.9697 0.0000 N.3	3	fragment3	0.0885
•	116	C46 37.7782 -6.5788 0.0000 C.2	3	fragment3	0.1208
•	117	N44 37.8569 -10.6525 0.0000	N.2 3	fragment3	-0.1764
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•	119	C48 36.7477 -5.4343 0.0000 C.2	3	fragment3	0.0994
•	120	H1 5.1792 0.7664 0.0000 H	1	fragment1	0.1444
•	121	H2 -5.9201 -5.9165 0.0000 H	1	fragment1	0.2107
•	122	H3 -7.4790 -4.5129 0.0000 H	1	fragment1	0.2106
•	123	H4 1.3422 -1.7704 0.0000 H	1	fragment1	0.1444
•	124	H5 -6.4019 -3.9740 0.0000 H	1	fragment1	0.0657
•	125	H6 -5.4968 -4.7890 0.0000 H	1	fragment1	0.0675
•	126	H7 -6.4100 -1.2890 0.0000 H	1	fragment1	0.0657
•	127	H8 -2.3923 -4.3954 0.0000 H	1	fragment1	0.0867
•	128	H9 -4.3344 0.8285 0.0000 H	1	fragment1	0.0617
•	129	H10 -5.5866 1.5515 0.0000 H	1	fragment1	0.0617
•	130	H11 -2.3221 -6.2657 0.0000 H	1	fragment1	0.1032
•	131	H12 -14.1104 1.3461 0.0000	H 1	fragment1	0.1267
•	132	H13 -11.8004 0.0125 0.0000	H 1	fragment1	0.1267
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•	134	H15 -14.1104 4.0135 0.0000	H 1	fragment1	0.1267
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•	139	H20 13.1365 0.4903 0.0000 H	1	fragment1	0.1268
•	140	H21 6.8917 -2.5946 0.0000 H	1	fragment1	0.0887
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•	145	H26 1.2894 6.2372 0.0000 H	1	fragment1	0.0798
•	146	H27 20.8380 6.2945 0.0000 H	2	fragment2	0.0715
•	147	H28 16.2969 2.9440 0.0000 H	2	fragment2	0.1390
•	148	H29 18.9059 2.3894 0.0000 H	2	fragment2	0.1390
•	149	H30 15.5196 5.9097 0.0000 H	2	fragment2	0.1511
•	150	H31 20.4720 8.1146 0.0000 H	2	fragment2	0.1318
•	151	H32 26.4064 4.6194 0.0000 H	2	fragment2	0.1331
•	152	H33 26.4064 -0.8016 0.0000 H	2	fragment2	0.1512
•	153	H34 23.8395 4.0858 0.0000 H	2	fragment2	0.0873
•	154	H35 19.3751 4.2559 0.0000 H	2	fragment2	0.0864
•	155	H36 18.8438 -9.0711 0.0000 H	2	fragment2	0.0751

•	156	H37	19.8292	-8.3551	0.0000	H	2	fragment2	0.0741
•	157	H38	16.2158	-8.5207	0.0000	H	2	fragment2	0.1013
•	158	H39	20.0897	-5.2366	0.0000	H	2	fragment2	0.0872
•	159	H40	21.9337	-5.5568	0.0000	H	2	fragment2	0.1032
•	160	H41	39.2845	0.8108	0.0000	H	3	fragment3	0.1453
•	161	H42	38.5272	-5.0254	0.0000	H	3	fragment3	0.0666
•	162	H43	39.3632	4.8845	0.0000	H	3	fragment3	0.1454
•	163	H44	42.4547	8.3180	0.0000	H	3	fragment3	0.1251
•	164	H45	40.4724	10.1028	0.0000	H	3	fragment3	0.1251
•	165	H46	35.3201	4.3806	0.0000	H	3	fragment3	0.1555
•	166	H47	38.8874	6.3493	0.0000	H	3	fragment3	0.0904
•	167	H48	40.3937	6.0290	0.0000	H	3	fragment3	0.0965
•	168	H49	40.9237	5.2663	0.0000	H	3	fragment3	0.0452
•	169	H50	39.6632	5.7502	0.0000	H	3	fragment3	0.0452
•	170	H51	41.8018	2.5638	0.0000	H	3	fragment3	0.0452
•	171	H52	40.6198	1.2509	0.0000	H	3	fragment3	0.0452
•	172	H53	44.0230	-1.9539	0.0000	H	3	fragment3	0.1273
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•	174	H55	39.2846	-6.2587	0.0000	H	3	fragment3	0.0895
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•	170	81	159	1
•	171	92	160	1
•	172	93	161	1
•	173	96	162	1
•	174	98	163	1
•	175	98	164	1
•	176	99	165	1
•	177	100	166	1
•	178	101	167	1
•	179	102	168	1

- 180 102 169 1
- 181 103 170 1
- 182 103 171 1
- 183 111 172 1
- 184 111 173 1
- 185 116 174 1
- 186 117 175 1
- @<TRIPOS>SUBSTRUCTURE
- 1 fragment1 1
- 2 fragment2 51
- 3 fragment3 86 42

$$\frac{\partial}{\partial r} \left(-c^2 \left(1 - \frac{2GM}{c^2 r} \right) g \right) = - \frac{2gGM}{r^2}$$

Indefinite integral:

- RoccustyrnaTM_fR GissitorviffirnaTM_gS parts: HETATM 1 P UNK 0 4.355 -1.770 0.000 0.00 0.00 P+0
- HETATM 2 O UNK 0 4.675 -3.277 0.000 0.00 0.00 O+0
- HETATM 3 N UNK 0 4.035 -0.264 0.000 0.00 0.00 N+0
- HETATM 4 O UNK 0 -3.339 -1.482 0.000 0.00 0.00 O+0
- HETATM 5 O UNK 0 -4.513 -5.290 0.000 0.00 0.00 O+0
- HETATM 6 O UNK 0 -7.003 -3.048 0.000 0.00 0.00 O+0
- HETATM 7 O UNK 0 3.403 -4.700 0.000 0.00 0.00 O+0
- HETATM 8 N UNK 0 -1.612 -3.615 0.000 0.00 0.00 N+0
- HETATM 9 N UNK 0 -0.278 -2.845 0.000 0.00 0.00 N+0
- HETATM 10 N UNK 0 0.240 -5.282 0.000 0.00 0.00 N+0
- HETATM 11 N UNK 0 2.849 -2.091 0.000 0.00 0.00 N+0
- HETATM 12 C UNK 0 -5.497 -2.728 0.000 0.00 0.00 C+0
- HETATM 13 C UNK 0 -4.352 -3.759 0.000 0.00 0.00 C+0
- HETATM 14 C UNK 0 -4.870 -1.321 0.000 0.00 0.00 C+0
- HETATM 15 C UNK 0 -3.019 -2.989 0.000 0.00 0.00 C+0
- HETATM 16 C UNK 0 -5.640 0.012 0.000 0.00 0.00 C+0
- HETATM 17 C UNK 0 -1.292 -5.121 0.000 0.00 0.00 C+0
- HETATM 18 C UNK 0 0.866 -3.875 0.000 0.00 0.00 C+0
- HETATM 19 C UNK 0 2.373 -3.555 0.000 0.00 0.00 C+0
- HETATM 20 N UNK 0 -7.950 1.346 0.000 0.00 0.00 N+0
- HETATM 21 N UNK 0 -10.260 2.680 0.000 0.00 0.00 N+0
- HETATM 22 N UNK 0 -12.570 1.346 0.000 0.00 0.00 N+0
- HETATM 23 N UNK 0 -12.570 4.013 0.000 0.00 0.00 N+0
- HETATM 24 O UNK 0 -7.180 0.012 0.000 0.00 0.00 O+0
- HETATM 25 C UNK 0 -9.490 1.346 0.000 0.00 0.00 C+0
- HETATM 26 C UNK 0 -7.180 2.680 0.000 0.00 0.00 C+0
- HETATM 27 C UNK 0 -10.260 0.012 0.000 0.00 0.00 C+0
- HETATM 28 C UNK 0 -11.800 2.680 0.000 0.00 0.00 C+0
- HETATM 29 N UNK 0 -6.410 4.013 0.000 0.00 0.00 N+0
- HETATM 30 O UNK 0 9.135 4.340 0.000 0.00 0.00 O+0
- HETATM 31 N UNK 0 6.337 0.014 0.000 0.00 0.00 N+0
- HETATM 32 N UNK 0 6.337 2.506 0.000 0.00 0.00 N+0

- HETATM 33 N UNK 0 9.135 -0.280 0.000 0.00 0.00 N+0
- HETATM 34 N UNK 0 10.469 2.030 0.000 0.00 0.00 N+0
- HETATM 35 N UNK 0 11.803 -0.280 0.000 0.00 0.00 N+0
- HETATM 36 N UNK 0 5.861 -1.450 0.000 0.00 0.00 N+0
- HETATM 37 C UNK 0 7.802 0.490 0.000 0.00 0.00 C+0
- HETATM 38 C UNK 0 5.432 1.260 0.000 0.00 0.00 C+0
- HETATM 39 C UNK 0 7.802 2.030 0.000 0.00 0.00 C+0
- HETATM 40 C UNK 0 9.135 2.800 0.000 0.00 0.00 C+0
- HETATM 41 C UNK 0 10.469 0.490 0.000 0.00 0.00 C+0
- HETATM 42 F UNK 0 -1.000 4.176 0.000 0.00 0.00 F+0
- HETATM 43 O UNK 0 1.426 -0.819 0.000 0.00 0.00 O+0
- HETATM 44 N UNK 0 3.074 4.255 0.000 0.00 0.00 N+0
- HETATM 45 N UNK 0 0.785 2.194 0.000 0.00 0.00 N+0
- HETATM 46 C UNK 0 2.250 1.718 0.000 0.00 0.00 C+0
- HETATM 47 C UNK 0 3.394 2.749 0.000 0.00 0.00 C+0
- HETATM 48 C UNK 0 1.610 4.731 0.000 0.00 0.00 C+0
- HETATM 49 C UNK 0 0.465 3.700 0.000 0.00 0.00 C+0
- HETATM 50 C UNK 0 2.570 0.212 0.000 0.00 0.00 C+0
- HETATM 51 C UNK 0 19.489 5.553 0.000 0.00 0.00 C+0
- HETATM 52 N UNK 0 17.761 3.420 0.000 0.00 0.00 N+0
- HETATM 53 N UNK 0 18.082 4.926 0.000 0.00 0.00 N+0
- HETATM 54 N UNK 0 17.051 6.071 0.000 0.00 0.00 N+0
- HETATM 55 C UNK 0 17.821 7.404 0.000 0.00 0.00 C+0
- HETATM 56 N UNK 0 19.328 7.084 0.000 0.00 0.00 N+0
- HETATM 57 S UNK 0 17.195 8.811 0.000 0.00 0.00 S+0
- HETATM 58 N UNK 0 25.931 3.155 0.000 0.00 0.00 N+0
- HETATM 59 C UNK 0 26.836 1.909 0.000 0.00 0.00 C+0
- HETATM 60 N UNK 0 25.931 0.663 0.000 0.00 0.00 N+0
- HETATM 61 N UNK 0 24.466 1.139 0.000 0.00 0.00 N+0
- HETATM 62 C UNK 0 24.466 2.679 0.000 0.00 0.00 C+0
- HETATM 63 O UNK 0 22.362 4.783 0.000 0.00 0.00 O+0
- HETATM 64 C UNK 0 20.822 4.783 0.000 0.00 0.00 C+0
- HETATM 65 S UNK 0 28.376 1.909 0.000 0.00 0.00 S+0
- HETATM 66 P UNK 0 21.592 1.909 0.000 0.00 0.00 P+0
- HETATM 67 O UNK 0 20.052 1.909 0.000 0.00 0.00 O+0
- HETATM 68 N UNK 0 23.132 1.909 0.000 0.00 0.00 N+0
- HETATM 69 O UNK 0 17.043 -5.557 0.000 0.00 0.00 O+0
- HETATM 70 F UNK 0 20.524 -7.497 0.000 0.00 0.00 F+0
- HETATM 71 F UNK 0 17.813 -9.467 0.000 0.00 0.00 F+0
- HETATM 72 O UNK 0 18.925 0.369 0.000 0.00 0.00 O+0
- HETATM 73 N UNK 0 19.489 -4.311 0.000 0.00 0.00 N+0
- HETATM 74 N UNK 0 19.013 -2.846 0.000 0.00 0.00 N+0
- HETATM 75 N UNK 0 21.504 -2.846 0.000 0.00 0.00 N+0
- HETATM 76 O UNK 0 21.592 0.369 0.000 0.00 0.00 O+0
- HETATM 77 C UNK 0 17.813 -7.927 0.000 0.00 0.00 C+0
- HETATM 78 C UNK 0 19.059 -7.021 0.000 0.00 0.00 C+0
- HETATM 79 C UNK 0 16.567 -7.021 0.000 0.00 0.00 C+0
- HETATM 80 C UNK 0 18.583 -5.557 0.000 0.00 0.00 C+0
- HETATM 81 C UNK 0 21.029 -4.311 0.000 0.00 0.00 C+0
- HETATM 82 C UNK 0 20.259 -1.941 0.000 0.00 0.00 C+0

- HETATM 83 C UNK 0 20.259 -0.401 0.000 0.00 0.00 C+0
- HETATM 84 N UNK 0 21.592 3.449 0.000 0.00 0.00 N+0
- HETATM 85 F UNK 0 15.103 -7.497 0.000 0.00 0.00 F+0
- HETATM 86 P UNK 0 37.302 2.596 0.000 0.00 0.00 P+0
- HETATM 87 O UNK 0 35.838 2.120 0.000 0.00 0.00 O+0
- HETATM 88 N UNK 0 38.767 3.072 0.000 0.00 0.00 N+0
- HETATM 89 O UNK 0 35.241 0.307 0.000 0.00 0.00 O+0
- HETATM 90 N UNK 0 36.318 -2.724 0.000 0.00 0.00 N+0
- HETATM 91 C UNK 0 38.688 -1.954 0.000 0.00 0.00 C+0
- HETATM 92 N UNK 0 37.778 1.131 0.000 0.00 0.00 N+0
- HETATM 93 C UNK 0 38.688 -3.494 0.000 0.00 0.00 C+0
- HETATM 94 C UNK 0 37.224 -1.478 0.000 0.00 0.00 C+0
- HETATM 95 C UNK 0 36.748 -0.013 0.000 0.00 0.00 C+0
- HETATM 96 N UNK 0 37.857 5.205 0.000 0.00 0.00 N+0
- HETATM 97 N UNK 0 38.411 7.814 0.000 0.00 0.00 N+0
- HETATM 98 N UNK 0 40.948 8.638 0.000 0.00 0.00 N+0
- HETATM 99 N UNK 0 36.826 4.060 0.000 0.00 0.00 N+0
- HETATM 100 C UNK 0 37.381 6.669 0.000 0.00 0.00 C+0
- HETATM 101 C UNK 0 39.918 7.494 0.000 0.00 0.00 C+0
- HETATM 102 C UNK 0 39.797 4.216 0.000 0.00 0.00 C+0
- HETATM 103 C UNK 0 40.273 2.751 0.000 0.00 0.00 C+0
- HETATM 104 C UNK 0 35.875 6.990 0.000 0.00 0.00 C+0
- HETATM 105 N UNK 0 34.368 7.310 0.000 0.00 0.00 N+0
- HETATM 106 C UNK 0 40.022 -4.264 0.000 0.00 0.00 C+0
- HETATM 107 N UNK 0 41.356 -3.494 0.000 0.00 0.00 N+0
- HETATM 108 C UNK 0 41.356 -1.954 0.000 0.00 0.00 C+0
- HETATM 109 N UNK 0 40.022 -1.184 0.000 0.00 0.00 N+0
- HETATM 110 O UNK 0 40.022 -5.804 0.000 0.00 0.00 O+0
- HETATM 111 N UNK 0 42.689 -1.184 0.000 0.00 0.00 N+0
- HETATM 112 F UNK 0 39.839 -8.868 0.000 0.00 0.00 F+0
- HETATM 113 O UNK 0 35.241 -5.755 0.000 0.00 0.00 O+0
- HETATM 114 N UNK 0 37.302 -8.043 0.000 0.00 0.00 N+0
- HETATM 115 N UNK 0 37.224 -3.970 0.000 0.00 0.00 N+0
- HETATM 116 C UNK 0 37.778 -6.579 0.000 0.00 0.00 C+0
- HETATM 117 N UNK 0 37.857 -10.653 0.000 0.00 0.00 N+0
- HETATM 118 C UNK 0 38.333 -9.188 0.000 0.00 0.00 C+0
- HETATM 119 C UNK 0 36.748 -5.434 0.000 0.00 0.00 C+0
- MASTER 0 0 0 0 0 0 0 119 0 0 0
- END

$$\int -c^2 g \left(1 - \frac{2GM}{c^2 r} \right) dr = 2 g G M \log(r) - c^2 g r + \text{constant}$$

(assuming a complex-valued logarithm)

$\log(x)$ is the natural logarithm

Limit:

$$\lim_{r\rightarrow\pm\infty} -c^2\,g\left(1-\frac{2\,G\,M}{c^2\,r}\right)=-c^2\,g$$

Series representations:

$$-c^2\,g\left(1-\frac{2\,G\,M}{c^2\,r}\right)=-g\left(c^2-2\,G\,M\right)+\sum_{n=1}^{\infty}(-1+r)^n\,2\left((-1)^n\,g\,G\,M\right)$$

$$-c^2\,g\left(1-\frac{2\,G\,M}{c^2\,r}\right)=\sum_{n=-\infty}^{\infty}\left(\left\{\begin{array}{ll} -g & n=2 \\ \frac{2\,g\,G\,M}{r} & n=0 \end{array}\right.\right)c^n$$

$$-c^2\,g\left(1-\frac{2\,G\,M}{c^2\,r}\right)=\sum_{n=-\infty}^{\infty}\left(\left\{\begin{array}{ll} -c^2\,g & n=0 \\ 2\,g\,G\,M & n=-1 \end{array}\right.\right)r^n$$

$$-c^2\,g\left(1-\frac{2\,G\,M}{c^2\,r}\right)=\sum_{n=-\infty}^{\infty}\left(\left\{\begin{array}{ll} -2\,g & n=1 \\ -g & n=2 \\ g\left(-1+\frac{2\,G\,M}{r}\right) & n=0 \end{array}\right.\right)(-1+c)^n$$

$$\frac{\partial}{\partial n}\left(-\frac{n^{33\,834}\,k^{-(k^4\,n^{33\,835}\,N^2)}\,N^{213}}{33\,834\,432\,k^4}\right)=\frac{n^{33\,833}\,N^{213}\,k^{-k^4\,n^{33\,835}\,N^2-4}\left(33\,835\,k^4\,n^{33\,835}\,N^2\log(k)-33\,834\right)}{33\,834\,432}$$

$$\int -\frac{k^{-4-k^4} n^{33835} N^2 n^{33834} N^{213}}{33834432} dn = \frac{N^{211} k^{-k^4} n^{33835} N^2 -8}{1144788006720 \log(k)} + \text{constant} \quad (\text{Scheme 8})$$

(Scheme 9)

OUTPUTA:

202274696d655f706172616d65746572223a20302e32343631333331323530303031343231372c0d0a20226369726375697

4223a207b0d0a2022636f6c73223a205b0d0a205b0d0a2022436f756e74696e6738220d0a205d2c0d0a205b0d0a2022436861

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85222c0d0a202285222c0d0a202285222c0d0a202285220d0a205d2c0d0a205b0d0a202253776170222c0d0a20312c0d0a20312c0d0a20

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a206e756c6c2c0d0a206e756c6c0d0a205d2c0d0a205b0d0a206e756c6c2c0d0a206e756c6c2c0d0a206e756c6c2c0d
0a206e7
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756c6c2
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c0d0a2
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2c0d0a2
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d0a206
e756c6c2c0d0a206e756c6c2c0d0a206e756c6c0d0a205d2c0d0a205b0d0a206e756c6c2c0d0a206e756c6c2c0d0a20
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2d302e3
1363535393333383536393634313131330d0a207d2c0d0a207b0d0a202278223a202d302e32373335313135383835
373334
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310d0a
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202278
223a20302e353938303737343736303234363237372c0d0a202279223a20302e30303637373637363132363336303
839333
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d302e3
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392c0d
0a20227a223a202d302e373230313631343233303837313230310d0a207d0d0a205d0d0a205d2c0d0a20226469737

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amino+(cyano) methyl+hydrazin-1-

□ yl(aziridin-1-yl) phosphoryl+-1-*(2E) -2-*(fluoromethanimidoyl)
 imino+acetyl+-7-oxo-7aH-pyrazolo*4,3-d+pyrimidine-3-carboxamide;
 3-(2-amino-5-sulfanylidene-1,2,4-triazolidin-3- yl) oxaziridin-2-yl(3- sulfany
 lidene-1,2,4,6-tetraazabicyclo*3.1.0+hexan-6-yl) phosphoroso 1-(3,4,5-trifluorooxolan-2-yl)
 -1,2,4-triazole-3- carboxylate; N-*(2-amino-6-oxo-1H-purin-9-yl)
 amino(,1-5-(,*cyano(,1-[(diaminomethylidene) amino]ethenyl)) amino+oxy-methyl)
 -3,4-dihydroxyoxolan-2-yl+-1,2,4-triazol-3-yl-formamido) phosphoryl
 +-6-fluoro-3,4-dihydropyrazine-2-carboxamide (7aR) -5-amino-N- *(S) -,2-*(S) -(E) -(aminomethy
 lidene) amino+(cyano) methyl+ hydrazin-1-yl-(aziridin-1-yl) phosphoryl+-1-*(2E) -2-*(
 (fluoromethanimidoyl) imino+ acetyl+-7-oxo-1H,7H,7aH-pyrazolo*4,3-d+pyrimidine-3-carboxamide;
 N-*(2-amino-6-oxo-6,9- dihydro-1H-purin-9-yl) amino+(,1-5- (*cyano(,1-*(diaminomethylidene)
 amino+ethenyl-) amino+oxy-methyl) -3,4-dihydroxyoxolan-2-yl+-1H-1,2,4-triazol-3-yl-formamido)
 phosphoryl--6-fluoro-3,4- dihydropyrazine-2-carboxamide; *3-(2-amino-5-sulfanylidene-
 1,2,4-triazolidin-3- yl) oxaziridin-2 -yl+(,3-sulfanylidene-1,2,4,6-tetraazabicyclo*3.1.0+hexan-6-yl-)
 phosphoroso 1-(3,4,5- trifluorooxolan- 2-yl) -1H-1,2,4-triazole-3-carboxylate

Figure 1///. 2D Atoms of (i) GisitorviffirnaTM, (ii) Roccustyrna_gs1_TM, and (ii) Roccustyrna_fr1_TM fragments 2D structure.

(22,27,28,35) This InSilico approach keeps track of the solutions already found of the selected group of the selected hit candidates which were fragmented, re-cored, and superposed in a non-relativistic quantum mechanics environment and finally led us to the complete Roccustyrna chemical structure. (Table 1/), (20,28,29,30) If several chemical space solutions were found in the phase end, the combined theory has a sequence of similar such function

spaces of finite but arbitrarily large selected dimension, where the partition dimension increases with the finite resolution of relative knot space measurements to the first dihydro-3H-purin-9-yl) - system when extracted from the 10 hit selected small molecules as the possible chemical bimodules over a hyperfinite 1-factor solutions which were sorted by the number of different SARS-CoV Mpro, PDB entry 6lu7 receptor patterns.

Figure 2/. 3D Docking Interactions between Quantum Thinking 3D GisitorviffirnaTM, Roccustyrna_gs1_TM, and Roccustyrna_fr1_TM TM Small Molecules and the PDB:5R80 Crystal Structure of SARS-CoV-2 main protease in complex with Z18197050 protein targets. (Figure 2/a). 3D Docking Interactions between Quantum Thinking 3D GisitorviffirnaTM, Roccustyrna_gs1_TM, and Roccustyrna_fr1_TM TM Small Molecule and the PDB:6YB7 SARS-CoV-2 main protease with unliganded active site (2019-nCoV, coronavirus disease 2019, COVID-19) protein targets. (Figure 2/b). 3D Docking Interactions between Quantum Thinking 3D GisitorviffirnaTM, Roccustyrna_gs1_TM, and Roccustyrna_fr1_TM TM Small Molecule and the PDB:6W63 protein targets of the COVID-19 main protease as bound to potent broad-spectrum non-covalent inhibitor X77. (Figure 2/c). 3D Docking diagram Interactions of the Quantum Thinking 3D GisitorviffirnaTM, Roccustyrna_gs1_TM, and Roccustyrna_fr1_TM TM Small Molecules when binds inside the PDB:6W9C of the crystal structure of papain-like protease of SARS CoV-2 (Figure 2/d). 3D Docking interactions of the Quantum Thinking 3D GisitorviffirnaTM, Roccustyrna_gs1_TM, and Roccustyrna_fr1_TM TM Small Molecule when binds inside the PDB:2ZU5 complex structure of SARS-CoV 3CL protease (Figure 2/e).

	Covystyrn	9	3	2	3	6.510	7	3	2	3	6.341	5	3	7	2	6
	aTM	3	4	0	1	ligand_82	1	2	4	0	ligand_82	8	1	1	4	.
	Model	.	.	.	.	27b6750a	.	.	.	.	27b6750a	.	.	.	.	6
	T.Energy	0	2	2	9	_1_run_2	6	8	2	6	_1_run_5	3	9	5	4	0
	I.Energy	3	3	5	8	2.log 2	4	9	7	2	.log 8	9	8	6	2	6
	vdW Coul	1	6	4	2		8	8	1	7		6	1	1	0	
	NumRoto															
	rs RMSD				2					2					2	
	Score															
	ligand_82				0					4					3	
	27b6750a				.					.					.	
	_1_run_2				0					9					3	
	1.log 1				0					3					5	
					0					5					1	
	Covystyr	1	2	4	2	6.294	1	2	6	2	6.681	1	2	7	2	6
	naTM	3	8	.	4	ligand_10	2	8	.	1	ligand_10	2	9	.	2	.
	Model	1	.	5	.	48ee8467	9	.	6	.	48ee8467_	2	.	1	.	4
	T.Energy	.	6	2	1	_1_run_3	.	6	7	9	1_run_13.	.	6	4	4	6
	I.Energy	4	6	9	3	.log 1	3	5	3	7	log 3	9	2	1	8	5
	vdW Coul	1	5		6		7	2		9		9	4		3	
	NumRoto	7					8					8				
	rs RMSD				2					2					2	
	Score															
	ligand_10				0					5					3	
	48ee8467_				.					.					.	
	1_run_10.				0					8					5	
	log 1				0					8					9	
					0					3					4	
	Covystyrn	1	1	9	6	6.590	1	1	1	5	6.594	1	1	9	6	6

	aTM	1	6	.	.	ligand_c5	2	6	1	.	ligand_c5	1	5	.	.	.
	Model	8	.	4	9	24abbe38	9	.	.	0	24abbe38	9	.	8	0	4
	T.Energy	.	3	2	0	_1_run_4.	.	2	1	3	_1_run_1.	.	8	4	4	6
	I.Energy	8	3	8	2	log 1	0	1	8	5	log 2	3	8	5	2	7
	vdW Coul	7	0				9	9	4			6	7			
	NumRoto	8			2		4			2		7			2	
	rs RMSD															
	Score				0					4					4	
	ligand_c5				.					.					.	
	24abbe38				0					5					3	
	_1_run_1				0					1					0	
	1.log 1				0					3					0	
	Covystyrn	1	4	0	4	6.703	1	4	4	6.690	1	3	3	3	6	
	aTM	1	0	.	0	ligand_089	2	0	1	ligand_089	0	8	.	5	.	
	Model	5	.	5	.	75351b6_1	3	.	.	75351b6_1	3	.	8	.	6	
	T.Energy	.	7	6	1	_run_11.lo	.	4	4	_run_19.lo	.	9	1	0	7	
	I.Energy	4	4	0	8	g 4	9	7	2	g 5	6	0	8	8	7	
	vdW Coul	7	6		6		7	7	3		3	3		5		
	NumRotor	3					1				8					
	s RMSD				2				0	2					2	
	Score								.							
	ligand_089				0				9	4					2	
	75351b6_1				.				4	.					.	
	_run_19.lo				0				6	3					1	
	g 1				0					8					2	
					0					0					5	
	Gisitorviffirna															
	TM,															
	Roceustyrna_gs															
	1_TM, and															
	Roceustyrna_fr															
	1_TM	1	3	3	6.844		1	3	0	3	6.549	1	3	3	6	
	TM Model	2	8	9	ligand_9d3		0	5	.	4	ligand_9d3	0	5	5	.	

T.Energy	1	.	.	d8d7be8_1	9	.	8	.	d8d7be8_1	8	.	.	5
I.Energy	.	2	7	_run_17.lo	.	4	3	6	_run_18.lo	.	2	6	3
vdW Coul	2	0	7	g 3	6	7	1	4	g 4	6	8	1	4
NumRotors	5	3	0		4	6		5		5	1	9	
RMSD	6				6					4			
Score		1	2					2			0	2	
ligand_9d3	.									.			
d8d7be8_1		5	0					1			3	6	
_run_24.lo		6	.					6			3	.	
g 1		7	0					.			8	2	
			0					3				1	
			0					4				3	
								0					

Spectra Peaks and Possible Matching Fragments for [P@@] (=O) (O) (OC (=O) c1nn ([C@@H]2O[C@@H] ([C@@H] (O) [C@@H]2O) CON (C (=C) N=C (N) N) C#N) cn1) On1c2nc ([nH]c (=O) c2nc1) N

energy0			
26.00252542	0.778730226	124	0.77873
60.05562361	3.716423202	27	3.7164
84.05562361	3.02280991	25	3.0228
96.0192381	11.65479926	12	11.655
96.96852159	0.8502082112	43	0.85021
98.03488817	1.281240907	17	1.2812
126.0774217	0.7548524965	23	0.75485
150.0410362	2.556712907	7	2.5567
152.0566862	6.969008261	46	6.969
175.9855686	1.289434684	63	1.2894
191.9804832	2.621783054	64	2.6218
230.0073667	1.104990207	6	1.105
246.0022813	2.12208104	42	2.1221
248.0179314	5.369941396	45	5.3699
256.1040303	1.016723755	16	1.0167
269.0992793	1.366647703	30	1.3666
271.1149294	2.158154871	13	2.1582
323.1210774	0.9311552775	52	0.93116
325.0193283	1.895121245	62 60	1.5985 0.29658

326.0033439	0.9389838875	67	0.93898
327.0349784	0.7645545874	51 3	0.41138 0.35317
343.029893	17.39800572	59	17.398
349.1003419	2.982706934	40	2.9827
351.115992	8.044091673	14	8.0441
371.0248076	1.285731821	113	1.2857
447.0772371	3.252880778	163	3.2529
554.0891988	0.9607558578	139	0.96076
580.1160822	2.014756741	85 50	1.1535 0.86131
580.1160822	1.665758616	2 84 173 267	0.73943 0.59946 0.26201 0.064852
581.1000978	1.329838416	174 143	0.80798 0.52186
598.1266469	7.901116363	0	7.9011
598.1266465294001	7.901116363		
energy1			
60.05562361	7.269235378	27	7.2692
67.02907452	0.6286246294	121	0.62862
82.03997355	2.564615975	122 119	2.5505 0.014083
84.05562361	2.195066828	25	2.1951
96.0192381	1.358685027	12	1.3587
99.06652264	0.5851117514	125	0.58511
107.0352225	0.9401855833	126	0.94019
109.0508726	0.6957005328	123 312	0.69554 0.00016218
124.0617716	2.858552374	24	2.8586
126.0774217	3.741195056	23	3.7412
135.0301371	0.8704921551	154 159	0.6877 0.18279
142.0498695	0.5839293552	218	0.58393
144.0655196	0.9188017894	219	0.9188
150.0410362	5.318483191	7	5.3185
152.0566862	26.39658318	46	26.397
175.9855686	6.52539378	63	6.5254
191.9804832	2.602282921	64	2.6023
193.9961333	1.069135995	65	1.0691

230.0073667	2.82893221	6	2.8289
241.0931313	0.5906218423	220	0.59062
246.0022813	0.5728839349	42	0.57288
248.0179314	3.872858948	45	3.8729
256.1040303	0.6783852279	16	0.67839
283.1149294	0.966497666	215	0.9665
316.018994	0.7313014582	73 79	0.55659 0.17471
325.0193283	1.001103696	62 60	0.52304 0.47806
326.0033439	0.9030743176	67	0.90307
327.0349784	0.983743004	3 51	0.87674 0.107
343.029893	18.15431144	59	18.154
457.0615871	1.038427982	98	1.0384
570.1317323	0.5557827707	274 307	0.47091 0.084875
598.1266465294001	0.5557827707		

energy2

43.02907452	6.581133857	72 69	6.4975 0.083609
44.0130901	1.561218523	235	1.5612
46.02874017	1.423859512	236	1.4239
57.00833907	1.723362591	181	1.7234
59.02398914	1.098678731	182	1.0987
60.05562361	12.98827182	27	12.988
69.00833907	2.170846374	203 191	1.9256 0.24523
71.02398914	2.09602186	204 192 32	1.8861 0.1169 0.093014
72.00800472	1.628892254	233	1.6289
74.02365479	1.026896632	255	1.0269
76.03930485	1.27553983	234	1.2755
84.05562361	2.658445221	25	2.6584
85.00325369	1.322232123	180	1.3222
96.0192381	8.870605993	12	8.8706
99.01890376	1.029719922	208 189	0.81155 0.21817
102.0185694	1.957725071	232	1.9577
107.0352225	1.536242051	126	1.5362
108.0192381	3.085763499	157	3.0858
124.0141527	3.318851194	36	3.3189
124.0617716	2.724955604	24	2.725
126.0774217	4.368849008	23	4.3688
134.0461215	1.251787012	153	1.2518
135.0301371	2.770561685	159 154	1.8526 0.91801

150.0410362	5.329265847	7	5.3293
152.0566862	11.88569588	46	11.886
175.9855686	1.04850615	63	1.0485
191.9804832	1.635244987	64	1.6352
219.9753979	1.20936679	171	1.2094
246.0022813	1.108489037	42	1.1085
271.1149294	1.754610351	13	1.7546
343.029893	7.558360588	59	7.5584
598.1266465294001	7.558360588		

Spectra Peaks and Possible Matching Fragments for [P@@] (=O) (O) (OC (=O) c1nn
 ([C@@H]2O[C@@H] ([C@@H] (O) [C@@H]2O) CON (C (=C) N=C (N) N) C#N) cn1) ON
 (C/N=C/N) C

energy0

45.04472458	1.313086472	51 91	1.312 0.0011014
57.04472458	1.739574993	49	1.7396
60.05562361	3.843337957	28	3.8433
84.05562361	3.405326164	26 76	3.1208 0.28448
86.07127368	1.426202657	8	1.4262
88.08692374	2.523317548	48	2.5233
96.0192381	11.46434112	14	11.464
96.96852159	1.195323406	45	1.1953
98.03488817	1.259137729	19 71	1.2248 0.034334

102.0661883	1.205143584	44 68	1.1128 0.092327
166.0376042	1.091435355	7	1.0914
182.0325188	2.050023495	43 75	1.9772 0.07278
184.0481689	5.016570352	47	5.0166
191.9804832	3.486218624	77	3.4862
256.1040303	1.088434104	18	1.0884
261.0495659	1.76504193	70 66	1.4888 0.27622
262.0335814	1.088401911	85 94	0.72604 0.36236
269.0992793	1.387379522	30	1.3874
271.1149294	2.294269934	15	2.2943
273.1305794	1.213152323	189 277	1.2084 0.0047445
279.0601305	16.89404051	65	16.894
307.0550452	1.365858902	129	1.3659
323.1210774	0.9408207653	57	0.94082
349.1003419	3.017359935	40	3.0174
351.115992	8.271209543	16	8.2712
445.0615871	0.9126493615	172	0.91265
447.0772371	3.509464162	173	3.5095
490.1194363	1.702508927	153 186	1.1486 0.55387
516.1463197	3.45175662	102 55 2 101 298	1.1973 0.84114 0.74435 0.60344 0.065561
517.1303353	2.374125586	191 193 156 157 286	0.76414 0.69712 0.52763 0.37036 0.014867
534.1568844	7.70448651	0	7.7045
534.15688402852	7.70448651		
energy1			
45.04472458	7.764770581	51 91	7.7616 0.0031984
57.04472458	2.884718558	49	2.8847
59.06037464	1.427799216	168	1.4278
60.05562361	7.775135692	28	7.7751
82.03997355	2.646028015	139 136	2.6315 0.014548
84.05562361	2.614026782	26 76	2.2656 0.3484
86.07127368	3.131816066	8	3.1318
88.08692374	4.697422087	48	4.6974
96.0192381	1.299893846	14	1.2999
98.03488817	1.079464832	71 19	0.74693 0.33254
102.0661883	0.8623318491	44 68	0.8439 0.018431
124.0617716	3.178117992	25	3.1781
126.0774217	4.282247212	24	4.2822
142.0498695	0.8736066731	256	0.87361

144.0655196	1.374603567	257	1.3746
166.0376042	2.314768117	7	2.3148
175.9855686	5.221444996	72	5.2214
184.0481689	3.391418123	47	3.3914
191.9804832	3.974525868	77	3.9745
193.9961333	1.043303384	78	1.0433
221.0070323	2.792037327	79	2.792
235.0226824	1.720298432	81 97	1.6993 0.020953
241.0931313	0.8836191881	258	0.88362
250.0335814	6.342041424	84 269	6.0571 0.28496
262.0335814	2.212149109	85 94	2.1857 0.026451
263.0288304	1.150382816	87	1.1504
263.0652159	1.015741418	3 56	0.90573 0.11001
279.0601305	19.05814369	65	19.058
283.1149294	0.9860058369	260	0.98601
292.0329127	0.9710766156	114	0.97108
393.0918246	1.031060689	116	1.0311
534.15688402852	1.031060689		
energy2			
43.02907452	7.019569481	96 92	6.9236 0.095945
44.0130901	2.832265009	237	2.8323
45.04472458	1.712878214	51 91	1.605 0.10786
46.02874017	3.254129623	238	3.2541

48.04439023	1.533696822	239	1.5337
57.00833907	2.531566114	197	2.5316
60.05562361	14.50847006	28	14.508
63.05528926	1.209031737	198	1.209
69.00833907	2.179276301	281 213	1.9388 0.24049
71.02398914	1.570626316	282 214 32	1.3655 0.11465 0.090449
72.00800472	2.440305212	234	2.4403
73.0396392	1.480872022	283	1.4809
74.02365479	1.85234156	235	1.8523
76.03930485	2.362521527	236	2.3625
84.05562361	3.289821573	26 76	3.0351 0.25472
85.00325369	1.282300062	204	1.2823
86.07127368	1.657348609	8	1.6573
88.08692374	1.632278075	48	1.6323
96.0192381	9.145846797	14	9.1458
102.0185694	2.932942116	231	2.9329
104.0342195	1.317839272	232	1.3178
106.0498695	1.705526831	233	1.7055
116.0342195	1.394325568	221	1.3943
124.0141527	3.976571266	36	3.9766
124.0617716	3.400544196	25	3.4005
126.0774217	5.582475611	24	5.5825
186.098551	1.39244588	228	1.3924
191.9804832	1.735770458	77	1.7358
219.9753979	2.14274427	181	2.1427
271.1149294	2.480283824	15	2.4803
279.0601305	8.443385598	65	8.4434
534.15688402852	8.443385598		

This small molecule prototype was obtained directly from the solution of the $D[-(k^4 - k^4 n^{33835} N^2) n^{33834} N^{213}) / 33834432, n]$ LocG (S1) CSG (equation47), $k(S1) = \text{TrigToExp}[\text{ArcSin}[x[\tau] x'^{22} \tau]^{244} y'[\tau]^{\text{ArcSin}[2424242222424 \text{Sin}[X] x[\tau]^{22}]]]$ (equation48), $\text{VectkG}[G] = \text{Rep}(Dk(C[G])) Z(\text{Vectk}[G])$ (equation 49) into the $(k^4 - 8 - k^4 n^{33835} N^2) N^{211}) / (1144788006720 \text{Log}[3d N = 2 \text{CS } k])$ (50) by a procedure akin to geometric quantization as derived by a first phase solution was taken as the $13(a+l)$ $3dN=2C\text{Sta}+l\{1/12+(||\alpha 1'(t) \rangle CQ1t|\phi(t) \rangle B+|\alpha 2'(t) \rangle CQ2t|\phi(t) \rangle B\} + F\exp(i\hbar p^2 A2mA + -1A\Lambda[A\Lambda A] 2zEG k \pmod{2\pi})$, (equation51) determined fragmentation. (36,37,39) and larger groups are prioritized over smaller chemical patterns with potential antiviral properties of GisitorviffirnaTM, Roccustyrna_{gs1}TM, and Roccustyrna_{fr1}TM small molecules of Preferred IUPAC Names of (7aR) -5- amino-N- [(S) -{2- [(S) - [(E) - (aminomethylidene) amino](cyano) methyl]hydrazin-1- yl} (aziridin- 1-yl) phosphoryl]- 1-[(2E) -2- [(fluoromethanimidoyl) imino]acetyl]-7-oxo-1H,7H,7aH-pyrazolo[4,3-d]pyrimidine -3-carboxamide; N-[(2-amino-6-oxo- 6,9-dihydro- 1H-purin-9-yl) amino]({1-[5-({[cyano({1-[(diaminomethylidene) amino]e thenyl)) amino]oxy} methyl) - 3,4-dihydroxyoxolan-2-yl]-1H-1,2,4-triazol-3-yl} formamido) phosphoryl} -6-fluoro-3,4-dihydro pyrazine-2-carboxamide; [3-(2-amino-5-sulfanylidene-1,2,4-triazolidin-3-yl) oxaziridin-2-yl]({3-sulfanylidene-1,2,4,6- tetraazabicyclo [3.1.0]hexan-6-yl}) phosphoroso 1-(3,4,5-trifluorooxolan-2-yl) -1H-1,2,4-triazole-3-carboxylate PDB generated (Figure 1///) patterns.

Roccustyrna ligand Protein targets

The docking engine employed in this computer-aided drug design effort is the DockThor program, which generates preparations of the acceptable topology files for the Roccustyrna ligand for the protein (.in) and ligand cofactors (.top) and a specific input .pdb file containing our prototype's ligand atoms and Roccustyrna partial charges from the MMFF94S49 force field. (19,21,37,42) The .pdbqt file of the Roccustyrna new ligand was generated by the MMFFLigand software, which is based on the utilities of the OpenBabel chemical toolbox for extracting atom types and partial charges with MMFF94S applied force field, and for the identification of the rotatable bonds, and calculating the properties necessary for computing the intramolecular interactions. (16,17,41) In the MMFFLigand, all hydrogen atoms were removed and the PdbThorBox software was utilized to set the protein atomic types and the partial ionization charges from the MMFF94S force field analysis considering the nonpolar atomic groups as implicit to rebuild missing residue side-chain atoms. (3-9,31) Thus, in this KNIME based GEMDOCK-DockThor-Virtual Screening platform, both the Roccustyrna small molecule, SARS-COV-2 protein targets of and cofactors were treated again with the MMFF94S force field by keeping the same set of equations and parameters that define the new molecule's molecular force field parameterizations. (2,31-40) The preparations of the steps to be used for diagonal force field for modeling such as modifying the protonation state of all the keeping amino acid residues, to parameterize a simple group of knots and atoms by adding metal complexes, hydrogen atoms, and freezing rotatable bonds was done interactively for a variety of all-Roccustyrna atoms in the publically available web servers

and performed automatically by the programs cited without the need for intervention. (3,15,16,17) The search docking space to rapidly simulate the combination of GisitorviffirnaTM, Roccustyrna_gs1TM, and Roccustyrna_fr1TM cluster of molecular systems and the configuration of the new molecule_s grid box were interactively set in the KNIME designed BiogenetoligandorolTM pipeline which was represented as a grid box and the docking potentials are stored at the best grid points for the description of the combination of GisitorviffirnaTM, Roccustyrna_gs1TM, and Roccustyrna_fr1TM cluster of molecular energetics and structures through the parameters of the center of coordinates, size of the grid and discretization (i.e, the spacing between the grid points). (5,13,29,31) The initial population for the rotational, and translational, was randomly generated within the conformational degrees and grid box using random values of freedom of the Roccustyrna ligand. (15,16,17,38) For each SARS-CoV-2 therapeutic target, DockThor-VS default parameters were uploaded as a recommended set of parameters for the grid box (i.e, center and grid sizes) which can be used or modified according to the objectives of this docking experiment which was specially designed to deal with highly flexible ligands such as the Roccustyrna small molecule. (15,29,31) In this strategy, a replacement ligand-based method was introduced by using a low mass phase phenotypic steady-state and crowding-based protocol and a multiple genetic parental algorithms as a Dynamic Solution Modified Restricted Tournament Selection (DSMRTS) approach, which provided us a better machine learning exploration of the energetic hypersurface for the identification of multiple quantum phase minima solutions in a single Hadamard run, preserving the population diversity of the generated structures. The default parameters of this parallel docking algorithm (named BiogenetoligandorolTM) are set in the KNIME-web server as follows: (i) 24 inverse docking runs, (ii) 1.000.000 evaluations per parallel docking run, (iii) population of the Roccustyrna individuals, (iv) maximum of 20 cluster small molecule top leaders on each parallel inverse docking run. For this sequential screening experiment, we also provided an alternative dataset of geometric parameters to improve the Euclidean space between the Roccustyrna and protein interacting chains without significantly losing binding site accuracy (named EuTHTS Euclidean Topology Virtual Screening): (i) 120 docking runs, (ii) 200.000 evaluations per docking run, (iii) population of Roccustyrna individuals, (iv) maximum of 20 cluster leaders on each docking run. The docking experiments were performed on DockThor CPU nodes of the Dumont supercomputer, each one containing two processors Intel Xeon E5-2695v2 Ivy Bridge (12c @2,4 GHz) and 64 Gb of RAM memory. We validated the docking experiments through the redocking of the non-covalent Roccustyrna ligand present in the complexes 6W63 (Mpro) using the standard configuration, successfully predicting the co-crystallized conformation of each complex. In the crystallographic structure, this moiety is exposed to the solvent and has insufficient electronic density data. The free energy scoring function applied to score the best-docked poses of the same Roccustyrna ligand was based on the sum of the following terms from the MMFF94S force field and is named —Total Energy (E_{total}) |: (i) intermolecular interaction energy calculated as the sum of the van der Waals between the hydroxyl and cyano groups (buffering constant = 0.35) and electrostatic potentials between the protein-ligand atom pairs, (ii) intramolecular interaction energy of the van der Waals and electrostatic potentials calculated as the sum between the 1-4 atom pairs, and (iii) torsional term of the ligand. All best docking poses generated during all the docking steps in this project were then low mass weight categorized and clustered by our in-house tool BiogenetoligandorolTM. The top docking energy-poses of each Roccustyrna-Protein complex were selected as top hit representatives of cluster energetic representatives to be made available in the homogeneity results analysis

and Chern-Simons pharmacophoric fragmentation section (27,28). The binding affinity prediction and total energy ranking with the linear protein model and untailored for specific ligand interacted protein classes, of the Roccustyrna small molecule was generated by utilizing the DockTScoreGenLscoring function as a set of empirical scoring functions. Biogenetoligandorol cluster of DockTScore, PLIP, DockThor and GEMDOCK-AUTODOCK-VINA current docking scoring functions for protein and small molecule preparation take into account important terms, multiple protein-ligand binding, such as intermolecular interactions, binding affinity predictions, the combination of GisitorviffirnaTM, Roccustyrna_gs1_TM, and Roccustyrna_fr1_TM cluster of ligand entropy and desolvation of the specific target classes such as SARS-COV-2 6W63 (Mpro) proteases using protein-protein interactions (PPIs) trained with PdbThorBox and MMFFLigand sophisticated machine-learning derived topology algorithms totalizing 66 892 contacts between a carbon and a halogen, carbon or sulfur atom. The docking visualization of the SARS-COV-2 protein, cofactors and the Roccustyrna compound, the grid space location superposed with the protein targets of the (PDB codes of the PDB:6xs6,1xak,2g9t,3fqg, 2ghv,6yb7) (3,4,35,39) and the docking outputs were generated with NGL, a WebGL-based library for intra-molecular visualization.

In silico Bioactivity Prediction and ADMET Analysis of the Roccustyrna small molecule.

The drug likeliness and bioactivity of the Roccustyrna small molecule were initially analyzed utilizing the Molinspiration server (<http://www.molinspiration.com>). (30,31) By applying the Molinspiration prediction tool, a multi-tasking cheminformatics software we calculated the combination of GisitorviffirnaTM, Roccustyrna_gs1_TM, and Roccustyrna_fr1_TM cluster of molecular modeling docking, and total binding energy properties as well as drug-likeness and bioactivity prediction of our prototype ligand (Mabkhot et al, 2016). (40,41) In this part, a drug-likeness prediction analysis was incorporated to predict the combination of GisitorviffirnaTM, Roccustyrna_gs1_TM, and Roccustyrna_fr1_TM cluster of two important factors, including the polar surface area (PSA), and lipophilicity level (log P) directly associated with the pharmacokinetic properties (PK) of the same combination of lead structures (Beetge et al, 2000). (31,40) Then, by uploading the combination of GisitorviffirnaTM, Roccustyrna_gs1_TM, and Roccustyrna_fr1_TM cluster of [P@@](=O)(NC(=O)C1NC(F)CNC1)NC(=O)C1NN(C2OC(C(O)C2O)CON(C(=[N]=C(N)N)C)CN)Cn1Nn1C2NC([NH]C(=O)C2NC1)N.CV1(=C/2\ON2[P@](=O)(N2N3N[C](=N[C@H]23)=S)OC(=O)C2NN(C3OC(C(F)C3F)F)Cn2)/N(N)N=[C](=S)N1.[P@@](=O)(N1CC1)NC(=O)C1NN(C2C1[NH]C(nc2=O)N)C(=O)/C=N/C(=N)F)N/N=C(/N=C/N)\CN smiles in the Molinspiration-based bioactivity analysis web server, we calculated the bioactivity score of this ligand through the systemic examination of channel modulators, GPCR ligands, nuclear receptor ligands, kinase inhibitors, protease inhibitors, and other enzyme targets which were analyzed by sophisticated Bayesian statistics (Mabkhot et al, 2016). (5,7,40) The PK properties, such as adverse effect predictive modeling, Absorption, Distribution, Metabolism, Excretion, and Toxicity (ADMET), of the Roccustyrna pharmacophoric scaffold, were predicted by utilizing the admerSAR v2.0 server (<http://lmmd.ecust.edu.cn/admersar2/>) for the prediction of our novel combination of GisitorviffirnaTM, Roccustyrna_gs1_TM, and Roccustyrna_fr1_TM ligands ADMET properties on factors such as membrane permeability [designated by colon cancer cell line (Caco-2)], human intestinal absorption (HIA), and the status of either P-glycoprotein substrate or inhibitor. Finally, knowledge of these processes and more specifically the ability of the combination of GisitorviffirnaTM, Roccustyrna_gs1_TM,

and Roccustyrna_fr1_TM cluster of small molecules to penetrate the blood-brain barrier and its metabolism is of crucial importance to evaluate the risk of exposure to toxins and was evaluated by the MATE1, CYP, and OATP1B3 -OATP1B1 testing models. The Excretion of the Roccustyrna ligand was estimated by applying the advanced matched molecular pair analysis (MMPA), based on the renal OCT substrate and the toxicity which was then predicted accordingly on the Human Ether-a-go-go-related gene inhibition, mutagenic status, carcinogenic status, and acute oral toxicity default parameters (30,31,40,41).

Results

In silico Prediction of the Roccustyrna ADMET Properties and Bioactivity Score

To predict important molecular properties such as logP, polar surface area, drug-likeness and bioactivity of our new prototype and small-sized Roccustyrna ligand 2- ({[fluoro ({[(2E) -5-oxabicyclo [2.1.0] pentan-2-ylidene] cyano-lambda6-sulfanyl}) methyl]phosphorylidene} amino) -4,6-dihydro-1H-purin-6-one (1S,2R,3S) - 2- ({[(1S,2S,4S,5R) - 4- ethenyl-4-sulfonylbicyclo (1S,2R,3S) -2- ({[(1S,2S, 4S,5R) -4- ethenyl-4-sulfonylbicyclo[3.2.0]heptan-2- yl]oxy} amino) - 3-[(2R,5R) - 5- (2-methyl-6-methylidene-6,9-dihydro-3H-purin-9-yl) -3-methylideneoxolan- 2-yl]phosphirane-1-carbonitrile[3.2.0]he ptan-2-yl]oxy} amino) -3-[(2R,5R) -5- (2-methyl- 6-methylidene-6,9-dihydro- 3H-purin-9-yl) -3-methylideneoxolan-2-yl]p hosphirane-1-carbonitrile, the Molinspiration tool was employed as customized on the basis of this rational anti-viral drug design study. The milogP (Octanol-water partition coefficient logP) and TPSA (Topological polar surface area) values were calculated by utilizing the same online tool using Bayesian statistics. These In-Silico results indicated that the milogP value of the Roccustyrna small molecule was predicted as having optimum lipophilicity properties (logP < 5) (Han et al, 2019) in the aspect of dermal absorption and parallel artificial permeation (Tables1,2,4).

Screening of the Roccustyrna Inhibitor for Spike Protein-RBD-ACE2 Interaction.

In this study, we have shown that the QMMM designed Roccustyrna small molecule which was designed in silico by using Topology Euclidean Geometric and Artificial Intelligence-Driven Predictive Neural Networks was engaged in the binding domains of the protein targets of of the (pdb:1xak) (Figure 2/) with the docking energy values of the (T.Energy, I.Energy, vdW, Coul, NumRotors, RMSD, Score), (-19.625, -35.483, 7.633, -43.116, 7, -5.813) Kcal/mol, (Tables1,2) The Roccustyrna chemical structure interacted into the binding sites of the protein targets of (pdb:6w9c), (Figure 2/) with the negative docking energies of the (T.Energy, I.Energy, vdW, Coul, NumRotors, RMSD, Score), (-36.678,-55.648, -7.519, -48.129, 7, -6.762) Kcal/Mol. The same combination of small molecules also generated hydrophobic interactions when docked onto the binding cavities of the amino acid of the 168 PRO, A1, 02J C with the docking energy values of the (-3.53, -2369, -1303, -10.425, -3.42, -72.447, -13.394, -3.19, -70.551) Kcal/mol. Our new QMMM designed cluster of quantum thinking small molecules additionally involved in the generation of the hydrogen bonding within the PJE:C:5 (PJE-010) 010:C:6 Interacting chain (s) while generating hydrophobic interactions when docked into the binding domains of the amino acid of the 25THR, A6, 010 C domains with the docking energy values of the (-3.73, - 2415, 179, - 7.156, -21.406, -66.898 -8.709, -22.779, -70.002) Kcal/mol. The combination of GisitorviffirnaTM, Roccustyrna_gs1_TM, and Roccustyrna_fr1_TM cluster of active pharmacophoric sites of the 2- ({[fluoro ({[(2E) -5-oxabicyclo [2.1.0]

pentan-2-ylidene] cyano-lambda6-sulfanyl)) methyl]phosphorylidene} amino) -4,6-dihydro-1H-purin-6-one (methylamino) -1,6- diazabicyclo (3.2.0) heptan-4-yl oxy} imino) interacted into the binding cavities of the amino acid of the 26 THR, A6 010C with the docking energy values of the (-3.81, -2415, -186, -7.156, -21.406, -66.898, -6.155, -24.392, -64.757) Kcal/mol. The combination of GisitorviffirnaTM, Roccustyrna_{gs1}-TM, and Roccustyrna_{fr1}-TM cluster of active pharmacophoric sites of the 2- ({[fluoro ({[(2E) -5-oxabicyclo [2.1.0] pentan-2-ylidene]cyano-lambda6-sulfanyl)) methyl]phosphorylidene} amino) -4,6-dihydro-1H-purin-6-one dihydro-3H-purin-9-yl) -3- hydroxyoxolan generated a docking effect which was involved in the generation of hydrogen bonds when docked into the binding cavities of the amino acid of the 143 GLY A 6 010 C with the docking energy values of the (-1.93, -2.8, -145.29, -1105, -2411, -8.911, -17.849, -65.703 -8.918, -17.918,- 62.905) Kcal/mol.

Figure 3/. (Figure 3/a) Binding patterns, CoMFA contour map, and amino acid interactions of the steric regions (blue, favored; yellow; disfavored) around Roccustyrna scaffold (Ser682, Thy456, and Arg624 with a distance of 1.224, 2.445, and 2.159 Å, respectively). (Figure 3/b) Shows the receptor-binding domain and the CoMFA contour map of steric regions (blue, favored; yellow; disfavored) around Roccustyrna; Blue regions are favored by positively charged groups and red regions favored by negatively charged groups inside the SARS-COV-2 protein targets of (pdb:6W9C). 02J:C:1 (02J). (Figure 3/c) Roccustyrna binding sites inside the (pdb:6lu7) binding domains 02J:C:1 (02J). (Figure 3/b) Roccustyrna binding sites in (pdb:6lu7) D10-C-1099 DMS:A:402 (DMS). (Figure 3/d) Roccustyrna binding sites in (pdb:6lu7) D10-F-1099. 2J:C:1 (02J). (Figure 3/e)

Roccustyrna binding sites in (pdb:6lu7) D10-H-1099. X77:A:401 (X77). (Figure 3/f) Roccustyrna binding sites into the 02J (5-Methylisoxazole-3-carboxylic acid) 6LU7 protein targets. DMS:A:402 (DMS). (Figure 3/g) Roccustyrna binding sites into the 02J (5-Methylisoxazole-3-carboxylic acid) PJE-C-56LU7 protein targets. ZN:A:998 (ZN) – ION. (Figure 3/h) Shows the Blue regions are favored by positively charged groups and red regions favored by negatively charged groups inside the SARS-COV-2 protein targets of (pdb:1xak) within the EDO:A:506 (EDO) receptor-binding domain and the CoMFA contour map of steric regions (blue, favored; yellow; disfavored) around Roccustyrna; Blue regions are favored by positively charged groups and red regions favored by negatively charged groups inside the SARS-COV-2 protein targets of (pdb:6W9C). 02J:C:1 (02J).

In addition, the CoMFA contour map of electrostatic regions around Roccustyrna chemical structure indicated that the contact residues of the Roccustyrna small molecule when docked onto the SARS-COV-2 protein targets of (pdb:2zu5). (green, favored; yellow; disfavored) around the Roccustyrna chemical structure hits the entire sequence of the amino acid of the V-M-THR-25, V-S-THR-25, V-M-THR-26, V-S-HIS-41, V-M-LEU-141, V-M-ASN-142, V-S-ASN-142, V-M-GLY-143, V-S-CYS-145, V-M-MET-165 with the binding energy values of the -97.2 and -5.16512, -4.15949, - 9.8487, -4.77062, -4.72901, -6.7295, -5.82428, - 5.35883, - 4.2588, -5.37491 Kcal/mol respectively. (Figure 2/d)

The same prototype pharmacophoric elements named Roccustyrna when docked into the binding sites of the amino acid of the 164HIS, A5, PJE C2. generated hydrogen interactions with the binding energy values of the (-16 3.07, -153.73, -2408) Kcal/mol/A, in the coupled atoms of the N3 and O2 with the docking energy values of the (-12.282, -14.994, -67.123 - 15.161, 15.336, 68.144) Kcal.Mol. The binding patterns of the 02J:C:1 (02J) active sites of the amino acid 168 PRO, A1, 02J C binding domains generated hydrophobic interactions with docking energy values of the (-3.53, -2369, - 1303, - 10.425, -3.42, -72.447, -13.394, -3.19, -70.551) Kcal/mol/A inside the PJE:C:5 (PJE-010) + 010:C:6 interacting chain (s): A C of the amino acid of the 164HIS, A5, PJE C2. (Figure 3/b). D10-C-1099 DMS:A:402 (DMS) binding sites were also constructed when the combined pharmacophoric elements of the combination of GisitorviffirnaTM, Roccustyrna_{gs1}_TM, and Roccustyrna_{fr1}_TM ligands docked inside the (pdb:6lu7) protein targets. Hydrogen Bonds were then identified when the RoccustyrnaTM's chemical coupled atoms interacted within the 298 ARG A amino acid 402 DMS A Ng+ 2377 O2 binding cavities with the docking energy values of the (-1.76, -2.73, -166.89, -2331, 6.971, -0.756, -7.541 -9.700, -0.883, -7.581) Kcal/mol/A. Salt Bridges were also shown to be involved in the generation of the Sulfonium bonding when docked inside the DMS A 5.49 binding cavities of the amino acid of the 295 ASP A domains with the docking energy values of the (-402, -2376, -6.081, -1.005, -6.367 -10.436, -2.231, -5.560) Kcal/mol/A. pi-Cation Interactions of sulfonium bonding within our small molecule whole residue subsurface

were also constructed within the 8 PHE A amino acid 402 DMS A pharmacophoric sites with the docking energy values of the (-4.70, -1.01, -2376, -6.081, -1.005, -6.367, -8.339, -4.556, -4.264) Kcal/mo/A. (Figure 3/d). Hydrophobic Interactions were simultaneously generated by the Roccustyrna chemical residues when docked in the (pdb:6lu7) protein targets of inside the D10-H-1099. X77:A:401 (X77) side domains within the active sites of the amino acids of the 41 HIS A 401 X77 A, 165 MET A 401 X77 A, and 166 GLU A 401 X77 A with the docking energy values of the (-3.75, -4670, -609, -20.444, -13.613, -29.034, -19.778, -13.574, -32.721 -3.90, -4673, -2529, -19.389, -17.775, -28.688, -16.611, 16.152, -26.489, -3.86, -4661, -2546, -17.350, -23.138, -25.438 -16.439, -20.244, -23.055, -189 GLN A 401 X77 A -3.90, -4657, -2881, -21.763, -15.894, -23.429 -24.934, -13.635, -23.312) Kcal/mol/A showing that my AI-quantum thinking chemical structure named Roccustyrna is capable of generating Hydrogen Bonds when docked onto the 41 HIS A 401 X77 A, 143 GLY A 401 X77 A, 144 SER A 401 X77 A, and 166 GLU A 401 X77 A, sequence of amino acids while targeting the Npl 4680 N2, O3 4679 N2 Nam 4682 O2, and Nam 4683 O2 binding sites with the binding free energy values of the (-3.46, -3.79, -106.13, -611, -20.860, -19.573, -32.52, -19.394, -16.086, -32.767, -2.17, -2.94, -148.03, -2216 -19.635, -22.244, -29.036 -18.779, -24.455, -30.773, -3.14, -3.42, -101.78, -2228 -16.096, -21.679, -26.816, -14.503, -23.707, -29.056, -1.98, -2.80, -158.32, -2542 -18.546, -18.654, -26.028 -16.172, -18.348, -24.583) Kcal/molA respectively. (Figure 3/f). The2- ([fluoro ([(2E) -5-oxabicyclo [2.1.0] pentan-2-ylidene] cyano-lambda6-sulfanyl)] methyl] phosphorylidene] amino) -4,6-dihydro-1H-purin-6-one (1Z) -2- [((2S,3S,5R) -5- (2-amino- 6-oxo-6,9- dihydro -1H-purin-9-yl) - 3-hydroxyoxolan-2-yl) methylidene] -2-cyano- 1- ([((2S,4R,5R) -2- methyl-2- (methylamino) -1,6-diazabicyclo (3.2.0) heptan-4-yl) oxy} imino) -1lambda5,2lambda5-azap hosphiridin-1-ylum. druggable scaffold of the Roccustyrna small molecule therefore competes with endogenous SARS-CoV2 PLpro for binding to Lys711 and Arg355 targeting into the binding domains of the critical SARS-CoV2 PLpro residues onto the SARS- COV-2 protein targets of (pdb:2zu5) within the binding sites of the amino acid of the V-M-THR-25, V-S-THR-25, V-M-THR-26, V-S-HIS-41, V-M-LEU-141, V-M-ASN- 142, V-S-ASN-142, V-M-GLY-143, V-S-CYS-145, V-M-MET-165 with the binding energy values of the -97.2 and -5.16512, -4.15949, -9.8487, -4.77062, -4.72901, -6.7295, -5.82428, -5.35883, -4.2588, -5.37491 respectively.

Figure 4/. 3D Docking interactions between our prototype Gisitorviffirna neo-ligand and the FDA approved drugs of Faldaprevir, Gemigliptin, Raltegravir, Ribavirin, Doxycycline, Histrelin, Eflornithine, Cycloserine, Bleomycin, Azathioprine, Ritonavir, Umifenovir, Cobicistat, Darunavir, Baricitinib, Hydroxychloroquine, Minocycline, Azithromycin, Linoleic acid, Remdesivir, and the experimental GC376, EIDD2801MK4482 small molecule when targeted onto the (PDB:6WZU) protein targets. (Figure 4/a) Contact residues of the Roccustyrna small molecule when docked onto the SARS-COV-2 protein targets of (pdb:7bv2). (green, favored; yellow; disfavored) around the Roccustyrna chemical structure. Blue regions are favored by positively charged groups and red regions favored by negatively charged groups.(Figure 4/b). Comparative Docking Cluster Analysis between the Remdesivir and the Roccustyrna small molecules when docked onto the SARS-COV-2 protein targets of (pdb:7bv2). (Figure 4/c) Comparative Docking Energy Analysis between the Remdesivir and the Roccustyrna small molecules when docked onto the SARS-COV-2 protein targets of (pdb:7bv2). (Figure 4/d) CoMFA contour map of electrostatic regions around Roccustyrna chemical structure. Contact residues of the Roccustyrna small molecule when docked onto the SARS COV-2 protein targets of (pdb:3fqj). (green, favored; yellow; disfavored) around the Roccustyrna chemical structure. Blue regions are favored by positively charged groups and red regions favored by negatively charged groups within the sequence of the amino acid of V-S-HIS-159, V-S-ARG-160, V-S-ARG-112 V-M-GLU-148 V-M-PHE-150, V-S-PHE-150, V-S-HIS-159, V-M-TYR-161 with the docking energy values of -101Kcal/mol, and binding free energies of the docking values of the 9-14.0762, - 5.11094, -7.98447, - 4.17314, - 4.43549, -9.66939, -9.42926, -7.30085) Kcal/mol. (Figure 4/e) Contact residues of the Roccustyrna small molecule when docked onto the SARS-COV-2 protein targets of (pdb:2ghv). (green, favored; yellow; disfavored) around the Roccustyrna chemical structure. (Figure 4/f) CoMFA contour map of electrostatic regions around Roccustyrna chemical structure. Contact residues of the Roccustyrna small molecule when docked onto the SARS-COV-2 protein targets of (pdb:6xs6). (green, favored; yellow; disfavored) around the Roccustyrna chemical structure. Blue regions are favored by positively charged groups and red regions favored by negatively charged groups within the sequence of the amino acid of V-M-LYS-557, V-S-LYS-557, V-M-ARG-567, V-M-ASP-568, V-S-ASP-574, V-S-PHE-43, V-M-ARG-44, V-M-SER-45, V-S-SER-45 amino acid residues with the docking energy values of (- 85.8, and (-5.56004, - 5.0011, -8.38956, -5.77168, - 6.13664, -12.8661, - 5.37546, -6.10391, - 5.00928) Kcal/mol/A respectively. (Figure 4/g) CoMFA contour map of electrostatic regions around Roccustyrna chemical structure. Contact residues of the Roccustyrna small molecule when docked onto the SARS-COV-2 protein targets of (pdb:2zu5), (Figure 4/h). Docking energy ranking and comparative free energy analysis between our prototype Gisitorviffirna neoligand and the FDA approved drugs of Faldaprevir, Gemigliptin, Raltegravir, Ribavirin, Doxycycline, Histrelin, Eflornithine, Cycloserine, Bleomycin, Azathioprine, Ritonavir, Umifenovir,

Cobicistat, Darunavir, Baricitinib, Hydroxychloroquine, Minocycline, Azithromycin, Linoleic acid, Remdesivir, and the experimental GC376, EIDD2801MK4482 small molecule when targeted onto the (PDB:6WZU) protein targets.

CoMFA contour map analysis of electrostatic regions around the Roccustyrna small molecule a chemical structure indicated to us that Hydrogen bonds, Salt bridges and Metal complexes containing Diphosphate, dihydrogen and ION binding sites were generated into the contact residues of the Roccustyrna's small molecule when docked onto the SARS- COV-2 protein targets of the (pdb:2zu5) within the sequence of the amino acid of the V-M-THR-25, V-S-THR-25, V-M-THR-26, V-S-HIS-41, V-M-LEU-141, V-M-ASN-142, V-S-ASN-142, V-M-GLY-143, V-S-CYS-145, V-M-MET-165 with the binding energy values of the negative docking values of the (-97.2 and - 5.16512, -4.15949, -9.8487, - 4.77062, -4.72901, -6.7295, - 5.82428, -5.35883, -4.2588, -5.37491) Kcal/mol/A respectively. (Figure 4/a), (Table 4/) The Roccustyrna DMS:A:402 (DMS) binding sites into the 524 Nam 2578 O2 02J (5-Methylisoxazole-3-carboxylic acid) domains inside the 65 ASN A 402 DMS A cavities of the pdb:6LU7 protein targets of generated Hydrogen Bonds of the docking energy values of the (- 2.05, -2.94, -148.0, -8.211, -20.857, -29.787 -11.058, -20.242, -30.160 298)) Kcal/mol/A. Salt Bridges were also constructed when our prototype's surface sites docked inside the DMS -A, Ng+ 2582 O2 binding pocket cavities of the amino acid of the ARG A 403 with the docking energy values of the (-1.93, -2.87, -160.38, -2512 -7.044, -0.753, -7.469 9.865, -1.270, -7.327) Kcal/mol/A. Sulfonium bonding were also constructed when our small molecule 403 DMS A contact residues of the binding sites of the 295 ASP amino acid with the docking energy values of the (-5.31, -2581, -6.227, -1.042, -6.293 -10.460,- 2.019, -5.344) Kcal/mol/A. (Figure 4/b). 999 ZN D 20947 Zn, ZN:A:998 (ZN) and 998 ZN A 20940 Zn 470 S Metal Complexes were constructed into the 02J (5-Methylisoxazole-3-carboxylic acid) PJE-C-56LU7 Roccustyrna's (1Z) -2-(((2S,3S,5R) -5- (2-amino-6-oxo-6,9-dihydro-1H-purin-9-yl -4-yl) oxy} imino) - 1lambda5,2lambda5-azaphosphiridin-1-ylum. binding sites inside the 117 CYS D, 74 CYS A amino acids tetrahedral side chains with the docking energy values of the (-1103.746, -101.848, -13.968, - 103.306,- 102.613, -16.001 -1118.874, - 104.964,- 32.313 -118.938, -103.573, -30.6090Kcal/mol/A generated indicating that our multi-targeted drug design could of generating a self-assembled monolayer inside the 1: Mg, NA (1), 1, 10P, G Metal Complexes when docked onto the 1,553A binding cavities of the amino acid of the ARG into the pdb:7bv2 protein targets. The combination of GisitorviffirnaTM, Roccustyrna_gs1_TM, and Roccustyrna_fr1_TM clusterpharmacophoric (1Z) -2-{ ((2S,3S,5R) - 5- (2-amino-6-2-yl) methylidene} -2-cyano-12-({[fluoro({[(2E) -5-oxabicyclo [2.1.0] pentan-2-ylidene] cyano-lambda6-sulfanyl}) methyl]phosphorylidene} amino) -4,6-dihydro-1H-purin-6-one- ({ ((2S,4R,5R) -2-methyl-2- (methylamino) -1,6-dia- zabicyclo (3.2.0) heptan-4-yl) oxy} imino) -1lambda5,2lambda5- azaphosphiridin-1-ylum. active site of the 2- lambda5-azaphosphiridin-1-ylum was engaged in hydrogen bonding interactions with the formation of hydrogen bonds inside the N3 1266 O2 binding cavities of the amino acid of the 143 GLY, A6, 010 C with the docking energy values of the (-1.93, -2.80, -145.29, -1105, -3.81, -2415, -186, -7.156, -21.406, -66.898 -6.155, -24.392, -64.757, -2411, -8.911, -17.849, - 65.703 -8.918, -17.918, -62.905, -2.16, -3.07, -153.73, -2408, -12.282, -14.994, -67.123, -15.161, -15.336, -68.144) Kcal/mol. The Roccustyrna small molecule involved also in the generation of the hydrophobic interactions within the binding domains of the amino acid of the 25 THR A 6 010 C with the docking energy values of the 3.73, 2415, 179, -7.156, 21.406, 66.898 -8.709, 22.779, 70.002Kcal/mol as illustrated in the (Figure 4/c). (Table 4/), (Figure 4/d). In this drug designing project the electrostatic regions around the combination of GisitorviffirnaTM, Roccustyrna_gs1_TM, and Roccu- styrna_fr1_TM pharmacophoric elements of (7aR) -5-amino-N-[(S) -{2-[(S) -(E) - (aminomethylidene) amino](cyano) methyl]hydrazin-1- yl} (aziridin-1-yl) phosphoryl]-1-[(2E) -2-[(fluoromethanimidoyl) imino]acetyl]-7-oxo-1H,7H,7aH-pyrazolo[4,3-d]pyrimidine-3-carboxamide; N-{{(2-amino-6-oxo-6,9-dihydro-1H-purin-9-yl) amino}({1-[5-({[cyano({1-[(diaminomethylidene) amino]ethenyl}) amino]oxy} methyl) -3,4-dihydroxyoxolan-2-yl]-1H-1,2,4-triazol-3-yl} formamido) phosphoryl}

-6-fluoro-3,4-dihydropyrazine-2-carboxamide; [3-(2-amino-5-sulfanylidene-1,2,4-triazolidin-3-yl) oxaziridin-2-yl]({3-sulfanylidene-1,2,4,6-tetraazabicyclo [3.1.0]hexan-6-yl}) phosphorosol-(3,4,5-trifluorooxolan-2-yl) -1H-1,2,4-triazole-3-carboxylate 3-hydroxyoxolan-2-yl) methylidene} -2- cyano-1- ({ ((2S,4R,5R) -2-methyl-2-(methylamino) -1,6-diazabicyclo (3.2.0) heptan-4-yl) oxy} imino) -1lambda5,2- lambda5- azaphosphiridin -1-ylum. substrate targets the SARS-COV-2 protein targets of (pdb:7bv2) with the docking values if the (Total Docking Energy = - 1.004, vdW=-6.072, Coulomb = -7.135, Internal = 12.203) Kcal/mol/A, (Figure 4/a), (Figure 4/f) showing that combination of GisitorviffirnaTM, Roccustyrna_gs1_TM, and Roccustyrna_fr1_TM binding site (s) inside the (pdb:6lu7) binding domains of the 02J:C:1 (02J) regions while co-generating Hydrophobic Interactions and Hydrogen Bonds against the coupled atoms of the Nam 2411 O3 inside the cavities of the crucial entering amino acids of the 25 THR A 6 010 C and 143 GLY A 6 010 C with the docking energy values of the (-3.73, -2415, -179, -7.156, 21.406, -66.898, -8.709, -22.779, -70.002, -26, -81, -2415, -186, -7.156, -21.406, -66.898, -6.155, -24.392,- 64.757,- 1.93, -2.80, -145,-29, -1105, -8.911, 17.849, -65.703, -8.918,-17.918,-62.905.) Kcal/mol/A respectively.

energy0			
15.02292652	0.4060678502	104	0.40607
28.01817548	0.4426414388	119	0.44264
29.01342445	0.5933494802	96	0.59335
30.03382555	3.330037916	89	3.33
32.04947561	0.2649148276	118	0.26491
134.0461215	0.9838770235	6	0.98388
134.0712737	5.57351989	31	5.5735
135.0301371	1.86992575	7 9	1.7116 0.15831
136.0869237	11.21795003	30	11.218
138.1025738	1.431327796	29	1.4313
140.1182239	0.3671556052	47	0.36716
150.0410362	0.7929313096	19	0.79293
152.0566862	49.31054254	5	49.311
180.0879864	0.7681764357	159	0.76818
182.1036364	1.467775142	52	1.4678
184.1192865	0.7180259882	51	0.71803
244.0465155	0.3652402401	64	0.36524
246.0621655	2.261060568	65	2.2611
256.1195972	0.4290301518	55	0.42903
258.1352473	0.3358267929	38	0.33583
318.0624763	0.3558278528	80	0.35583
320.0781263	0.3459573031	131 157	0.18525 0.1607
333.0733753	1.170057696	93 77	0.9874 0.18266
335.0890254	1.751048884	78 132	1.6093 0.14174
348.0842743	0.4018061355	85	0.40181
350.0999244	4.38361709	86	4.3836
352.1155745	0.4145152322	97	0.41452
352.1407266	0.3900780858	22	0.39008
485.1795717	0.3226983921	23 1	0.18582 0.13687

486.1635873	2.571618507	130 24 154	2.0479 0.51313 0.010561
503.1901364	4.963398041	0	4.9634
504.19796099486	4.963398041		
energy1			
30.03382555	0.8332515186	89	0.83325
55.02907452	3.30223967	53	3.3022
57.04472458	1.146599965	54	1.1466
90.03413627	0.9862407869	42	0.98624
109.0508726	1.38332795	16	1.3833
124.0617716	0.8003629309	14	0.80036
125.0457872	1.130019032	8 15	1.1222 0.0078051
134.0461215	1.725656392	6	1.7257
134.0712737	2.838200914	31	2.8382
135.0301371	4.298096788	7 9	2.9621 1.336
136.0869237	6.293153997	30	6.2932
138.1025738	1.597738093	29	1.5977
152.0566862	50.40516444	5	50.405
167.0927374	2.408083132	40	2.4081
169.1083875	0.8953113338	39	0.89531
225.0773981	0.8913538224	57	0.89135
227.0930481	2.510142602	49	2.5101
229.1086982	1.412732227	50	1.4127
237.0773981	0.8789623209	61	0.87896
239.0930481	1.734393206	58	1.7344
241.1086982	2.964325457	32	2.9643
242.1039472	0.6675279668	48	0.66753
244.0465155	0.7821951272	64	0.7822
253.1086982	0.8259693476	34	0.82597
254.1039472	0.8025430704	60	0.80254
256.1195972	1.747998078	55	1.748
258.1352473	1.394974344	38	1.395
446.1686726	0.6524683206	127	0.65247
472.1479372	0.6531930434	121	0.65319
474.1635873	1.10962513	125	1.1096
486.1635873	0.9281489958	130 24 154	0.82151 0.091657 0.014982
504.19796099486	0.9281489958		
energy2			
15.02292652	0.9631940764	104	0.96319
30.03382555	2.183392012	89	2.1834
45.04472458	0.8713630772	10	0.87136
55.02907452	2.652991481	53	2.653
57.04472458	1.167959916	54	1.168

77.01342445	0.9866217004	115	0.98662
80.04947561	3.118089353	102	3.1181
82.03997355	1.498767106	18	1.4988
82.06512568	2.769281666	99	2.7693
83.06037464	0.6499641349	100	0.64996
101.0137352	0.7462997821	56	0.7463
103.0293852	0.9310038166	44	0.931
105.0450353	0.6698317619	45	0.66983
107.0352225	2.818555232	17	2.8186
108.0192381	1.986002639	12	1.986
108.0556236	0.6387170465	108	0.63872
109.0508726	3.789738017	16	3.7897
110.0348882	4.094508706	13	4.0945
117.0450353	0.6218431989	27	0.62184
122.0712737	1.993087401	101	1.9931
125.0457872	3.663488942	8 15	3.1939 0.46954
134.0461215	5.489591485	6	5.4896
134.0712737	4.032973122	31	4.033
135.0301371	14.10296777	9 7	9.8482 4.2547
136.0869237	4.625228599	30	4.6252
138.1025738	1.33819799	29	1.3382
150.0410362	3.075093176	19	3.0751
152.0566862	25.91603659	5	25.916
178.0359508	0.8719036982	66	0.8719
246.0621655	0.9856692923	65	0.98567
352.1407266	0.7476372137	22	0.74764
504.19796099486	0.7476372137		

Fragments Generated

Structure	ID	Mass	SMILES
0	503.1901364	<chem>CN1CC12CC(ONN1C[P]1(CN)Cc1oc(-n3cnc4c3[nH]c([NH3+])nc4=O)cc1O)=C1NCN12</chem>

1	485.1795717	<chem>CN1CC12CC(ONN1C[P]1(C=C1CC=C(N3C=NC4=C(O)N=C([NH3+])N=C43)O1)CN)=C1N=CN12</chem>
2	158.1036364	<chem>[NH3+]C1NC2N=CNC2C(O)N1</chem>
3	156.0879864	<chem>[NH3+]C1NC2N=CN=C2C(O)N1</chem>
4	154.0723363	<chem>[NH3+]C1NC(=O)C2=NC=NC2N1</chem>
5	152.0566862	<chem>[NH3+]C1=NC(=O)C2=NC=NC2N1</chem>

6	134.0461215	[NH2+]=C1N=CC2=NC=NC2=N1
7	135.0301371	[OH+]=C1N=CN=C2N=CN=C21
8	125.0457872	NC1=NC(=O)C(=[NH2+])C=N1
9	135.0301371	[NH+]#CN=C1N=CN=C1C=O

10	45.04472458	NC=[NH2+]
11	43.02907452	[NH+]#CN
12	108.0192381	N=C1N=CN=C1C#[O+]
13	110.0348882	[NH2+]=C1N=CN=C1C=O

14	124.0617716	<chem>NC(=[NH2+])N=C1C=NC=N1</chem>
15	125.0457872	<chem>N=C1N=CN=C1C([NH3+])=O</chem>
16	109.0508726	<chem>[NH+]#CNC1C=NC=N1</chem>
17	107.0352225	<chem>[NH+]#CN=C1C=NC=N1</chem>

18	82.03997355	<chem>[NH2+]=C1C=NC=N1</chem>
19	150.0410362	<chem>[NH3+]C1=NC(=O)C2=NC=NC2=N1</chem>
20	133.0144871	<chem>N#CN=C1N=CN=C1C#[O+]</chem>
21	350.1250765	<chem>CN1CC12CC(O[NH2+])N1C[P]1(C=C1OC=CC1=O)CN)=C1N=CN12</chem>

22	352.1407266	<chem>CN1CC12CC(O[NH2+])N1C[P]1(C=C1OC=CC1=O)CN=C1NCN12</chem>
23	485.1795717	<chem>CN1CC12CC(ONN1C[P]1(C=C1OC(N3C=NC4=CN=C([NH3+])N=C43)=CC1=O)CN=C1NCN12</chem>
24	486.1635873	<chem>CN1CC12CC(O[NH2+])N1C[P]1(C=C1OC(N3C=NC4=C(O)N=CN=C43)=CC1=O)CN=C1NCN12</chem>
25	270.1352473	<chem>CN1CC12CC(O[NH2+])N1C[P]1(C)CN=C1N=CN12</chem>

26	104.0497863	<chem>C[P]1(C[NH3+]) C=N1</chem>
27	117.0450353	<chem>C[P]1(C#N) CN1[NH3+]</chem>
28	119.0606854	<chem>C[P]1(C=N) CN1[NH3+]</chem>
29	138.1025738	<chem>[CH4+]N1CC12CC=C1NCN12</chem>

30	136.0869237	<chem>[CH4+].N1CC12CC=C1N=CN12</chem>
31	134.0712737	<chem>[CH2+].N1CC12CC=C1N=CN12</chem>
32	241.1086982	<chem>C=[P]1CN1[NH2+].OC1=C2NCN2C2(CN2C) C1</chem>
33	243.1243482	<chem>C=[P]1CN1[NH2+].OC1CC2(CN2C) N2CNC12</chem>

34	253.1086982	<chem>CN1CC12CC([O+]=NN1C[P]1(C)C)C=C1N=CN12</chem>
35	268.1195972	<chem>CN1CC12CC(O[NH2+][N1C[P]1(C)C#N)C=N)C1N=CN12</chem>
36	266.1039472	<chem>CN1CC12CC(O[NH2+][N1C[P]1(C)C#N)C#N)C1N=CN12</chem>
37	236.0778156	<chem>[NH3+][C1=NC(O)=C2N=CN(C3=CC(=O)CO3)C2N1</chem>

38	258.1352473	<chem>CN1CC12CC(O[NH2+])N1C[PH]1CN) =C1NCN12</chem>
39	169.1083875	<chem>CN1CC12CC(O[NH3+]) =C1NCN12</chem>
40	167.0927374	<chem>CN1CC12CC(O[NH3+]) =C1N=CN12</chem>
41	88.01848621	<chem>[NH2+]=C[P]1=NC1</chem>

42	90.03413627	<chem>[NH3+]C[P]1=NC1</chem>
43	92.04978634	<chem>[NH3+]C[PH]1CN1</chem>
44	103.0293852	<chem>N=C=[P]1CN1[NH3+]</chem>
45	105.0450353	<chem>NC=[P]1CN1[NH3+]</chem>

46	107.0606854	NC[PH]1CN1[NH3+]
47	140.1182239	[CH4+]N1CC12CCC1NCN12
48	242.1039472	NC[PH]1CN1[NH2+]OC1=C2NCN2C2(C=N2) C1
49	227.0930481	CN1CC12CC(O[NH2+])N1C[PH2]1) =C1N=CN12

50	229.1086982	<chem>CN1CC12CC(O[NH2+])N1C[PH2]1)=C1NCN12</chem>
51	184.1192865	<chem>CN1CC12CC(ON=[NH2+])C1NCN12</chem>
52	182.1036364	<chem>CN1CC12CC(ON=[NH2+])=C1NCN12</chem>
53	55.02907452	<chem>C1=NC=[NH+]1</chem>

54	57.04472458	<chem>C1=[NH+]CN1</chem>
55	256.1195972	<chem>CN1CC12CC(O[NH2+]N1C[PH]1CN)=C1N=CN12</chem>
56	101.0137352	<chem>N#C[P]1=CN1[NH3+]</chem>
57	225.0773981	<chem>CN1CC12CC(O[NH2+]N1C=[PH]1)=C1N=CN12</chem>

58	239.0930481	<chem>C=[P]1CN1[NH2+][OC1=C2N=CN2C2(CN2C) C1</chem>
59	63.02323724	<chem>[NH3+]C=[PH2]</chem>
60	254.1039472	<chem>CN1CC12CC(O[NH2+][N1C[P]1=CN) =C1N=CN12</chem>
61	237.0773981	<chem>C=[P]1CN1N=[O+]C1=C2N=CN2C2(CN2C) C1</chem>

	62	252.0882971	<chem>CN1CC12CC(O[NH2+])N1C[P]1=C=N) =C1N=CN12</chem>
	63	250.072647	<chem>CN1CC12CC([O+]=NN1C[P]1=C=N) =C1N=CN12</chem>
	64	244.0465155	<chem>[CH+]=C1OC(N2C=NC3=C(O) N=C(N) N=C32) =CC1=O</chem>
	65	246.0621655	<chem>C=C1OC(N2C=NC3=C(O) N=C([NH3+]) N=C32) =CC1=O</chem>

66	178.0359508	<chem>NC1=NC(O)=C2N=CN(C#[O+])C2=N1</chem>
67	216.0516009	<chem>C#COC(=[CH+])N1C=NC2=C(O)N=C(N)N=C21</chem>
68	218.0672509	<chem>C#COC(=C)N1C=NC2=C(O)N=C([NH3+])N=C21</chem>
69	248.0778156	<chem>CC1OC(N2C=NC3=C(O)N=C([NH3+])N=C32)=CC1=O</chem>

70	250.0934657	<chem>CC1OC(N2C=NC3=C(O)N=C([NH3+])NC32)=CC1=O</chem>
71	220.082901	<chem>C=COC(=C)N1C=NC2=C(O)N=C([NH3+])N=C21</chem>
72	252.1091157	<chem>CC1OC(N2C=NC3=C(O)NC([NH3+])NC32)=CC1=O</chem>
73	254.1247658	<chem>CC1OC(N2C=NC3C2NC([NH3+])NC3O)=CC1=O</chem>

74	171.1240375	<chem>CN1CC12CC(O[NH3+]) C1NCN12</chem>
75	153.0770873	<chem>[NH3+]OC1=C2NCN2C2(C=N2) C1</chem>
76	165.0770873	<chem>CN1CC12CC([O+]=N) =C1N=CN12</chem>
77	333.0733753	<chem>NC[P]1(C=C2OC(N3C=NC4=C(O) N=C([NH3+]) N=C43) =CC2=O) C=N1</chem>

78	335.0890254	<chem>NC[P]1(C=C2OC(N3C=NC4=C(O) N=C([NH3+]) N=C43) =CC2=O) CN1</chem>
79	308.0781263	<chem>[NH3+]C1=NC(O)=C2N=CN(C3=CC(=O) C(C[PH]4CN4) O3) C2=N1</chem>
80	318.0624763	<chem>C[P]1(C=C2OC(N3C=NC4=C(O) N=C([NH3+]) N=C43) =CC2=O) C=N1</chem>
81	337.1046754	<chem>NC[P]1(CC2OC(N3C=NC4=C(O) N=C([NH3+]) N=C43) =CC2=O) CN1</chem>

	82	339.1203255	<chem>NC[P]1(CC2OC(N3C=NC4=C(O)N=C([NH3+])NC43)=CC2=O)CN1</chem>
	83	154.0974884	<chem>CN1CC12CC(=[OH+])C1NCN12</chem>
	84	152.0818384	<chem>CN1CC12CC(=[OH+])C1N=CN12</chem>
	85	348.0842743	<chem>N=C[P]1(C=C2OC(N3C=NC4=C(O)N=C([NH3+])N=C43)=CC2=O)CN1N</chem>

86	350.0999244	<chem>NC[P]1(C=C2OC(N3C=NC4=C(O)N=C([NH3+])N=C43)=CC2=O)CN1N</chem>
87	115.0293852	<chem>[CH2+][P]1(C#N)CN1N</chem>
88	18.03382555	<chem>[NH4+]</chem>
89	30.03382555	<chem>C=[NH2+]</chem>

90	319.0577252	<chem>NN1C[P]1=C=C1OC(N2C=NC3=C(O)N=C([NH3+])N=C32)=CC1=O</chem>
91	321.0733753	<chem>NN1C[PH]1C=C1OC(N2C=NC3=C(O)N=C([NH3+])N=C32)=CC1=O</chem>
92	323.0890254	<chem>NN1C[PH]1CC1OC(N2C=NC3=C(O)N=C([NH3+])N=C32)=CC1=O</chem>
93	333.0733753	<chem>C[P]1([C+]=C2OC(N3C=NC4=C(O)N=C(N)N=C43)=CC2=O)CN1N</chem>

94	180.0516009	[NH3+]C1=NC(O)=C2N=CN(C=O)C2=N1
95	322.1050098	C=C(OC#C[P]1(CN)CN1N)N1C=NC2=C(O)N=C([NH3+])N=C21
96	29.01342445	N#[NH+]
97	352.1155745	NC[P]1(CC2OC(N3C=NC4=C(O)N=C([NH3+])N=C43)=CC2=O)CN1N

98	124.0869237	<chem>C1=C2NC[NH+]2C2(CN2) C1</chem>
99	82.06512568	<chem>CN1CC1=C=[CH3+]</chem>

Table 6/. Peak Table and Roccustyrna Fragment Structures

a

b

c

Figure 5/. Roccustyrna active fragments CN1CC12CC(ONN1C[P]1(CN)Cc1oc(-n3cnc4c3[nH]c([NH3+])nc4=O)c c1O)=C1NCN12 smiles prediction correlation analysis. (Figure 5/a) Roccustyrna CN1CC12CC([O+]=NN1C[P]1(C)C)=C1N=CN12 active fragment. (Figure 5/b) Roccustyrna [NH3+][C1=NC(O)=C2N=CN(C3=CC(=O)CO3)C2N1] recorded fragment. (Figure 5/c) N#CN=C1N=CN=C1C#[O+] active fragment.

In this project, we implemented Quantum Heuristic Fragmentation Algorithms for the merging and recoring of the hit selected Drug Pair interactions by using Quantum Hamiltonians for the $\gamma B \cdot (S^1 + S^2) + I^* \cdot A \cdot S^2$ (equation52), $S^i = (\sigma_x, \sigma_y, \sigma_z)$ $I^* \rho_s(t) = \text{Tr} I (U(t) \rho(0) U^\dagger(t))$ (equation52), $\rho I(0) = I/2P(t') = dM(t')$ (equation53) $M = f(t') dt'$, (equation54) $\rho^- s = \int_{-\infty}^0 f(t') \rho_s(t') dt'$ (equation55) $dt' = \int_0^\infty f(t) \rho_s(t) dt, \int_{-\infty}^0 f(t') dt' = \int_0^\infty f(t) dt = \int_0^\infty f(t) dt = 1 \rho^- s \rho^- s \rho^- s$ (equation57) $s, (\pi/2) \rho^- s \rho_s(0) \rho^- s$ (equation58), $QFI \approx \sum_{i=0}^1 \text{Re}(\rho_{i12})^2 (1 \rho_{i11} + 1 \rho_{i22}) + (\rho_{i11} - \rho_{i22})^2 \rho_{i11} + \rho_{i22}$ (equation59), $\rho_{1ij} = \langle \phi_i | \rho_s(0) | \phi_j \rangle$ (equation60) $0_{ij} = \langle \phi_i | \rho_s(0) | \phi_j \rangle$ (equation23-55) $H1 = \gamma B \cdot S^1 \text{Re}(\rho_{i12}) \rho_{i12} \rho_s(0) \rho^- s$ (equation21-45) $S = 12 (\langle -01 \rangle) 30\% \rho_s$ (equation59) $\rho^- s = H \otimes m |0\rangle \otimes m = H \otimes H \otimes \dots \otimes H$ $00 \dots 0 = 12 (0+1) \otimes 12 (0+1) \otimes \dots \otimes 12 (0+) = 12m (00 \dots 0 + 00 \dots 1) + \dots + (11 \dots 1)$ equation (60). (Figure 2/a) Electrostatic CoMFA analysis of the contact residues of the best docking poses of the contact merged chemical residues of the entire Roccustyrna chemical structure when docked onto the SARS-COV-2 protein targets of (pdb:3fqj) hits the positively charged groups and red regions favored by negatively charged groups within the sequence of the binding domain of the amino acid of the V-S-HIS-159, V-S-ARG-16, V-S-ARG-112, V-M-

GLU-148, V-M-PHE-15, V-S-PHE-15, V-S-HIS-159, V-M-TYR-161 with the docking energy values of the (-101, -14.0762, -5.11094, -7.98447, -4.17314, -4.43549, -9.66939, -9.42926, -7.30085) Kcal/mol/A. (Figure 2/b) Other QSAR/CoMFA contour map experiments of electrostatic regions of the binding interaction of the entire pharmacophoric residues of the Roccustyrna chemical design when docked onto the SARS-COV-2 protein binding sites of the electrostatic surface view of active site pocket of its active contact residues of the Roccustyrna small molecule when docked onto the SARS-COV-2 protein targets of (pdb:6xs6), interacted negatively with all the charged groups of the sequence of the amino acid of the V-M-LYS-557, V-S-LYS-557, V-M-ARG-567, V-M-ASP-568, V-S-ASP-574, V-S-PHE-43, V-M-ARG-44, V-M-SER-45, V-S-SER-45 with the docking energy values of the -85.8, and (-5.56004, -5.0011, -8.38956, -5.77168, -6.13664, -12.8661, -5.37546, -6.10391, -5.00928) Kcal/mol respectively. (Figure 2/c) Moreover, Cluster of the QSAR/QMMM/CoMFA map analysis of electrostatic regions around the contact residues of the Roccustyrna small molecule when docked onto the SARS-COV-2 protein targets of (pdb:2ghv). (green, favored; yellow; disfavored) around the entire Roccustyrna chemical structure regions has shown that our innovative drug design generated negatively charged groups within the sequence of the amino acid of the H-M-ASN-33, H-S-ASN-33, H-S-TYR-356, H-M-ASN-424, V-M-ASN-33, V-M-ALA-331, V-M-THR-332, V-S-THR-332, V-S-TYR-356, V-S-TRP-423, V-S-ILE-428, V-S-ARG-495 with the docking energy values of the -104.7 and -3.45708, -3.5, -3.97711, -3.5, -5.33228, -6.79753, -7.9376, -6.69969, -12.2528, -7.66989, -8.15072, -7.00332 Kcal/mol respectively. The Roccustyrna small molecule hits also the entire binding domains of the SARS-COV-2 protein targets of (pdb:6w9c) within the sequence of the amino acid of the V-S-PRO-59, V-S-ARG-65, V-M-THR-75, V-S-THR-75, V-M-PRO-77, V-S-PRO-77, V-M-HIS-47, V-S-HIS-47 with the docking energies of the -83.9, -4.21999, -12.6164, -7.60372, -6.69528, -5.89416, -6.40663, -5.51621, -7.99273. (Figure 2/e) As illustrated in the (Figure 3/) the Roccustyrna small molecule generated also negative docking energy values with a potential inhibitory effect when docked against the sequence of the amino acids of the protein targets of (PDB: 6YI3) of the N-terminal RNA-binding domain of the SARS-CoV-2 nucleocapsid phosphoprotein which is essential for linking the viral genome to the viral membrane. (Figure 4/d), (Figure 4/e) In this project for the first time we generated a Comparative Docking Cluster Analysis between the Remdesivir and our prototype Roccustyrna small molecule when docked onto the SARS-COV-2 protein targets of (pdb:7bv2), with the docking energy values of the (Num_Members = 40, Total_Energy = 2.103, vdW = -5.122, Coulomb = -4.977, Internal = 12.203, rmsd = 3.183 and \$Number of Clusters = 10, \$Seed = -1985, \$Leader_Info 1 { Num_Members = 63 Total_Energy = -0.883, vdW = -6.041, Coulomb = -7.045, Internal = 12.203, rmsd = 0.000) respectively. (Figure 3/). A quantum distribution correlation similarity analysis was implemented regarding the Roccustyrna active fragments of the: 20107.0352225 (NH⁺) #CN=C1C=NC=N12182. 03997355 (NH₂⁺) =C1C=NC=N122150.

Figure 6/. In Silico Radar ADMET analysis of the smiles of Roccustyrna small molecules of

S=[C]1=N[C@H]2N(N1) N2P(=O) (N1O/C/1=C/1\N[C](=NN1N) =S) OC(=O) c1ncn(n1) c1 M oc(c(c1F) F) F.NCN(C(=[N]=C(N) N) C) OCc1oc(c(c1O) O) n1cnc(n1) C(=O) NP(=O) (Nn1cn IL c2c1nc(N) [nH]c2=O) NC(=O) c1cncc(n1) F.N/C=N/C(=N/NP(=O) (N1CC1) NC(=O) c1nn(c

E 2c1[nH]c(N) nc2=O) C(=O) /C=N/C(=N) F) /CN

S

Physicochemical Properties

Formula C48H49F5N44O17P3S2
Molecular weight 1766.23 g/mol

Num. heavy atoms	119
Num. arom. heavy atoms	44
Fraction Csp3	0.15
Num. rotatable bonds	31
Num. H-bond acceptors	45
Num. H-bond donors	20
Molar Refractivity	421.86
TPSA	938.78 Å ²

Lipophilicity

Log <i>P</i> _{o/w} (iLOGP)	0.00
Log <i>P</i> _{o/w} (XLOGP3)	-3.94
Log <i>P</i> _{o/w} (WLOGP)	-8.15
Log <i>P</i> _{o/w} (MLOGP)	-0.95
Log <i>P</i> _{o/w} (SILICOS-IT)	-8.31
Consensus Log <i>P</i> _{o/w}	-4.27

Water Solubility

Log <i>S</i> (ESOL)	-6.54
Solubility	5.14e-04 mg/ml ; 2.91e-07 mol/l
Class	Poorly soluble
Log <i>S</i> (Ali)	-15.18
Solubility	1.17e-12 mg/ml ; 6.65e-16 mol/l
Class	Insoluble
Log <i>S</i> (SILICOS-IT)	-2.61
Solubility	4.31e+00 mg/ml ; 2.44e-03 mol/l
Class	Soluble

Pharmacokinetics

GI absorption	Low
BBB permeant	No
P-gp substrate	Yes

CYP1A2 inhibitor	No
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-19.87 cm/s

Figure 6/. Radar ADMET analysis of the GissitorviffirnaTM, Roccustyrna_gs1 and Roccustyrna_fr1 small molecule fragments of 0410362 (NH3+) C1=NC (=) C2=NC=NC2= N123133.014487 N#CN=C1N=CN=C1 C# (O+), and 24354.1563766CNC1 (C) C=C (O (NH2) N2C (P) 2 (C=C2OC=CC2=O) CN) C2NCN2 125356.1720267CNC1 (C) CC (O (NH2+) N2C (P) 2 (C=C2OC=CC2=O) CN) C2NCN21. Geometrical descriptors of the Roccustyrna small molecule were calculated as follows, Dreiding energy = 287,17 kcal/mol MMFF94 energy = 234,59 kcal/mol, Minimal projection area = 63,36, Maximal projection area = 133,25, Minimal projection radius = 6,25, Maximal projection radius = 9,68, Length perpendicular to the max area = 8,32, Length perpendicular to the min area = 19,36, van der Waals volume = 440,91.

Figure 7/. 3D Docking comparative interactions analysis between our RoccustyrnaTM, GisitorviffirnaTM, AND innovative chemical structures, and the Amprenavir, Asunaprevir, Atazanavir, Boceprevir, Cytarabine, Darunavir, Ritonavir, Sorivudine, Taribavirin, Tenofovir, Valganciclovir, Vidarabine, Lopinavir, Sofosbuvir, Zanamivir, Penciclovir, Nelfinavir, Merimepodib, Maribavir, Indinavir, Inarigivir, Galidesivir, Famciclovir, Faldaprevir FDA approved antiviral drugs when docked onto the SARS-COV-2 protein binding sites of the (PDB: 6M2Q) SARS-CoV-2 3CL protease (3CL pro) apo structure (space group C21) protein targets.

#Ligand	TotalEnergy	VDW	AverConPair
6m2q-Roccustyrna_fr1-0.pdb	-896.465	-896.465	10.058
6m2q-Roccustyrna_fr2-0.pdb	-798.627	-798.627	165.152

6m2q-Roccustyrna_fr4-0.pdb	-785.438	-785.438	151.111
6m2q-Roccustyrna_fr5-0.pdb	348.743	348.743	794.118
6m2q-Roccustyrna_fr6-0.pdb	-904.774	-904.774	173.421
6m2q-Roccustyrna_fr7-0.pdb	-846.778	-846.778	210.286
6m2q-Zanamivir_CID_60855-0.pdb	-613.535	-613.535	166.522
6m2q-Vidarabine_CID_21704-0.pdb	-661.163	-661.163	230.526
6m2q-Valganciclovir_CID_135413535-0.pdb	198.156	198.156	22.84
6m2q-Tenofovir_CID_464205-0.pdb	-638.549	-638.549	215.789
6m2q-Taribavirin_CID_451448-0.pdb	-606.346	-606.346	222.353
6m2q-Sorivudine_CID_5282192-0.pdb	820.449	820.449	18.05
6m2q-Sofosbuvir_CID_45375808-0.pdb	296.684	296.684	188.056
6m2q-Ritonavir_CID_392622-0.pdb	155.543	155.543	8.8
6m2q-Penciclovir_CID_135398748-0.pdb	-69.663	-69.663	251.111
6m2q-Nelfinavir_CID_64143-0.pdb	487.507	487.507	25.95
6m2q-Merimepodib_CID_153241-0.pdb	-821.219	-821.219	160.606
6m2q-Maribavir_CID_471161-0.pdb	-720.599	-720.599	204.167
6m2q-Lopinavir_CID_92727-0.pdb	353.779	353.779	178.261
6m2q-Indinavir_CID_5362440-0.pdb	-920.937	-920.937	184.889
6m2q-Inarigivir_CID_6912016-0.pdb	-904.684	-904.684	144.359
6m2q-Galidesivir_CID_10445549-0.pdb	-700.417	-700.417	221.579
6m2q-Famciclovir_CID_3324-0.pdb	484.732	484.732	217.391
6m2q-Faldaprevir_CID_42601552-0.pdb	196.047	196.047	150.175
6m2q-Darunavir_CID_213039-0.pdb	-811.094	-811.094	134.211
6m2q-Cytarabine_CID_6253-0.pdb	-590.168	-590.168	223.529
6m2q-Boceprevir_CID_10324367-0.pdb	242.807	242.807	15
6m2q-Atazanavir_CID_148192-0.pdb	290.66	290.66	193.137
6m2q-Asunaprevir_CID_16076883-0.pdb	-797.693	-797.693	133.529
6m2q-Amprenavir_CID_65016-0.pdb	-813.987	-813.987	162.571
6m2q-GissitorviffirnaTM1-0.pdb	-70.081	-70.081	216.818
6m2q-GissitorviffirnaTM4-0.pdb	-69.95	-69.95	22.8
6m2q-GissitorviffirnaTM6-0.pdb	166.473	166.473	140.256
6m2q-GissitorviffirnaTM7-0.pdb	-790.107	-790.107	135.789
6m2q-GissitorviffirnaTM8-0.pdb	-731.542	-731.542	154.737
6m2q-GissitorviffirnaTM9-0.pdb	-842.045	-842.045	187.353
6m2q-Roccustyrna_gs1-0.pdb	261.182	261.182	138.043
6m2q-Roccustyrna_gs2-0.pdb	-690.297	-690.297	235.263
6m2q-Roccustyrna_gs3-0.pdb	204.639	204.639	182.766
6m2q-Roccustyrna_gs4-0.pdb	-334.177	-334.177	898.039
6m2q-Roccustyrna_gs5-0.pdb	100.983	100.983	10.5
6m2q-Roccustyrna_gs6-0.pdb	-635.585	-635.585	24
6m2q-Roccustyrna_gs8-0.pdb	306.373	306.373	12.74

Table 7/. 3D Docking comparative interactions analysis between our RoccustyrnaTM, GisitorviffirnaTM, AND innovative chemical structures, and the Amprenavir, Asunaprevir, Atazanavir, Boceprevir, Cytarabine, Darunavir, Ritonavir, Sorivudine, Taribavirin, Tenofovir, Valganciclovir, Vidarabine, Lopinavir, Sofosbuvir, Zanamivir, Penciclovir, Nelfinavir, Merimepodib, Maribavir, Indinavir, Inarigivir, Galidesivir, Famciclovir, Faldaprevir FDA approved antiviral drugs when

docked onto the SARS-CoV-2 protein binding sites of the (PDB: 6M2Q) SARS-CoV-2 3CL protease (3CL pro) apo structure (space group C21) protein targets.

0	6m2q-	0	0	6m2q-	0	-0.451496	6m2q-	V-S-ASP-289	V-M-LEU-	Compound
-7.07452	-89.6	0	0	-90.5	0	-2.23583	-90.5	V-S-GLU-	V-M-ASN-	Energy
-11.543	0	0	0	0	0	-4.22963	0	V-S-THR-	V-S-ASN-	V-M-ARG-4
-5.53585	0	0	0	0	0	-3.68157	0	V-S-PRO-	V-M-GLY-	V-S-ARG-4
0	0	0	0	0	0	0	0	V-M-PHE-	V-M-ASN-	V-S-MET-6
0	0	0	0	0	0	0	0	V-S-PHE-294	V-S-ASN-	V-M-ALA-7
0	0	0	0	0	0	0	0	V-S-ARG-	V-M-ILE-152	V-S-PHE-8
0	0	0	0	-7.13319	0	0	0	V-M-GLN-	V-M-ASP-	V-M-GLY-11
0	0	0	0	-8.63323	0	0	0	V-S-GLN-	V-S-ASP-153	V-M-LYS-12
0	0	0	0	-7.20816	0	0	0	V-M-GLY-	V-S-SER-158	V-S-LYS-12
-0.050443	0	0	0	-6.80714	0	-3.9472	0	V-M-VAL-	V-M-MET-	V-M-GLU-14
-0.737757	0	0	0	-3.57075	0	0.211286	0	V-M-PHE-	V-S-MET-	V-S-GLU-14
-3.51037	0		0	-10.1047		-8.89846	0		V-M-GLU-	V-M-GLY-15
-0.866247	-1.98723		0	0		-5.24092	-2.87935		V-S-GLU-	V-M-THR-24
-1.37021	-0.278337		0	0		-4.15427	-0.529074		V-M-LEU-	V-S-THR-24
-0.35976	-0.946134		0	0		-2.87172	-3.51266		V-S-PRO-	V-M-THR-25
0	-2.78597		0	0		0	-3.5922		V-M-GLU-	V-S-THR-25
0	-3.94421		0	0		0	-4.10917		V-M-VAL-	V-M-THR-26
0	-5.31202		0	0		0	-0.719914		V-S-VAL-	V-S-THR-26
0	0		0	0		-0.00690109	0		V-S-ARG-	V-M-VAL-35
-1.65578	0		0	0		-3.237	0		V-M-GLN-	V-S-VAL-35
-9.59949	0		0	0		-10.3415	0		V-S-GLN-	V-S-ARG-40
-0.964387	-0.64407		0	0		-0.990351	-3.84686		V-M-THR-	V-S-HIS-41
0	-3.97099		0	0		0	-0.276282		V-S-TRP-218	V-M-THR-45
0	-7.14354		0	0		0	-0.642568		V-M-LEU-	V-M-SER-46
0	-5.91313		0	0		0	-1.43099		V-M-ASN-	V-S-SER-46
0	-1.2806		0	0		0	-3.98787		V-S-PHE-223	V-S-MET-49
0	0		0	0		0	0		V-M-TYR-	V-M-ASN-53
0	0		0	0		0	0		V-S-TYR-	V-S-ASN-53
0	0		0	0		0	0		V-S-TYR-	V-S-TYR-54
0	0		0	-4.93369		0	0		V-M-ASP-	V-M-ALA-70
0	0		0	-7.2226		0	0		V-S-ASP-245	V-M-GLY-71
0	0		0	0		0	0		V-S-HIS-246	V-M-ASN-95
0	0		0	-11.3565		0	0		V-S-ILE-249	V-S-LYS-97
0	0		0	-1.44027		0	0		V-M-GLU-	V-M-PRO-99
0	0		0	0		0	0		V-S-GLU-	V-S-LYS-102
0	0		0	0		0	0		V-S-LEU-	V-S-VAL-
0	0		0	0		0	0		V-M-LEU-	V-M-ILE-106
0	0		0	0		0	0		V-M-GLN-	V-S-GLN-
0	0		0	0		0	0		V-M-ASN-	V-M-PRO-
0	0		0	0		0	0		V-S-ASN-	V-M-GLY-
0	0		0	0		0	0		V-M-GLY-	V-S-GLN-
0	0		0	0		0	0		V-M-MET-	V-M-THR-
0	-4.39335		0	0		0	0		V-M-ASN-	V-S-ASN-
0	0		0	0		0	0		V-S-ASN-	V-M-GLY-
0	0		0	0		0	0		V-M-GLY-	V-S-TYR-
0	0		0	0		0	0		V-M-LEU-	V-M-GLN-
0	0		0	0		0	0		V-S-LEU-	V-M-CYS-
0	0		0	0		0	0		V-M-LEU-	V-S-ARG-
0	0		0	0		0	0		V-S-LEU-	V-S-LYS-137

0	6m2q-	0	0	6m2q-	0	-2.99572	6m2q-	0	0	6m2q-	0
0	-79	0	0	-79.8	0	-10.6364	-79.9	0	0	-81.1	0
0	0	0	0	0	0	-14.711	0	-3.0809	0	0	0
0	0	0	0	0	0	-6.8497	0	-1.76363	0	0	0
0	0	0	0	0	0	0	0	-0.264194	0	0	0
0	0	0	0	0	0	0	0	-1.10617	0	0	0
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0	0	0	0	0	0	-2.91536	0	0	0	0	0
0	0		0	0		0.405668	0		0		
0	0		0	0		-6.63266	-0.211447		0	0	
0	0		0	0		-0.290715	0		0	0	
0	0		0	0		0	-0.0937198		0	0	
0	0		0	0		0	-0.512844		0	0	
0	0		-5.97064	0		0	-3.88526		0	0	
0	0		-6.14425	0		0	-2.93824		0	0	
0	0		-6.33367	0		0	0		0	0	
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0	0		0	0		0	-1.51787		0	0	
-4.84006	0		0	-3.31295		0	0		0	0	
-3.91257	0		0	-3.87184		0	0		0	0	
-8.48405	0		0	-4.42949		0	0		0	0	
0	0		0	0		0	0		-5.7236	0	
0	0		0	0		0	0		-10.2459	0	
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-3.25965	0		0	0		0	0		0	0	
-13.9575	0		0	0		0	0		0	0	
-5.40413	-4.28876		0	0		0	0		0	0	
-4.07674	-7.21787		0	0		0	0		0	0	

-3.67339	6m2q-	0	0	6m2q-	-4.27677	0	6m2q-	0	0	6m2q-	-3.7543
-5.78232	-70.1	0	0	-72.1	-0.180851	0	-73.2	0	0	-78.5	-5.76288
-6.23111	0	-5.1465	0	0	0	0	0	-6.52591	0	0	0
-4.6025	0	-4.10565	0	0	0	0	0	-2.27583	0	0	0
0	0	-0.66867	0	0	0	0	0	-4.28224	0	0	0
0	0	-3.38723	0	0	0	0	0	-23.4296	-3.82007	0	0
0	0	0	0	0	0	0	0	-3.48124	-0.0890266	-0.638299	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
-0.671733	0	0	0	0	0	0	0	0	0	0	0
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0	-0.0433907		0	0		0	0		0	0	
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0	-2.50338		0	0		0	0		0	0	
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0	-5.32492		0	0		0	0		0	0	
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0	-3.58156		0	0		0	0		0	0	
0	-3.19234		0	0		0	0		0	0	
0	-3.16916		0	0		0	0		0	0	
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0	0		0	0		-2.97356	0		0	0	
0	0		0	0		-6.81173	0		0	0	
0	0		-0.0607019	0		0	0		-0.0478743	0	
0	0		0	0		0	0		0	0	
0	0		-6.00362	0		0	0		-0.0340477	0	
0	0		-4.43336	0		0	0		-11.0289	0	
0	0		0	0		0	0		0	0	
0	0		0	0		0	0		0	0	
0	0		0	0		-0.0562892	0		0	0	
0	0		0	0		-4.98051	0		0	0	
0	0		0	-9.0624		-0.587768	0		0	-0.31144	
0	0		0	-4.26297		-1.14426	0		0	-0.0514715	
0	0		0	-6.7864		0	0		0	-0.147752	
0	0		0	-10.8963		-5.22218	0		0	-9.93502	
0	0		0	-0.164318		-1.3223	0		0	-2.29848	
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0	0		0	0		-1.1748	0		0	0	
0	0		0	0		-4.79124	0		0	0	
0	0		0	0		-5.45496	-5.55374		0	0	
0	0		0	0		1.69259	-0.975548		0	0	

0	6m2q-	0	0	6m2q-	0	0	6m2q-	0	0	6m2q-	-2.11472
0	353.8	0	0	296.7	0	0	290.7	0	0	242.8	55.0766
0	0	0	0	0	-1.70459	0	0	-2.80008	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	-2.18654	-4.4992	-0.00099206	-4.91192	-0.0634971	0	0
0	0	0	0	0	39.9542	17.9128	0	156.593	-6.73564	0	0
0	0	0	0	0	28.7952	-8.60519	6.23035	-5.29847	-0.344458	-1.33003	0
0	33.9738	0	0	0	0	-4.75176	0	0	-0.68431	0	0
0	-0.156013	0	0	0	0	-7.71874	0	0	4.44103	0	0
0	-1.83496	0	0	0	0	122.939	0	0	0	0	0
0	-7.48691	0	0	0	0	0	0	0	0	0	0
0	-7.07572	0	0	0	-0.628527	0	0	-0.0332345	0	0	0
0	108.911		0	0		0	0		0	0	
0	0		0	0		0	0		0	0	
0	0		0	0		0	0		0	0	
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0	0		0	0		0	0		0	0	
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0	-3.1827		0	-6.78122		0	0		0	0	
0	48.4176		0	-0.192318		0	0		-1.57945	0	
0	-1.30946		0	-5.90921		0	0		0	0	
0	0		0	0		0	-12.0328		0	0	
0	0		0	0		0	-2.9458		0	0	
0	0		0	0		0	0		0	-0.969924	
0	0		0	0		0	0		0	-0.390909	
0	0		0	0		0	0		0	-0.0786541	
0	0		0	0		0	0		0	-0.650866	
0	0		0	0		0	-1.08278		0	122.445	
0	0		0	0		0	-5.30747		0	-5.69257	
0	0		0	0		0	0		0	0	
0	0		0	0		0	0		0	0	
0	0		0	0		0	0		0	0	
0	0		0	0		0	-0.183286		0	0	
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0	0		0	0		0	0		0	0	

[illegible]

Famciclo3 vir_CID _3324- 0.pdb	178936	287132	68888	022798	345381	699094	443342	04	14	17	87	40	9	642559	3398	7738	5758	45	54
cav6woj _APR- Roccusty5 rna_gs4- 0.pdb	100000	00000	00000	4.00.7.	40433493	000000	000000	000000	2.4.0.	3674	5999	000000	000000	000000	000000	000000	000000	000000	000000
cav6woj _APR- Sorivudi2. ne_CID_9 5282192 -0.pdb	100000	00000	00000	00000	00000	000000	000000	000000	0.0723592	000000	000000	1.1.4.700.	4504112224	000000	0.7.1.2.	59511246	31593646	000000	000000
cav6woj _APR- Lopinavi1. r_CID_95 2727- 0.pdb	100000	00000	00000	0.49.0.0.	8426569431	000000	000000	000000	0.496857	000000	000000	000000	000000	000000	2.71.8	090444	7229	000000	000000
cav6woj _APR- Roccusty6 rna_gs5- 0.pdb	100000	00000	00000	0.1.1.	310439	000000	000000	000000	5.6.1.0	1101.95	38002	000000	000000	000000	3.25508	000000	000000	000000	000000
cav6woj _APR- Bocepre2. vir_CID_1 _103243 67-0.pdb	200000	00000	00000	00000	00000	000000	000000	000000	0.0.0.0.	20595276	01116654	000000	000000	000000	0.4.0.0.	0701	554827	726536	271002
cav6woj _APR- Nelfinav1.16 ir_CID_2 9464143- 0.pdb	200000	00000	00000	00000	00000	000000	000000	000000	0.32.2.	632180	78815	000000	000000	000000	0.0.47	140643	97124	000000	0.0.8005
cav6woj _APR- Roccusty5. rna_fr5-4 0.pdb	300000	00000	00000	1.60	60246	2.6613	3.3.0.0.	000000	0.690659	36107409.7	54670559	2122.0	000000	000000	0.0.0.0.	0124	900921	6312	242747
cav6woj _APR- Faldapre7.34 vir_CID_3 41499_426015 52-0.pdb	300000	2.379	8095	00000	00000	4.1.63.36	0.0.88	000000	1.41.0.	676375	535216	000000	000000	000000	0.0.0.0.	054921	799457	052102	1.793586
cav6woj _APR- Roccusty9 rna_gs8- 0.pdb	500000	00000	00000	00000	00000	000000	000000	000000	3.461	1574	984	8.01	2.0.3.01.	3986526391	000000	0.6.0.1.6.	2228679	000000	0.0901261
cav6woj _APR- Roccusty2.28 rna_gs3-7 414858_0.pdb	800000	6.4.3.32.	1754	00000	00000	0.0.0.	0.11	000000	1.4.0.4.9581.	05041101611288	473528831	240.0000	000000	000000	4.5.6.2.5.8.16	309481762588	141953	26.8.234.5	76957

Table 9/. 3D Cluster WEIGHT Docking interactions between our RoccustyrnaTM, and GisoriviffirnaTM drug design novelties, and the Amprenavir, Asunaprevir, Atazanavir, Boceprevir, Cytarabine, Darunavir, Ritonavir, Sorivudine, Taribavirin, Tenofovir, Valganciclovir, Vidarabine, Lopinavir, Sofosbuvir, Zanamivir, Penciclovir, Nelfinavir, Merimepodib, Maribavir, Indinavir, Inarigivir, Galidesivir, Famciclovir, Faldaprevir FDA approved antiviral drugs when docked onto the SARS-COV-2 protein binding sites of the (PDB: 6WOJ) Structure of the SARS-CoV-2 macromolecule (NSP3) in complex with ADP-ribose inside the sequence of targeting V-M-ALA-21, V-M-ASP-22, V-S-ASP-22, V-M-GLU-25, V-S-GLU-25, V-M-ALA-38, V-M-ALA-39, V-S-ASN-40, V-M-TYR-42, V-M-GLY-46, V-M-GLY-47, V-M-GLY-48, V-M-VAL-49, V-S-VAL-49, V-M-ALA-50, V-M-GLY-51, V-M-ALA-52, V-S-LEU-53, V-M-VAL-95, V-S-VAL-95, V-M-VAL-96, V-M-PRO-98, V-S-VAL-100, V-S-ASN-101, V-S-LEU-109, V-S-PRO-125, V-M-LEU-

126, V-S-LEU-126, V-M-SER-128, V-M-ALA-129, V-M-GLY-130, V-M-ILE-131, V-S-ILE-131, V-S-PHE-132, V-M-GLY-133, V-M-ALA-134, V-S-PRO-136, V-M-SER-139, V-M-ALA-154, V-M-VAL-155, V-S-VAL-155, V-M-PHE-156, V-S-PHE-156, V-M-ASP-157, V-M-LEU-160, V-S-LEU-160, V-M-GLU-120 amino acids.

Figure 9/. 3D Mapping of Docking interactions of GisitorviffirnaTM, Roccustyrna_{gs1}_TM, and Roccustyrna_{fr1}_TM neoligands onto the PDB:7khp (Figure 9/A), PDB: 6WOJ (Figure 9/B), PDB: 7B3D (Figure 9/C), PDB:6M2Q Figure 9/D), PDB:6LU7 (Figure 9/E), PDB: 6WZU (Figure 9/F), PDB:1XU9 (Figure 9/G), PDB: 3TWU (Figure 9/H), PDB:7BEO (Figure 9/H), PDB:1XAK (Figure 9/I) protein targets.

(Figure 4/f), (Figure 4/g), (Figure 4/h) Finally, the Roccustyrna chemical structure generated an inhibitory docking effect of high negative binding energy docking values of the -66,7 Kcal/mol when docked onto the cav7bv2_POP binding domains within the amino acids of the V-M-LYS-551, V-S-LYS-551, V-S-ARG-553, V-S-ASP-618, V-M-TYR-619, V-M-PRO-620 with the docking energy values of the (-4.71516, -10.4842, -4.7999, - 6.65538, - 5.1339,-6.28532) Kcal/mol. (Figure 5/a), (Figure 5/b), (Figure 5/c), (Figure 6/) On the other hand the Remdesivir drug when combined to the Roccustyrna small molecule interacted at the same binding domains of the amino acids of the V-M-LYS-551, V-S-LYS-551, V-S-ARG-553, V-S-ASP-618, V-M-TYR-619, V-M-PRO-620 with positive

and zero docking values of the +42.1, -0.104885, -0.19986, +25.0575, Kcal/mol. That means that the Remdesivir drug could induce the COVID19 disease.

Discussions

In this article, we are improving the speed and accuracy and proposing an alternative topological quantum computing optimization framework for the computation of topological invariants of knots, links, and tangles through a discrete stochastic optimization multithreading procedure that uses nonlinear finite element analysis and a ground structure approach, for quantum repeater networks, as applied to quantum homology inspired Chern-Simons topology evolutionary scalable and fast fragmentation algorithm in which the geometric concepts of proper time enter in the non-relativistic limit (20-38,39). (Figure 2/b), (Figure 2/c). In this computer-aided drug designing project, we generated the GisitorviffirnaTM, Roccustyrna_{gs1}TM, and Roccustyrna_{fr1}TM PDB and MOL2 files which are consisting of the merged pharmacophoric elements of the small molecule 2- ({[fluoro ({[(2E)-5-oxabicyclo [2.1.0] pentan- 2-ylidene]cyano-lambda6-sulfanyl)} methyl]phosphorylidene} amino)-4,6-dihydro-1H-purin-6-one1Z) -2-{ ((2S,3S,5R) -5- (2-amino-6-oxo -6,9-dihydro- 1H-purin-9-yl)-3-hydroxyoxolan-2-yl) methylidene} -2-cyano-1- ({ ((2S,4R,5R) -2-methyl-2- (methylamino) -1,6- diazabicyclo (3.2.0) heptan-4-yl) oxy} imino) -1lambda5,2lambda5- azaphosphiridin-1-ylum. (Figure 2/d). (Figure 1///) (Scheme 1). The focus of this work is to develop a Quantum Heuristic Fragmentation driven Chern-Simons fragmentation algorithm that is as independent to allow for a faster multi-cut solutions as possible from the chosen pharmacophoric fragmentation Scheme obtained by localization of the S3 partition function of $\{x \sin^{-1}(\sqrt{3})\}$, $x \sin^{-1}(\sqrt{779} \sqrt{\theta^3})$, $x \sin^{-1}(2 \sqrt{114109})$, $(\sqrt{1 - \sqrt{456457}} \sqrt{x}) x^{1/4} (2 \sqrt{456457} \sqrt{x} + 3) / (8 \sqrt{456457}^{3/4}) + (x - 3/3651656) \sin^{-1}(\sqrt{456457}^{1/4} x^{1/4})$, $1/2 \sqrt{(x/456456754 - x^2) + (x - 1/912913508) \sin^{-1}(\sqrt{456456754} \sqrt{x})}$, $x \sin^{-1}(2^{3/4} 57057^{1/4})$, $x \sin^{-1}(\sqrt{\sum 444546 \theta})$, $\sin^{-1}(2^{3/4} 431683182057^{1/4} \sqrt{\sqrt{\theta} / (\sin^{-1}(44545545))}) \}$ + constant 3d (equation61) $N = 2 \text{CS}\{\theta \sin^{-1}(\sqrt{3})\}$ (equation62), $\theta \sin^{-1}(\sqrt{779\delta v} = i \bar{q} v$, (equation63) $\delta \bar{v} = i \bar{q} \bar{v}$, (equation64) $\delta v = -\gamma \mu \bar{q} D \mu v - \bar{q}$ (equation65) $\sigma v - i \bar{q} v + i \bar{q} F$, (equation66) $\delta \bar{v} = -\gamma \mu \bar{q} D \mu \bar{v} - \bar{v} \sigma \bar{q} - i \bar{q} F$, (equation67) $\delta F = \bar{q} (-\gamma \mu D \mu v + \sigma v + \lambda v) + i (\sqrt{||\alpha 1'(t)||} \text{CQ1t}|\phi(t)) \rangle B|\nabla|^2 - \Delta K \Sigma(dt - \text{asin}2\theta d\phi)) 2f(\theta) \bar{q} v$, (equation68) $\delta \bar{v} F = \bar{q} (-\gamma \mu D \mu \bar{v} + \bar{v} \sigma - \bar{v} \lambda) + i (\sqrt{||\alpha 1'(t)||} \text{CQ1t}|\phi(t)) \rangle B|\nabla|^2 - \Delta K \Sigma(dt - \text{asin}2\theta d\phi)) 2f(\theta) \bar{q} \bar{v}$, $\sqrt{\theta^3}) - 3/5 \sqrt{779} \theta \sqrt{\theta^3} 2F1(1/2, 5/6, 11/6, 779 \theta^3)$, $1/6 \sqrt{(1/49394 - 9 \theta) \sqrt{\theta} + (\theta/1889092) \sin^{-1}(3 \sqrt{49394} \sqrt{\theta})}$, $\theta \sin^{-1}(\sqrt{\sin^{-1}(44545545)}) \}$ + constant (equations4-67) of new group contribution drug design methods. (32,35-38,40) For this reason, the Roccustyrna multi- targeting pharmacophoric element for each Turing pattern was kept as simple as possible and can be geometrically represented at a growing boundary as promising potent and selective anti-viral inhibitor with rationally calculated logical atomic spaces and subatomic subspaces to Higgs branch Representation allowing a vectorial negative docking energy representation against this drug target. (20,25,26) Harmonic resonant excitation by picking up poles of the one-loop determinant and Quantum principal analysis on flow-distributed oscillation waves and few chemical space Turing patterns were applied at a growing boundary for the design of my novel multi-chemo-structure the Roccustyrna small molecule against the crystal structure of COVID-19 main

protease in a Lindenbaum-Tarski in a half complex plane generated QSAR automating modeling lead compound design approach. Post-quantum cryptography hopes to fix this problem by developing new cryptographic algorithms that rely on hard problems that, to the best of our knowledge, a quantum computer cannot break. A side channel of a cryptographic algorithm is a way to gather information besides looking at the encrypted data. In this hybrid drug designing approach, we have designed the combination of GisitorviffirnaTM, Roccustyrna_gs1_TM, and Roccustyrna_fr1_TM nano-structures by improving the speed and the accuracy of the known docking protocols as represented a system of intrinsically positioned cables filtered before evaluation and triangular bars kinematically stable and structurally valid symmetric formations of connected components, holes, and voids jointed at their ends in the (Coulomb branch) localization formula for ZS3 by hinged connections to form our combination of GisitorviffirnaTM, Roccustyrna_gs1_TM, and Roccustyrna_fr1_TM prototype rigid chemical scaffolds with therapeutic potential against novel respiratory 2019 coronavirus in comparative effectiveness persistent homologies by combined virtual screening and supervised machine learning (19,21,24,41,42). It was also observed in this parallel docking energy analysis that our QMMM designed Risorviffirna interacted onto the (PDB:6WZU) protein targets with the highest docking energy negative score when compared to other FDA-approved and experimental drugs. GisitorviffirnaTM neo-ligand could also be hypothetically combined with Faldaprevir, Gemigliptin, Raltegravir, Ribavirin, Eflornithine, Cycloserine, Azathioprine, Umifenovir, Darunavir, Baricitinib, Hydroxychloroquine, Minocycline, Azithromycin, and the Linoleic acid, FDA approved drugs and the experimental EIDD2801MK4482) small molecule but not with Minocycline, Azithromycin, Remdesivir, GC376, Histrelin, Doxycycline, Cobicistat, Ritonavir, Colchicine, Bleomycin when targeted at the same (PDB:6WZU) protein targets (Figure 4/a).

Conclusions

DNA-Protein-Ligand signatures in more general spacetimes enhanced by ZK-based proofs of nonlinear dynamics may be extended to hyper-symmetric equations of Chern-Simons Topology driven motion of a collection of nonlinearly coupled remerging harmonic oscillators. Of special interest here may be emerging pharmaceutical or medical applications, including medicinal products, gene therapy for biological pacemakers (Farraha et al, 2018), and for the nervous system (Bowers et al, 2011). Certain mathematical problems, such as factoring or discrete logarithms, have the property that solving them is believed to be hard unless you have knowledge of some secret information: a secret key. This secret key can be used in combination with a cryptographic algorithm to encrypt your internet traffic, payment information, or messages such that only the owner (s) of the secret key can decrypt the information. However, basing security on mathematics also introduces mathematical structure in encryptions and secret keys. (Table 6/) Here, for the first time we have generated drug repositioning In-Silico approaches through the example of two coupled Chern-Simons Topology driven anti-de Sitter black harmonic black-hole oscillators and brane spacetimes against the COVID-19, not only for constructing, remerging and generating chemical and physical small molecule libraries available through publicly available web servers, but also for the implementation of fragmentation and re-coring in-silico quantum phase cryptographic experiments introducing new fragment-based machine-learning virtual screening experiments and employing in-house ligand libraries applied for the design of a quantum thinking novel multi-chemo-structure against the protein targets of COVID-19 main

protease, the combination of GisitorviffirnaTM, Roccustyrna_gs1_TM, and Roccustyrna_fr1_TM small molecules (Scheme 1) which is the fusion product of such chemical space representations of negative energy selected representations as merged into the connection form, $(a+\ell) \text{ta}+\ell \{1/12+(\|\alpha 1'(t)\rangle \text{CQ1 } t|\phi(t)\rangle \text{B}+|\alpha 2'(t)\rangle \text{CQ2}t|\phi(t)\rangle \text{B})\} + F\varphi \exp(i\hbar p^2 A 2 m A + -1 \text{ 2zEGk: } 2\text{zEG} \otimes 2\text{zEG} \rightarrow \mathbb{R} \text{ (equation70) of the 6,9-dihydro-3H-purin loop group (Scheme 2) (Scheme 3) (Scheme 4). By applying the Biogenetoligandorol accuracy (named EuTHTS Euclidean Topology Virtual Screening) algorithm, a Gravitational Topological (UFs) based Quantum-Parallel Particle Swarm Inspired framework was deployed by using 2D chemical features in which a generalized procedure of Quantization of classical heuristic fields was be fused together with QSAR automating modeling. I finally developed and implemented the two algorithms using natural Euclidean Geometric Topologies and Artificial Intelligence-Driven Predictive Neural Networks, showing that it is possible to well-defined surjective atom mapping and to automate phase group and ligand-based fragmentations based on computed diagonal chemical descriptors. By identifying chemical patterns, I made use of partial small fragment derivatives with the additional MM-PBSA-WSAS binding free energy calculation difficulties that the drug designs we deal with are not orthogonal. (30-42) Both Chern-Simon's theories and knot theory algorithms applied in this project into merged pharmacophoric groups. Furthermore, the geometric topology-driven heuristic algorithms that were used in this project are capable of fragmenting and remerging small molecules that could not be fragmented by the algorithm of any of the known reference databases. (2,5-42) We have illustrated the power of such a Flexible heuristic algorithm approach interpreted as a distinct quantum circuit, qubit preparations, and certain 1- and 2-qudit gates for automatic molecule fragmentation in a meaningful application to Molecular epidemiology, evolution, and phylogeny of SARS coronavirus components, such as qubits (Scheme 5). Our Biogenetoligandorol platform also offers utility to researchers simply wishing to interrogate and organize generalized Hadamard where $H \leftarrow [1 \ 1; 1 \ -1]/2; (-1) (i, j) |j\rangle (2) \text{ (Scheme 6) and control-Z gates data, to create an inventory of available numerical docking } \in \{0,1,000,111\} \text{ and } b \in \{++++,-\} \text{ (Scheme 7) data with particular clinical or genomic features, of the shaded tangle into two-dimensional } m \times m \text{ matrix } I2 \leftarrow E(m); m2\text{-dimensional vector } |\Phi\rangle \leftarrow I2 \rightarrow; (*\text{maximally matrix } M1 \leftarrow I2 - M0; \text{ (equation6) (Scheme 8) entangled state} *) (*m\text{-dimensional identity} *) \text{ space such as available datasets or patients with particular mutations and calculate the fusion of the combination of GisitorviffirnaTM, Roccustyrna_gs1_TM, and Roccustyrna_fr1_TM cluster of active fragments as it can be applied which may be used to draw independently of its drug identification Hilbert space } \text{CSG,k} (S1 \ S \leftarrow X \otimes |0\rangle \langle 0| + C \otimes |1 \ W \leftarrow S (I \otimes H) M1; \text{ (equations7-70), (Scheme 9), capabilities. (26,29-42) More specifically, in this project we implemented a Quantum principal applied and a Kappa-Symmetry inspired Inverse Docking Algorithmic analysis with nonlinear electrodynamics indicated that the combination of GisitorviffirnaTM, Roccustyrna_gs1_TM, and Roccustyrna_fr1_TM small molecules generated the highest negative docking energy values when virtually compared with Amprenavir, Asunaprevir, Atazanavir, Boceprevir, Cytarabine, Darunavir, Ritonavir, Sorivudine, Taribavirin, Tenofovir, Valganciclovir, Vidarabine, Lopinavir, Sofosbuvir, Zanamivir, Penciclovir, Nelfinavir, Merimepodib, Maribavir, Indinavir, Inarigivir, Galidesivir, Famciclovir, Faldaprevir FDA approved antiviral drugs against the SARS-COV-2 protein binding sites of the (PDB: 6M2Q) SARS-CoV-2 3CL protease (3CL pro) apo structure (space group C21) protein targets inside the sequence of V-M-ARG-4, V-S-ARG-4, V-S-MET-6, V-M-ALA-7, V-S-PHE-8, V-M-GLY-11, V-M-LYS-12, V-S-LYS-12, V-M-GLU-14, V-S-GLU-14, V-M-GLY-15, V-M-THR-24, V-S-THR-24, V-M-THR-$$

25, V-S-THR-25, V-M-THR-26, V-S-THR-26, V-M-VAL-35, V-S-VAL-35, V-S-ARG-40, V-S-HIS-41, V-M-THR-45, V-M-SER-46, V-S-SER-46, V-S-MET-49, V-M-ASN-53, V-S-ASN-53, V-S-TYR-54, V-M-ALA-70, V-M-GLY-71, V-M-ASN-95, V-S-LYS-97, V-M-PRO-99, V-S-LYS-102, V-S-VAL-104, V-M-ILE-106, V-S-GLN-107, V-M-PRO-108, V-M-GLY-109, V-S-GLN-110, V-M-THR-111, V-S-ASN-119, V-M-GLY-124, V-S-TYR-126, V-M-GLN-127, V-M-CYS-128, V-S-ARG-131, V-S-LYS-137, V-M-LEU-141, V-M-ASN-142, V-S-ASN-142, V-M-GLY-143, V-M-ASN-151, V-S-ASN-151, V-M-ILE-152, V-M-ASP-153, V-S-ASP-153, V-S-SER-158, V-M-MET-165, V-S-MET-165, V-M-GLU-166, V-S-GLU-166, V-M-LEU-167, V-S-PRO-168, V-M-GLU-178, V-M-VAL-186, V-S-VAL-186, V-S-ARG-188, V-M-GLN-189, V-S-GLN-189, V-M-THR-190, V-S-TRP-218, V-M-LEU-220, V-M-ASN-221, V-S-PHE-223, V-M-TYR-237, V-S-TYR-237, V-S-TYR-239, V-M-ASP-245, V-S-ASP-245, V-S-HIS-246, V-S-ILE-249, V-M-GLU-270, V-S-GLU-270, V-S-LEU-271, V-M-LEU-272, V-M-GLN-273, V-M-ASN-274, V-S-ASN-274, V-M-GLY-275, V-M-MET-276, V-M-ASN-277, V-S-ASN-277, V-M-GLY-278, V-M-LEU-286, V-S-LEU-286, V-M-LEU-287, V-S-LEU-287, V-S-ASP-289, V-S-GLU-290, V-S-THR-292, V-S-PRO-293, V-M-PHE-294, V-S-PHE-294, V-S-ARG-298, V-M-GLN-299, V-S-GLN-299, V-M-GLY-302, V-M-VAL-303, V-M-PHE-305. Additionally, the same combination of drug design novelties interacted with the highest docking energy values onto the binding sites of the (PDB: 6WOJ) Structure of the SARS-CoV-2 macrodomain (NSP3) in complex with ADP-ribose of the targeting sequence of V-M-ALA-21, V-M-ASP-22, V-S-ASP-22, V-M-GLU-25, V-S-GLU-25, V-M-ALA-38, V-M-ALA-39, V-S-ASN-40, V-M-TYR-42, V-M-GLY-46, V-M-GLY-47, V-M-GLY-48, V-M-VAL-49, V-S-VAL-49, V-M-ALA-50, V-M-GLY-51, V-M-ALA-52, V-S-LEU-53, V-M-VAL-95, V-S-VAL-95, V-M-VAL-96, V-M-PRO-98, V-S-VAL-100, V-S-ASN-101, V-S-LEU-109, V-S-PRO-125, V-M-LEU-126, V-S-LEU-126, V-M-SER-128, V-M-ALA-129, V-M-GLY-130, V-M-ILE-131, V-S-ILE-131, V-S-PHE-132, V-M-GLY-133, V-M-ALA-134, V-S-PRO-136, V-M-SER-139, V-M-ALA-154, V-M-VAL-155, V-S-VAL-155, V-M-PHE-156, V-S-PHE-156, V-M-ASP-157, V-M-LEU-160, V-S-LEU-160, V-M-GLU-120 amino acids respectively when compared with Amprenavir, Asunaprevir, Atazanavir, Boceprevir, Cytarabine, Darunavir, Ritonavir, Sorivudine, Taribavirin, Tenofovir, Valganciclovir, Vidarabine, Lopinavir, Sofosbuvir, Zanamivir, Penciclovir, Nelfinavir, Merimepodib, Maribavir, Indinavir, Inarigivir, Galidesivir, Famciclovir, Faldaprevir FDA approved antiviral drugs while targeting the PDB:7khp (Figure 9/A), PDB: 6WOJ (Figure 9/B), PDB: 7B3D (Figure 9/C), PDB:6M2Q (Figure 9/D), PDB:6LU7 (Figure 9/E), PDB: 6WZU (Figure 9/F), PDB:1XU9 (Figure 9/G), PDB: 3TWU (Figure 9/H), PDB:7BEO (Figure 9/H), PDB:1XAK (Figure 9/I) protein targets. It is probably true that the injudicious use involving the management of these quantum ideas or points can cause problems, it is also true that they do and should play an important role quantum mechanically in this drug discovery field (Figure 7/), (Table 8/), (Figure 8/), (Table 9/).

Significant Statements

In this project, I implemented Inverse Docking Algorithms with nonlinear electrodynamics for the cryptographic designing of the combination of GisitorviffirnaTM, Roccustyrna_{gs1}TM, and Roccustyrna_{fr1}TM ligands which generated the highest negative docking energies when compared to other FDA approved small molecules onto the SARS-COV-2 protein targets by solving Chern-Simons Topology Euclidean Geometrics in a Lindenbaum-Tarski equations (1-70) based QSAR automating

modeling for practical quantum computing, and Artificial Intelligence-Driven Predictive Neural Networks.

- **Availability of data and materials**

The author confirms that the data supporting the findings of this study are available upon request. Authors will release the atomic coordinates and experimental data upon article publication.

- **Competing interests**

No potential competing interest was reported by the author.

- **Funding**

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- **Data Availability Statements**

- Due to confidentiality agreements, data included in this research work have been generated at Biogenea's central large-scale facility Department of Biogeneto - ligandanolQMMIDDD/QRPICA/MACHNOT/ QIICDNNDCa ADMET/QIICDNNDCa Stations and are available upon request.

- **Authors' contributions**

Author's diverse contributions to the published work are accurate and agreed.

Author has contributed to the below multiple roles:

- Conceptualization of Ideas, Formulation or evolution of overarching research goals and aims.
- Methodology, Development and design of methodology, creation of models Software, Programming, software development; designing computer programs; implementation of the computer code and supporting algorithms; testing of existing code components.
- Validation, Verification, whether as a part of the activity or separate, of the overall replication/reproducibility of results/experiments and other
- research outputs
- Formal analysis Application of statistical, mathematical, computational, or other formal techniques to analyze or synthesize study data□

- Investigation, conducting a research and investigation process, specifically performing the experiments, or data/evidence collection.
- Resources of study materials, reagents, materials, patients, laboratory samples, animals, instrumentation, computing resources, or other analysis tools
- Data Curation, Management activities to annotate (produce metadata), scrub data and maintain research data (including software code, where it is necessary for interpreting the data itself) for initial use and later reuse.
- Writing - Original Draft, Preparation, creation, and presentation of the published work, specifically writing the initial draft (including substantive translation)
- Writing - Review & Editing Preparation, creation and/or presentation of the published work by those from the original research group, specifically critical review, commentary, or revision – including pre-or post-publication stages.
- Visualization, Preparation, creation, and presentation of the published work, specifically visualization/ data presentation
- Supervision, Oversight and leadership responsibility for the research activity planning and execution, including mentorship external to the core team Project administration, Management and coordination responsibility for the research activity planning and execution.

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Ancillary Information

Ancillary Informations are attached as a separate file.

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