Improved (DFT) Generalized k-nearest information systems on Molecular QSAR-QMMM Cryptographic Mining and Chern-Simons Weighted ℓ neuron(l):= $\varphi \otimes D \otimes R^2 \otimes S \otimes R^1$ Topologies for the generation of the Roccustyrna Ligand Targeting SARS-COV-2 D614G Binding Sites.

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Research Article

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Improved (DFT) Generalized k-nearest information systems on Molecular QSAR-QMMM Cryptographic Mining and Chern-Simons Weighted ℓ neuron(ι):= $\varphi \circ D \circ R_2 \circ S \circ R_1$ Topologies for the generation of the Roccustyrna Ligand Targeting SARS-COV-2 D614G Binding Sites.

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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 for generalized formalisms of k-nearest neighbors as a Tipping–Ogilvie and Machine Learning application within the quantum computing context targeting the atomistic level of the protein apparatus of the SARS-COV-2 viral characteristics. In this effort, we 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 AI-Quantum designed molecules of GisitorviffirnaTM, Roccustyrna_{gs1}TM, and Roccustyrna_{fr1}TM ligands targeting the COVID-19-SARS-COV-2 SPIKE D614G mutation by unifying Molecular Pairs (MMP), Lindenbaum-Tarski logical spaces and Adaptive Weighted KNN Positioning for Matched Bemis and Murko (BM) driven eigenvalue statements into Shannon entropy quantities as composed by Tipping–Ogilvie driven Machine Learning potentials on a (DFT) ℓ neuron(ι):= $\varphi \circ D \circ R_2 \circ S \circ R_1$ $c_0 \zeta_2(1 + \sum i) = [A \wedge A'(p)] \otimes [\partial \hat{v} \partial \hat{q}, \partial \hat{u} \partial \hat{p}] - [\partial \hat{v} \otimes \partial \hat{p}, \otimes \partial \hat{u} \otimes \partial \hat{q}] = 1 c i \xi i \{ - \hbar 2 0 < \equiv \equiv \equiv \langle \psi * || \psi * \rangle = [A \wedge A'(p)] \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi) (xp), D(\alpha): (xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r): (xp) \mapsto (e - r 0 0 e r)(xp), BS(\theta): x_1 x_2 p_1 p_2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 0 0 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v = 0, 1, 2, \dots \lambda = 1/2 + \gamma_2 + 1/4 c_1 \langle \psi || (1 - \rho^0) || \psi \rangle [A \wedge A'(p)] \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi) (xp), D(\alpha): (xp) \mapsto (x + Re(\alpha)p + \int_{\mathbb{R}^3} \langle \psi || \rho^0 || \psi \rangle a_{22} v K S_1(r) = v_{ext}(r) + \int dr' \rho(r') || r - r' || + v X C_1(r) m b_2 r_2 e d_2 \pi^2 B_2 m B V [P - \sqrt{Q} - (r r y v \Gamma(b + v) \Gamma(c) v! c_0 a_2 \sqrt{-} - \sqrt{Q} - (r r y v \Gamma(b + v) \Gamma(c) v! c_0 a_2 Q - \sqrt{P} - \sqrt{Q})] \equiv |C m d \pi C d \pi_2 | \phi(W \hat{x} + \alpha)\rangle, dy_2 \Sigma \Sigma^Q \otimes \bar{\sigma} - \bar{\sigma} \sigma^q - i_- + c_0 a_2 [1 - y y]_2 \} \psi(y) v) \text{ improver for Chern-Simons Topology Euclidean Geometrics.}$

1

PDB:6WZU

3D Docking Interactions of the combination of GisitorviffirnaTM, 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

Illustration1. 3D Docking representations of (i) GisitorviffirnaTM, (ii) Roccustyrna_gs1_TM, and (ii) Roccustyrna_fr1_TM fragments when targeted onto the PDB:6WZU SARS-Cov-2 protein targets.

Introduction

(1,2,3) The COVID-19 viral infectious which emerged in China at the end of 2019 previously provisionally named 2019-nCoV or 2019 novel coronavirus was officially 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) in the range 2.0-6.0 with a reproductive number (RN) 5,4 higher than SARS and Middle East Respiratory Syndrome Coronavirus (MERS) respectively (8) with more than 44,000 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 have 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 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 drug-protein-gene interactions of personalized intervention options for control, characterize, and prevention of viral outbreaks, and 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 (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 a common approach as a quantum-many body premium technique and semi-empirical computational scheme in place (24) of the quantum processor and docking energy used for studying molecule structure under QM simulated sampling error among other quantitative understanding observables. Density Field Theories (DFT) is continuously increasing for more systematic and less expensive methods (25) when compared to traditional drug development approaches to repositioning drugs and physical extracts and represent the similarities (26) and dissimilarities (27) between drugs and repurposed viral proteins, respectively. (28) However, the Schrödinger equations 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 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. Molecular Pairs (MMP), Lindenbaum-Tarski logical spaces, and Adaptive Weighted KNN Positioning Matched Bemis and Murko (BM) driven eigenvalue statements were incorporated in this project when analyzing pharmacological data allowing a well-defined superposition for each fragmented pharmacophore. This shows that the application to quantum computing as orthogonally applied for the design of small molecules may allow pure mechanical computations both for re-generating Lipinski rules and quantum 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 associated axiomatic formulations (AQFT) for Lindenbaum-Tarski guided Adaptive Weighted KNN Positioning 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 subbase supersymmetric solutions have 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 Molecular Pairs (MMP) as a core part of contemporary physics (Minkowski-type, wave-edge, etc), (20,27,32-33) including von Neumann and Dirac formulation states as well as probabilistic transformations on Murko (BM) driven eigenvalue statements for algebraic multi-metrics (Triangle area, Bond-angle, etc) were incorporated in this project to treat Tipping-Ogilvie and Machine Learning observables as foundational according to the interaction information theory (QIT) reference frames. (20,33,34,35) In this project, we show an original strategy and demonstrate the utility and the mechanics of this (32) unified molecular formalism as a Tipping-Ogilvie and Machine Learning QMMMP application within the quantum computing context as perturbed asymptotically through the example of 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 Quasi-helical 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. To demonstrate its flexibility, we tackle a hugely different objective issued from the organic molecular materials domain. We show that our method can generate sets of optimized critical molecules having high energy or low energy, starting only from penicillamine derivatives. We can also set constraints on a synthesizability score and structural features. The basic idea developed in Levine (2004) incorporates critical components of what is to be expected from a —real|| 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. Maximum Common Substructure (MCS) topologies for generalized k-nearest neighbors on Tipping–Ogilvie and Machine Learning generated Molecular Pairs (MMP), and an Adaptive Weighted KNN Positioning Matched Bemis and Murko (BM) approach for Predictive Neural Networks and Quantum- Inspired frameworks were employed for supercritical entanglements introducing an advanced quantum mechanical inverse docking algorithm providing further insight to confirm the practicality of docking energy predictions. In this protocol, tools from conventional cryptography for wild type and selected mutations for Nsp3 (papain-like, PLpro domain), Nsp5 Nsp15 (NendoU), (Mpro, 3CLpro), Nsp12 (RdRp), N protein and Spike were combined as inputs and the key element functions of SARS-CoV-2 protein pathways in understanding and designing possible novel antiviral agents, from both a quantum algebraic and a cheminformatic perspective along with the principles of the regulation of computer-aided drug discovery methodologies. This paper concentrates on the unification of quantum mechanics fundamental theories into a master wave equation for a generalized k-nearest molecular oscillator described by the second-order term of the Tipping–Ogilvie potential expansion with Chern Simons connections over compact of $\psi(y)v=Ev=y\lambda\exp[-\beta vy]F(\lambda-\gamma 2/\beta v, 2\lambda, 2\beta vy)F(c,b;y)=\sum_{v=0}^{\infty}\Gamma(c+v)\Gamma(b)y^v\Gamma(b+v)\Gamma(c)v!c0a2[1-\gamma 2(v+\lambda)2]v=0,1,2,\dots\lambda=1/2+\gamma 2+1/4c0a2[1-yy]2\psi(y)v(\phi k)\otimes k1mCQ2t|\phi(t)c0\zeta 2(1+\sum i)=[\Lambda\Lambda'(p)]\otimes[\partial v^{\wedge}\partial q^{\wedge},\partial u^{\wedge}\partial p^{\wedge}]-[\partial v^{\wedge}\otimes\partial p^{\wedge},\otimes\partial u^{\wedge}\otimes\partial q^{\wedge}]=1ci\xi i\{-\hbar 20<\equiv\equiv\equiv\langle\psi*||\psi*\rangle=[\Lambda\Lambda'(p)]\mapsto(\cos\phi-\sin\phi\sin\phi\cos\phi)\frac{\partial}{\partial t}\hat{P}\psi(t)|\partial\theta(t)/\partial t\rangle\int 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20<\equiv\equiv\equiv\langle\psi*||\psi*\rangle=[\Lambda\Lambda'(p)]\mapsto(\cos\phi-\sin\phi\sin\phi\cos\phi)(xp),D(\alpha):(xp)\mapsto(x+Re(\alpha)p+Im(\alpha)),S(r):(xp)\mapsto(e-r00er)(xp),BS(\theta):x1x2p1p2\mapsto\cos\theta\sin\theta-\sin\theta\cos\theta\cos\theta\sin\theta00-\sin\theta\cos\theta x1x2p1p2v=0,1,2,\dots\lambda=1/2+\gamma 2+1/4c1\langle\psi||(\mathbb{1}^{\wedge}-\rho^{\wedge}0)||\psi\rangle)[\Lambda\Lambda'(p)]\mapsto(\cos\phi-\sin\phi\sin\phi\cos\phi)(xp),D(\alpha):(xp)\mapsto(x+Re(\alpha)p+Im(\alpha)),S(r):(xp)\mapsto(e-r00er)(xp),BS(\theta):x1x2p1p2\mapsto\cos\theta\sin\theta-\sin\theta\cos\theta\cos\theta\sin\theta00-\sin\theta\cos\theta x1x2p1p2v=0,1,2,\dots\lambda=1/2+\gamma 2+1/4c1\delta ij-[\Lambda\Lambda'(p)]\mapsto(\cos\phi-\sin\phi\sin\phi\cos\phi)(xp),D(\alpha):(xp)\mapsto(x+Re(\alpha)p+Im(\alpha)),S(r):(xp)\mapsto(e-r00er)(xp),BS(\theta):x1x2p1p2\mapsto\cos\theta\sin\theta-\sin\theta\cos\theta\cos\theta\sin\theta00-\sin\theta\cos\theta 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2+1/4c1\psi||(\mathbb{1}^{\wedge}-\rho^{\wedge}0)||\psi\rangle)[\Lambda\Lambda'(p)]\mapsto(\cos\phi-\sin\phi\sin\phi\cos\phi)(xp),D(\alpha):(xp)\mapsto(x+Re(\alpha)p+Im(\alpha)),S(r):(xp)\mapsto(e-r00er)(xp),BS(\theta):x1x2p1p2\mapsto\cos\theta\sin\theta-\sin\theta\cos\theta\cos\theta\sin\theta00-\sin\theta\cos\theta x1x2p1p2v=0,1,2,\dots\lambda=1/2+\gamma 2+1/4c1\psi||(\mathbb{1}^{\wedge}-\rho^{\wedge}0)||\psi\rangle)[\Lambda\Lambda'(p)]\mapsto(\cos\phi-\sin\phi\sin\phi\cos\phi)(xp),D(\alpha):(xp)\mapsto(x+Re(\alpha)p$

$2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x_1 x_2 p_1 p_2 v = 0, 1, 2, \dots, \lambda = 1/2 + \gamma_2 + 1/4 c_1 \delta_{ij} - [A\Lambda A'(p)]$
 $\mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi) \quad (xp), D(\alpha):(xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r):(xp) \mapsto (e - r00er)(xp), BS(\theta):x_1 x_2 p_1 p_2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x_1 x_2 p_1 p_2 v = 0, 1, 2, \dots, \lambda = 1/2 + \gamma_2 + 1/4 c_1 \langle \psi || \rho^0 || \psi \rangle N - Tr[\rho^0] - \sum N_i = 1, j \neq i \langle \psi || \rho^0 || \psi \rangle 1 - 2\Re \sum N_i = 1 \quad \text{where } A < irr7\Gamma jIP[N](a_4 \cos 4\theta) - j < i \langle \psi || \rho^0 || \psi \rangle a_{22} v_{KS1}(r) a_4 \cos 2\theta + a_2 r_2 + r_4 \rangle \Sigma_3' \langle \psi || \rho^0 || \psi \rangle a_{22} v_{KS1}(r) = v_{ext}(r) + \int dr' \rho(r') ||r - r'|| + v_{XC1}(r) m b_2 r_2 e d_2 \pi^2 B_2 m B V[P^- \sqrt{Q^-} (rr_y v \Gamma(b+v) \Gamma(c) v! c_0 a_2 \sqrt{-\sqrt{Q^-} (rr_y v \Gamma(b+v) \Gamma(c) v! c_0 a_2 Q^- \sqrt{P^-} \sqrt{P^-}})] \equiv |C m d \pi C d \pi_2 | \phi(W x^+ + \alpha) \rangle, (17 \partial t \hat{P} \psi(t) | \partial \theta(t) / \partial t) \int M_3 \psi A] = (\nabla p k)^2 / p k + 4 m_2 \hbar^2 0 < \equiv = = \langle \psi_* || \psi_* \rangle = [A\Lambda A'(p)] \mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi) (xp), D(\alpha):(xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r):(xp) \mapsto (e - r00er)(xp), BS(\theta):x_1 x_2 p_1 p_2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x_1 x_2 p_1 p_2 v = 0, 1, 2, \dots, \lambda = 1/2 + \gamma_2 + 1/4 c_1 \langle \psi || (\hat{1} - \rho^0) || \psi \rangle [A\Lambda A'(p)]$
 $\mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi) \quad (xp), D(\alpha):(xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r):(xp) \mapsto (e - r00er)(xp), BS(\theta):x_1 x_2 p_1 p_2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x_1 x_2 p_1 p_2 v = 0, 1, 2, \dots, \lambda = 1/2 + \gamma_2 + 1/4 c_1 \delta_{ij} - [A\Lambda A'(p)]$
 $\mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi) \quad (xp), D(\alpha):(xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r):(xp) \mapsto (e - r00er)(xp), BS(\theta):x_1 x_2 p_1 p_2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x_1 x_2 p_1 p_2 v = 0, 1, 2, \dots, \lambda = 1/2 + \gamma_2 + 1/4 c_1 \langle \psi || \rho^0 || \psi \rangle N - j < i \langle \psi || \rho^0 || \psi \rangle a_{22} v_{KS1}(r) a_4 \cos 2\theta + a_2 r_2 + r_4 \rangle \Sigma_3' \langle \psi || \rho^0 || \psi \rangle j j_2 k p k \wedge d A) k + 13 \psi \langle A(\nabla R k)^2 + R_2 k \nabla \phi k \wedge [A\Lambda A] \hbar^2 0 < \equiv = = \langle \psi_* || \psi_* \rangle = [A\Lambda A'(p)] \mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi) (xp), D(\alpha):(xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r):(xp) \mapsto (e - r00er) \quad (xp), BS(\theta):x_1 x_2 p_1 p_2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x_1 x_2 p_1 p_2 v = 0, 1, 2, \dots, \lambda = 1/2 + \gamma_2 + 1/4 c_1 \langle \psi || (\hat{1} - \rho^0) || \psi \rangle [A\Lambda A'(p)]$
 $\mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi) \quad (xp), D(\alpha):(xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r):(xp) \mapsto (e - r00er)(xp), BS(\theta):x_1 x_2 p_1 p_2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x_1 x_2 p_1 p_2 v = 0, 1, 2, \dots, \lambda = 1/2 + \gamma_2 + 1/4 c_1 \delta_{ij} - [A\Lambda A'(p)] \mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi) \quad (xp), D(\alpha):(xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r):(xp) \mapsto (e - r00er)(xp), BS(\theta):x_1 x_2 p_1 p_2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x_1 x_2 p_1 p_2 v = 0, 1, 2, \dots, \lambda = 1/2 + \gamma_2 + 1/4 c_1 \langle \psi || \rho^0 || \psi \rangle N - Tr[\rho^0] - \sum N_i = 1, j \neq i \langle \psi || \rho^0 || \psi \rangle 1 - 2\Re j i \langle \psi || \rho^0 || \psi \rangle a_{22} v_{KS1}(r) a_4 \cos 2\theta + a_2 r_2 + r_4 \rangle \Sigma_3' \langle \psi || \rho^0 || \psi \rangle dy_2 \Sigma \Sigma^Q \otimes \bar{\sigma} - \bar{\sigma} \sigma^Q - i_+ c_0 a_2 [1 - yy]_2 \} \psi(y) v) R_2(\phi k) \otimes k_1 m C Q_2 t | \phi(t) \text{ to be a better representation of the realistic potentials in computation of energy eigenvalues.}$

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, 3fqg, 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, 3fqg, 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 Biogenetoligandorol™. 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 Biogenetoligandorol™ (Biogenetoligandorol™, Synthocure™, 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 Roccustyrna small molecule using the Biogenetoligandorol™ cluster of algorithms.

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 (Tab s1/) after exhaustive virtual screening analysis was obtained accordingly, Colchicine, Raltegravir, Hexacosanol, Benzoxazolinon, Carboxy-Pentadic 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([N]H]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 [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([N]H)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) (Fig s1/). 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

-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) Therefore, from a mathematical perspective, a TQFT that recovers the above AI-Quantum Hilbert symmetric spaces may be called –Chern–Simon’s theory. The generative model featured an embedding layer followed by three gated recurrent units (GRU) [37] with 356 dimensions, and finally a linear layer that reshaped the outputs to the size of all possible tokens. The loss function is the Negative Log-Likelihood (NLL): where “xt” is a random variable representing the probability for all possible tokens of the vocabulary at step “t” and “xt-1” is the token chosen at the previous step. 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 $\partial t \hat{P}$

$$\psi(t)|\partial\theta(t)/\partial t\rangle \int M_3\psi A] = (\nabla pk)^2/pk + 4m_2\hbar^2 0 < \equiv = \langle \psi_* || \psi_* \rangle = [A\Lambda A'(p)] \mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi)$$

$$(xp), D(\alpha):(xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r):(xp) \mapsto (e - r00er)(xp), BS(\theta):x_1x_2p_1p_2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x_1x_2p_1p_2v=0,1,2 \dots \lambda=1/2+\gamma^2+1/4c_1\langle\psi||(\mathbb{1}^{\wedge}-\rho^{\wedge}0)||\psi\rangle][A\Lambda A'(p)]$$

$$\mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi) (xp), D(\alpha):(xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r):(xp) \mapsto (e - r00er)(xp), BS(\theta):x_1x_2p_1p_2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x_1x_2p_1p_2v=0,1,2 \dots \lambda=1/2+\gamma^2+1/4c_1\delta_{ij} - \sum N_i, j=1\langle\psi||\rho^{\wedge}0||\psi\rangle N - Tr[\rho^{\wedge}0] - \sum N_i=1, j \neq i\langle\psi||\rho^{\wedge}0||\psi\rangle 1 - 2\Re \sum N_i=1 \text{ where}$$

$$A < irr7\Gamma jIP[N](a_4\cos 4\theta) - j < i\langle\psi||\rho^{\wedge}0||\psi\rangle a_{22}vKS_1(r)a_4\cos 2\theta + a_2r_2 + r_4 \Sigma_3' \langle\psi||\rho^{\wedge}0||\psi\rangle jj_2kp_k \wedge dA)k + 13$$

$$\psi \langle A(\nabla Rk)^2 + R_2k \nabla \phi k \wedge [A\Lambda A] \hbar^2 0 < \equiv = \langle \psi_* || \psi_* \rangle = [A\Lambda A'(p)] \mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi)$$

$$(xp), D(\alpha):(xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r):(xp) \mapsto (e - r00er)(xp), BS(\theta):x_1x_2p_1p_2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x_1x_2p_1p_2v=0,1,2 \dots \lambda=1/2+\gamma^2+1/4c_1\langle\psi||(\mathbb{1}^{\wedge}-\rho^{\wedge}0)||\psi\rangle][A\Lambda A'(p)]$$

$$\mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi) (xp), D(\alpha):(xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r):(xp) \mapsto (e - r00er)(xp), BS(\theta):x_1x_2p_1p_2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x_1x_2p_1p_2v=0,1,2 \dots \lambda=1/2+\gamma^2+1/4c_1\delta_{ij} - [A\Lambda A'(p)] \mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi) (xp), D(\alpha):(xp) \mapsto (x + Re(\alpha)p + Im(\alpha)),$$

$$S(r):(xp) \mapsto (e - r00er)(xp), BS(\theta):x_1x_2p_1p_2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x_1x_2p_1p_2v=0,1,2 \dots \lambda=1/2+\gamma^2+1/4c_1\langle\psi||\rho^{\wedge}0||\psi\rangle N - Tr[\rho^{\wedge}0] - \sum N_i=1, j \neq i\langle\psi||\rho^{\wedge}0||\psi\rangle 1 - 2\Re \sum N_i=1 \text{ where}$$

$$A < irr7\Gamma jIP[N]i\langle\psi||\rho^{\wedge}0||\psi\rangle a_{22}vKS_1(r)a_4\cos 2\theta + a_2r_2 + r_4 \Sigma_3' \langle\psi||\rho^{\wedge}0||\psi\rangle (25,29). \text{ 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^{i\{rt\}}(p(r', t)\partial t \hat{P} \psi(t)|\partial\theta(t)/\partial t\rangle \int M_3\psi A] = (\nabla pk)^2/pk + 4m_2\hbar^2 0 < \equiv = \langle \psi_* || \psi_* \rangle = [A\Lambda A'(p)] \mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi) (xp), D(\alpha):(xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r):(xp) \mapsto (e - r00er)(xp), BS(\theta):x_1x_2p_1p_2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x_1x_2p_1p_2v=0,1,2 \dots \lambda=1/2+\gamma^2+1/4c_1\langle\psi||(\mathbb{1}^{\wedge}-\rho^{\wedge}0)||\psi\rangle][A\Lambda A'(p)] \mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi) (xp), D(\alpha):(xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r):(xp) \mapsto (e - r00er)(xp), BS(\theta):x_1x_2p_1p_2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x_1x_2p_1p_2v=0,1,2 \dots \lambda=1/2+\gamma^2+1/4c_1\delta_{ij} - [A\Lambda A'(p)] \mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi) (xp), D(\alpha):(xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r):(xp) \mapsto (e - r00er)(xp), BS(\theta):x_1x_2p_1p_2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x_1x_2p_1p_2v=0,1,2 \dots \lambda=1/2+\gamma^2+1/4c_1\langle\psi||(\mathbb{1}^{\wedge}-\rho^{\wedge}0)||\psi\rangle][A\Lambda A'(p)] \mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi) (xp), D(\alpha):(xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r):(xp) \mapsto (e - r00er)(xp), BS(\theta):x_1x_2p_1p_2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x_1x_2p_1p_2v=0,1,2 \dots \lambda=1/2+\gamma^2+1/4c_1\delta_{ij} - [A\Lambda A'(p)] \mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi)$$

$(xp), D(\alpha):(xp) \mapsto (x + \text{Re}(\alpha)p + \text{Im}(\alpha)), S(r):(xp) \mapsto (e - r00er)(xp), BS(\theta):x1x2p1p2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x1x2p1p2v=0,1,2 \dots \lambda=1/2+\gamma 2+1/4c1\langle \psi||\rho^0||\psi \rangle N - \text{Tr}[\rho^{\wedge} \rho^0] - \sum Ni=1, j \neq i \langle \psi||\rho^0||\psi \rangle$
 $1-2\Re \sum Ni=1$ where $A < irr7\Gamma jIP[N](a4\cos 4\theta) - j < i \langle \psi||\rho^0||\psi \rangle a22vKS1(r)$
 $a4\cos 2\theta + a2r2 + r4) \Sigma 3' \langle \psi||\rho^0||\psi \rangle$ (equation2) $V'ip = (V'ip + iV'f)$ eif, (equation3) $\rho^{-s}QFI \approx \sum i=01 \text{Re}(\rho i12)$
 $2(1\rho i11 + 1\rho i22) + (\rho i11 - \rho i22) 2\rho i11 + \rho i22$, (equation4) $\rho 1ij = \langle v_i \langle 1 \rho s$ (equation5) $v_j \rangle 1 \rangle$
(equation6) $\rho 0ij = \langle v_i \langle 0 \rho s(0) v_j \rangle 0 \rangle 0 \rangle \partial t \hat{P} \psi(t) |\partial \theta(t) / \partial t \rangle \int M3 \psi A = (\nabla pk) 2 / pk + 4m2 \hbar 20 < \equiv =$
 $= \langle \psi * || \psi * \rangle = [A \wedge A'(p)] \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi) (xp), D(\alpha):(xp) \mapsto (x + \text{Re}(\alpha)p + \text{Im}(\alpha)),$
 $S(r):(xp) \mapsto (e - r00er)(xp), BS(\theta):x1x2p1p2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x1x2p1p2v=0,1,2$
 $\dots \lambda=1/2+\gamma 2+1/4c1\langle \psi||(\hat{1} - \rho^0)||\psi \rangle [A \wedge A'(p)] \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi) (xp), D(\alpha):(xp) \mapsto$
 $(x + \text{Re}(\alpha)p + \text{Im}(\alpha)), S(r):(xp) \mapsto (e - r00er)(xp), BS(\theta):x1x2p1p2 \mapsto \cos\theta \sin\theta -$
 $\sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x1x2p1p2v=0,1,2 \dots \lambda=1/2+\gamma 2+1/4c1\delta ij - \sum Ni,$
 $j=1 \langle \psi||\rho^0||\psi \rangle N - \text{Tr}[\rho^{\wedge} \rho^0] - \sum Ni=1, j \neq i \langle \psi||\rho^0||\psi \rangle 1 - 2\Re \sum Ni=1$ where $A < irr7\Gamma jIPi \langle \psi||\rho^0||\psi \rangle$
 $a22vKS1(r) a4\cos 2\theta + a2r2 + r4) \Sigma 3' \langle \psi||\rho^0||\psi \rangle jj2kpk \wedge dA) k + 13 \psi \langle A(\nabla Rk) 2 + R2k \nabla \phi k \wedge [A \wedge A] \hbar 201 \rangle$
Molecular scaffolds are generally used to describe the common core structures of the molecules [25]. The selected herbs are classified into structural classes using the characteristic scaffolds of each group [14]. In medicinal chemistry, a molecular scaffold is used to represent the core structure of a group of active compounds. Since the compounds with the same scaffold may influence a particular metabolic pathway, the molecular scaffolds can effectively contribute to the prediction of biological activities [16]. The scaffold of molecule groups is defined as a common sub-graph of the graphs of the molecule groups. Representatively, Maximum Common Substructure (MCS), Matched Molecular Pairs (MMP), and Bemis and Murko (BM) are the commonly used methods to produce molecular scaffolds [22–30]. In addition to exact carbon skeleton matching, we also evaluated a fuzzy skeleton filter. The fuzzy scaffold filter was based on the carbon skeleton but used the atom pair fingerprint [36] for similarity assessment to compare carbon skeletons instead of exact scaffold match. For each generated carbon skeleton, an atom pair fingerprint was calculated, and different carbon skeletons were compared using the Tanimoto coefficient. If the coefficient value was at least 0.6, the two scaffolds were considered similar and the corresponding compound was added to the same bucket. The scaffold, as per the MMP method, is defined as the common part among molecules that have different molecular fragments at the same single specific site [38, 39]. MCS method defines a scaffold as the maximum common edge subgraph of the graphs of molecule groups [30]. Unlike the MMP and MCS methods, the scaffolds produced by the BM method reveal a hierarchical structure [31]. (equation7) $H1 = \gamma B0 \cdot S^1 \text{Re}(\rho i12) \rho i12 \rho s(0) \rho^{-s}$ (equation8) $S^1 = 12 \langle \rangle - 01 \rangle$) 30% ρs (equation9) $\rho^{-s} = H \otimes m$ (equation10) $V'2ip = \{V'2ip + 2iV'f \cdot V' (p + (pV'2f + W \leftarrow S(I \otimes H) (equation11) M1; \langle p(V'f) (equation12) e\phi f, i \rangle = \langle \Phi | MT$
 $(I3 - NT) - 2(\rho \otimes I2) | \Phi \rangle (f + if \langle p) (equation13) \text{eif}$, and the Schrödinger equation becomes $n \geq 2m(V, z(p + 2iV'f \cdot V' (p + i(pV'f - M = \{M0, M1\} (equation14) (V'fY \langle p) = ifi I3 \leftarrow E(m2) (equation15) (*m2 - dimensional identity*) ((\langle p + if(p) - g.(V' (p + i(pv'f))$ 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 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-Pentadic acid, Ursane, Antheraxanthin, RA-XIII, Crotonate and Byrsonima coccolobifolia. (Tab s1/), (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) $\partial t \hat{P}$
 $\psi(t) |\partial \theta(t) / \partial t \rangle \int M3 \psi A = (\nabla pk) 2 / pk + 4m2 \hbar 20 < \equiv = \langle \psi * || \psi * \rangle = [A \wedge A'(p)] \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$
 $(xp), D(\alpha):(xp) \mapsto (x + \text{Re}(\alpha)p + \text{Im}(\alpha)), S(r):(xp) \mapsto (e - r00er)(xp), BS(\theta):x1x2p1p2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x1x2p1p2v=0,1,2 \dots \lambda=1/2+\gamma 2+1/4c1\langle \psi||(\hat{1} - \rho^0)||\psi \rangle [A \wedge A'(p)]$
 $\mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$
 $(xp), D(\alpha):(xp) \mapsto (x + \text{Re}(\alpha)p + \text{Im}(\alpha)), S(r):(xp) \mapsto (e - r00er)(xp), BS(\theta):x1x2p1p2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x1x2p1p2v=0,1,2 \dots \lambda=1/2+\gamma 2+1/4c1\delta ij - [A \wedge A'(p)] \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$
 $(xp), D(\alpha):(xp) \mapsto (x + \text{Re}(\alpha)p + \text{Im}(\alpha)), S(r):(xp) \mapsto (e - r00er)(xp), BS(\theta):x1x2p1p2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x1x2p1p2v=0,1,2 \dots \lambda=1/2+\gamma 2+1/4c1\langle \psi||\rho^0||\psi \rangle N - \text{Tr}[\rho^{\wedge} \rho^0] - \sum Ni=1, j \neq i \langle \psi||\rho^0||\psi \rangle$

$1-2\Re\sum N_i=1$ where $A<irr7\Gamma jIP[N](a4\cos4\theta)\langle\psi||\rho^0||\psi\rangle jj2kpk\wedge dA)k+$
 $13\psi\langle A(\nabla Rk)^2+R2k\nabla\phi k\wedge[A\wedge A]\hbar20<\equiv\equiv\equiv\langle\psi*||\psi*\rangle=[A\wedge A'(p)]\mapsto(\cos\phi-\sin\phi\sin\phi\cos\phi)$
 $(xp),D(\alpha):(xp)\mapsto(x+Re(\alpha)p+Im(\alpha)),S(r):(xp)\mapsto(e-r00er)(xp),$
 $BS(\theta):x1x2p1p2\mapsto\cos\theta\sin\theta-\sin\theta\cos\theta\cos\theta\sin\theta00-\sin\theta\cos\theta x1x2p1p2v=0,1,2....\lambda=1/2+\gamma2+1/4c1\langle\psi||(\mathbb{1}^{\wedge}-\rho^0)||\psi\rangle[A\wedge A'(p)]\mapsto(\cos\phi-\sin\phi\sin\phi\cos\phi)$ $(xp),D(\alpha):(xp)\mapsto(x+Re(\alpha)p+Im$
 $(\alpha)),S(r):(xp)\mapsto(e-r00er)(xp),BS(\theta):x1x2p1p2\mapsto\cos\theta\sin\theta-\sin\theta\cos\theta\cos\theta\sin\theta00-\sin\theta\cos\theta x1x2p1p2v=0$
 $,1,2....\lambda=1/2+\gamma2+1/4c1\delta ij-[A\wedge A'(p)]\mapsto(\cos\phi-\sin\phi\sin\phi\cos\phi)$
 $(xp),D(\alpha):(xp)\mapsto(x+Re(\alpha)p+Im(\alpha)),S(r):(xp)\mapsto(e-r00er)(xp),BS(\theta):x1x2p1p2\mapsto\cos\theta\sin\theta-\sin\theta\cos\theta\cos$
 $\theta\sin\theta00-\sin\theta\cos\theta x1x2p1p2v=0,1,2....\lambda=1/2+\gamma2+1/4c1\langle\psi||\rho^0||\psi\rangle N-\text{Tr}[\rho^p^0]-\sum N_i=1,j\neq i\langle\psi||\rho^0||\psi\rangle$
 $1-2\Re\sum N_i=1$ where $A<irr7\Gamma jIPi\langle\psi||\rho^0||\psi\rangle a22vKS1(r)a4\cos2\theta+a2r2+r4)\Sigma3'\langle\psi||\rho^0||\psi\rangle$ Then one can
choose $n\ g\{t\}$ such as to eliminate the purely time-dependent terms, and one finally arrives at, $= (2mV'2(p$
 $+mf; r'(p=ih(p,ipir,t)=-ea\ h\ J(pir',t)$ (equation17) $\partial t\hat{P}$
 $\psi(t)|\partial\theta(t)/\partial t)\int M3\psi A]=(\nabla pk)^2/pk+4m2\hbar20<\equiv\equiv\equiv\langle\psi*||\psi*\rangle=[A\wedge A'(p)]\mapsto(\cos\phi-\sin\phi\sin\phi\cos\phi)$
 $(xp),D(\alpha):(xp)\mapsto(x+Re(\alpha)p+Im(\alpha)),S(r):(xp)\mapsto(e-r00er)(xp),BS(\theta):x1x2p1p2\mapsto\cos\theta\sin\theta-\sin\theta\cos\theta\cos$
 $\theta\sin\theta00-\sin\theta\cos\theta x1x2p1p2v=0,1,2....\lambda=1/2+\gamma2+1/4c1\langle\psi||(\mathbb{1}^{\wedge}-\rho^0)||\psi\rangle[A\wedge A'(p)]$
 $\mapsto(\cos\phi-\sin\phi\sin\phi\cos\phi)$ $(xp),D(\alpha):(xp)\mapsto(x+Re(\alpha)p+Im(\alpha)),S(r):(xp)\mapsto(e-r00er)(xp),B$
 $S(\theta):x1x2p1p2\mapsto\cos\theta\sin\theta-\sin\theta\cos\theta\cos\theta\sin\theta00-\sin\theta\cos\theta x1x2p1p2v=0,1,2....\lambda=1/2+\gamma2+1/4c1\delta ij-[A\wedge$
 $A'(p)]\mapsto(\cos\phi-\sin\phi\sin\phi\cos\phi)$ $(xp),D(\alpha):(xp)\mapsto(x+Re(\alpha)p+Im(\alpha)),$
 $S(r):(xp)\mapsto(e-r00er)(xp),BS(\theta):x1x2p1p2\mapsto\cos\theta\sin\theta-\sin\theta\cos\theta\cos\theta\sin\theta00-\sin\theta\cos\theta x1x2p1p2v=0,1,2$
 $....\lambda=1/2+\gamma2+1/4c1\langle\psi||\rho^0||\psi\rangle N-\text{Tr}[\rho^p^0]-\sum N_i=1,j\neq i\langle\psi||\rho^0||\psi\rangle$ $1-2\Re\sum N_i=1$ where
 $\langle A(\nabla Rk)^2+R2k\nabla\phi k\wedge[A\wedge A]\hbar20<\equiv\equiv\equiv\langle\psi*||\psi*\rangle=[A\wedge A'(p)]\mapsto(\cos\phi-\sin\phi\sin\phi\cos\phi)$
 $(xp),D(\alpha):(xp)\mapsto(x+Re(\alpha)p+Im(\alpha)),S(r):(xp)\mapsto(e-r00er)(xp),BS(\theta):x1x2p1p2\mapsto\cos\theta\sin\theta-\sin\theta\cos\theta\cos$
 $\theta\sin\theta00-\sin\theta\cos\theta x1x2p1p2v=0,1,2....\lambda=1/2+\gamma2+1/4c1\langle\psi||(\mathbb{1}^{\wedge}-\rho^0)||\psi\rangle[A\wedge A'(p)]$
 $\mapsto(\cos\phi-\sin\phi\sin\phi\cos\phi)$ $(xp),D(\alpha):(xp)\mapsto(x+Re(\alpha)p+Im(\alpha)),S(r):(xp)\mapsto(e-r00er)$
 $(xp),BS(\theta):x1x2p1p2\mapsto\cos\theta\sin\theta-\sin\theta\cos\theta\cos\theta\sin\theta00-\sin\theta\cos\theta x1x2p1p2v=0,1,2....\lambda=1/2+\gamma2+1/4c1\delta i$
 $j-[A\wedge A'(p)]\mapsto(\cos\phi-\sin\phi\sin\phi\cos\phi)$ $(xp),D(\alpha):(xp)\mapsto(x+Re(\alpha)p+Im(\alpha)),S(r):(xp)\mapsto$
 $(e-r00er)(xp),BS(\theta):x1x2p1p2\mapsto\cos\theta\sin\theta-\sin\theta\cos\theta\cos\theta\sin\theta00-\sin\theta\cos\theta x1x2p1p2v=0,1,2....\lambda=1/2+\gamma$
 $2+1/4c1\langle\psi||\rho^0||\psi\rangle N-\text{Tr}[\rho^p^0]-\sum N_i=1,j\neq i\langle\psi||\rho^0||\psi\rangle$ $1-2\Re\sum N_i=1$ where $A<irr7\Gamma jIP[N](a4\cos4\theta)-$
 $j<i\langle\psi||\rho^0||\psi\rangle a22vKS1(r)a4\cos2\theta+a2r2+r4)\Sigma3'\langle\psi||\rho^0||\psi\rangle jj2kpk\wedge dA)k+13\psi\langle A(\nabla Rk)^2+R2k\nabla\phi k\wedge[A\wedge A]$
 $\hbar201\rangle$ (equation7) $H1=\gamma B0\cdot S^1Re(\rho i12)\rho i12ps(0)\rho^s$ (equation8) $S\rangle=12(\rangle-01\rangle)$ 30%ps
(equation9) $\rho^s=H\otimes m$ (equation10) $V'2ip=\{V'2ip+2iV'f-V'(p+(pV'2f+W\leftarrow S(I\otimes H)$ (equation11) $M1;$
 $<p(V'f)$ (equation12) $e\phi f,i>=\langle\Phi|MT(I3-NT)-2(\rho\otimes I2)|\Phi\rangle(f)+if<p$ (equation13) eif , and the
Schrödinger equation becomes $n\ 2\ 2\ m(V,z(p+2iV'f-V'(p+i(pVf-M=\{M0,M1\}$ (equation14) $(V'fY<p)$
 $=ifi\ I3\leftarrow E(m2)$ (equation15) (*m2-dimensional identity*) $((<p+if(p)-g.(V'(p+i(pv'f))$ 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 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-Pentatic acid, Ursane,
Antheraxanthin, RA-XIII, Crotonate and Byrsonima coccolobifolia. (Tab s1/), (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 $n\ g\{t\}$ 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.

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 .pdqt 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. Subsequently, substructure analysis was performed using DataWarrior 4.2.2, on the proposed SARS-COV-2 multi-target penicillamine derivative ligands predicted by both ligand-based and structure-based techniques (considering docking scores less than or equal to the threshold of the best F measure for each docking model

$$\partial t \hat{P} \psi(t) |\partial \theta(t) / \partial t| \int M^3 \psi A = (\nabla p k)^2 / p k + 4 m^2 \hbar^2 0 < \equiv \equiv = \langle \psi^* || \psi^* \rangle = [A \wedge A'(p)] \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$$

$$(xp), D(\alpha): (xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r): (xp) \mapsto (e - r 0 0 er)(xp), BS(\theta): x_1 x_2 p_1 p_2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 0 0 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v = 0, 1, 2, \dots \lambda = 1/2 + \gamma^2 + 1/4 c_1 \quad \langle \psi || \quad |(\hat{1} - \rho^0) || \psi \rangle [A \wedge A'(p)]$$

$$\mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi) \quad (xp), D(\alpha): (xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r): (xp) \mapsto (e - r 0 0 er)(xp), BS(\theta): x_1 x_2 p_1 p_2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 0 0 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v = 0, 1, 2, \dots \lambda = 1/2 + \gamma^2 + 1/4 c_1 \delta_{ij} - [A \wedge A'(p)] \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi) \quad (xp), D(\alpha): (xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r): (xp) \mapsto (e - r 0 0 er)(xp), BS(\theta): x_1 x_2 p_1 p_2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 0 0 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v = 0, 1, 2, \dots \lambda = 1/2 + \gamma^2 + 1/4 c_1 \langle \psi || \rho^0 || \psi \rangle N - Tr[\rho^0] - \sum N_i = 1, j \neq i \langle \psi || \rho^0 || \psi \rangle 1 - 2 \Re \sum N_i = 1 \quad \text{where}$$

$$A < irr 7 \Gamma j I P \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 0 0 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v = 0, 1, 2, \dots \lambda = 1/2 + \gamma^2 + 1/4 c$$

$$[N](a_4 \cos 4 \theta) - j < i \langle \psi || \rho^0 || \psi \rangle a_{22} v_{KS1}(r)$$

$$a_4 \cos 2 \theta + a_2 r^2 + r^4 \rangle \Sigma 3' \langle \psi || \rho^0 || \psi \rangle j j 2 k p k \wedge d A) k + 13 \psi \langle A(\nabla R k)^2 + R^2 k \nabla \phi k \wedge [A \wedge A] \hbar^2 0 < \equiv \equiv = \langle \psi^* || \psi^* \rangle = [A \wedge A'(p)] \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi) \quad (xp), D(\alpha): (xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r): (xp) \mapsto (e - r 0 0 er)(xp), BS(\theta): x_1 x_2 p_1 p_2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 0 0 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v = 0, 1, 2, \dots \lambda = 1/2 + \gamma^2 + 1/4 c_1 \langle \psi || (\hat{1} - \rho^0) || \psi \rangle [A \wedge A'(p)] \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$$

$$(xp), D(\alpha): (xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r): (xp) \mapsto (e - r 0 0 er)$$

$$(xp), BS(\theta): x_1 x_2 p_1 p_2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 0 0 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v = 0, 1, 2, \dots \lambda = 1/2 + \gamma^2 + 1/4 c_1 \delta_i j - [A \wedge A'(p)] \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$$

$$(xp), D(\alpha): (xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r): (xp) \mapsto (e - r 0 0 er)(xp), BS(\theta): x_1 x_2 p_1 p_2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 0 0 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v = 0, 1, 2, \dots \lambda = 1/2 + \gamma^2 + 1/4 c_1 \langle \psi || \rho^0 || \psi \rangle N - Tr[\rho^0] - \sum N_i = 1, j \neq i \langle \psi || \rho^0 || \psi \rangle 1 - 2 \Re \sum N_i = 1 \quad \text{where} \quad A < irr 7 \Gamma j I P [N](a_4 \cos 4 \theta) - j < i \langle \psi || \rho^0 || \psi \rangle a_{22} v_{KS1}$$

(r) $a_4 \cos 2 \theta + a_2 r^2 + r^4 \rangle \Sigma 3' \langle \psi || \rho^0 || \psi \rangle$. The chemical series found were (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 in addition to various compounds consisting of the common and frequent heterocycles identified originally in the substructural analysis of the extracted ChEMBL compounds. (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 publicly 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_gs1_TM, and Roccustyrna_fr1_TM cluster of molecular systems and the configuration of the new molecules 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_gs1_TM, and

Roccustyrna_fr1_TM 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 $\partial t \hat{P} \psi(t) | \partial \theta(t) / \partial t$)

$$\int M3 \quad \psi A] = (\nabla p k) 2 / p k + 4 m 2 \hbar 2 0 \equiv \equiv \langle \psi * || \psi * \rangle = [A \Lambda A'(p)] \quad \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$$

$$(x p), D(\alpha):(x p) \mapsto (x+R e(\alpha) p+I m(\alpha)), S(r):(x p) \mapsto (e-r 0 0 e r)(x p), B S(\theta): x 1 x 2 p 1 p 2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 0 0 - \sin \theta \cos \theta x 1 x 2 p 1 p 2 v=0,1,2 \dots \lambda=1 / 2+\gamma 2+1 / 4 c 1\langle \psi ||(\hat{1}-\rho^{\wedge} 0)|| \psi\rangle)[A \Lambda A'(p)]$$

$$\mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$$

$$(x p), D(\alpha):(x p) \mapsto (x+R e(\alpha) p+I m(\alpha)), S(r):(x p) \mapsto (e-r 0 0 e r)(x p), B S(\theta): x 1 x 2 p 1 p 2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 0 0 - \sin \theta \cos \theta x 1 x 2 p 1 p 2 v=0,1,2 \dots \lambda=1 / 2+\gamma 2+1 / 4 c 1 \delta i j-[A \Lambda A'(p)] \quad \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$$

$$(x p), D(\alpha):(x p) \mapsto (x+R e(\alpha) p+I m(\alpha)), S(r):(x p) \mapsto (e-r 0 0 e r)(x p), B S(\theta): x 1 x 2 p 1 p 2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 0 0 - \sin \theta \cos \theta x 1 x 2 p 1 p 2 v=0,1,2 \dots \lambda=1 / 2+\gamma 2+1 / 4 c 1\langle \psi || \rho^{\wedge} 0 || \psi\rangle N-\operatorname{Tr}[\rho^{\wedge} \rho^{\wedge} 0]-\sum N i=1, j \neq i\langle \psi || \rho^{\wedge} 0 || \psi\rangle$$

$$1-2 \Re \sum N i=1 \quad \text { where } \quad A< \operatorname{irr} 7 \Gamma j I P[N](a 4 \cos 4 \theta)-j< i\langle \psi || \rho^{\wedge} 0 || \psi\rangle a 2 2 v K S 1$$

$$(r) a 4 \cos 2 \theta+a 2 r 2+r 4) \Sigma 3'\langle \psi || \rho^{\wedge} 0 || \psi\rangle j j 2 k p k \wedge A) k+13 \psi\langle A(\nabla R k) 2+R 2 k \nabla \phi k \wedge[A \Lambda A] \hbar 2 0 \equiv \equiv \langle \psi * || \psi * \rangle=[$$

$$A \Lambda A'(p)] \quad \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi) \quad (x p), D(\alpha):(x p) \mapsto (x+R e(\alpha) p+I m(\alpha)), S(r):(x p) \mapsto$$

$$(e-r 0 0 e r)(x p), B S(\theta): x 1 x 2 p 1 p 2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 0 0 - \sin \theta \cos \theta x 1 x 2 p 1 p 2 v=0,1,2 \dots \lambda=1 / 2+\gamma$$

$$2+1 / 4 c 1\langle \psi ||(\hat{1}-\rho^{\wedge} 0)|| \psi\rangle)[A \Lambda A'(p)] \quad \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi) \quad (x p), D(\alpha):(x p) \mapsto (x+R e(\alpha) p+I m(\alpha)), S$$

$$(r):(x p) \mapsto (e-r 0 0 e r)(x p), B S(\theta): x 1 x 2 p 1 p 2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 0 0 - \sin \theta \cos \theta x 1 x 2 p 1 p 2 v=0,1,2 \dots$$

$$\lambda=1 / 2+\gamma 2+1 / 4 c 1 \delta i j-[A \Lambda A'(p)] \quad \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi) \quad (x p), D(\alpha):(x p) \mapsto (x+R e(\alpha) p+I m(\alpha)),$$

$$S(r):(x p) \mapsto (e-r 0 0 e r)(x p), B S(\theta): x 1 x 2 p 1 p 2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 0 0 - \sin \theta \cos \theta x 1 x 2 p 1 p 2 v=0,1,2$$

$$\dots \lambda=1 / 2+\gamma 2+1 / 4 c 1\langle \psi || \rho^{\wedge} 0 || \psi\rangle N-\operatorname{Tr}[\rho^{\wedge} \rho^{\wedge} 0]-\sum N i=1, j \neq i\langle \psi || \rho^{\wedge} 0 || \psi\rangle 1-2 \Re \sum N i=1 \quad \text { where }$$

$$A< \operatorname{irr} 7 \Gamma j I P[N](a 4 \cos 4 \theta)-j< i\langle \psi || \rho^{\wedge} 0 || \psi\rangle a 2 2 v K S 1(r) a 4 \cos 2 \theta+a 2 r 2+r 4) \Sigma 3'\langle \psi || \rho^{\wedge} 0 || \psi\rangle(5,13,29,31)$$

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 (Etotal) ||: (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 Biogenetoligandrol™. 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

$$\psi(t)|\partial\theta(t)/\partial t|\int M_3\psi A]=(\nabla pk)^2/pk+4m^2\hbar^2<=====\langle\psi_*||\psi_*\rangle=[A\wedge A'(p)]$$

$$\mapsto(\cos\phi-\sin\phi\sin\phi\cos\phi)$$

$$(xp),D(\alpha):(xp)\mapsto(x+Re(\alpha)p+Im(\alpha)),S(r):(xp)\mapsto(e-r00er)(xp),BS(\theta):x1x2p1p2\mapsto\cos\theta\sin\theta-\sin\theta\cos\theta\cos\theta\sin\theta00-\sin\theta\cos\theta x1x2p1p2v=0,1,2....\lambda=1/2+\gamma^2+1/4c1\langle\psi||(\mathbb{1}^{\wedge}-\rho^{\wedge}0)||\psi\rangle[A\wedge A'(p)]$$

$$\mapsto(\cos\phi-\sin\phi\sin\phi\cos\phi)$$

$$(xp),D(\alpha):(xp)\mapsto(x+Re(\alpha)p+Im(\alpha)),S(r):(xp)\mapsto(e-r00er)(xp),BS(\theta):x1x2p1p2\mapsto\cos\theta\sin\theta-\sin\theta\cos\theta\cos\theta\sin\theta00-\sin\theta\cos\theta x1x2p1p2v=0,1,2....\lambda=1/2+\gamma^2+1/4c1\delta_{ij}-[A\wedge A'(p)]$$

$$\mapsto(\cos\phi-\sin\phi\sin\phi\cos\phi)$$

$$(xp),D(\alpha):(xp)\mapsto(x+Re(\alpha)p+Im(\alpha)),S(r):(xp)\mapsto(e-r00er)(xp),BS(\theta):x1x2p1p2\mapsto\cos\theta\sin\theta-\sin\theta\cos\theta\cos\theta\sin\theta00-\sin\theta\cos\theta x1x2p1p2v=0,1,2....\lambda=1/2+\gamma^2+1/4c1\langle\psi||\rho^{\wedge}0||\psi\rangle N-\text{Tr}[\rho^{\wedge}p^{\wedge}0]-\sum Ni=1,j\neq i\langle\psi||\rho^{\wedge}0||\psi\rangle 1-2\Re\sum Ni=1$$

where

$$A\mapsto\cos\theta\sin\theta-\sin\theta\cos\theta\cos\theta\sin\theta00-\sin\theta\cos\theta x1x2p1p2v=0,1,2....\lambda=1/2+\gamma^2+1/4c$$

$$<irr7\Gamma jIP[N](a4\cos4\theta)-j<i\langle\psi||\rho^{\wedge}0||\psi\rangle a22vKS1(r)a4\cos2\theta+a2r^2+r4)\Sigma3'\langle\psi||\rho^{\wedge}0||\psi\rangle jj2kpk\wedge dA)k+13\psi\langle$$

$$A(\nabla Rk)^2+R2k\nabla\phi k\wedge[A\wedge A']\hbar^2<=====\langle\psi_*||\psi_*\rangle=[A\wedge A'(p)]$$

$$\mapsto(\cos\phi-\sin\phi\sin\phi\cos\phi)$$

$$(xp),D(\alpha):(xp)\mapsto(x+Re(\alpha)p+Im(\alpha)),S(r):(xp)\mapsto(e-r00er)(xp),BS(\theta):x1x2p1p2\mapsto\cos\theta\sin\theta-\sin\theta\cos\theta\cos\theta\sin\theta00-\sin\theta\cos\theta x1x2p1p2v=0,1,2....\lambda=1/2+\gamma^2+1/4c1\langle\psi||(\mathbb{1}^{\wedge}-\rho^{\wedge}0)||\psi\rangle[A\wedge A'(p)]$$

$$\mapsto(\cos\phi-\sin\phi\sin\phi\cos\phi)$$

$$(xp),D(\alpha):(xp)\mapsto(x+Re(\alpha)p+Im(\alpha)),S(r):(xp)\mapsto(e-r00er)(xp),BS(\theta):x1x2p1p2\mapsto\cos\theta\sin\theta-\sin\theta\cos\theta\cos\theta\sin\theta00-\sin\theta\cos\theta x1x2p1p2v=0,1,2....\lambda=1/2+\gamma^2+1/4c1\delta_{ij}-[A\wedge A'(p)]$$

$$\mapsto(\cos\phi-\sin\phi\sin\phi\cos\phi)$$

$$(xp),D(\alpha):(xp)\mapsto(x+Re(\alpha)p+Im(\alpha)),S(r):(xp)\mapsto(e-r00er)(xp),BS(\theta):x1x2p1p2\mapsto\cos\theta\sin\theta-\sin\theta\cos\theta\cos\theta\sin\theta00-\sin\theta\cos\theta x1x2p1p2v=0,1,2....\lambda=1/2+\gamma^2+1/4c1\langle\psi||\rho^{\wedge}0||\psi\rangle N-\text{Tr}[\rho^{\wedge}p^{\wedge}0]-\sum Ni=1,j\neq i\langle\psi||\rho^{\wedge}0||\psi\rangle$$

$$1-2\Re\sum Ni=1$$

where

$$A<irr7\Gamma jIP[N](a4\cos4\theta)-j<i\langle\psi||\rho^{\wedge}0||\psi\rangle$$

$$a22vKS1(r)a4\cos2\theta+a2r^2+r4)\Sigma3'\langle\psi||\rho^{\wedge}0||\psi\rangle$$

The binding affinity prediction and total energy ranking with the linear protein model and untailed 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. Biogenetoligandrol 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 Gisitorviffirna™, 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,3fq, 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>)

$$\psi(t)|\partial\theta(t)/\partial t|\int M_3\psi A]=(\nabla pk)^2/pk+4m^2\hbar^2<=====\langle\psi_*||\psi_*\rangle=[A\wedge A'(p)]$$

$$\mapsto(\cos\phi-\sin\phi\sin\phi\cos\phi)$$

$$(xp),D(\alpha):(xp)\mapsto(x+Re(\alpha)p+Im(\alpha)),S(r):(xp)\mapsto(e-r00er)(xp),BS(\theta):x1x2p1p2\mapsto\cos\theta\sin\theta-\sin\theta\cos\theta\cos\theta\sin\theta00-\sin\theta\cos\theta x1x2p1p2v=0,1,2....\lambda=1/2+\gamma^2+1/4c1\langle\psi||(\mathbb{1}^{\wedge}-\rho^{\wedge}0)||\psi\rangle[A\wedge A'(p)]$$

$$\mapsto(\cos\phi-\sin\phi\sin\phi\cos\phi)$$

$$(xp),D(\alpha):(xp)\mapsto(x+Re(\alpha)p+Im(\alpha)),S(r):(xp)\mapsto(e-r00er)(xp),BS(\theta):x1x2p1p2\mapsto\cos\theta\sin\theta-\sin\theta\cos\theta\cos\theta\sin\theta00-\sin\theta\cos\theta x1x2p1p2v=0,1,2....\lambda=1/2+\gamma^2+1/4c1\delta_{ij}-[A\wedge A'(p)]$$

$$\mapsto(\cos\phi-\sin\phi\sin\phi\cos\phi)$$

$$(xp),D(\alpha):(xp)\mapsto(x+Re(\alpha)p+Im(\alpha)),S(r):(xp)\mapsto(e-r00er)(xp),BS(\theta):x1x2p1p2\mapsto\cos\theta\sin\theta-\sin\theta\cos\theta\cos\theta\sin\theta00-\sin\theta\cos\theta x1x2p1p2v=0,1,2....\lambda=1/2+\gamma^2+1/4c1\langle\psi||\rho^{\wedge}0||\psi\rangle N-\text{Tr}[\rho^{\wedge}p^{\wedge}0]-\sum Ni=1,j\neq i\langle\psi||\rho^{\wedge}0||\psi\rangle$$

$\gamma_1 - 2\Re \sum_{N_i=1}^{\infty}$ where
 $A < \text{irr} 7 \Gamma j I P [N] (a_4 \cos 4\theta) - j < i \langle \psi || \rho^0 || \psi \rangle a_{22} v_{KS1}(r) a_4 \cos 2\theta + a_2 r^2 + r^4 \rangle \Sigma_3' \langle \psi || \rho^0 || \psi \rangle j j_2 k p k \wedge d A) k + 13$
 $\psi \langle A(\nabla R k) 2 + R 2 k \nabla \phi k \wedge [A \wedge A] \hbar 20 < \equiv \equiv \equiv \langle \psi * || \psi * \rangle = [A \wedge A'](p)] \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$
 $(x p), D(\alpha):(x p) \mapsto (x + \text{Re}(\alpha) p + \text{Im}(\alpha)), S(r):(x p) \mapsto (e - r 00 e r)(x p), B S(\theta):x_1 x_2 p_1 p_2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos$
 $\theta \sin \theta 00 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v=0,1,2, \dots \lambda=1 / 2+\gamma_2+1 / 4 c 1\langle \psi ||(\mathbb{1}^{\wedge}-\rho^{\wedge} 0)|| \psi \rangle)[A \wedge A'](p)]$
 $\mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$
 $(x p), D(\alpha):(x p) \mapsto (x + \text{Re}(\alpha) p + \text{Im}(\alpha)), S(r):(x p) \mapsto (e - r 00 e r)(x p), B S(\theta):x_1 x_2 p_1 p_2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos$
 $\theta \sin \theta 00 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v=0,1,2, \dots \lambda=1 / 2+\gamma_2+1 / 4 c 1 \delta_{i j}-[A \wedge A'](p)] \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$
 $(x p), D(\alpha):(x p) \mapsto (x + \text{Re}(\alpha) p + \text{Im}(\alpha)), S(r):(x p) \mapsto (e - r 00 e r)(x p), B S(\theta):x_1 x_2 p_1 p_2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos$
 $\theta \sin \theta 00 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v=0,1,2, \dots \lambda=1 / 2+\gamma_2+1 / 4 c 1\langle \psi || \rho^0 || \psi \rangle N - \text{Tr}[\rho^{\wedge} \rho^{\wedge} 0] - \sum N_i=1, j \neq i \langle \psi || \rho^0 || \psi \rangle$
 $\gamma_1 - 2\Re \sum_{N_i=1}^{\infty}$ where
 $A < \text{irr} 7 \Gamma j I P [N] (a_4 \cos 4\theta) - j < i \langle \psi || \rho^0 || \psi \rangle a_{22} v_{KS1}(r) a_4 \cos 2\theta + a_2 r^2 + r^4 \rangle \Sigma_3' \langle \psi || \rho^0 || \psi \rangle j j_2 k p k \wedge d A) k + 13$ 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) $\partial t \hat{P}$
 $\psi(t) | \partial \theta(t) / \partial t \int M_3 \psi A] = (\nabla p k) 2 / p k + 4 m_2 \hbar 20 < \equiv \equiv \equiv \langle \psi * || \psi * \rangle = [A \wedge A'](p)] \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$
 $(x p), D(\alpha):(x p) \mapsto (x + \text{Re}(\alpha) p + \text{Im}(\alpha)), S(r):(x p) \mapsto (e - r 00 e r)(x p), B S(\theta):x_1 x_2 p_1 p_2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos$
 $\theta \sin \theta 00 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v=0,1,2, \dots \lambda=1 / 2+\gamma_2+1 / 4 c 1\langle \psi ||(\mathbb{1}^{\wedge}-\rho^{\wedge} 0)|| \psi \rangle)[A \wedge A'](p)]$
 $\mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$
 $(x p), D(\alpha):(x p) \mapsto (x + \text{Re}(\alpha) p + \text{Im}(\alpha)), S(r):(x p) \mapsto (e - r 00 e r)(x p), B S(\theta):x_1 x_2 p_1 p_2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos$
 $\theta \sin \theta 00 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v=0,1,2, \dots \lambda=1 / 2+\gamma_2+1 / 4 c 1 \delta_{i j}-[A \wedge A'](p)] \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$
 $(x p), D(\alpha):(x p) \mapsto (x + \text{Re}(\alpha) p + \text{Im}(\alpha)), S(r):(x p) \mapsto (e - r 00 e r)(x p), B S(\theta):x_1 x_2 p_1 p_2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos$
 $\theta \sin \theta 00 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v=0,1,2, \dots \lambda=1 / 2+\gamma_2+1 / 4 c 1\langle \psi || \rho^0 || \psi \rangle N - \text{Tr}[\rho^{\wedge} \rho^{\wedge} 0] - \sum N_i=1, j \neq i \langle \psi || \rho^0 || \psi \rangle$
 $\gamma_1 - 2\Re \sum_{N_i=1}^{\infty}$ where
 $A < \text{irr} 7 \Gamma j I P [N] (a_4 \cos 4\theta) - j < i \langle \psi || \rho^0 || \psi \rangle a_{22} v_{KS1}(r) a_4 \cos 2\theta + a_2 r^2 + r^4 \rangle \Sigma_3' \langle \psi || \rho^0 || \psi \rangle j j_2 k p k \wedge d A) k + 13$
 $\psi \langle A(\nabla R k) 2 + R 2 k \nabla \phi k \wedge [A \wedge A] \hbar 20 < \equiv \equiv \equiv \langle \psi * || \psi * \rangle = [A \wedge A'](p)] \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$
 $(x p), D(\alpha):(x p) \mapsto (x + \text{Re}(\alpha) p + \text{Im}(\alpha)), S(r):(x p) \mapsto (e - r 00 e r)(x p), B S(\theta):x_1 x_2 p_1 p_2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos$
 $\theta \sin \theta 00 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v=0,1,2, \dots \lambda=1 / 2+\gamma_2+1 / 4 c 1\langle \psi ||(\mathbb{1}^{\wedge}-\rho^{\wedge} 0)|| \psi \rangle)[A \wedge A'](p)]$
 $\mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$
 $(x p), D(\alpha):(x p) \mapsto (x + \text{Re}(\alpha) p + \text{Im}(\alpha)), S(r):(x p) \mapsto (e - r 00 e r)(x p), B S(\theta):x_1 x_2 p_1 p_2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos$
 $\theta \sin \theta 00 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v=0,1,2, \dots \lambda=1 / 2+\gamma_2+1 / 4 c 1 \delta_{i j}-[A \wedge A'](p)] \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$
 $(x p), D(\alpha):(x p) \mapsto (x + \text{Re}(\alpha) p + \text{Im}(\alpha)), S(r):(x p) \mapsto (e - r 00 e r)(x p), B S(\theta):x_1 x_2 p_1 p_2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos$
 $\theta \sin \theta 00 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v=0,1,2, \dots \lambda=1 / 2+\gamma_2+1 / 4 c 1\langle \psi || \rho^0 || \psi \rangle N - \text{Tr}[\rho^{\wedge} \rho^{\wedge} 0] - \sum N_i=1, j \neq i \langle \psi || \rho^0 || \psi \rangle$
 $\gamma_1 - 2\Re \sum_{N_i=1}^{\infty}$ where
 $A < \text{irr} 7 \Gamma j I P [N]$
 $\mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 00 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v=0,1,2, \dots \lambda=1 / 2+\gamma_2+1 / 4 c$
 $(a_4 \cos 4\theta) - j < i \langle \psi || \rho^0 || \psi \rangle a_{22} v_{KS1}(r) a_4 \cos 2\theta + a_2 r^2 + r^4 \rangle \Sigma_3' \langle \psi || \rho^0 || \psi \rangle j j_2 k p k \wedge d A) k + 13$ 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) $\partial t \hat{P}$
 $\psi(t) | \partial \theta(t) / \partial t \int M_3 \psi A] = (\nabla p k) 2 / p k + 4 m_2 \hbar 20 < \equiv \equiv \equiv \langle \psi * || \psi * \rangle = [A \wedge A'](p)] \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$
 $(x p), D(\alpha):(x p) \mapsto (x + \text{Re}(\alpha) p + \text{Im}(\alpha)), S(r):(x p) \mapsto (e - r 00 e r)(x p), B S(\theta):x_1 x_2 p_1 p_2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos$
 $\theta \sin \theta 00 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v=0,1,2, \dots \lambda=1 / 2+\gamma_2+1 / 4 c 1\langle \psi ||(\mathbb{1}^{\wedge}-\rho^{\wedge} 0)|| \psi \rangle)[A \wedge A'](p)]$
 $\mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$
 $(x p), D(\alpha):(x p) \mapsto (x + \text{Re}(\alpha) p + \text{Im}(\alpha)), S(r):(x p) \mapsto (e - r 00 e r)(x p), B S(\theta):x_1 x_2 p_1 p_2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos$
 $\theta \sin \theta 00 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v=0,1,2, \dots \lambda=1 / 2+\gamma_2+1 / 4 c 1 \delta_{i j}-[A \wedge A'](p)] \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$
 $(x p), D(\alpha):(x p) \mapsto (x + \text{Re}(\alpha) p + \text{Im}(\alpha)), S(r):(x p) \mapsto (e - r 00 e r)(x p), B S(\theta):x_1 x_2 p_1 p_2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos$
 $\theta \sin \theta 00 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v=0,1,2, \dots \lambda=1 / 2+\gamma_2+1 / 4 c 1\langle \psi || \rho^0 || \psi \rangle N - \text{Tr}[\rho^{\wedge} \rho^{\wedge} 0] - \sum N_i=1, j \neq i \langle \psi || \rho^0 || \psi \rangle$

$$)1-2\Re\sum N_i=1(k)$$

$$I((T_{plain}, T_{cipher}), K_{prvite}) = \sum p((T_{plain}, T_{cipher}), K_{prvite}) \times \log p(K_{prvite} | (T_{plain}, T_{cipher})) p(K_{prvite})$$

$$\varphi \circ D \circ R_2 \circ S \circ R_1 < i \langle \psi || \rho^0 || \psi \rangle a_{22} v_{KS1}(r) a_4 \cos 2\theta + a_2 r^2 + r^4 \rangle \Sigma_3' \langle \psi || \rho^0 || \psi \rangle / 2m \int (\nabla R_0) 2 drr + \int R_{20} v drr \equiv$$

$$Ev[R_0, \phi_0] = (\hbar^2 \omega_0 \equiv \langle \psi^* || \psi^* \rangle = [A \wedge A'](p)) \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$$

$$(xp), D(\alpha): (xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r): (xp) \mapsto (e - r_0 0er)(xp), BS(\theta): x_1 x_2 p_1 p_2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 00 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v = 0, 1, 2, \dots \lambda = 1/2 + \gamma_2 + 1/4 c_1 \langle \psi || (\mathbb{1}^{\wedge} - \rho^0) || \psi \rangle [A \wedge A'](p)]$$

$$\mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$$

$$(xp), D(\alpha): (xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r): (xp) \mapsto (e - r_0 0er)(xp), BS(\theta): x_1 x_2 p_1 p_2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 00 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v = 0, 1, 2, \dots \lambda = 1/2 + \gamma_2 + 1/4 c_1 \delta_{ij} \quad \text{where}$$

$$A \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 00 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v = 0, 1, 2, \dots \lambda = 1/2 + \gamma_2 + 1/4 c$$

$$< irr 7 \Gamma j IP[N] (a_4 \cos 4\theta) - j < i \langle \psi || \rho^0 || \psi \rangle a_{22} v_{KS1}(r) a_4 \cos 2\theta + a_2 r^2 + r^4 \rangle \Sigma_3' \langle \psi || \rho^0 || \psi \rangle jj 2 k p k \wedge d A) k + 13 \psi$$

$$\langle A(\nabla R_k)^2 + R_2 k \nabla \phi k \wedge [A \wedge A] \hbar^2 \omega_0 \equiv \langle \psi^* || \psi^* \rangle = [A \wedge A'](p) \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$$

$$(xp), D(\alpha): (xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r): (xp) \mapsto (e - r_0 0er)(xp), BS(\theta): x_1 x_2 p_1 p_2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 00 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v = 0, 1, 2, \dots \lambda = 1/2 + \gamma_2 + 1/4 c_1 \langle \psi || (\mathbb{1}^{\wedge} - \rho^0) || \psi \rangle [A \wedge A'](p)] \mapsto (\cos \phi -$$

$$\sin \phi \sin \phi \cos \phi) \quad (xp), D(\alpha): (xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r): (xp) \mapsto (e - r_0 0er)(xp), BS(\theta):$$

$$: x_1 x_2 p_1 p_2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 00 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v = 0, 1, 2, \dots \lambda = 1/2 + \gamma_2 + 1/4 c_1 \delta_{ij} - [A \wedge A']$$

$$\mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi) \quad (xp), D(\alpha): (xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r): (xp) \mapsto (e - r_0 0er)(xp), BS(\theta):$$

$$(e - r_0 0er)(xp), BS(\theta): x_1 x_2 p_1 p_2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 00 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v = 0, 1, 2, \dots \lambda = 1/2 +$$

$$\gamma_2 + 1/4 c_1 \langle \psi || \rho^0 || \psi \rangle N - Tr[\rho^{\wedge} \rho^0] - \sum N_i = 1, j \neq i \langle \psi || \rho^0 || \psi \rangle 1 - 2 \Re \sum N_i = 1 \quad \text{where}$$

$$A < irr 7 \Gamma j IP[N] (a_4 \cos 4\theta) - j < i \langle \psi || \rho^0 || \psi \rangle a_{22} v_{KS1}(r) a_4 \cos 2\theta + a_2 r^2 + r^4 \rangle \Sigma_3' \langle \psi || \rho^0 || \psi \rangle \quad (31,40) \quad \text{Then, by}$$

uploading the combination of GisitorviffirnaTM, Roccustyrna_gs1_TM, and Roccustyrna_fr1_TM cluster of

[P@@](=O) (NC(=O) c1nc(F) cnc1) (NC(=O) c1nn(c2o c(c(O) c2O) CON(C(=[N])=C(N) N) C) CN) cn1)

Nn1c2nc([N]H)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 smiles in the Molinspiration-based bioactivity

analysis web server, we calculated the bioactivity score of this ligand through the systemic examination cf

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/admetSar2/>) 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 -OATP1B1testing 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]-phospho-rylidene} 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-

sulfonyl-bicyclo[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]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, 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 (Tab s1),(Tab s2), (Tab s3), (Tab s4).

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) (Fig s2/) 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, (Tab s4),(Tab s5) The Roccustyrna chemical structure interacted into the binding sites of the protein targets of (pdb:6w9c), (Fig s2/) 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]phosphor-rylidene} amino) -4,6- dihydro-1H-purin-6-onedihydro-3H-purin-9-yl) -3- hydroxy-oxolan 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.

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. (Fig s2/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. (Fig s3/) D10-C-1099 DMS:A:402 (DMS) binding sites were also constructed when the combined pharmacophoric elements of the combination of GisorviffirnaTM, 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. (Fig s3/), for $j=1\langle\psi||(\hat{1}-\rho^0)||\psi_j\rangle[A\Lambda A'(p)] \mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi)(xp), D(\alpha):(xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r):(xp) \mapsto (e - r00er)(xp), BS(\theta):x1x2p1p2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x1x2p1p2v=0,1,2 \dots \lambda=1/2 + \gamma 2 + 1/4c1\delta ij - [A\Lambda A'(p)] \mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi)(xp), D(\alpha):(xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r):(xp) \mapsto (e - r00er)(xp), BS(\theta):x1x2p1p2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x1x2p1p2v=0,1,2 \dots \lambda=1/2 + \gamma 2 + 1/4c1\langle\psi||\rho^0||\psi_j\rangle N - Tr[\rho^p \rho^0] - \sum_{Ni=1, j \neq i} \langle\psi||\rho^0||\psi_j\rangle 1 - 2\Re \sum_{Ni=1} A < irr7\Gamma jIP[N](a4\cos4\theta) - j < i \langle\psi||\rho^0||\psi_j\rangle a22vKS1(r)a4\cos2\theta + a2r2 + r4) \Sigma 3' \langle\psi||\rho^0||\psi_j\rangle$ 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. (Fig s3/) 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 (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

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. (Fig s4/a), (Tab s4/), (Tab s5/) The Roccustyrna DMS:A:402 (DMS) binding sites into the 524 Nam 2578 O2 O2J (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. (Fig s4/) when solved the $\hat{b}t\hat{P} \psi(t)|\partial\theta(t)/\partial t\rangle \int M3\psi A\rangle=(\nabla pk)^2/pk+4m2\hbar20<\equiv\equiv\langle\psi*||\psi*\rangle=[\Lambda\Lambda'(p)]\mapsto(\cos\phi-\sin\phi\sin\phi\cos\phi)$
 $(xp),D(\alpha):(xp)\mapsto(x+Re(\alpha)p+Im(\alpha)),S(r):(xp)\mapsto(e-r00er)(xp),BS(\theta):x1x2p1p2\mapsto\cos\theta\sin\theta-\sin\theta\cos\theta\cos\theta\sin\theta00-\sin\theta\cos\theta x1x2p1p2v=0,1,2....\lambda=1/2+\gamma2+1/4c1\langle\psi||(\hat{1}-\rho^0)||\psi\rangle[\Lambda\Lambda'(p)]$
 $\mapsto(\cos\phi-\sin\phi\sin\phi\cos\phi)(xp),D(\alpha):(xp)\mapsto(x+Re(\alpha)p+Im(\alpha)),S(r):(xp)\mapsto(e-r00er)(xp),BS(\theta):x1x2p1p2\mapsto\cos\theta\sin\theta-\sin\theta\cos\theta\cos\theta\sin\theta00-\sin\theta\cos\theta x1x2p1p2v=0,1,2....\lambda=1/2+\gamma2+1/4c1\delta_{ij}-[\Lambda\Lambda'(p)]\mapsto(\cos\phi-\sin\phi\sin\phi\cos\phi)(xp),D(\alpha):(xp)\mapsto(x+Re(\alpha)p+Im(\alpha)),S(r):(xp)\mapsto(e-r00er)(xp),BS(\theta):x1x2p1p2\mapsto\cos\theta\sin\theta-\sin\theta\cos\theta\cos\theta\sin\theta00-\sin\theta\cos\theta x1x2p1p2v=0,1,2....\lambda=1/2+\gamma2+1/4c1\langle\psi||\rho^0||\psi\rangle N-\text{Tr}[\rho^0]-\sum N_i=1, j\neq i\langle\psi||\rho^0||\psi\rangle 1-2\Re v \text{ for } (k)$
 $I((Tplain,Tcipher),Kprvite)\equiv\sum p((Tplain,Tcipher),Kprvite)\times\log p(Kprvite|(Tplain,Tcipher))p(Kprvite)\sum p(Tplain,Tcipher)*p(Kprvite|(Tplain,Tcipher))\times\log p(Kprvite|(Tplain,Tcipher))p(Kprvite)$
 $\varphi\circ D\circ R2\circ S\circ R1<i\langle\psi||\rho^0||\psi\rangle a22vKS1(r)a4\cos2\theta+a2r2+r4)\Sigma3'\langle\psi||\rho^0||\psi\rangle/2m)\int(\nabla R0)2drr+\int R20vdrr\equiv Ev[R0,\phi0]=(\hbar20<\equiv\equiv\langle\psi*||\psi*\rangle=[\Lambda\Lambda'(p)]\mapsto(\cos\phi-\sin\phi\sin\phi\cos\phi)$
 $(xp),D(\alpha):(xp)\mapsto(x+Re(\alpha)p+Im(\alpha)),S(r):(xp)\mapsto(e-r00er)(xp),BS(\theta):x1x2p1p2\mapsto\cos\theta\sin\theta-\sin\theta\cos\theta\cos\theta\sin\theta00-\sin\theta\cos\theta x1x2p1p2v=0,1,2....\lambda=1/2+\gamma2+1/4c1\langle\psi||(\hat{1}-\rho^0)||\psi\rangle[\Lambda\Lambda'(p)]$
 $\mapsto(\cos\phi-\sin\phi\sin\phi\cos\phi)$
 $(xp),D(\alpha):(xp)\mapsto(x+Re(\alpha)p+Im(\alpha)),S(r):(xp)\mapsto(e-r00er)(xp),BS(\theta):x1x2p1p2\mapsto\cos\theta\sin\theta-\sin\theta\cos\theta\cos\theta\sin\theta00-\sin\theta\cos\theta x1x2p1p2v=0,1,2....\lambda=1/2+\gamma2+1/4c1\delta_{ij}$
 $A<irr7\Gamma jIP[N](a4\cos4\theta)-j<i\langle\psi||\rho^0||\psi\rangle a22vKS1(r)a4\cos2\theta+a2r2+r4)\Sigma3'\langle\psi||\rho^0||\psi\rangle jj2kpk\Lambda dA)k+13$
 $\psi(A(\nabla Rk)2+R2k\nabla\phi k\Lambda[\Lambda\Lambda]\hbar20<\equiv\equiv\langle\psi*||\psi*\rangle=[\Lambda\Lambda'(p)]\mapsto(\cos\phi-\sin\phi\sin\phi\cos\phi)$
 $(xp),D(\alpha):(xp)\mapsto(x+Re(\alpha)p+Im(\alpha)),S(r):(xp)\mapsto(e-r00er)(xp),BS(\theta):x1x2p1p2\mapsto\cos\theta\sin\theta-\sin\theta\cos\theta\cos\theta\sin\theta00-\sin\theta\cos\theta x1x2p1p2v=0,1,2....\lambda=1/2+\gamma2+1/4c1\langle\psi||(\hat{1}-\rho^0)||\psi\rangle[\Lambda\Lambda'(p)]$
 $\mapsto(\cos\phi-\sin\phi\sin\phi\cos\phi)$
 $(xp),D(\alpha):(xp)\mapsto(x+Re(\alpha)p+Im(\alpha)),S(r):(xp)\mapsto(e-r00er)(xp),BS(\theta):x1x2p1p2\mapsto\cos\theta\sin\theta-\sin\theta\cos\theta\cos\theta\sin\theta00-\sin\theta\cos\theta x1x2p1p2v=0,1,2....\lambda=1/2+\gamma2+1/4c1\delta_{ij}-[\Lambda\Lambda'(p)]\mapsto(\cos\phi-\sin\phi\sin\phi\cos\phi)$
 $(xp),D(\alpha):(xp)\mapsto(x+Re(\alpha)p+Im(\alpha)),S(r):(xp)\mapsto(e-r00er)(xp),BS(\theta):x1x2p1p2\mapsto\cos\theta\sin\theta-\sin\theta\cos\theta\cos\theta\sin\theta00-\sin\theta\cos\theta x1x2p1p2v=0,1,2....\lambda=1/2+\gamma2+1/4c1\langle\psi||\rho^0||\psi\rangle N-\text{Tr}[\rho^0]-\sum N_i=1, j\neq i\langle\psi||\rho^0||\psi\rangle 1-2\Re\sum N_i=1$
 $A<irr7\Gamma jIP[N](a4\cos4\theta)-j<i\langle\psi||\rho^0||\psi\rangle a22vKS1(r)a4\cos2\theta+a2r2+r4)\Sigma3'\langle\psi||\rho^0||\psi\rangle 999 \text{ ZN D } 20947$
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-azaphosphoridin-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 GisorviffirnaTM, Roccustyrna_gs1_TM, and Roccustyrna_fr1_TM cluster of pharmacophoric (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 (Fig s4/) when $\int \psi(t) |\partial \theta(t) / \partial t| \int M_3 \psi A = (\nabla p k)^2 / p k + 4 m^2 \hbar^2 0 < \equiv \equiv \equiv = \langle \psi^* | | \psi^* \rangle = [A \Lambda A' (p)]$

$\mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi) (xp), D(\alpha): (xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r): (xp) \mapsto (e - r00er)(xp), BS(\theta): x1x2p1p2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 00 - \sin \theta \cos \theta x1x2p1p2v=0,1,2 \dots \lambda = 1/2 + \gamma^2 + 1/4c1 \langle \psi | | \rho^0 | | \psi \rangle [A \Lambda A' (p)] \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$

$(xp), D(\alpha): (xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r): (xp) \mapsto (e - r00er)(xp), BS(\theta): x1x2p1p2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 00 - \sin \theta \cos \theta x1x2p1p2v=0,1,2 \dots \lambda = 1/2 + \gamma^2 + 1/4c(k)$

$I((Tplain, Tcipher), Kprvite) = \sum p((Tplain, Tcipher), Kprvite) \times \log p(Kprvite | (Tplain, Tcipher)) p(Kprvite) \sum p(Tplain, Tcipher) * p(Kprvite | (Tplain, Tcipher)) \times \log p(Kprvite | (Tplain, Tcipher)) p(Kprvite)$

$\varphi \circ D \circ R_2 \circ S \circ R_1 < i \langle \psi | | \rho^0 | | \psi \rangle a_{22} v_{KS1}(r) a_4 \cos 2\theta + a_2 r^2 + r_4 \rangle \Sigma_3' \langle \psi | | \rho^0 | | \psi \rangle / 2m \int (\nabla R_0)^2 drr + \int R_2 v drr \equiv$

$Ev[R_0, \phi_0] = (\hbar^2 0 < \equiv \equiv \equiv \langle \psi^* | | \psi^* \rangle = [A \Lambda A' (p)] \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$

$(xp), D(\alpha): (xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r): (xp) \mapsto (e - r00er)(xp), BS(\theta): x1x2p1p2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 00 - \sin \theta \cos \theta x1x2p1p2v=0,1,2 \dots \lambda = 1/2 + \gamma^2 + 1/4c1 \langle \psi | | (\hat{1} - \rho^0) | | \psi \rangle [A \Lambda A' (p)]$

$\mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi) (xp), D(\alpha): (xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r): (xp) \mapsto (e - r00er)(xp), BS(\theta): x1x2p1p2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 00 - \sin \theta \cos \theta x1x2p1p2v=0,1,2 \dots \lambda = 1/2 + \gamma^2 + 1/4c1 \delta_{ij} - \sum N_i$

Ni, is parallel solved with $j = 1 \langle \psi | | \rho^0 | | \psi \rangle N - Tr[\rho^0 \rho^0] - \sum N_i = 1, j \neq i \langle \psi | | \rho^0 | | \psi \rangle 1 - 2\Re \sum N_i = 1, j < i \langle \psi | | \rho^0 | | \psi \rangle j j \quad 2kpk \wedge dA) k + 13\psi \quad \langle A(\nabla R k)^2 + R_2 k \nabla \phi k \wedge [A \Lambda A] \hbar^2 0 < \equiv \equiv \equiv \langle \psi^* | | \psi^* \rangle = [A \Lambda A' (p)]$

$\mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi) (xp), D(\alpha): (xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r): (xp) \mapsto (e - r00er)(xp), BS(\theta): x1x2p1p2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 00 - \sin \theta \cos \theta x1x2p1p2v=0,1,2 \dots \lambda = 1/2 + \gamma^2 + 1/4c1 \langle \psi | | (\hat{1} - \rho^0) | | \psi \rangle [A \Lambda A' (p)]$

$\mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi) (xp), D(\alpha): (xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r): (xp) \mapsto (e - r00er)(xp), BS(\theta): x1x2p1p2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 00 - \sin \theta \cos \theta x1x2p1p2v=0,1,2 \dots \lambda = 1/2 + \gamma^2 + 1/4c1 \delta_{ij} - [A \Lambda A' (p)] \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$

$(xp), D(\alpha): (xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r): (xp) \mapsto (e - r00er)(xp), BS(\theta): x1x2p1p2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 00 - \sin \theta \cos \theta x1x2p1p2v=0,1,2 \dots \lambda = 1/2 + \gamma^2 + 1/4c1 \langle \psi | | \rho^0 | | \psi \rangle N - Tr[\rho^0 \rho^0] - \sum N_i = 1, j \neq i \langle \psi | | \rho^0 | | \psi \rangle 1 - 2\Re \sum N_i = 1$

where $A < irr 7 \Gamma j IP[N] (a_4 \cos 4\theta) - j < i \langle \psi | | \rho^0 | | \psi \rangle a_{22} v_{KS1}(r) a_4 \cos 2\theta + a_2 r^2 + r_4 \rangle \Sigma_3' \langle \psi | | \rho^0 | | \psi \rangle$ (Tab s4/), (Fig s4/), for $j = 1 \langle \psi | | (\hat{1} - \rho^0) | | \psi \rangle \sum N_i, \quad j = 1 \delta_{ij} - [A \Lambda A' (p)] \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$

$(xp), D(\alpha): (xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r): (xp) \mapsto (e - r00er)(xp), BS(\theta): x1x2p1p2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 00 - \sin \theta \cos \theta x1x2p1p2v=0,1,2 \dots \lambda = 1/2 + \gamma^2 + 1/4c1 \langle \psi | | \rho^0 | | \psi \rangle N - Tr[\rho^0 \rho^0] - \sum N_i = 1, j \neq i \langle \psi | | \rho^0 | | \psi \rangle 1 - 2\Re \sum N_i = 1$

where $A < irr 7 \Gamma j IP[N] (a_4 \cos 4\theta) - j < i \langle \psi | | \rho^0 | | \psi \rangle a_{22} v_{KS1}(r) a_4 \cos 2\theta + a_2 r^2 + r_4 \rangle \Sigma_3' \langle \psi | | \rho^0 | | \psi \rangle$ eigenvalues. In this drug designing project the electrostatic regions around the combination of GisorvifirnaTM, Roccustyrna_{gs1}TM, and Roccustyrna_{fr1}TM pharmacophoric elements of (7aR) -5-amino-N-[(S) -{2-[(S) -[(E) - (amino-methylidene) amino](cyano) methyl]hydrazin-1-yl} (aziridin-1-yl) phosphoryl]-1-[(2E) -2-[(fluoro-methanimidoyl) 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 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, (Fig s4/a), (Fig s4/f) showing that combination of GisorviffirnaTM, 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 03 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. 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 $\gamma B \cdot (S^1 + S^2) + \Gamma \cdot A \cdot S^2$ (equation52), $S^i = (\sigma_x, \sigma_y, \sigma_z)$ $\Gamma \rho_s(t) = \text{Tr} I(U(t) \rho(0) U^\dagger(t))$ (equation52), $\rho I(0) = I/2P(t') = d M(t')$ (equation53) $M = f(t') dt'$, (equation54) $\rho^- s = \int -\infty f(t') \rho_s(t')$ (equation55) $dt' = \int_0^\infty f(t) \rho_s(t) dt, \int -\infty f(t')$ (equation56) $dt = \int_0^\infty f(t) dt = 1 \rho^- s \rho^- s \rho^- s$ (equation57) $s(\pi/2) \rho^- s \rho_s(0) \rho^- s$ (equation58), $QFI \approx \sum_i \rho_i(12) \frac{1}{2} (1 \rho_{i11} + 1 \rho_{i22}) + (\rho_{i11} - \rho_{i22}) \frac{1}{2} \rho_{i11} + \rho_{i22}$ (equation59), $\rho_{1ij} = \langle \phi_i | \rho_s(0) | \phi_j \rangle$ ρ (equation60) $0_{ij} = \langle \phi_i | \rho_s(0) | \phi_j \rangle$ $0 = 0$ $\partial t \hat{P} \psi(t) |\partial \theta(t) / \partial t \rangle \int M^3 \psi A = (\nabla p k)^2 / p k + 4 m^2 \hbar^2 0 < \equiv = \langle \psi_* || \psi_* \rangle = [A \Lambda A'(p)] \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$ $(xp), D(\alpha): (xp) \mapsto (x + \text{Re}(\alpha)p + \text{Im}(\alpha)), S(r): (xp) \mapsto (e - r 0 0 e r)(xp), BS(\theta): x_1 x_2 p_1 p_2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 0 0 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v = 0, 1, 2, \dots \lambda = 1/2 + \gamma 2 + 1/4 c 1 \langle \psi || (\hat{1} - \rho^0) || \psi \rangle [A \Lambda A'(p)]$ $\mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$ $(xp), D(\alpha): (xp) \mapsto (x + \text{Re}(\alpha)p + \text{Im}(\alpha)), S(r): (xp) \mapsto (e - r 0 0 e r)(xp), BS(\theta): x_1 x_2 p_1 p_2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 0 0 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v = 0, 1, 2, \dots \lambda = 1/2 + \gamma 2 + 1/4 c 1 \delta_{ij} - [A \Lambda A'(p)] \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$ $(xp), D(\alpha): (xp) \mapsto (x + \text{Re}(\alpha)p + \text{Im}(\alpha)), S(r): (xp) \mapsto (e - r 0 0 e r)(xp), BS(\theta): x_1 x_2 p_1 p_2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 0 0 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v = 0, 1, 2, \dots \lambda = 1/2 + \gamma 2 + 1/4 c 1 \langle \psi || \rho^0 || \psi \rangle N - \text{Tr}[\rho^0] - \sum_{N=1, j \neq i} \langle \psi || \rho^0 || \psi \rangle$ $1 - 2 \Re \sum_{N=1}$ where $A < \text{irr} 7 \Gamma j P[N] (a 4 \cos 4 \theta) - j < i \langle \psi || \rho^0 || \psi \rangle a 2 2 v K S 1(r) a 4 \cos 2 \theta + a 2 r^2 + r 4 \rangle \Sigma 3' \langle \psi || \rho^0 || \psi \rangle j j 2 k p k \wedge d A) k + 13$ $\psi \langle A(\nabla R k)^2 + R 2 k \nabla \phi k \wedge [A \Lambda A] \hbar^2 0 < \equiv = \langle \psi_* || \psi_* \rangle = [A \Lambda A'(p)] \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$ $S \rangle = 12 \langle -01 \rangle$ 30% ρ_s (equation59) $\rho^- s = H \otimes m 0 \rangle \otimes m = H \otimes H \otimes \dots \otimes H$ $0 0 \dots 0 = 12 (0 + 1) \otimes 12 (0 + 1) \otimes \dots \otimes 12 (0 + 1) = 12 m (0 0 \dots 0) + 0 0 \dots 1 \rangle + \dots + (1 1 \dots 1)$ equation (60) $\partial t \hat{P} \psi(t) |\partial \theta(t) / \partial t \rangle \int M^3 \psi A = (\nabla p k)^2 / p k + 4 m^2 \hbar^2 0 < \equiv = \langle \psi_* || \psi_* \rangle = [A \Lambda A'(p)] \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$ $(xp), D(\alpha): (xp) \mapsto (x + \text{Re}(\alpha)p + \text{Im}(\alpha)), S(r): (xp) \mapsto (e - r 0 0 e r)(xp), BS(\theta): x_1 x_2 p_1 p_2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 0 0 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v = 0, 1, 2, \dots \lambda = 1/2 + \gamma 2 + 1/4 c 1 \langle \psi || (\hat{1} - \rho^0) || \psi \rangle [A \Lambda A'(p)]$ $\mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$ $(xp), D(\alpha): (xp) \mapsto (x + \text{Re}(\alpha)p + \text{Im}(\alpha)), S(r): (xp) \mapsto (e - r 0 0 e r)(xp), BS(\theta): x_1 x_2 p_1 p_2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 0 0 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v = 0, 1, 2, \dots \lambda = 1/2 + \gamma 2 + 1/4 c 1 \delta_{ij} - [A \Lambda A'(p)] \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$ $(xp), D(\alpha): (xp) \mapsto (x + \text{Re}(\alpha)p + \text{Im}(\alpha)), S(r): (xp) \mapsto (e - r 0 0 e r)(xp), BS(\theta): x_1 x_2 p_1 p_2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 0 0 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v = 0, 1, 2, \dots \lambda = 1/2 + \gamma 2 + 1/4 c 1 \langle \psi || \rho^0 || \psi \rangle N - \text{Tr}[\rho^0] - \sum_{N=1, j \neq i} \langle \psi || \rho^0 || \psi \rangle$ $1 - 2 \Re \sum_{N=1}$ where $A < \text{irr} 7 \Gamma j P[N] (a 4 \cos 4 \theta) - j < i \langle \psi || \rho^0 || \psi \rangle a 2 2 v K S 1(r) a 4 \cos 2 \theta + a 2 r^2 + r 4 \rangle \Sigma 3' \langle \psi || \rho^0 || \psi \rangle j j 2 k p k \wedge d A) k + 13$ $\psi \langle A(\nabla R k)^2 + R 2 k \nabla \phi k \wedge [A \Lambda A] \hbar^2 0 < \equiv = \langle \psi_* || \psi_* \rangle = [A \Lambda A'(p)] \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$ $(xp), D(\alpha): (xp) \mapsto (x + \text{Re}(\alpha)p + \text{Im}(\alpha)), S(r): (xp) \mapsto (e - r 0 0 e r)(xp), BS(\theta): x_1 x_2 p_1 p_2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 0 0 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v = 0, 1, 2, \dots \lambda = 1/2 + \gamma 2 + 1/4 c 1 \langle \psi || (\hat{1} - \rho^0) || \psi \rangle [A \Lambda A'(p)]$ $\mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$ $(xp), D(\alpha): (xp) \mapsto (x + \text{Re}(\alpha)p + \text{Im}(\alpha)), S(r): (xp) \mapsto (e - r 0 0 e r)(xp), BS(\theta): x_1 x_2 p_1 p_2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 0 0 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v = 0, 1, 2, \dots \lambda = 1/2 + \gamma 2 + 1/4 c 1 \delta_{ij} - [A \Lambda A'(p)] \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$ $(xp), D(\alpha): (xp) \mapsto (x + \text{Re}(\alpha)p + \text{Im}(\alpha)), S(r): (xp) \mapsto (e - r 0 0 e r)(xp), BS(\theta): x_1 x_2 p_1 p_2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 0 0 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v = 0, 1, 2, \dots \lambda = 1/2 + \gamma 2 + 1/4 c 1 \langle \psi || \rho^0 || \psi \rangle N - \text{Tr}[\rho^0] - \sum_{N=1, j \neq i} \langle \psi || \rho^0 || \psi \rangle$ $1 - 2 \Re \sum_{N=1}$ where

$A < \text{irr}7\Gamma jIP[N](a4\cos4\theta) - j < i \langle \psi_i || \rho^0 || \psi_j \rangle a22vKS1(r)a4\cos2\theta + a2r2 + r4) \Sigma 3' \langle \psi_i || \rho^0 || \psi_j \rangle$ (Fig s2/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:3fqg) 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. (Fig s2/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. (Fig s2/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) as output when $\partial t \hat{P} \psi(t) | \partial \theta(t) / \partial t \int M3\psi A = (\nabla pk)^2 / pk + 4m2\hbar20 < \equiv \equiv \equiv \langle \psi^* || \psi^* \rangle = [A\Lambda A'(p)] \mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi)$

$(xp), D(\alpha): (xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r): (xp) \mapsto (e - r00er)(xp), BS(\theta): x1x2p1p2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x1x2p1p2v=0,1,2 \dots \lambda = 1/2 + \gamma2 + 1/4c1 \langle \psi_i || (\mathbb{1}^{\wedge} - \rho^0) || \psi_j \rangle \Sigma Ni, j=1\delta ij - [A\Lambda A'(p)] \mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi)$

$(xp), D(\alpha): (xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r): (xp) \mapsto (e - r00er)(xp), BS(\theta): x1x2p1p2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x1x2p1p2v=0,1,2 \dots \lambda = 1/2 + \gamma2 + 1/4c1 \langle \psi_i || \rho^0 || \psi_j \rangle N - \text{Tr}[\rho^{\wedge} p^0] - \Sigma Ni = 1$, is parallel solved to $j \neq i \langle \psi_i || \rho^0 || \psi_j \rangle 1 - 2\Re \Sigma Ni = 1$ where

$A < \text{irr}7\Gamma jIP[N](a4\cos4\theta) - j < i \langle \psi_i || \rho^0 || \psi_j \rangle a22vKS1(r)a4\cos2\theta + a2r2 + r4) \Sigma 3' \langle \psi_i || \rho^0 || \psi_j \rangle jj2kpk\wedge dA)k+13$

$\psi \langle A(\nabla Rk)^2 + R2k \nabla \phi k \wedge [A\Lambda A] \hbar20 < \equiv \equiv \equiv \langle \psi^* || \psi^* \rangle = [A\Lambda A'(p)] \mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi)$

$(xp), D(\alpha): (xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r): (xp) \mapsto (e - r00er)(xp), BS(\theta): x1x2p1p2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x1x2p1p2v=0,1,2 \dots \lambda = 1/2 + \gamma2 + 1/4c1 \langle \psi_i || (\mathbb{1}^{\wedge} - \rho^0) || \psi_j \rangle [A\Lambda A'(p)] \mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi)$

$(xp), D(\alpha): (xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r): (xp) \mapsto (e - r00er)(xp), BS(\theta): x1x2p1p2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x1x2p1p2v=0,1,2 \dots \lambda = 1/2 + \gamma2 + 1/4c1 \delta ij - [A\Lambda A'(p)] \mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi)$

$(xp), D(\alpha): (xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r): (xp) \mapsto (e - r00er)(xp), BS(\theta): x1x2p1p2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x1x2p1p2v=0,1,2 \dots \lambda = 1/2 + \gamma2 + 1/4c1 \langle \psi_i || \rho^0 || \psi_j \rangle N - \text{Tr}[\rho^{\wedge} p^0] - \Sigma Ni = 1, j \neq i \langle \psi_i || \rho^0 || \psi_j \rangle 1 - 2\Re \Sigma Ni = 1(k)$

$I((Tplain, Tcipher), Kprvite) = \Sigma p((Tplain, Tcipher), Kprvite) \times \log p(Kprvite | (Tplain, Tcipher)) p(Kprvite) \Sigma p(Tplain, Tcipher) * p(Kprvite | (Tplain, Tcipher)) \times \log p(Kprvite | (Tplain, Tcipher)) p(Kprvite)$

$\varphi \circ D \circ R2 \circ S \circ R1 < i \langle \psi_i || \rho^0 || \psi_j \rangle a22vKS1(r)a4\cos2\theta + a2r2 + r4) \Sigma 3' \langle \psi_i || \rho^0 || \psi_j \rangle / (2m) \int (\nabla R0)^2 drr + \int R20v drr \equiv Ev[R0, \phi0] = (\hbar20 < \equiv \equiv \equiv \langle \psi^* || \psi^* \rangle = [A\Lambda A'(p)] \mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi)$

$(xp), D(\alpha): (xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r): (xp) \mapsto (e - r00er)(xp), BS(\theta): x1x2p1p2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x1x2p1p2v=0,1,2 \dots \lambda = 1/2 + \gamma2 + 1/4c1 \langle \psi_i || (\mathbb{1}^{\wedge} - \rho^0) || \psi_j \rangle [A\Lambda A'(p)] \mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi)$

$(xp), D(\alpha): (xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r): (xp) \mapsto (e - r00er)(xp), BS(\theta): x1x2p1p2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x1x2p1p2v=0,1,2 \dots \lambda = 1/2 + \gamma2 + 1/4c1 \delta ij$ where

$A < \text{irr}7\Gamma jIP[N](a4\cos4\theta) - j < i \langle \psi_i || \rho^0 || \psi_j \rangle a22vKS1(r)a4\cos2\theta + a2r2 + r4) \Sigma 3' \langle \psi_i || \rho^0 || \psi_j \rangle$ (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. (Fig s2/e) As illustrated in the (Fig s3/) 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. (Fig s4/d), (Fig s4/e) In this project for the first time we generated a Comparative Docking Cluster Analysis between the Remdesivir and our prototype Roccustyrnas 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.

(Fig s4/f), (Fig s4/g), (Fig s4/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. (Fig s5/a), (Fig s5/b), (Fig s5/c), (Fig s6/) 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 through the example of coupled anti-de Sitter black harmonic black-hole oscillators and brane spacetimes 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) $\partial_t \hat{P} \psi(t) | \partial \theta(t) / \partial t$ $\int M_3 \psi A = (\nabla p k)^2 / p k + 4 m^2 \hbar^2 < \equiv \equiv \equiv \langle \psi^* | | \psi^* \rangle = [A \wedge A'](p)] \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$ $(xp), D(\alpha): (xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r): (xp) \mapsto (e - r00er)(xp), BS(\theta): x1x2p1p2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 00 - \sin \theta \cos \theta x1x2p1p2 v=0,1,2 \dots \lambda = 1/2 + \gamma^2 + 1/4 c1 \langle \psi | | \rho^0 | | \psi \rangle [A \wedge A'](p)] \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$ $(xp), D(\alpha): (xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r): (xp) \mapsto (e - r00er)(xp), BS(\theta): x1x2p1p2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 00 - \sin \theta \cos \theta x1x2p1p2 v=0,1,2 \dots \lambda = 1/2 + \gamma^2 + 1/4 c1 \delta_{ij} - [A \wedge A'](p)] \mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$ $(xp), D(\alpha): (xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r): (xp) \mapsto (e - r00er)(xp), BS(\theta): x1x2p1p2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 00 - \sin \theta \cos \theta x1x2p1p2 v=0,1,2 \dots \lambda = 1/2 + \gamma^2 + 1/4 c1 \langle \psi | | \rho^0 | | \psi \rangle N - Tr[\rho^p \rho^0] - \sum N_i = 1,$ (k) $I((Tplain, Tcipher), Kprvite) = \sum p((Tplain, Tcipher), Kprvite) \times \log p(Kprvite | (Tplain, Tcipher)) p(Kprvite) \sum p(Tplain, Tcipher) * p(Kprvite | (Tplain, Tcipher)) \times \log p(Kprvite | (Tplain, Tcipher)) p(Kprvite) \quad \varphi \circ D \circ R_2 \circ S \circ R_1 < i \langle \psi | | \rho^0 | | \psi \rangle a_{22} v_{KS1}(r) a_4 \cos 2\theta + a_2 r^2 + r^4 \rangle \Sigma_3' \langle \psi | | \rho^0 | | \psi \rangle / 2m \int (\nabla R_0) 2 drr + \int R_2 v drr \equiv Ev[R_0, \phi_0] = (\hbar^2 < \equiv \equiv \equiv \langle \psi^* | | \psi^* \rangle = [A \wedge A'](p)].$ 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-2yl) 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-
ylium. (Fig s2/), $j=1\langle\psi||(\mathbb{1}-\rho^0)||\psi\rangle[A\Lambda A'(p)] \mapsto (\cos\phi-\sin\phi\sin\phi\cos\phi)$
 $(xp),D(\alpha):(xp)\mapsto(x+Re(\alpha)p+Im(\alpha)),S(r):(xp)\mapsto(e-r00er)(xp),BS(\theta):x1x2p1p2\mapsto\cos\theta\sin\theta-\sin\theta\cos\theta\cos$
 $\theta\sin\theta00-\sin\theta\cos\theta x1x2p1p2v=0,1,2,\dots,\lambda=1/2+\gamma2+1/4c1\delta ij-[A\Lambda A'(p)] \mapsto (\cos\phi-\sin\phi\sin\phi\cos\phi)$
 $(xp),D(\alpha):(xp)\mapsto(x+Re(\alpha)p+Im(\alpha)),S(r):(xp)\mapsto(e-r00er)(xp),BS(\theta):x1x2p1p2\mapsto\cos\theta\sin\theta-\sin\theta\cos\theta\cos$
 $\theta\sin\theta00-\sin\theta\cos\theta x1x2p1p2v=0,1,2,\dots,\lambda=1/2+\gamma2+1/4c1\langle\psi||\rho^0||\psi\rangle N-\text{Tr}[\rho^p^0]-\sum_{Ni=1,j\neq i}\langle\psi||\rho^0||\psi\rangle$
 $1-2\Re\sum_{Ni=1}$ where
 $A<irr7\Gamma jIP[N](a4\cos4\theta)-j<i\langle\psi||\rho^0||\psi\rangle a22vKS1(r)a4\cos2\theta+a2r2+r4)\Sigma3'\langle\psi||\rho^0||\psi\rangle$ (Fig s1) (Scheme
1), $\partial_t\hat{P}\psi(t)|\partial\theta(t)/\partial t\rangle\int M3\psi A=(\nabla pk)2/pk+4m2\hbar20<\equiv\equiv\equiv\langle\psi*||\psi*\rangle=[A\Lambda A'(p)] \mapsto (\cos\phi-\sin\phi\sin\phi\cos\phi)$
 $(xp),D(\alpha):(xp)\mapsto(x+Re(\alpha)p+Im(\alpha)),S(r):(xp)\mapsto(e-r00er)(xp),BS(\theta):x1x2p1p2\mapsto\cos\theta\sin\theta-\sin\theta\cos\theta\cos$
 $\theta\sin\theta00-\sin\theta\cos\theta x1x2p1p2v=0,1,2,\dots,\lambda=1/2+\gamma2+1/4c1\langle\psi||(\mathbb{1}-\rho^0)||\psi\rangle[A\Lambda A'(p)]$
 $\mapsto (\cos\phi-\sin\phi\sin\phi\cos\phi)$
 $(xp),D(\alpha):(xp)\mapsto(x+Re(\alpha)p+Im(\alpha)),S(r):(xp)\mapsto(e-r00er)(xp),BS(\theta):x1x2p1p2\mapsto\cos\theta\sin\theta-\sin\theta\cos\theta\cos$
 $\theta\sin\theta00-\sin\theta\cos\theta x1x2p1p2v=0,1,2,\dots,\lambda=1/2+\gamma2+1/4c1\delta ij-[A\Lambda A'(p)] \mapsto (\cos\phi-\sin\phi\sin\phi\cos\phi)$
 $(xp),D(\alpha):(xp)\mapsto(x+Re(\alpha)p+Im(\alpha)),S(r):(xp)\mapsto(e-r00er)(xp),BS(\theta):x1x2p1p2\mapsto\cos\theta\sin\theta-\sin\theta\cos\theta\cos$
 $\theta\sin\theta00-\sin\theta\cos\theta x1x2p1p2v=0,1,2,\dots,\lambda=1/2+\gamma2+1/4c1\langle\psi||\rho^0||\psi\rangle N-\text{Tr}[\rho^p^0]-\sum_{Ni=1,j\neq i}\langle\psi||\rho^0||\psi\rangle$
 $1-2\Re\sum_{Ni=1}$ where
 $A<irr7\Gamma jIP[N](a4\cos4\theta)-j<i\langle\psi||\rho^0||\psi\rangle a22vKS1(r)a4\cos2\theta+a2r2+r4)\Sigma3'\langle\psi||\rho^0||\psi\rangle jj2kpk\wedge dA)k+13$
 $\psi\langle A(\nabla Rk)2+R2k\nabla\phi k\wedge[A\Lambda A]$ (44) 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 $\{x\sin^(-1)(\sqrt{3})\}, x\sin^(-1)(\sqrt{779}\sqrt{\theta^3})\}, x\sin^(-1)(2\sqrt{114109})$
 $\}, (\sqrt{1-\sqrt{456457}}\sqrt{x})x^{(1/4)}(2\sqrt{456457}\sqrt{x}+3)/(8456457^{(3/4)}+(x-3/3651656)\sin^(-1)(456457^{(1/4)}x^{(1/4)}), 1/2\sqrt{(x/456456754-x^2)}+(x-1/912913508)\sin^(-1)$
 $(\sqrt{456456754}\sqrt{x}), x\sin^(-1)(2^{(3/4)}57057^{(1/4)}), x\sin^(-1)(\sqrt{\sum 444546\theta}), \sin^(-1)$
 $(-1)(2^{(3/4)}431683182057^{(1/4)}\sqrt{\sqrt{\theta}/(\sin^(-1)(44545545))})\} + \text{constant } 3d$ (equation61)
 $N=2CS\{\theta\sin^(-1)(\sqrt{3})\}$ (equation62), $\theta\sin^(-1)(\sqrt{779\delta v}=i\bar{\rho}v, \text{ (equation63)} \delta^{\sim}v=i\bar{q}^{\sim}v,$
(equation64) $\delta v=-\gamma\mu\bar{q}D\mu v-\bar{q}$ (equation65) $\sigma v-\text{if}(\theta) \bar{q}v+i\bar{\rho}F, \text{ (equation66)} \delta^{\sim}v=-\gamma\mu^{\sim}\bar{q}D\mu^{\sim}v-\bar{v}\sigma^{\sim}\bar{q}$
 $-\text{if}(\theta) \bar{v}^{\sim}\bar{q}+i\bar{v}^{\sim}F\bar{q}, \text{ (equation67)} \delta F=\bar{q}(-\gamma\mu D\mu v+\sigma v+\lambda v)+i(43)\sqrt{(|\alpha1'(t)y'(k)=\{\otimes k=1m'\varphi(\lambda k)\otimes k$
 $=1m'D(\alpha k)\otimes k=1\psi(y)v=Ev=y\lambda\exp[-\beta v y]F(\lambda-\gamma2/\beta v,2\lambda,2\beta v y)F(c,b;y)=\sum v=0\infty\Gamma(c+v)\Gamma(b)yv\Gamma(b+v)\Gamma(c)$
 $v!c0a2[1-\gamma2(v+\lambda)2]v=0,1,2,\dots,\lambda=1/2+\gamma2+1/4c0a2[1-y y]2\}\psi(y)v(\phi k)\otimes k1mCQ2t|\phi(t)$ (44)
 $c0\zeta2(1+\sum i)=[A\Lambda A'(p)] \otimes [\partial v^{\sim}\partial q^{\sim},\partial u^{\sim}\partial p^{\sim}]-[\partial v^{\sim}\otimes\partial p^{\sim},\otimes\partial u^{\sim}\otimes\partial q^{\sim}]=1ci\xi i\{-\hbar20<\equiv\equiv\equiv\langle\psi*||\psi*\rangle=[A\Lambda A'(p)]$
 $\mapsto (\cos\phi-\sin\phi\sin\phi\cos\phi)$ $(xp),D(\alpha):(xp)\mapsto(x+Re(\alpha)p+Im(\alpha)),$
 $S(r):(xp)\mapsto(e-r00er)(xp),BS(\theta):x1x2p1p2\mapsto\cos\theta\sin\theta-\sin\theta\cos\theta\cos\theta\sin\theta00-\sin\theta\cos\theta x1x2p1p2v=0,1,2$
 $\dots,\lambda=1/2+\gamma2+1/4c1\delta ij$ (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
procedures of QSAR modeling Quantization for generalized heuristic fields when fused together with von
Neumann and Dirac formulation states on eigenvalue statements equipped with a natural "inclusion" functor
 $T\rightarrow T''$ for algebraic multi-metrics hope to fix this chemical space 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) was also observed in this parallel docking energy analysis that our QMMM designed Risitorviffirna 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. In this Schrödinger picture for the system minimum-energy of quantum mechanics the dynamics of quantum states for the $S[p0,\phi]=S[p0]+S[p0,\phi]$ and $I[p0,\phi]=I[p0]+I[p0,\phi]$ non-classical Shannon entropy is governed by the system energy operator $\hat{H} : i\hbar\partial|\psi(t)\rangle/\partial t = \hat{H} |\psi(t)\rangle$ (42,43,44) which gives the following expression for the time derivative of the conditional probability $P[\theta(t)|\psi(t)]$ in question:

$$\begin{aligned} \partial P[\theta(t)|\psi(t)]/\partial t &= \{22mb2r\partial t\hat{P} \psi(t)|\partial\theta(t)/\partial t\rangle(k) \\ I((Tplain,Tcipher),Kprvite) &= \sum p((Tplain,Tcipher),Kprvite) \times \log p(Kprvite|(Tplain,Tcipher)) p(Kprvite) \\ &\quad \sum p(Tplain,Tcipher) * p(Kprvite|(Tplain,Tcipher)) \times \log p(Kprvite|(Tplain,Tcipher)) p(Kprvite) \\ \varphi \circ D \circ R2 \circ S \circ R1 &< i(\psi||\rho^0||\psi_j) a22vKS1(r) a4\cos 2\theta + a2r^2 + r^4 \rangle \Sigma 3' \langle \psi||\rho^0||\psi_j \rangle / 2m \int (\nabla R0) 2drr + \int R20vdrr \equiv \\ Ev[R0,\phi0] &= (\hbar 20 < \equiv \equiv \equiv \langle \psi * || \psi * \rangle = [A\Lambda A'(p)] (xp), D(\alpha): (xp) \mapsto (x + Re(\alpha)p + Im(\alpha)), S(r): (xp) \\ \mapsto (e - r00er)(xp), BS(\theta): x1x2p1p2 &\mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x1x2p1p2v = 0, 1, 2 \dots \lambda = 1/2 \\ + \gamma 2 + 1/4c & \quad 1\delta ij - [A\Lambda A'(p)] \quad \mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi) \\ (xp), D(\alpha): (xp) &\mapsto (x + Re(\alpha)p + Im(\alpha)), S(r): (xp) \mapsto (e - r00er)(xp), BS(\theta): x1x2p1p2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos \\ \theta \sin\theta 00 - \sin\theta \cos\theta x1x2p1p2v &= 0, 1, 2 \dots \lambda = 1/2 + \gamma 2 + 1/4c 1 \langle \psi||\rho^0||\psi_j \rangle N - \text{Tr}[\rho^{\wedge} \rho^0] - \sum Ni = 1, j \neq i \langle \psi||\rho^0||\psi_j \rangle \\ 1 - 2\Re \sum Ni &= 1 \quad \text{where} \\ A < irr7\Gamma jIP[N] &(a4\cos 4\theta) - j < i(\psi||\rho^0||\psi_j) a22vKS1(r) a4\cos 2\theta + a2r^2 + r^4 \rangle \Sigma 3' \langle \psi||\rho^0||\psi_j \rangle a22vKS[p0,\phi] = S[\\ p0] + S[p0,\phi] &\text{AND } I[p0,\phi] = I[p0] + I[p0,\phi] 1(r) = vext(r) + \int dr' \rho(r') ||r - r'|| + vXC1,(r) mb2r2ed2\pi^2 B2mBV[P^- \\ \sqrt{Q^-} &(rryv\Gamma(b+v)\Gamma(c)v!c0a2\sqrt{-}\sqrt{Q^-}(rryv\Gamma(b+v)\Gamma(c)v!c0a2Q^-\sqrt{P^-}\sqrt{Q^-}) \equiv |Cmd\pi C\pi 2|\phi(Wx^{\wedge} + \alpha), \\ dy2\Sigma\Sigma^Q \otimes \quad \sigma &- \quad \sigma\sigma^q \quad -i_+ + c0a2[1 - yy]2] \psi(y) v < \quad q^{\wedge}u, \quad |\nabla[P^-\sqrt{Q^-}\sqrt{-}Q^-\sqrt{P^-}\sqrt{Q^-}] \equiv |2 \text{where } Q \\ \text{refer } S[p0,\phi] &= S[p0] + S[p0,\phi] \text{ and } I[p0,\phi] = I[p0] + I[p0,\phi] \text{ to } \neq wx^{\wedge}(j) = \int_{-\infty}^{\infty} xj|xj\rangle \langle xj| dxj. \text{ By the way, (j)} \\ \text{represents the } j\text{th } R2(\phi k) \otimes k(x * p *) &\mapsto (\text{input of the neuron or the } j\text{th } wx^{\wedge}(j) = \int_{-\infty}^{\infty} \text{output of a neuron in the} \\ \text{last layer, } y^{\wedge}(k) &\text{represents the } k\text{th output of the Pharmacophoric system A: S4- cyano-1- (}\{ \{ (2S,4R,5R) \text{-2-} \\ \text{methyl-2-2- (}\{ \{ \text{fluoro (}\{ \{ (2E) \text{-5- oxabicyclo [2.1.0] pentan- 2-ylidene} \} \text{cyano-lambda6-sulfanyl}} \} \} \\ \text{methyl} \} \text{phosphorylidene} \} \text{amino) -4,6-dihydro-1H-purin-6-one (methylamino) -1,6-diazabicyclo (3.2.0) } \\ \text{heptan-4-yl) (1S,2R,3S) -2- (}\{ \{ (1S,2S,4S,5R) \text{-4-ethenyl-4- sulfonylbicyclo[3.2.0]heptan-2-yl} \} \text{oxy} \} \text{amino) -3-} \\ \text{2- (}\{ \{ \text{fluoro (}\{ \{ (2E) \text{-5-oxabicyclo [2.1.0] pentan-2-ylidene} \} \text{cyano-lambda6-sulfanyl}} \} \} \\ \text{methyl} \} \text{phosphorylidene} \} \text{amino) -4,6-dihydro-1H-purin-6-one[(2R,5R) -5- (2-methyl-6-methylidene-6,9-} \\ \text{dihydro-3H-purin-9-yl) -3-methylideneoxolan-2-yl]phosphirane-1-carbonitrile-oxy} \} \text{imino) -1lambda5,} \\ \text{2lambda5-azaphosphiridin-1-ylum input of a fragmented compounds in the next pharmacophoric system B:} \\ \text{S4- cyano-1- (}\{ \{ (2S,4R,5R) \text{-2-methyl-2-2- (}\{ \{ \text{fluoro (}\{ \{ (2E) \text{-5- oxabicyclo [2.1.0] pentan- 2-ylidene} \} \text{cyano-} \\ \text{lambda6-sulfanyl}} \} \} \text{methyl} \} \text{phosphorylidene} \} \text{amino) S4- cyano-1- (}\{ \{ (2S,4R,5R) \text{-2-methyl-2-2- (}\{ \{ \text{fluoro (}\{ \{ (2E) \text{-5-} \\ \text{oxabicyclo [2.1.0] pentan- 2-ylidene} \} \text{cyano-lambda6-sulfanyl}} \} \} \text{methyl} \} \text{phosphorylidene} \} \text{amino) -} \\ \text{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) \text{-4-ethenyl-4-} \\ \text{sulfonylbicyclo[3.2.0]heptan-2-yl} \} \text{oxy} \} \text{amino) -3- 2- (}\{ \{ \text{fluoro (}\{ \{ (2E) \text{-5-} \end{aligned}$$

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 -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. αk represents the parameters of displacement $D(\alpha(k))$ and $\phi(\cdot)$ is nonlinear function. (42,43,44)

Conclusions

DNA-Protein-Ligand signatures in more general spacetimes enhanced by ZK-based proofs of nonlinear dynamics in an extended cryptography model to encrypt and decrypt chemical data which may be extended to hyper-symmetric equations of Chern-Simons Topology driven motion on a collection of nonlinearly coupled remerging harmonic oscillators. Of special interest here is the fusion pharmacophoric product of quantum reference frame representations from the Hopf algebra structure on U_{qg} , when the universal R matrix may provide the 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) To keep the method as simple as possible, we choose to generate the best docking-scoring individuals and to replace the worst docking-scoring of integrable highest-weight modules with functionalities on the wave equation for the molecular oscillator described by the second-order term of the Tipping-Ogilvie potential expansion with connections over compact of $\psi(y)v=Ev=y\lambda\exp[-\beta v y]F(\lambda-\gamma/2/\beta v, 2\lambda, 2\beta v y)F(c, b; y)=\sum_{v=0}^{\infty} \Gamma(c+v)\Gamma(b)y^v\Gamma(b+v)\Gamma(c)v!c_0a_2[1-\gamma^2(v+\lambda)^2] \mapsto (\cos\phi-\sin\phi\sin\phi\cos\phi)(xp), D(\alpha):(xp)\mapsto(x+Re(\alpha)p+Im(\alpha)), S(r):(xp)\mapsto(e-r00er)(xp), BS(\theta):x_1x_2p_1p_2\mapsto\cos\theta\sin\theta-\sin\theta\cos\theta\cos\theta\sin\theta00-\sin\theta\cos\theta x_1x_2p_1p_2v=0,1,2,\dots,\lambda=1/2+\gamma^2+1/4c_0a_2[1-yy]^2\psi(y)v(\phi k)\otimes k_1mCQ_2t|\phi(t)c_0\zeta_2(1+\partial t\tilde{P} \psi(t)|\partial\theta(t)/\partial t)\int M_3\psi A]=(\nabla pk)^2/pk+4m^2\hbar^20<\equiv\equiv\equiv\langle\psi_*||\psi_*\rangle=[A\wedge A'](p)]\mapsto(\cos\phi-\sin\phi\sin\phi\cos\phi) \forall i, y\in Y_i, \tilde{y}\in\tilde{Y}_i\tilde{\xi}_i(y, \tilde{y})\geq 0, \forall i, y\in Y_i, \tilde{y}\in\tilde{Y}_iWTe=1; W\geq 0f_{LL}(1)(x, y) f_{LH}(1)(x, y) f_{HL}(1)(x, y) f_{HH}(1)(x, y) f_1, \dots, 6=\max\{f_{LH}(l)(x, y), f_{LH}(l)(x, y), f_{LH}(l)(x, y)\}, \forall l=1, 2 f_7, \dots, 12=\min\{f_{LH}(l)(x, y), f_{LH}(l)(x, y), f_{LH}(l)(x, y)\}, \forall l=1, 2 f_{13}, \dots, 18=\text{mean}\{f_{LH}(l)(x, y), f_{LH}(l)(x, y), f_{LH}(l)(x, y)\}, \forall l=1, 2 f_{19}, \dots, 24$ of maximum fixed number of times through two coupled Chern-Simons Topology driven anti-de Sitter black harmonic black-hole oscillator by means of ordinary differential equation over the moduli space of four-punctured spheres. This secret Machine Learning improver key introduces the conditional probabilities between quantum reference frames, which generalize a network of electronic structure communications and can be used in combination with cryptographic algorithms for every connected group G and level $k \geq 0$ modular tensor categories that are additively equivalent to $\text{Rep}_k(LG)$ to encrypt and decrypt chemical information. (Tab s6/) Here, for the first time we have generated molecular information systems transmitting “drug repositioning signals” of electron allocations to quantum refence frames by using Chern-Simons harmonic oscillators on anti-de Sitter brane spacetimes for constructing, remerging, and generating chemical and physical small molecule libraries available through publicly web servers. Implementations of in-silico quantum phase cryptographic experiments and fragmentations via the molecular network of the occupied electronic orbitals were re-cored as introduced in this fragment-based and machine-learning virtual screening experiment by employing in-house ligand libraries for the design of a quantum thinking novel multi-chemo-structure against the protein targets of COVID-19 main protease. A combination of GisitorviffirnaTM, Roccustyrna_{gs1}TM, and Roccustyrna_{fr1}TM small molecules (Scheme 1) was generated as the fusion product of chemical space representations when merged into the connection form of $(a+\ell)ta+\ell\{1/12+(\|\alpha_1'(t)\rangle CQ_1$ of the external search: $\min\Psi\langle\P|\hat{H}|\Psi\rangle=\min\rho Ev[\rho]=\min\rho\{\int v(rr)\rho(rr)drr+\text{inf}\Psi\rightarrow\rho\langle\P|\hat{F}|\Psi\rangle\}=Ev[\rho_0]Ev[\rho_0]=\int v(rr)\rho_0(rr)drr+\text{inf}\Psi\rightarrow\rho_0\langle\P|\hat{F}|\Psi\rangle$ $\text{Min}\phi I [\phi_0]= I[\rho_0]+\min\phi I[\rho_0, \phi]=I[\rho_0]|\Psi\rangle=Vne[\rho_0]+Vee[\rho_0]+\text{inf}\Psi\rightarrow\rho_0\langle\P|\hat{T}|\Psi\rangle=Vne[\rho_0]+Vee[\rho_0]+T[\rho_0]=Vne[\rho_0]+$

$$Vee[\rho_0] + (\hbar/2) \langle \psi^* | \psi \rangle = [A\Lambda A'(p)] \mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi)$$

$$(xp), D(\alpha): (xp) \mapsto (x + \operatorname{Re}(\alpha)p + \operatorname{Im}(\alpha)), S(r): (xp) \mapsto (e - r00er)(xp), BS(\theta): x1x2p1p2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x1x2p1p2v=0,1,2,\dots,\lambda=1/2+\gamma/2+1/4c1\langle\psi||(\mathbb{1}^\wedge-\rho^\wedge 0)||\psi\rangle[A\Lambda A'(p)]$$

$$\mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi)$$

$$(xp), D(\alpha): (xp) \mapsto (x + \operatorname{Re}(\alpha)p + \operatorname{Im}(\alpha)), S(r): (xp) \mapsto (e - r00er)(xp), BS(\theta): x1x2p1p2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x1x2p1p2v=0,1,2,\dots,\lambda=1/2+\gamma/2+1/4c1\delta_{ij} - [A\Lambda A'(p)] \mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi)$$

$$(xp), D(\alpha): (xp) \mapsto (x + \operatorname{Re}(\alpha)p + \operatorname{Im}(\alpha)), S(r): (xp) \mapsto (e - r00er)(xp), BS(\theta): x1x2p1p2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x1x2p1p2v=0,1,2,\dots,\lambda=1/2+\gamma/2+1/4c1\langle\psi||\rho^\wedge 0||\psi\rangle N - \operatorname{Tr}[\rho^\wedge \rho^\wedge 0] - \sum_{Ni=1,j \neq i} \langle\psi||\rho^\wedge 0||\psi\rangle$$

$$1 - 2\Re \sum_{Ni=1} \text{ where}$$

$$A < \operatorname{irr} 7 \Gamma j IP[N] (a4 \cos 4\theta) - j < i \langle\psi||\rho^\wedge 0||\psi\rangle a22vKS1(r) a4 \cos 2\theta + a2r2 + r4) \Sigma 3' \langle\psi||\rho^\wedge 0||\psi\rangle 8m) I[\rho_0]. t \phi(t)$$

$$\rangle B + |\alpha 2'(t) \rangle CQ2t \phi(t) \quad c0\zeta 2(1 + \sum i) = [A\Lambda A'(p)] \quad \otimes [\partial v^\wedge \partial q^\wedge, \partial u^\wedge \partial p^\wedge] -$$

$$[\partial v^\wedge \otimes \partial p^\wedge, \otimes \partial u^\wedge \otimes \partial q^\wedge] = 1ci\zeta i\{-\hbar/2) \langle \psi^* | \psi \rangle = [A\Lambda A'(p)] \mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi)$$

$$(xp), D(\alpha): (xp) \mapsto (x + \operatorname{Re}(\alpha)p + \operatorname{Im}(\alpha)), S(r): (xp) \mapsto (e - r00er)(xp), BS(\theta): x1x2p1p2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x1x2p1p2v=0,1,2,\dots,\lambda=1/2+\gamma/2+1/4c1\langle\psi||(\mathbb{1}^\wedge-\rho^\wedge 0)||\psi\rangle[A\Lambda A'(p)]$$

$$\mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi)$$

$$(xp), D(\alpha): (xp) \mapsto (x + \operatorname{Re}(\alpha)p + \operatorname{Im}(\alpha)), S(r): (xp) \mapsto (e - r00er)(xp), BS(\theta): x1x2p1p2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x1x2p1p2v=0,1,2,\dots,\lambda=1/2+\gamma/2+1/4c1\delta_{ij} - [A\Lambda A'(p)] \mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi)$$

$$(xp), D(\alpha): (xp) \mapsto (x + \operatorname{Re}(\alpha)p + \operatorname{Im}(\alpha)), S(r): (xp) \mapsto (e - r00er)(xp), BS(\theta): x1x2p1p2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x1x2p1p2v=0,1,2,\dots,\lambda=1/2+\gamma/2+1/4c1\langle\psi||\rho^\wedge 0||\psi\rangle N - \operatorname{Tr}[\rho^\wedge \rho^\wedge 0] - \sum_{Ni=1,j \neq i} \langle\psi||\rho^\wedge 0||\psi\rangle$$

$$1 - 2\Re \sum_{Ni=1} \text{ where}$$

$$A < \operatorname{irr} 7 \Gamma j IP[N] (a4 \cos 4\theta) - j < i \langle\psi||\rho^\wedge 0||\psi\rangle a22vKS1(r) a4 \cos 2\theta + a2r2 + r4) \Sigma 3' \langle\psi||\rho^\wedge 0||\psi\rangle a22vKS1(r) = \operatorname{vext}($$

$$r) + \int dr' \rho(r') ||r - r'|| + vXC1, (r) mb2r2ed2\pi^2 B2mBV[P - \sqrt{Q} - (rr\gamma v \Gamma(b+v) \Gamma(c) v! c0a2\sqrt{-} - \sqrt{Q} - (rr\gamma v \Gamma(b+v)$$

$$\Gamma(c) v! c0a2Q - \sqrt{P} - \sqrt{Q}] = |\operatorname{Cmd} \pi C d \pi 2| \phi(Wx^\wedge + \alpha), dy2\Sigma\Sigma' Q \otimes \bar{\sigma} - \bar{\sigma} \sigma^\wedge q - i_- + c0a2[1 - yy]2\} \psi(y)v) \rangle B) \} +$$

$$Fq \exp(-i\hbar \hat{p}^2 A2mA + -1 \ 2zEGk: 2zEG \otimes 2zEG \rightarrow \mathbb{R} \text{ (equation70) into the 6,9-dihydro-3H-purin loop group}$$

scaffolding (Scheme 2), (Scheme 3), (Scheme 4). By applying EuTHTS Euclidean Topology accuracy algorithms on our Virtual Screening, and Gravitational Topological (UFs) scheme some of Quantum-Parallel Particle Swarm Inspired framework generated in which a generalized procedure of Quantization of classical heuristic fields fused together with QSAR automating modeling equipped with a natural “inclusion” functor $T \rightarrow T''$ of the electronic Hamiltonian $\hat{H} (N) = \hat{V} ne(N) + [\hat{T} (N) + \hat{V} ee(N)] \equiv \sum_{i=1}^N v(i) + \hat{F} (N) \partial t \hat{P}$

$$\psi(t) |\partial \theta(t) / \partial t \rangle \int M3 \psi A = (\nabla pk) 2 / pk + 4m2 \hbar/2) \langle \psi^* | \psi \rangle = [A\Lambda A'(p)] \mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi)$$

$$(xp), D(\alpha): (xp) \mapsto (x + \operatorname{Re}(\alpha)p + \operatorname{Im}(\alpha)), S(r): (xp) \mapsto (e - r00er)(xp), BS(\theta): x1x2p1p2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x1x2p1p2v=0,1,2,\dots,\lambda=1/2+\gamma/2+1/4c1\langle\psi||(\mathbb{1}^\wedge-\rho^\wedge 0)||\psi\rangle[A\Lambda A'(p)]$$

$$\mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi)$$

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 of general (variational) quantum states: $S[p0, \phi] = S[p0] + S[p0, \phi]$ and $I[p0, \phi] = I[p0] + I[p0, \phi]$. I made use of partial small fragment derivatives as well as probabilistic transformations on Murko (BM) circuit statements 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-Simons 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 $\partial t \hat{P}$

$$\psi(t) |\partial \theta(t) / \partial t \rangle \int M3 \psi A = (\nabla pk) 2 / pk + 4m2 \hbar/2) \langle \psi^* | \psi \rangle = [A\Lambda A'(p)] \mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi)$$

$$(xp), D(\alpha): (xp) \mapsto (x + \operatorname{Re}(\alpha)p + \operatorname{Im}(\alpha)), S(r): (xp) \mapsto (e - r00er)(xp), BS(\theta): x1x2p1p2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x1x2p1p2v=0,1,2,\dots,\lambda=1/2+\gamma/2+1/4c1\langle\psi||(\mathbb{1}^\wedge-\rho^\wedge 0)||\psi\rangle[A\Lambda A'(p)]$$

$$\mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi) \quad (xp), D(\alpha): (xp) \mapsto (x + \operatorname{Re}(\alpha)p + \operatorname{Im}(\alpha)), S(r):$$

$(xp) \mapsto (e-r00er)(xp), BS(\theta):x1x2p1p2 \mapsto \cos\theta\sin\theta - \sin\theta\cos\theta\cos\theta\sin\theta00 - \sin\theta\cos\theta x1x2p1p2v=0,1,2,\dots,\lambda=1/2+\gamma2+1/4c1\delta ij - [A\Lambda A'(p)] \mapsto (\cos\phi - \sin\phi\sin\phi\cos\phi)$
 $(xp), D(\alpha):(xp) \mapsto (x+Re(\alpha)p+Im(\alpha)), S(r):(xp) \mapsto (e-r00er)(xp), BS(\theta):x1x2p1p2 \mapsto \cos\theta\sin\theta - \sin\theta\cos\theta\cos\theta\sin\theta00 - \sin\theta\cos\theta x1x2p1p2v=0,1,2,\dots,\lambda=1/2+\gamma2+1/4c1\langle\psi||\rho^0||\psi\rangle N - \text{Tr}[\rho^*\rho^0] - \sum_{Ni=1,j \neq i} \langle\psi||\rho^0||\psi\rangle$
 $1-2\Re\sum_{Ni=1} \text{ for } A < irr7\Gamma jIP[N](a4\cos4\theta) - j < i \langle\psi||\rho^0||\psi\rangle a22vKS1(r)a4\cos2\theta+a2r2+r4)\Sigma3' \langle\psi||\rho^0||\psi\rangle$
 qubits (Scheme 5). We suggest that such ligand-protein binding site topology maps will be useful for building further understanding of the relationship between diagonal chemical descriptors, small molecules, and complex viral biological systems. (43, 44) This generalized Hadamard approach is potentially applicable to the discovery of hit matter for novel biological targets, with clinical or genomic features for predicting and rationalizing ligand poly-pharmacology and for predicting new ligand functions. In addition, we suggest that such an objective binding site symmetrized map, which encompasses unliganded cavities, will also be useful for optimizing compound screening collections towards a more complete chemical coverage of multi-targeted pharmacophoric space. Our Biogenetoligandorol platform may also offer utility to researchers to interrogate and organize generalized k-nearest neighbors on an Adaptive Weighted KNN Positioning of
 $D(p,q)=(p1-q1)^2+(p2-q2)^2+\dots+(pn-qn)^2$ Average Accuracy= $\sum_{i=1}^l TP_i + TN_i TP_i + FN_i + FP_i + TN_i / l$
 $\kappa = P(A) - P(E)1 - P(E)$ $\kappa = P(A) - P(E)1 - P(E) = 0.9 - 0.44041 - 0.4404 \approx 0.82$
 $D(p,q)=(p1-q1)^2+(p2-q2)^2+\dots+(pn-qn)^2$ Average Accuracy= $\sum_{i=1}^l TP_i + TN_i TP_i + FN_i + FP_i + TN_i / l$
 $\kappa = P(A) - P(E)1 - P(E)$ $(xp), D(\alpha):(xp) \mapsto (x+Re(\alpha)p+Im(\alpha)), S(r):(xp) \mapsto (e-r00er)(xp), BS(\theta):x1x2p1p2 \mapsto \cos\theta\sin\theta - \sin\theta\cos\theta\cos\theta\sin\theta00 - \sin\theta\cos\theta x1x2p1p2v=0,1,2,\dots,\lambda=1/2+\gamma2+1/4c1\delta ij - [A\Lambda A'(p)] \mapsto (\cos\phi - \sin\phi\sin\phi\cos\phi)$
 $(xp), D(\alpha):(xp) \mapsto (x+Re(\alpha)p+Im(\alpha)), S(r):(xp) \mapsto (e-r00er)(xp), BS(\theta):x1x2p1p2 \mapsto \cos\theta\sin\theta - \sin\theta\cos\theta\cos\theta\sin\theta00 - \sin\theta\cos\theta x1x2p1p2v=0,1,2,\dots,\lambda=1/2+\gamma2+1/4c1\langle\psi||\rho^0||\psi\rangle N - \text{Tr}[\rho^*\rho^0] - \sum_{Ni=1,j \neq i} \langle\psi||\rho^0||\psi\rangle$
 $1-2\Re\sum_{Ni=1}$ where $A < irr7\Gamma jIP[N](a4\cos4\theta) - j < i \langle\psi||\rho^0||\psi\rangle a22vKS1(r)a4\cos2\theta+a2r2+r4)\Sigma3' \langle\psi||\rho^0||\psi\rangle$ coefficients (26,29-42). More specifically, in this project we unified generalized k-nearest values and topology geometric methods for generalized formalisms of k-nearest neighbors of Molecular Pairs (MMP) and von Neumann formulations for Dirac formulation states as a Tipping-Ogilvie and Machine Learning application within the quantum computing context with algebraic multi-metrics characteristics targeting the atomistic level of the protein apparatus of the SARS-COV-2 viral characteristics. An Adaptive Weighted KNN Positioning approach through nonlinear electrodynamics to simulate an advanced quantum mechanical inverse docking algorithm were applied in this unified protocol by providing further insight on a $\ell_{neuron}(i) := \varphi \circ D \circ R2 \circ S \circ R1$ improver for Chern-Simons Topology Euclidean Geometrics for generating a negative docking energy effect of the highest docking energy value against a specific protein target. (Illustration1) As a result for Entangled Neural Networks and Quantum-Inspired Kappa-Symmetrizing frameworks and by using Chern-Simons normalized Shannon entropy quantities through Tipping-Ogilvie potentials we generated the combination of GisitorviffirnaTM, Roccustyrna_{gs1}TM, and Roccustyrna_{fr1}TM small molecules which were able of producing the highest rates of 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) inside the amino acid 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 our 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 (Fig s9/A), PDB: 6WOJ (Fig s9/B), PDB: 7B3D (Fig s9/C), PDB:6M2Q (Fig s9/D), PDB:6LU7 (Fig s9/E), PDB: 6WZU (Fig s9/F), PDB:1XU9 (Fig s9/G), PDB: 3TWU (Fig s9/H), PDB:7BEO (Fig s9/H), PDB:1XAK (Fig s9/I) protein targets. (44) 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 (Fig s7/), (Tab s8/), (Fig s8/), (Tab s9/), (Fig s10/), (Fig s11/).

Significant Statements

In this project, I implemented Inverse Docking Algorithms with nonlinear electrodynamics for the cryptographic designing of the combination of Gisitorviffirna_{TM}, 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. In this effort, we 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 AI-Quantum designed molecules of Gisitorviffirna_{TM}, Roccustyrna_{gs1}_{TM}, and Roccustyrna_{fr1}_{TM} ligands targeting the COVID-19-SARS-COV-2 SPIKE D614G mutation by unifying Molecular Pairs (MMP), Lindenbaum-Tarski logical spaces and Adaptive Weighted KNN Positioning for Matched Bemis and Murko (BM) driven eigenvalue statements into Shannon entropy quantities as composed by Tipping-Ogilvie driven Machine Learning potentials on a (DFT) $\ell_{\text{neuron}}(i) := \varphi \circ D \circ R_2 \circ S \circ R_1$ $c_0 \zeta^2 (1 + \sum i) = [A \wedge A'](p)$ $\otimes [\partial v^{\wedge} \partial q^{\wedge}, \partial u^{\wedge} \partial p^{\wedge}] - [\partial v^{\wedge} \otimes \partial p^{\wedge}, \otimes \partial u^{\wedge} \otimes \partial q^{\wedge}] = 1 c i \xi i \{-\hbar 20 < \equiv \equiv \equiv \langle \psi^* || \psi^* \rangle = [A \wedge A'](p)$ $\mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$ $(xp), D(\alpha): (xp) \mapsto (x + \text{Re}(\alpha)p + \text{Im}(\alpha)), S(r): (xp) \mapsto (e - r 00er)(xp), BS(\theta): x_1 x_2 p_1 p_2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 00 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v = 0, 1, 2, \dots \lambda = 1/2 + \gamma 2 + 1/4 c 1$ $\langle \psi || (1^{\wedge} - \rho^{\wedge} 0) || \psi \rangle \sum N_i, / \partial t \hat{P}$ $\psi(t) | \partial \theta(t) / \partial t \int M_3 \psi A] = (\nabla p k) 2 / p k + 4 m 2 \hbar 20 <$ $\equiv \equiv \equiv \langle \psi^* || \psi^* \rangle = [A \wedge A'](p)$ $\mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$ $(xp), D(\alpha): (xp) \mapsto (x + \text{Re}(\alpha)p + \text{Im}(\alpha)), S(r): (xp) \mapsto (e - r 00er)(xp), BS(\theta): x_1 x_2 p_1 p_2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 00 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v = 0, 1, 2, \dots \lambda = 1/2 + \gamma 2 + 1/4 c$ $1 \langle \psi || (1^{\wedge} - \rho^{\wedge} 0) || \psi \rangle [A \wedge A'](p)$ $\mapsto (\cos \phi - \sin \phi \sin \phi \cos \phi)$ $(xp), D(\alpha): (xp) \mapsto (x + \text{Re}(\alpha)p + \text{Im}(\alpha)), S(r): (xp) \mapsto (e - r 00er)(xp), BS(\theta): x_1 x_2 p_1 p_2 \mapsto \cos \theta \sin \theta - \sin \theta \cos \theta \cos \theta \sin \theta 00 - \sin \theta \cos \theta x_1 x_2 p_1 p_2 v = 0, 1, 2, \dots \lambda = 1/2 + \gamma 2 + 1/4 c 1 \delta_{ij} - [A \wedge A'](p)$

$\mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi) \quad (xp), D(\alpha): (xp) \mapsto (x + \text{Re}(\alpha)p + \text{Im}(\alpha)), S(r): (xp)$
 $\mapsto (e - r00er)(xp), BS(\theta): x1x2p1p2 \mapsto \cos\theta \sin\theta - \sin\theta \cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x1x2p1p2v=0,1,2$
 $\dots \lambda = 1/2 + \gamma^2 + 1/4c1\langle \psi || \rho^0 || \psi \rangle N - \text{Tr}[\rho^0] - \sum N_i = 1, j \neq i \langle \psi || \rho^0 || \psi \rangle 1 - 2\Re \sum N_i = 1$ where
 $A < \text{irr} 7\Gamma jIP[N](a4\cos 4\theta) - j < i \langle \psi || \rho^0 || \psi \rangle a22vKS1(r)a4\cos 2\theta + a2r2 + r4) \Sigma 3' \langle \psi || \rho^0 || \psi \rangle jj2kpk \wedge d$
 $A)k + 13\psi \langle A(\nabla Rk)2 + R2k \nabla \phi k \wedge [A \wedge A] \quad j = 1\delta ij - [A \wedge A'](p) \quad \mapsto (\cos\phi - \sin\phi \sin\phi \cos\phi)$
 $(xp), D(\alpha): (xp) \mapsto (x + \text{Re}(\alpha)p + \text{Im}(\alpha)), S(r): (xp) \mapsto (e - r00er)(xp), BS(\theta): x1x2p1p2 \mapsto \cos\theta \sin\theta - \sin\theta$
 $\cos\theta \cos\theta \sin\theta 00 - \sin\theta \cos\theta x1x2p1p2v=0,1,2 \dots \lambda = 1/2 + \gamma^2 + 1/4c1\langle \psi || \rho^0 || \psi \rangle N - \text{Tr}[\rho^0] - \sum N_i =$
 $1, j \neq i \langle \psi || \rho^0 || \psi \rangle \quad |\psi \rangle 1 - 2\Re \sum N_i = 1$ where
 $A < \text{irr} 7\Gamma jIP[N](a4\cos 4\theta) - j < i \langle \psi || \rho^0 || \psi \rangle a22vKS1(r)a4\cos 2\theta + a2r2 + r4) \Sigma 3' \langle \psi || \rho^0 || \psi \rangle a22vKS1$
 $(r) = \text{vext}(r) + \int dr' \rho(r') ||r - r'|| + vXC1, (r) mb2r2ed2\pi^2 B2mB \nabla [P - \sqrt{Q} - (rryv\Gamma(b+v)\Gamma(c)v!c0a2\sqrt{-}$
 $-\sqrt{Q} - (rryv\Gamma(b+v)\Gamma(c)v!c0a2Q - \sqrt{P} - \sqrt{Q}) \equiv |Cm d\pi C d\pi 2|\phi(Wx^{\wedge} + \alpha)\rangle, dy \quad 2\Sigma \Sigma^- Q \quad \otimes \quad \bar{\sigma} \quad - \quad \bar{\sigma} \sigma^- q$
 $-i_- + c0a2[1 - yy]2\psi(y)v$ improver for Chern-Simons Topology Euclidean Geometrics.

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- **Conflicts of interest/Competing interests.**

No potential competing interest was reported by the author.

- **Availability of data and material**

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.

- **Code availability**

Due to confidentiality agreements, data included in this research work have been generated at Biogenea's central large-scale facility Department of Biogeneto - ligandorolQMMIDDD/QPRPICA/MACHNOT/ QIICDNDCA ADMET/QIICDNDCA 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 Information's are attached as a separate file.

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