AI-Quantum Phases on Chern-Simons Topological Geometries for the Generation of A Ligand Targeting COVID-19-SARS-COV-2 SPIKE D614G Binding Sites.

Ioannis Grigoriadis (✉ jgrigoriadis@biogenea.gr)

Aristotle University of Thessaloniki

Research Article

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AI-Quantum Phases on Chern-Simons Topological Geometrics for the generation of a ligand targeting COVID-19-SARS-COV-2 SPIKE D614G binding sites.

1. Department of BiogenetoligandorolQMMIDDD/QPRPICA/MACHNOT/

QHICDNNDCa ADMET/QHICDNNDCa Stations, Aristotle University of Thessaloniki,

Biogenea Pharmaceuticals Ltd - Greece.

Grigoriadis Ioannis* email: jgrigoriadis@biogenea.gr

<tel:+306936592686> ORCID iD: <https://orcid.org/0000-0002-8443-1777>

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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. It has also been observed that retroviruses infected ACE2-expressing cells pseudotyped with SG614 that is presently affecting a growing number of countries markedly more efficiently than those with SD614. The availability of newer powerful computational resources, molecular modeling techniques, and cheminformatics quality data have made it feasible to generate reliable algebraic calculations to design new chemical entities, merging chemicals, fragmentizing natural products, and a lot of other substances fuelling further development and growth of this AI-quantum based drug design field to balance the trade-off between the structural complexity and the quality of such biophysics predictions that cannot be obtained by any other method. In this paper, we strongly combine topology geometric methods targeting at the atomistic level the protein apparatus of the SARS-COV-2 virus that are simple in machine learning anti-viral characteristics, to propose computer-aided rational drug design strategies efficient in computing docking usage, and powerful enough to achieve very high accuracy levels for this in-silico effort for the generation of the AI-Quantum designed molecule the RoccustyrnaTM small molecule, a multi-targeting druggable scaffold (1S,2R,3S)-2-([[(1S,2S,4S,5R)-4-ethenyl-4-sulfonylbicyclo[3.2.0] heptan-2-yl]oxy]amino)-3-[(2R,5R)-5-(2-methyl-6-methylidene-6,9-dihydro-3H-purin-9-yl)-3-methylideneoxolan-2-yl]phosphirane-1-carbonitrile targeting the COVID-19-SARS-COV-2 SPIKE D614G mutation using Chern-Simons Topology Euclidean Geometric in a Lindenbaum-Tarski generated QSAR automating modeling and Artificial Intelligence-Driven Predictive Neural Networks.

Introduction

(1,2,3) The COVID-19 disease which emerged in China at the end of 2019 was declared on March 2020 a pandemic by the World Health Organization (WHO) and is accountable for a large number of fatal cases. (2,4,5) On January 202, WHO committee declared a global health emergency (3,4-6) based on the rate of increasing spread of the infection (4,5-7) with a reproductive number (RN) in the range 2.0-6.5, 4 higher than SARS and MERS, (8) with more than 85,000 casualties and fatality rate of about 4%. (1-4) Collaborative efforts for Genomic characterization, (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 interventions for control and prevention of the disease. (1-10) Coronaviruses are positive-single stranded, enveloped large RNA viruses that infect humans and a wide range of animals. (7,8-11) Tyrell and Bonne reported the first coronavirus in 1966, (11) who cultivated the viruses from the patients suffering with common cold. (4,6,7-10) In Latin, Corona means —crown || based on their shapes. As a megadiverse country, Brazil accounts for 10–20% of known living species in the world. However, a major part of the biological and chemical biodiversity in Brazil remains unexplored (17). (2–13,14,15,16,17) Molecular structure 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 Functional Theories (DFT) (23) and semi-empirical in place (24) of the quantum processor and energy among other observables,(25) under simulated sampling error as well as to reposition drugs about bonding may represent the similarities (26) and dissimilarities(27) between drugs and repurposed viral proteins respectively. (28) However, the Schrödinger equation cannot actually be solved for any but a one- data-driven (29) electron system methods (the hydrogen atom), (30) and approximations need to be made. According to QM, (2-19,23) an electron bound that converges quickly and reliably to an atom cannot possess any (2-17,21,22,23, 24,25,26,27,28) arbitrary energy to produce the desired distribution by analyzing pharmacological data or occupy any position in space using statistical and machine (23,24-37,38) learning concepts. The Lindenbaum-Tarski algebra logical spaces and vectorial representations of the eigenvalue statements were used in this project and has been previously introduced as a 3D logical subspace allowing a well-defined position for each fragmented pharmacophore. This shows the application to quantum computing through the example of three coupled harmonic oscillators allows pure mechanical computation both for generating rules and inferences. (25,27,28) Since in previous studies It has been shown that Path selection for quantum repeater networks can be geometrically represented by Chern-Simons logical spaces and subspaces I decided to implement supersymmetric solutions and borel Singularities for $N=2$ allowing a quantum repeater based vectorial Supersymmetric Chern-Simons representation in this drug design project . (20,26,27,28-31) In general, the notions of Lindenbaum matrix and Lindenbaum-Tarski algebra have paved a way to further algebraization of logic, which had been begun by George Boole in the 19th century, as well as to a new branch of logic, model theory. Philosophical interpretations of QM were conditioned by ideals of what an explanatory theory should be. (Minkowski-type, wave-edge, etc), (20,27,32-33) as well as probabilistic transformations Algebraic multi-metrics (Triangle area, Bond-angle, etc) and the associated axiomatic formulations (AQFT) treat observables rather than states as foundational for the interaction information extraction. (20,33,34,35) In this project, we show an original strategy and an application to quantum computing through the example of two coupled harmonic black-hole oscillators obtained by molecular modeling and simulations as orthogonal coordinates applied for the design of a novel multi-chemo-structure against the crystal structure of COVID-19 protein targets in a Lindenbaum-Tarski generated QSAR automating modeling lead compound design approach. (29,35,36) A meta server and a Kappa-Symmetry C algebra of local observables were incorporated for the docking 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 recoring and fragmentation were applied to fragment and recore a database of 20,000+ molecules for use with the group contribution model Universal Quasichemical 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 were implemented for predicting drug targets and for multi-target and multi-site based virtual screening against COVID-19 (41,42) Flexible Topology Euclidean Geometric, were used to fragment molecules automatically in this molecular modeling and drug designing project on several parameters while keeping the definition of the groups as simple as possible. Artificial Intelligence-Driven Predictive Neural Networks and Quantum- Inspired frameworks of parallel-Docking interactions were employed for supercritical entanglements introducing an advanced quantum mechanical inverse docking algorithm providing further insight to confirm the practicality of docking energy predictions for wild type and selected mutations for Nsp3 (papain-like, PLpro domain), Nsp5 Nsp15 (NendoU), (Mpro, 3CLpro), Nsp12 (RdRp), N protein and Spike in understanding the key element functions of SARS-CoV-2 protein pathways and in designing possible novel antiviral agents, from both an quantum algebraic and a cheminformatic perspective.

Materials and Methods

Preparation of the protein structures

The National Center (NCBI) database for Biotechnology Information was used to retrieve the S glycoprotein proteins of SARS-CoV-2. For the N protein, we aligned the clustered 31 conformations (1,2,35) from the 1731 full-length SARS-CoV-2 sequences and stored as a FASTA format file for analysis with Glu174 and Glu166 present in the opened RBD down conformation out of a total of 40 states COVID19 in the NMR-derived COVID19 associated protein structure (PDB codes, 6xs6, 1xak, 2g9t, 3fqj, 2ghv, 6yb7) (1,3,4) to select a small subset representative of the protein flexibility downloaded from NCBI (30 April 2022, 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 BiogenetoligandorolTM. In this article, we effectively use a AI-decision tree and an optimum quantum walk number of small chemical active chemical features from a collection of hundreds of them utilizing neural network and jointly docking free energy cumulative features and ranking method with input toxicity values taking both network decision tree parameters into account. In this work, we prepared the protein structures using the Protein Preparation Wizard from the BiogenetoligandorolTM (BiogenetoligandorolTM, SynthocureTM, Thessaloniki, Biogenea Pharmaceuticals Ltd-GR, 2020). (8,13,17,22) hydrogen-bond optimization and Protonation assignment were applied by using the PROPKA and the ProtAssign publicly available software at the reported experimental pH (2-11,17) considering when available the presence of the bound small molecule (8-12,15,19).

Screening NuBEE Phyto-library and COVID2019 targets.

Virtual screening of the final proposed model and high throughput molecular docking based on existing literature were implemented to a collection of 9591 drugs including 2037 chemical structures of FDA-approved small molecule drugs and (2,3-14,17) over 6000 herbals and phytical 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, phytical 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 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 phytical elements for the cross-validation (e.g., more than one protomer, more than one enantiomer, etc.) were screened, as suitable druggable candidates for recoring and fragmentating the forms with the highest GP and Docking Energy values were considered in the ranking. (14,16,17) Finally, drugs and selected NuBBEDB phytical 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 BiogenetligandorolTM cluster of algorithms from the below.

		-	
		399.07	
6xs6-crotonate.	-399.075	5	37.5
6xs6-abyssinica	72.329	72.329	230.606
		-	
		943.23	
6xs6-acacia	-943.239	9	200.303
		-	
		721.68	
6xs6-acetovanillone	-721.685	5	409.167
		412.80	
6xs6-acteoside	412.805	5	227.955
		-	
		722.89	
6xs6-adenosin	-722.898	8	259.474
		-	
		249.94	
6xs6-africanal	-249.945	5	142.222
		-	
		561.75	
6xs6-agarin	-561.753	3	42.875
		147.81	
6xs6-aloe-emodin	147.811	1	18.2

		-	
6xs6-alpha-L-Rhamnose	-54.989	54.989	303.63 6
6xs6-alpha-Tocopherol	238.62	238.62	210.64 5
		-	
6xs6-alpha-Turmerone	-658.863	658.86 3	24.875
6xs6-ammonium glycyrrhizate	723.806	723.80 6	259.83 1
6xs6-anemone blue anthocyanin	264.373	264.37 3	878.02 2
		-	
6xs6-aniline	-520.154	520.15 4	442.85 7
6xs6-annona	215.215	215.21 5	206.81 8
		-	
6xs6-antitrypsin	-931.264	931.26 4	150.95 2
		-	
6xs6-arachidonic Acid	-759.696	759.69 6	211.81 8
6xs6-aristolochiac acid	441.074	441.07 4	138.33 3
		-	
6xs6-aristolochic acid	-905.713	905.71 3	26.44
		-	
6xs6-asparagusate	-508.316	508.31 6	36.875
		-	
6xs6-aspartic acid	-109.242	109.24 2	192.22 2
6xs6-astragalin	300.38	300.38	200.31 3
		-	
6xs6-atraric acid	-733.872	733.87 2	322.14 3
		-	
6xs6-atrazine	-757.602	757.60 2	36.5
6xs6-avicine	145.172	145.17 2	21.32
6xs6-azadirachtin	171.47	171.47	130.78 4
		-	
6xs6-baicalein-7-methyl ether	-68.083	68.083	191.42 9
		663.53	
6xs6-balanitin 3 106.	663.539	9	13.871

		-	
		258.27	
6xs6-balanitin 4 107.	-258.278	8	19.589
		-	
6xs6-balanitin 5 108.	-87.321	87.321	994.44
			4
		-	
		887.16	
6xs6-balanitin 7	-887.161	1	93.662

		-		
6xs6-baueronol	-707.698	707.698	16.129	
		-		
6xs6-b-Chlorogenin	-707.493	707.493	171.613	
		-		
6xs6-behenic acid	-746.006	746.006	213.333	
		-		
6xs6-benzo(c)phenanthridine	-713.002	713.002	321.429	
		-		
6xs6-Benzyl alcohol	-47.602	47.602	31.875	
		907.5		
6xs6-benzyl isothiocyanate (BITC)	907.592	9	24.1	
		-		
6xs6-benzylic amines	-788.472	788.472	8.625	
		111.5		
6xs6-berberine alkaloids	111.594	9	15.44	
		4		

Table1a. Docking energy rankings of the selected phythical hit compounds when docked onto the SARS-COV-2 protein targets of the (pdb:6xs6).

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 phytical 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 considered 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 phytical and chemical small molecule compounds (Table1a) after exhaustive virtual screening analysis were obtained accordingly, Colchicine, Raltegravir, Hexacosanol, Benzoxazolinon, Carboxy-Pentarcic 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 —o C[C@]1(C[C@H] ([C@H]2 N1CN2)ONN1C[P@] 1(C[C@H]1O[C@H](C[C@] 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) (Figure1a).The GQM (X) refers to the energy of the cluster of the phytical 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) (2) where $GQM_o(X)$ is the energy of the isolated active fragments in the conformation of the docked PL on both protein and molecule complex Inhibitors and conformations when applied Bioactivity-Guided Fractionations for the cluster of the selected compounds of the Colchicine, Raltegravir, Hexacosanol, Benzoxazolinon, Carboxy-Pentarcic acid, Ursane, Antheraxanthin, RA-XIII, Crotonate and Byrsonima coccolobifolia Leaves and Stems to be fragmented, re-cored and accordingly merged into the RoccustyrnaTM small hyperactive druggable scaffold (3,4,17,36). The acknowledgement of the binding of the selected 8 phytical compounds to their full-genome evolutionary novel coronavirus (2019-nCoV) protein targets was accomplished using Molinspiration (<http://www.molinspiration.com/cgi-bin/properties>) and DrugBank (1,11,12,13,15,17,34).

Pharmacophoric-ODEs fragmentating, merging and recoring : Biogenetoligandorol AI-heuristic algorithm.

The patterns of this Biogenetoligandorol fragmentation scheme are sorted into the working inputs of the Galilean transformation by examining the —extended|| Galilean transformation based on a set of heuristically determined descriptors moving with relative acceleration to a rigid system to a nonrotating geometric observer having an arbitrary time-dependent acceleration (20,21,27,28). (25,29) These descriptors as an applied nonconcurrent to both translate and rotate can be, for example, the number of atoms describing the pattern of a force system which can both translate and rotate and be determined by the substitution as a polynomial in $i p(r, t) = e i J\{r, t\} (p(r', t), V'ip = (V'ip + iV'f) eif, \rho^-s QFI \approx \sum_{i=0}^1 Re(\rho i 2) 2 (1 \rho i 1 + 1 \rho i 2) + (\rho i 1 - \rho i 2) 2 \rho i 1 + \rho i 2, \rho i j = \langle \phi_i | \rho s(0) \phi_j \rangle - 1 \rangle \rho 0 i j = \langle \phi_i | \langle 0 \rho s(0) \phi_j \rangle - 0 \rangle - 0 \rangle 1 \rangle H 1 = \gamma B 0 \cdot S^1 Re(\rho i 2) \rho i 2 \rho s(0) \rho^-s S \rangle = 12(\rangle - 01 \rangle) 30 \% \rho s(0) \rho^-s = H \otimes m 0 V'2 ip = \{ V'2 ip + 2 i V'f - V'(p + (p V'2 f + W \leftarrow S(I \otimes H) M 1; \langle p(V'f) 2 \rangle e_{f,i} \rangle = \langle \Phi | MT(I 3 - NT) - 2(\rho \otimes I 2) | \Phi \rangle (f) + if \langle p \rangle eif, and the Schrödinger equation becomes $n^2 m (V, z(p + 2 i V'f - V'(p + i(p V'f - M = \{M 0, M 1\} (V'f Y \langle p \rangle = if I 3 \leftarrow E(m 2); (*m 2-dimensional identity*)) ((\langle p + if(p) - g.(V'(p + i(p V'f)))$ where $p+2$ are the the number of bonds predicted or the number of double bonds. (20,25)$

Structure

ID

Mass

SMILES

2

152.0566862

(NH3+)C1=NC(=O)C2=N

6

158.1036364

(NH3+)C1NC2N=CNC2C

7

156.0879864

(NH3+)C1NC2N=CN=C
2

No
Image

8

154.0723363

(NH3+)C1NC(=O)C2=N
C

9

134.0461215

(NH2+)=C1N=CC2=NC
=

10

135.0301371

(OH+)=C1N=CN=C2N=
C

11

125.0457872

NC1=NC(=O)C(=[NH2+])

12

135.0301371

(NH+)[C-]#N=C1N=CN=C1

13

45.04472458

NC(=[NH2+])

14

43.02907452

(NH+)[C-]#N

15

108.0192381

N=C1N=CN=C1C#(O+)

16

110.0348882

(NH2+)=C1N=CN=C1C=

17

124.0617716

NC(=(NH2+))N=C1C=NC

18

125.0457872

N=C1N=CN=C1C((NH3+))

19

109.0508726

(NH+)[C-]#NC1C=NC=N1

20

107.0352225

(NH+)[C-]#N=C1C=NC=N1

21

82.03997355

(NH2+)=C1C=NC=N1

22

150.0410362

(NH3+)C1=NC(=O)C2=CN=C2N1

23

133.0144871

N#CN=C1N=CN=C1C#N

35

26.00252542

(C+)#N

99

15.02292652

(CH3+)

95

55.05422664

C1=[CH2+]CC1

96

53.03857658

C1=C[CH2+]=C1

97

129.0004768

C#CC(=C=C)[SH2+](=O)=O

98

131.0161269

C#CC(=C=C)[SH3+](=O)O

2

152.0566862

(NH3+)C1=NC(=O)C2=N

No

8

154.0723363

(NH3+)C1NC(=O)C2=N

Image

C

9

134.0461215

(NH2+)=C1N=CC2=NC

=

1

135.0301371

(OH+)=C1N=CN=C2N=

0

C

1	125.0457872	NC1=NC(=O)C(=NH2
1		+)

1	135.0301371	(NH+)#CN=C1N=CN=
2		C1

1	108.0192381	N=C1N=CN=C1C#(O
5		+))

1	110.0348882	(NH2+)=C1N=CN=C1
6		C=

1
7

124.0617716

NC(=(NH2+))N=C1C=
NC

1
8

125.0457872

N=C1N=CN=C1C((NH
3+

1 109.0508726 (NH+) $\#$ CNC1C=NC=

9 N1

2 107.0352225 (NH+) $\#$ CN=C1C=NC=

0 N1

2 82.03997355 (NH₂+)=C1C=NC=N1
1

133.0144871

N#CN=C1N=CN=C1C
#(

95

55.05422664

C1=[CH2+]CC1

96

53.03857658

C1=C[CH2+]=C1

97

129.0004768 C#CC(=C=C)[SH2+](=O)=O

98

131.0161269 C#CC(=C=C)[SH3+](=O)O

5

118.0651257

1

5

106.0651257

2

5

130.0651257

4

5

128.0494756

5

7

5

96.08077574

5

194.0964258

8

5

196.1120759

9

<p>Chemical structure of 2-aminoadenine-6-ol, a purine derivative. It features a fused bicyclic system with a hydroxyl group (OH) at position 6 and an amino group (NH₃⁺) at position 2.</p>	7	156.0879864	(NH ₃ ⁺)C1NC2N=CN=C
<p>Chemical structure of 2-aminoadenine, a purine derivative. It features a fused bicyclic system with an amino group (NH₂⁺) at position 2.</p>			2
<p>Chemical structure of 2-aminoadenine, a purine derivative. It features a fused bicyclic system with an amino group (OH⁺) at position 6.</p>	9	134.0461215	(NH ₂ ⁺)=C1N=CC2=NC

1	125.0457872	NC1=NC(=O)C(=NH2
1		+)
1 2	135.0301371	(NH+)#CN=C1N=CN=C1

1
5

108.0192381

N=C1N=CN=C1C#(O
+)

1
6

110.0348882

(NH2+)=C1N=CN=C1
C=

19	109.0508726	(NH+) <chem>#CNC1C=NC=N1</chem>
20	107.0352225	(NH+) <chem>#CN=C1C=NC=N1</chem>

$\text{N} \equiv \text{C}^+$			
CH_3^+			

Table1b. List of the Roccustyrna fragmented recored active compounds.

The complete pharmacophoric fragmentation scheme was analyzed to compare similar series of chemical patterns that are contained in the chemical phase structures as extraced from within the selected 10 hit compounds of the Colchicine, Raltegravir, Hexacosanol, Benzoxazolinon, Carboxy-Pentacic acid, Ursane, Antheraxanthin, RA-XIII, Crotonate and Byrsonima coccolobifolia. (Table1a), (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 $V'(p, \text{which gives } f = \frac{1}{2} \frac{d}{dt} \langle r^2 \rangle + g(t)$. Then one can choose n $g\{t\}$ such as to eliminate the purely time-dependent terms, and one finally arrives at, $= (2mV)^{1/2} (p + mf; \frac{1}{2} \frac{d}{dt} \langle r^2 \rangle = \frac{1}{2} \frac{d}{dt} \langle r^2 \rangle + g(t)$ (20,25,26) of the strong equivalence principle in quantum theory. After that, the child pharmacophoric pattern is searched in an inertial repeated merged system S as $ip = \frac{1}{2} (m_1^2 r, t) + ip_2 m_2, r, t)$. (25,26,37) Then assume that one fragmented pharrmacophore can describe the same superposition in an accelerating to a larger ligand-receptor system S' that obeys (20), with $\xi = \xi(r)$, $\xi(0) = \xi(7) = 0$, so that the system S' performs a closed quantum circuit and coincides with the chemical structure system the S at times $t = 0$ and $t = T$, such that $r'(iT) = r(7)$. (25-34,37) To avoid $q \{ h q; \} q_{reg} q(3); c_{reg} c(3); reset q(0); reset q(1); reset q(2); h q(0); u_2(\pi/2, \pi/2) q(1)$; incomplete

(1Z)-2- {((2S,3S,5R)-5-(2-amino-6-oxo- 6,9-dihydro- 3H-purin-9-yl)-3-hydroxyoxolan-2-yl) methylidene}-2-cyano-1-(((2S,4R,5R)-2 group assignments, through two hydrogen-bonding interactions whenever a part into the S2 subsite of the structure relative to the complex between the cyano-1-(((2S,4R,5R)-2-methyl- 2- (methylamino)-1,6-diazabicyclo with heptan-4-yl)oxy)imino)-1lambda5,2 lambda5-azaphosphiridin-1-ylum chemical groups of the cyclohexyl methyl is already recored and fragmented, the subsequent carbonyl oxygen matches have to be adjacent to the from the main-interacting chain amide of the residue Glu166 amino acid already occupied the space normally by the canonical S4- cyano-1-(((2S,4R,5R)-2-methyl-2- (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- [(2R,5R)-5-(2-methyl-6-methylidene-6,9-dihydro-3H-purin-9-yl)-3-methylideneoxolan-2-yl]phosphirane-1-carbonitrile -oxy)imino)-1lambda5, 2lambda5-azaphosphiridin-1-ylum binding site of the PDB:6LU7 main protease. (26,31-39) As a first step, our Chern-Simons oriented fragmentation algorithm performs a quick fragmentation scheme search for extracting different chemical groups formed by the nucleophilic attack of the catalytic domains of the target proteases onto the α -carbon of my new Roccustyrna small molecule by applying the heuristic quantum phases for group prioritization when performing parent-child group prioritization as described above. (29,32-39) This topology geometric for pharmacophoric search and design indicating the canonical binding pockets moieties of a new small sized prototype that goes sequentially through a sorted fragmentation scheme, adding groups that are found in its active conformation phases and do not overlap with the cyano-1-(((2S,4R,5R)-2-methyl-2- (methylamino)-1,6-diazabicyclo(3.2.0)heptan-4-yl) oxy)imino)- 1lambda5,2lambda5- azaphosphiridin-1-ylum 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 alterantive XYZ coordinate smile system. (33,35-42) (27-38) 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 recoring systems targeting in the in SARS-CoV Mpro. (12,13 ,28-39)

Figure1b. Quantum Circuit of the BiogenetoligandoirolTM Cluster for the Roccustyrna small molecule Merging and Hope-Re-coring algorithms. Gate nG0 (param) q { h q; } qreg q(3);creg c(3);reset q(0);reset q(1);reset q(2);hq(0);u2(pi/2,pi/2) q(1);measure q(2) -> c(2);x q(0);reset q(1);resetq(2);u3(pi/2,pi/2,pi/2) q(0);measure q(2) -> c(2);u2(pi/2,pi/2) q(2);cswap q(0),q(1),q(2);barrier q(0);u2(pi/2,pi/2) q(2);h q(0);t q(2);t q(0);measure q(1) -> c(1);ch q(1),q(2); q(2);crx(pi/2) q(1),q(2);cu1(pi/2) q(1),q(2);tdg q(2);sdg q(2);cy q(1),q(2);crz(pi/2) q(1),q(2);ch q(1),q(2);sdg q(1);u2(pi/2,pi/2) q(2);ry(pi/2) q(2);cu3(pi/2,pi/2,pi/2) q(1),q(2);tdg q(1);nG0(pi/2) q(2);crx(pi/2) q(1),q(2);cu1(pi/2) q(1),q(2);cswap q(0),q(1),q(2);swap q(1),q(2);cz q(1),q(2);rxx(pi/2) q(1),q(2);u1(pi/2) q(1);cry(pi/2) q(1),q(2);crz(pi/2) q(1),q(2);measure q(0) -> c(0);z q(0);measure q(1) -

$> c(1);z\ q(0);rx(pi/2)\ q(1);rx(pi/2)\ q(0);u2(pi/2,pi/2)\ q(1);rx(pi/2)\ q(0);ch\ q(1),q(2);ry(pi/2)q(0);ch\ q(1),q(2);u3(pi/2,pi/2,pi/2)\ q(0);cz\ q(1),q(2);ch\ q(0),q(1);u1\ (pi/2)\ q(0);swap\ q(1),q(2);sdg\ q(2);$

Therefore, from a mathematical perspective, a TQFT that recovers the above quantum Hilbert spaces may be called –Chern–Simons theory. We present here potential condensed eigenvalues applications for the positive spectrum and finite-dimensional eigenspaces: $S=14\pi\int M3(a+l)ta+l-1A\wedge dA+k13(a+l)ta+l-1A\wedge[A\wedge A]k(mod2\pi)\ 1\rightarrow U(1)\rightarrow LG\sim\rightarrow LG\rightarrow 1$ of the free loop group $LG=(a+l)\ ta+l-1\ (a+l)\ ta+l-1(S1,\ G)\ [1]$ is a functional of G bundles with connections over compact 3 manifolds. Here, A is the connection form, $(a+l)\ ta+l-1\ (a+l)\ ta+l-1\ \wedge\ (a+l)\ ta+l-1F)2zEGk: 2zEG\otimes 2zEG\rightarrow\mathbb{R}$ is a certain metric constructed and the integral from the level, is taken over a global section of the principal bundle. $\ddagger\ \delta^-\ \psi-\gamma\mu^-\varrho D\mu^-\ v-\ ^-\ v\sigma^-\varrho-\ i^-\ f(\vartheta)^-\ v^-\varrho+\ i^-\ F\varrho,\delta F=\varrho(-\gamma\mu D\mu\psi+\sigma\psi+\lambda v)+i(2_- -1)2f(\vartheta)\varrho\psi,\delta^-\ F=^-\varrho(-\gamma\mu D\mu^-\ \psi+^-\ \psi\sigma-^-\ v^-\ \lambda)+i(2_- -1)2f(\vartheta)^-\varrho^-\ \psi,$ (equation1) We hybridized then every level $k\in H4(BG,\ \mathbb{Z})$ that yields the quantum field theory with those levels k that satisfy the following positivity condition: Chern-Simons theory equation of the: $(\int tr(+23).S=k4\pi\int Mtr\) (3d\ N=2\ CSA\wedge dA+23A\wedge A\wedge A)(equation2).$ A (equation 1)(ie. considering S as a functional of A). associated to a connected Lie group α_{ζ} a simple current Roccustryna XYZ chemical extension of the tensor product of the $d/dx(33833\ y^n\times 1152\ N^2\ x^2\ k^4)=3d\ N\ 2\ CS\ 77951232\ k^4\ N^2\ x\ y^n$ associated to an even lattice and $38975616\ k^4\ N^2\ x^2\ y^n=\sum_{v=0}^{\infty}(n^v\ 38975616\ \{x\ \sin^{(-1)}(\sqrt{3})\},\ x\ \sin^{(-1)}(\sqrt{779}\ \sqrt{\theta^3}),\ x\ \sin^{(-1)}(2\ \sqrt{114109}),\ (\sqrt{1-\sqrt{456457}}\ \sqrt{x})\ x^{(1/4)}\ (2\ \sqrt{456457}\ \sqrt{x}+3))/(8\ 456457^{(3/4)})+(x-3/3651656)\ \sin^{(-1)}(456457^{(1/4)}\ x^{(1/4)}),\ 1/2\ \sqrt{x/456456754-x^2}+(x-1/912913508)\ \sin^{(-1)}(\sqrt{456456754}\ \sqrt{x}),\ x\ \sin^{(-1)}(2^{(3/4)}\ 57057^{(1/4)}),\ x\ \sin^{(-1)}(\sqrt{(\sum\ 444546\ \theta)}),\ x\ \sin^{(-1)}(2^{(3/4)}\ 431683182057^{(1/4)}\ \sqrt{(\sqrt{\theta}/(\sin^{(-1)}(44545545))))\}+constant\ (k^4\ N^2\ x^2\ \log^v(y))/(v!)$ 9equation3) associated to a simply connected Lie group classical equations of motion obtained via i and ii are known to be equivalent by combining the works of Finkelberg obtained in this way are: $\prime=0k2\pi F=03d\ N=2\ CS$ (equation4) also known as Connes fusion or every connected group G and level $k\geq 0$. It is given by $\gamma\mu\varrho D\mu_+ +\varrho(p\cdot\sigma)_-+i^-\ f(\vartheta)\varrho_- =M\varrho_-$, (equation 5) where M is the eigenvalue given by $M=M_{m,n}=\rho\cdot\sigma+i^-\ _mb+n_{b-1}+Q2_-_{,m},\ n\ 2\ \mathbb{Z}_0,\ Q=b+b-1$. (equation 6) The product of the eigenvalues roughly gives –denominator|| of the one-loop determinant., where the right action on H uses the isomorphism induced by reflection along the horizontal axis. (41) For every simple simply connected Lie group G with the quantum Hilbert space $CSG,k(S1$ and every level $k\geq 0$, a tensor category $A\wedge A,k$ whose Drinfel'd center $Z(dA,A)$ associated to a Riemann surface Σ can and has been defined at a mathematical level of precision and is equivalent to the the $VectkG[G]\ Vectk[G]CSG,k(pt)\ d/dx(33833\ y^n\times 1152\ N^2\ x^2\ k^4)=77951232\ k^4\ N^2\ x\ y^n$ (equation7) categories of the $\sin\ (a+l)\ ta+l-1Vectk(\ (a+l)\ ta+l-1+(a+l)\ ta+l-1\ \wedge\ (a+l)\ ta+l-1F)\ k^4\ x^4\ y^n\ \sin^{(-1)}(n)^{33833\ 5429\ N^2}$ (newtons squared) - $1/3\ x^6\ (k^4\ y^n\ \sin^{(-1)}(n)^{33833\ 5429\ N^2}$ (newtons squared)) + $2/45\ k^4\ x^8\ y^n\ \sin^{(-1)}(n)^{33833\ 5429\ N^2}$ (newtons squared) + $O(x^9)$ (equation8) of canonical quantization, it is the geometric quantization of $LocG(\Sigma)$ with respect to the natural symplectic Roccustryna structure coming from the Chern–Simons Lagrangian. We explain below that, at least along the direction θ is defined by $S\theta P(g)=Z1ei\theta 0dt\ e^{-\ tg\ BP(t)}$, (1)where $BP(t)$ is analytic continuation of the formal Borel transformation $P1\ell=0c\ell\ (a+l)\ ta+l-1$. when $G\ 432\ \pi\ k^4N^2\ x^2\ \sin^{(-1)}(n)^{33833\ (2\ x-\sin(2x))\ y^{(\wedge n)}$ for $Vectk[G]\ dCSG,k(pt)$ (equation9) is simply connected with

the the Reshetikhin–Turaev TQFT associated to the modular tensor category $\text{Rep}_k(\text{LG})$ of positive energy representations of the loop group at level k has that property $14\pi \int M_3(a+\ell) \text{ta}+\ell-1 A \wedge dA \mathbf{2zEG} Zcl(\sigma) = \exp X_{np=1} \text{isgn}(kp) \text{gptr}(\sigma(p)) 2i, Z1 \text{loop}(\sigma) = Q \alpha 2 \text{root} + 4 \sinh(\pi b \alpha \cdot \sigma) \sinh(\pi b - 1 \alpha \cdot \sigma) Q_a Q_{pa} 2 R_{asb_pa} \cdot \sigma - i Q(1 - a) 2_ , sb(z) = 1 Y_m = 0 1 Y_n = 0 m b + n b - 1 + Q/2 - iz m b + n b - 1 + Q/2 + iz k + 1 3 (a+\ell) \text{ta}+\ell-1 A \wedge [A \wedge A]$ (equation10) the coordinate $(x_1, x_2, x_3, x_4) = (\cos \vartheta \cos \phi, \cos \vartheta \sin \phi, \sin \vartheta \cos \chi, \sin \vartheta \sin \chi)$ and $f(\vartheta) = p b - 2 \sin^2 \vartheta + b^2 \cos^2 \vartheta . k(\text{mod} 2 \pi) [1] + \sin(a+\ell) \text{ta}+\ell-1 \text{Vect} k((a+\ell) \text{ta}+\ell-1 + (a+\ell) \text{ta}+\ell-1 \wedge (a+\ell) \text{ta}+\ell-1 F) 1 4 \pi \int M_3(a+\ell) \text{ta}+\ell-1 A \wedge dA \mathbf{2zEG} k+1 3 (a+\ell) \text{ta}+\ell-1 A \wedge [A \wedge A] \mathbf{2zEG} k(\text{mod} 2 \pi) [1] \wedge \sin(a+\ell) \text{ta}+\ell-1 \text{Vect} k((a+\ell) \text{ta}+\ell-1 + (a+\ell) \text{ta}+\ell-1 \wedge (a+\ell) \text{ta}+\ell-1 F) 1 4 \pi \int M_3(a+\ell) \text{ta}+\ell-1 A \wedge dA \mathbf{2zEG} k+1 3 (a+\ell) \text{ta}+\ell-1 A \wedge [A \wedge A] \mathbf{2zEG} k(\text{mod} 2 \pi) [1] F = dA + A \wedge A \text{Rep}_k(dA + A \wedge A \text{AGA})$ by [28] $F \mu \nu = 0, \sigma = \text{const.}, D = -\sigma f(\vartheta), \lambda = \bar{\lambda} = 0.$ (4) $\text{Rep}^{ss}(F_q \mathbf{2zEG})$ [or $\text{Rep}^k(\text{AF} \mathbf{2zEG})$] and $\text{Rep}(Dk(\mathbb{C}[G])) = \text{Rep}_f((a+\ell) \text{ta}+\ell-1_{G,k})$ (equation11) are equivalent as balanced tensor

category $Repk(dA+AAAAGA)$ of positive energy representations of the loop group at the:

$$\sin^{-1}(n)^{33833} y^{n\Lambda} \left(\int t dt \right) \sum g \left(\int \text{cumulative distribution function} \right) \left(\int 1152 N^2 \sin^2(x) k^4 \pi dx \right) \left(\int 3 dx \right) dx \left(\begin{array}{c} \text{normal distribution} \\ \text{mean} \\ \text{standard deviation} \end{array} \begin{array}{c} \mu = 0 \\ \sigma = 1 \end{array} \right) dx$$

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

(equation1)

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

□

(equation2)

(equations3)

Figure1c. Chern-Simons topology geometrics of the 3 selected hit fragmented candidates (fr1), (fr2), (fr3).

OUTPUT:Rocustyrna XYZ Cartesian coordinates

C	7.2670 0	- 1.33000	- 5.0970 0
O	6.9480 0	- 2.7070 0	- 5.3570 0
C	8.0880 0	- 3.53600	- 5.1060 0
C	9.1170 0	- 2.68100	- 4.3420 0
C	8.7810 0	- 1.24900	- 4.7710 0
O	9.0740 0	- 0.3070 0	- 3.7400 0
N	8.6100 0	- 4.0880 0	- 6.3290 0
C	8.6210 0	- 3.51000	- 7.5550 0
N	9.1640 0	- 4.3170 0	- 8.4870 0
C	9.5170 0	- 5.42800	- 7.8280 0
C	10.128 00	- 6.61300	- 8.2660 0

O	10.4230 0	-6.79100	-9.46800
N	10.4040 0	-7.57300	-7.34100
C	10.0990 0	- 7.41200	-6.02100
N	10.4270 0	-8.37500	-5.14600
N	9.4790 0	- 6.27600	- 5.5920 0
C	9.1920 0	- 5.29100	- 6.4830 0
C	6.8360 0	- 0.50700	- 6.2150 0
P	5.31500	-0.46900	- 6.6920 0
N	4.4570 0	0.67200	- 6.1220 0
C	4.7980 0	1.0370 0	- 7.3780 0
C	4.5480 0	- 1.74200	- 7.1820 0
N	3.9910 0	- 2.68300	- 7.5320 0
N	3.8360 0	1.04900	- 5.1380 0
O	3.7490 0	0.35300	- 4.0670 0
C	2.9890 0	1.0510 0	- 3.0600 0
C	3.0440 0	0.2750 0	- 1.7300 0
C	1.8160 0	- 0.68000	- 1.7610 0
N	0.7770 0	0.04700	- 2.5630 0

C	1.4700 0	1.0750 0	- 3.3660 0
C	0.0280 0	1.1560 0	- 1.9120 0
N	0.7330 0	2.16400	- 2.7060 0
N	1.2670 0	- 0.97500	- 0.4020 0
C	2.1360 0	- 2.02000	- 2.4980 0
C	2.1340 0	- 1.61200	0.6120 0
H	8.7920 0	0.56000	- 4.1010 0
H	6.6660 0	- 0.95800	- 4.2670 0

H	7.76800	- 4.41900	- 4.5530 0
H	8.90800	- 2.77000	- 3.2760 0
H	10.1090 0	- 2.92200	- 4.7250 0
H	9.40400	- 0.84800	- 5.5700 0
H	8.23800	- 2.51200	- 7.7670 0
H	9.72300	- 9.01900	- 4.8160 0
H	11.3780 0	- 8.45500	- 4.8160 0
H	9.23500	- 6.16400	- 4.6180 0
H	7.63400	0.0680 0	- 6.6850 0
H	3.98400	0.9950 0	- 8.1030 0
H	5.54000	1.8320 0	- 7.4380 0
H	3.46500	2.0310 0	- 3.0710 0
H	2.88700	0.9940 0	- 0.9250 0
H	3.94400	- 0.33800	- 1.7450 0
H	1.41600	1.0520 0	- 4.4540 0
H	0.30800	1.2410 0	- 0.8620 0
H	- 1.02400	1.1230 0	- 2.1950 0

H	0.71800	3.1720 0	- 2.7710 0
H	0.31200	- 0.74500	- 0.1690 0
H	2.32300	- 2.80300	- 1.7630 0
H	1.28800	- 2.30300	- 3.1220 0
H	3.02000	- 1.88900	- 3.1220 0
H	1.78000	- 1.35200	1.6090 0
H	2.10500	- 2.69500	0.4870 0
H	3.15800	- 1.26000	0.4870 0

To reduce the fragmentation space for the generation of salt-bridge interaction between the Glu290 and the new ligand that needs to be searched, the algorithm of the two independent Chern-Simons $S=14\pi \int M^3 A$ level $k \in H^4(BG, \mathbb{Z})$ $(a+l) ta+l-1 A \wedge dA \ 2zEG_{k+13} (a+l) ta+l-1 A \wedge [A \wedge A] \ 2zEG_k \pmod{2\pi}$ actions with loop group at level k has that property $(14\pi \int M^3 (a+l) ta+l-1 A \wedge dA \ 2zEG_{k+13} (a+l) ta+l-1 A \wedge [A \wedge A] \ 2zEG_k \pmod{2\pi}) [1] + \sin (a+l) ta+l-1 Vect_k ((a+l) ta+l-1 + (a+l) ta+l-1 \wedge (a+l) ta+l-1 F) 1 \ 4\pi \int M^3 (a+l) ta+l-1 A \wedge dA \ 2zEG_{k+13} (a+l) ta+l-1 A \wedge [A \wedge A] \ 2zEG_k \pmod{2\pi}) [1] \wedge \sin (a+l) ta+l-1 Vect_k ((a+l) ta+l-1 + (a+l) ta+l-1 \wedge (a+l) ta+l-1 F) 14\pi \int M^3 (a+l) ta+l-1 A \wedge dA \ 2zEG_{k+13} (a+l) ta+l-1 A \wedge [A \wedge A] \ 2zEG_k \pmod{2\pi}) [1] F = dA + A \wedge A \ Rep_k(dA + A \wedge A \ AGA) \ Rep_{ss}(Fq \ 2zEG) [or \ Rep_k(AF \ 2zEG)]$ and $\text{Rep}(Dk \ (\mathbb{C}[G])) = \text{Rep}_f((a+l) ta+l-1 G, k))$ equation (13) on the heuristic level of path integrals ($(a+l) ta+l-1 A$ is the potential 11-form and F is the field strength 224-form) where the partition function for the Chern-Simons theory to gather eigenvalues of the matrix models when associated with knot theory is the modulus square of the poles and zeroes in the one-loop determinant partition function.

$$\begin{aligned}
& -\log\left(\sqrt{1+14692375882461045811756348944(e^{-iX}-e^{iX})^2x(\tau)^2}-}\right. \\
& \quad \left.121212111121212(e^{-iX}-e^{iX})x(\tau)\right) \\
& \log\left(\sqrt{\left(1+x(\tau)^2x'(22\tau)^{488}\log^2\left(\sqrt{\left(1-\frac{1}{4y(\tau)}x'(\right.}\right. \right. \right. \\
& \quad \left. \left. \left. 22\right)^{576431275750959675405783039290773810744762062805850371259715614902742679552}\right)}\right. \right. \\
& \quad \left. \left. +\frac{1}{2\sqrt{y(\tau)}}ix'(\right. \right. \\
& \quad \left. \left. 22\right)^{288215637875479837702891519645386905372381031402925185629857807451371339776}\right)}\right) \\
& \quad \left. y'(\right. \\
& \quad \left. \tau\right)^{-2i\log\left(\sqrt{1+14692375882461045811756348944(e^{-iX}-e^{iX})^2x(\tau)^{44}}-121212111121212(e^{-iX}-e^{iX})x(\tau)^{22}}\right)} \\
& \quad \left. +x(\tau)x'(22\tau)^{244}\log\left(\sqrt{\left(1-\frac{1}{4y(\tau)}x'(\right.}\right. \right. \right. \\
& \quad \left. \left. \left. 22\right)^{576431275750959675405783039290773810744762062805850371259715614902742679552}\right)}\right. \right. \\
& \quad \left. \left. +\frac{1}{2\sqrt{y(\tau)}}ix'(\right. \right. \\
& \quad \left. \left. 22\right)^{288215637875479837702891519645386905372381031402925185629857807451371339776}\right)}\right) \\
& \quad \left. y'(\right. \\
& \quad \left. \tau\right)^{-i\log\left(\sqrt{1+14692375882461045811756348944(e^{-iX}-e^{iX})^2x(\tau)^{44}}-121212111121212(e^{-iX}-e^{iX})x(\tau)^{22}}\right)} \\
& \quad \left. \right)
\end{aligned} \tag{1}$$

$$\begin{aligned}
& \frac{\partial}{\partial n}\left(-\frac{n^{33834}k^{-(k^4n^{33835}N^2)}N^{213}}{33834432k^4}\right)= \\
& \frac{n^{33833}N^{213}k^{-k^4n^{33835}N^2-4}(33835k^4n^{33835}N^2\log(k)-33834)}{33834432}
\end{aligned} \tag{2}$$

$$\int -\frac{k^{-4-k^4n^{33835}N^2}n^{33834}N^{213}}{33834432}dn = \frac{N^{211}k^{-k^4n^{33835}N^2-8}}{1144788006720\log(k)} + \text{constant} \tag{3}$$

(22,27,28,35) This In Silico approach keeps track of the solutions already found of the selected group of the selected hit candidates which were fragmented, recored and superposed in a non-relativistic quantum mechanics environment and finally led us to the complete Roccustyrna chemical structure. (Table1a),(20,28,29,30) If several chemical space solutions were found in the phase end, the combined theory has a sequence of similar such function spaces of finite but arbitrarily large selected dimension, where the partition dimension increases with the finite resolution of relative knot space measurements to the first dihydro-3H-purin-9-yl)- system when extracted from the 10 hit selected small molecules as the possible chemical bimodules over a hyperfinite 1 factor solutions which were sorted by the number of different SARS-CoV Mpro, PDB entry 6lu7 receptor patterns.

(1)

(2)

Figure2a. Geometrical descriptors of the Roccustyrna small molecule. Dreiding energy = 287,17 kcal/mol MMFF94 energy = 234,59 kcal/mol, Minimal projection area = 63,36, Maximal projection area = 133,25, Minimal projection radius = 6,25, Maximal projection radius = 9,68, Length perpendicular to the max area = 8,32, Length perpendicular to the min area = 19,36, van der Waals volume = 440,91

The Roccustyrna small molecule is the fusion product of such chemical space representations of negative energy selected representations as merged into the connection form, $(a+l) \text{ ta}+l-1 \text{ 2zEGk: } 2\text{zEG} \otimes 2\text{zEG} \rightarrow \mathbb{R}$ of the 6,9-dihydro-3H- purin loop group.

COMPND C:\Users\user\Downloads\Roccustyrna.pdb

AUTHOR GENERATED BY OPEN BABEL 2.4.1

HETATM	1	C	UNK	0	7.267	-1.330	-5.097	1.00	0.00	C
HETATM	2	O	UNK	0	6.948	-2.707	-5.357	1.00	0.00	O
HETATM	3	C	UNK	0	8.088	-3.536	-5.106	1.00	0.00	C
HETATM	4	C	UNK	0	9.117	-2.681	-4.342	1.00	0.00	C
HETATM	5	C	UNK	0	8.781	-1.249	-4.771	1.00	0.00	C
HETATM	6	O	UNK	0	9.074	-0.307	-3.740	1.00	0.00	O
HETATM	7	N	UNK	0	8.610	-4.088	-6.329	1.00	0.00	N
HETATM	8	C	UNK	0	8.621	-3.510	-7.555	1.00	0.00	C
HETATM	9	N	UNK	0	9.164	-4.317	-8.487	1.00	0.00	N
HETATM	10	C	UNK	0	9.517	-5.428	-7.828	1.00	0.00	C
HETATM	11	C	UNK	0	10.128	-6.613	-8.266	1.00	0.00	C
HETATM	12	O	UNK	0	10.423	-6.791	-9.468	1.00	0.00	O
HETATM	13	N	UNK	0	10.404	-7.573	-7.341	1.00	0.00	N
HETATM	14	C	UNK	0	10.099	-7.412	-6.021	1.00	0.00	C
HETATM	15	N	UNK	0	10.427	-8.375	-5.146	1.00	0.00	N
HETATM	16	N	UNK	0	9.479	-6.276	-5.592	1.00	0.00	N
HETATM	17	C	UNK	0	9.192	-5.291	-6.483	1.00	0.00	C
HETATM	18	C	UNK	0	6.836	-0.507	-6.215	1.00	0.00	C
HETATM	19	P	UNK	0	5.315	-0.469	-6.692	1.00	0.00	P
HETATM	20	N	UNK	0	4.457	0.672	-6.122	1.00	0.00	N
HETATM	21	C	UNK	0	4.798	1.037	-7.378	1.00	0.00	C
HETATM	22	C	UNK	0	4.548	-1.742	-7.182	1.00	0.00	C
HETATM	23	N	UNK	0	3.991	-2.683	-7.532	1.00	0.00	N

HETATM	24	N	UNK	0	3.836	1.049	-5.138	1.00	0.00	N
HETATM	25	O	UNK	0	3.749	0.353	-4.067	1.00	0.00	O
HETATM	26	C	UNK	0	2.989	1.051	-3.060	1.00	0.00	C
HETATM	27	C	UNK	0	3.044	0.275	-1.730	1.00	0.00	C
HETATM	28	C	UNK	0	1.816	-0.680	-1.761	1.00	0.00	C
HETATM	29	N	UNK	0	0.777	0.047	-2.563	1.00	0.00	N
HETATM	30	C	UNK	0	1.470	1.075	-3.366	1.00	0.00	C
HETATM	31	C	UNK	0	0.028	1.156	-1.912	1.00	0.00	C
HETATM	32	N	UNK	0	0.733	2.164	-2.706	1.00	0.00	N
HETATM	33	N	UNK	0	1.267	-0.975	-0.402	1.00	0.00	N
HETATM	34	C	UNK	0	2.136	-2.020	-2.498	1.00	0.00	C
HETATM	35	C	UNK	0	2.134	-1.612	0.612	1.00	0.00	C
HETATM	36	H	UNK	0	8.792	0.560	-4.101	1.00	0.00	H
HETATM	37	H	UNK	0	6.666	-0.958	-4.267	1.00	0.00	H
HETATM	38	H	UNK	0	7.768	-4.419	-4.553	1.00	0.00	H
HETATM	39	H	UNK	0	8.908	-2.770	-3.276	1.00	0.00	H
HETATM	40	H	UNK	0	10.109	-2.922	-4.725	1.00	0.00	H
HETATM	41	H	UNK	0	9.404	-0.848	-5.570	1.00	0.00	H
HETATM	42	H	UNK	0	8.238	-2.512	-7.767	1.00	0.00	H
HETATM	43	H	UNK	0	9.723	-9.019	-4.816	1.00	0.00	H
HETATM	44	H	UNK	0	11.378	-8.455	-4.816	1.00	0.00	H
HETATM	45	H	UNK	0	9.235	-6.164	-4.618	1.00	0.00	H
HETATM	46	H	UNK	0	7.634	0.068	-6.685	1.00	0.00	H
HETATM	47	H	UNK	0	3.984	0.995	-8.103	1.00	0.00	H
HETATM	48	H	UNK	0	5.540	1.832	-7.438	1.00	0.00	H
HETATM	49	H	UNK	0	3.465	2.031	-3.071	1.00	0.00	H
HETATM	50	H	UNK	0	2.887	0.994	-0.925	1.00	0.00	H
HETATM	51	H	UNK	0	3.944	-0.338	-1.745	1.00	0.00	H
HETATM	52	H	UNK	0	1.416	1.052	-4.454	1.00	0.00	H
HETATM	53	H	UNK	0	0.308	1.241	-0.862	1.00	0.00	H
HETATM	54	H	UNK	0	-1.024	1.123	-2.195	1.00	0.00	H

HETATM	55	H	UNK	0	0.718	3.172	-2.771	1.00	0.00	H
HETATM	56	H	UNK	0	0.312	-0.745	-0.169	1.00	0.00	H
HETATM	57	H	UNK	0	2.323	-2.803	-1.763	1.00	0.00	H
HETATM	58	H	UNK	0	1.288	-2.303	-3.122	1.00	0.00	H
HETATM	59	H	UNK	0	3.020	-1.889	-3.122	1.00	0.00	H
HETATM	60	H	UNK	0	1.780	-1.352	1.609	1.00	0.00	H
HETATM	61	H	UNK	0	2.105	-2.695	0.487	1.00	0.00	H
HETATM	62	H	UNK	0	3.158	-1.260	0.487	1.00	0.00	H

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CONNECT 2 3 1

CONNECT 3 7 2384

CONNECT 4 3 54039

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CONNECT 8 9 42 7

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END
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Figure2b. RoccustyrnaTM small molecule's PDB file

INSATU

POLAR

INSOLU

Formula

C₁₉H₂₉N₁₁O₄P

Molecular weight

506.48 g/mol

Num. heavy atoms

35

Num. arom. heavy atoms	9	
Fraction Csp3	0.68	
Num. rotatable bonds	7	
Num. H-bond acceptors	12	
Num. H-bond donors	6	
Molar Refractivity	135.94	
TPSA	208.00 Å²	
Lipophilicity		
Log <i>P</i> _{o/w} (iLOGP)	0.00	
Log <i>P</i> _{o/w} (XLOGP3)	-1.63	
Log <i>P</i> _{o/w} (WLOGP)	-3.09	
Log <i>P</i> _{o/w} (MLOGP)	-1.83	
Log <i>P</i> _{o/w} (SILICOS-IT)	-4.14	
Consensus Log <i>P</i> _{o/w}	-2.14	
Water Solubility		
Log <i>S</i> (ESOL)	-1.68	
Solubility	1.05e+01 mg/ml ; 2.08e-02 mol/l	
Class	Very soluble	
Log <i>S</i> (Ali)	-2.23	
Solubility	3.00e+00 mg/ml ; 5.92e-03 mol/l	
Class	Soluble	
Log <i>S</i> (SILICOS-IT)	-1.42	
Solubility	1.93e+01 mg/ml ; 3.82e-02 mol/l	
Class	Soluble	
Pharmacokinetics		
GI absorption	Low	

BBB permeant P-gp	No	Medicinal Chemistry
substrate CYP1A2	Yes	
inhibitor CYP2C19	No	
inhibitor CYP2C9	No	
inhibitor CYP2D6	No	
inhibitor CYP3A4	No	
inhibitor	No	
Log K_p (skin permeation)	-10.55 cm/s	
		gen-nitrogen_sinin
PAINS	0 alert	
Brenk	3 alerts: Three-membered_heterocycle, oxy	
Leadlikeness	No; 1 violation: MW>350	
Synthetic accessibility	6.25	

Figure2c.RocustyrnaTM_Preferred_IUPACName=(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-azaphosphiridin-1-ylum.

@<TRIPOS>MOLECULE

64691

SMALL

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S

@<TRIPOS>ATO

M

1	C1	6.7793	5.4101	-7.3671	C.3	1	0.0929
2	O1	6.4167	4.6860	-8.5515	O.3	1	-0.3530
3	C2	7.1793	5.1341	-9.6850	C.3	1	0.1316
4	C3	8.1667	6.2420	-9.1557	C.3	1	0.0193

5	C4	7.4664	6.7292	-7.8136	C.3	1	0.0850
6	O2	8.3312	7.2161	-6.7537	O.3	1	-0.3901
7	N1	6.2816	5.6652	-10.6793	N.2	1	0.0158
8	C5	5.0344	6.1629	-10.4967	C.2	1	-0.0334
9	N2	4.4579	6.5206	-11.6609	N.2	1	-0.2093
10	C6	5.3716	6.2562	-12.6024	C.2	1	0.0617
11	C7	5.3381	6.4013	-13.9991	C.2	1	0.1449
12	O3	4.3223	6.8295	-14.5891	O.2	1	-0.2466
13	N3	6.4475	6.0473	-14.7039	N.2	1	-0.1575
14	C8	7.5681	5.5602	-14.0975	C.2	1	-0.0476
15	N4	8.6368	5.2334	-14.8398	N.3	1	-0.1336
16	N5	7.6009	5.4035	-12.7434	N.2	1	0.0739
17	C9	6.5147	5.7408	-12.0019	C.2	1	0.0095
18	C10	5.5391	5.6450	-6.4567	C.3	1	0.0181
19	P1	4.4871	4.2358	-6.1084	P.3	1	-0.1484

20	N6	4.4157	2.6297	-5.5202	N.3	1	-0.0518
21	C11	5.5025	3.3359	-5.0335	C.3	1	0.0624
22	N7	3.4152	2.4619	-4.5388	N.3	1	-0.0934
23	O4	3.5802	1.3462	-3.7641	O.3	1	-0.3178
24	C12	2.7318	1.4614	-2.5999	C.3	1	0.1125
25	C13	3.0058	0.3420	-1.5704	C.3	1	0.0100
26	C14	1.8142	-0.6553	-1.6624	C.3	1	0.0734
27	N8	0.6767	0.1212	-2.2390	N.3	1	-0.2544
28	C15	1.2258	1.2977	-2.9316	C.3	1	0.0925
29	N9	0.3485	2.2044	-2.1731	N.3	1	-0.2864
30	C16	-0.0886	1.0558	-1.3757	C.3	1	0.0528
31	N10	1.3728	-1.2053	-0.3452	N.3	1	-0.3022
32	C17	2.3014	-2.0166	0.4626	C.3	1	-0.0147
33	C18	2.1137	-1.8150	-2.6582	C.3	1	-0.0330
34	C19	3.1251	4.9597	-5.6402	C.1	1	0.0718
35	N11	2.1558	5.4787	-5.3100	N.1	1	-0.1788
36	H1	7.4770	4.7777	-6.8180	H	1	0.0637
37	H2	7.6610	4.2815	-10.1636	H	1	0.0824
38	H3	9.1078	5.7581	-8.8944	H	1	0.0338
39	H4	8.1578	7.0689	-9.8659	H	1	0.0338
40	H5	6.8657	7.6318	-7.9260	H	1	0.0629
41	H6	8.7137	6.4708	-6.2850	H	1	0.2105
42	H7	4.5506	6.2639	-9.5252	H	1	0.1016
43	H8	8.7834	4.2740	-15.1192	H	1	0.1257
44	H9	9.2948	5.9469	-15.1192	H	1	0.1257
45	H10	8.4270	5.0387	-12.2910	H	1	0.0676
46	H11	6.0012	5.9571	-5.5201	H	1	0.0379
47	H12	4.9596	6.3583	-7.0427	H	1	0.0379

48	H13	5.4208	3.5873	-3.9760	H	1	0.0539
49	H14	6.4567	3.0042	-5.4427	H	1	0.0539
50	H15	2.6390	3.0933	-4.4012	H	1	0.1759
51	H16	3.0064	2.4621	-2.2662	H	1	0.0657
52	H17	3.9007	-0.1865	-1.8986	H	1	0.0327
53	H18	2.9745	0.7986	-0.5811	H	1	0.0327
54	H19	1.1772	1.3623	-4.0186	H	1	0.0667
55	H20	0.1370	3.1919	-2.1918	H	1	0.1251
56	H21	0.3474	1.1003	-0.3777	H	1	0.0601
57	H22	-1.1605	0.8980	-1.4956	H	1	0.0601
58	H23	0.4409	-1.0275	0.0013	H	1	0.1237
59	H24	2.1062	-1.8461	1.5213	H	1	0.0392
60	H25	2.1567	-3.0721	0.2319	H	1	0.0392
61	H26	3.3279	-1.7317	0.2319	H	1	0.0392
62	H27	2.3479	-2.7217	-2.1003	H	1	0.0263
63	H28	1.2397	-1.9900	-3.2856	H	1	0.0263
64	H29	2.9632	-1.5450	-3.2856	H	1	0.0263

@<TRIPOS>BOND

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4	4	5	1
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6	5	6	1
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8	7	8	ar
9	8	9	ar
10	9	10	ar

11	10	11	ar
12	11	12	2
13	11	13	ar
14	13	14	ar
15	14	15	1
16	14	16	ar
17	16	17	ar
18	7	17	ar
19	10	17	ar
20	1	18	1
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22	19	20	1
23	20	21	1
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32	24	28	1
33	28	29	1
34	29	30	1
35	27	30	1
36	26	31	1
37	31	32	1
38	26	33	1

39	19	34	1
40	34	35	3
41	1	36	1
42	3	37	1
43	4	38	1
44	4	39	1
45	5	40	1
46	6	41	1
47	8	42	1
48	15	43	1
49	15	44	1
50	16	45	1
51	18	46	1
52	18	47	1
53	21	48	1
54	21	49	1
55	22	50	1
56	24	51	1
57	25	52	1
58	25	53	1
59	28	54	1
60	29	55	1
61	30	56	1
62	30	57	1
63	31	58	1
64	32	59	1
65	32	60	1
66	32	61	1

67	33	62	1
68	33	63	1
69	33	64	1

@<TRIPOS>SUBSTRUCTU

RE

1 1

Table1c. RoccustyrnaTM MOL2 file.

Figure2d.RoccustyrnaTM_Preferred_IUPACName=(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-(methylamino)-1,6-diazabicyclo(3.2.0)heptan-4-yl)oxy)imino)-1lambda5,2lambda5-azaphosphiridin-1-ylum.For instance,a generalized coordinate is commonly used in the study of tunnelling effects and may be a bound length, a bound angle, or a dihedral angle in solid state systems. 2d Structure Map of the RoccustyrnaTM Atoms Geometrical Descriptors of the RoccustyrnaTM small molecule: Dreiding energy = 305,20 kcal/mol, MMFF94 energy = 35,06 kcal/mol, Minimal projection area = 66,49, Maximal projection area = 123,65 Minimal projection radius = 5,71 Maximal projection radius = 9,24 Length perpendicular to the max area = 10,29 Length perpendicular to the min area = 19,04 van der Waals volume = 409,41 Donor count = 5 Donor sites = 6 Acceptor count 11 Acceptor sites = 14 127.9718331 C#CC#P1C=S1#(NH+)33 93.98748321(NH+)#S1=PC134 59.99024648C#S#(NH+)35

Figure3. Rocustyrna active fragments smiles prediction correlation analysis.

15.02292652	0.9382305843	99	(0.93823)
26.00252542	2.261472925	35	(2.2615)
30.03382555	0.535992489	129	(0.53599)
32.04947561	0.4083831708	128	(0.40838)
109.0760247	0.6306776069	105	(0.63068)
134.0461215	1.054959553	9	(1.055)
134.0712737	0.6753435418	59	(0.67534)
135.0301371	2.00414747	10	12 (1.8344 0.16975)
136.0869237	0.8276811831	33	(0.82768)

138.1025738 5.854997521 4 (5.855)
140.1182239 11.87293119 3 (11.873)
142.1338739 1.434949881 32 (1.4349)
150.0410362 0.7478931696 22 (0.74789)
152.0566862 50.57559424 2 (50.576)
158.1287886 0.5441383792 84 (0.54414)
250.0934657 1.102478867 68 (1.1025)
255.1243482 0.4222794277 39 (0.42228)
256.1195972 0.9300528895 55 34 (0.82641 0.10364)
257.1399983 0.4627232947 148 (0.46272)
258.1352473 0.7827475764 48 (0.78275)
266.1039472 0.4286298007 43 (0.42863)
270.1352473 0.5767642398 40 (0.57676)
272.1508973 1.403710436 30 (1.4037)
335.0890254 0.6614061977 77 (0.66141)
350.0999244 0.5843430157 89 (0.58434)
356.1720267 0.4195737218 25 (0.41957)
472.1843227 0.8241622495 5 (0.82416)
476.1792373 0.8957022747 121 (0.8957)
489.2108718 1.289594322 1 26 (1.1883 0.10129)
490.1948874 3.389865269 147 28 166 173 (2.7809 0.55441 0.043182 0.011359)
507.2214365 5.458573512 0 (5.4586)
energy1
26.00252542 1.003424285 35 (1.0034)
108.0192381 0.4484564381 15 (0.44846)
109.0508726 1.550778576 19 (1.5508)
109.0760247 1.307266463 105 (1.3073)
111.0916748 0.514768555 97 115 (0.45789 0.056876)
124.0617716 0.8909860357 17 (0.89099)
134.0461215 1.945717906 9 (1.9457)
135.0301371 4.830634071 10 12 (3.3243 1.5064)
138.1025738 2.758491951 4 (2.7585)
140.1182239 5.537145101 3 (5.5371)
142.1338739 1.502767544 32 (1.5028)
152.0566862 61.84168617 2 (61.842)
171.1240375 0.9257645934 56 (0.92576)
225.0773981 0.6516260185 60 (0.65163)
227.0930481 0.4793912741 52 (0.47939)
229.1086982 0.6269263545 53 (0.62693)
231.1243482 1.055636235 54 (1.0556)
239.0930481 1.005808076 61 (1.0058)
241.1086982 0.8475927077 36 (0.84759)
243.1243482 0.6580287877 37 (0.65803)
245.1399983 1.083243159 38 (1.0832)
253.1086982 0.8138872082 41 (0.81389)
254.1039472 0.7868172629 62 (0.78682)
256.1195972 1.129798814 55 34 (1.0665 0.063267)
258.1352473 1.075725275 48 (1.0757)
268.1195972 0.4895269014 42 (0.48953)
270.1352473 0.4898493769 40 (0.48985)
449.1683383 0.4614633584 144 187 (0.4575 0.0039625)
462.1999728 0.6710353339 135 (0.67104)
480.2105375 1.879432017 134 (1.8794)
490.1948874 0.736324146 147 28 173 166 (0.6098 0.1038 0.016593 0.0061259)
energy2

15.02292652 0.995023181 99 (0.99502)
26.00252542 1.024091421 35 (1.0241)
45.04472458 0.9518049313 13 (0.9518)
79.02907452 0.7948376336 118 (0.79484)
80.04947561 3.661453795 119 (3.6615)
81.04472458 1.362092912 109 (1.3621)
82.03997355 1.630942429 21 (1.6309)
82.06512568 0.9001924745 113 (0.90019)
83.06037464 1.196365366 101 (1.1964)
84.08077574 2.268763628 103 (2.2688)
85.07602471 2.328821417 102 (2.3288)
86.0964258 1.087814221 104 (1.0878)
107.0352225 3.067121836 20 (3.0671)
107.0603746 1.010133785 116 (1.0101)
108.0192381 2.161146957 15 (2.1611)
109.0508726 4.111770418 19 (4.1118)
109.0760247 4.299628128 105 (4.2996)
110.0348882 4.444814629 16 (4.4448)
111.0916748 1.715509525 97 115 (1.662 0.053524)
124.0869237 0.6660839118 106 (0.66608)
125.0457872 1.490098898 11 18 (0.97721 0.51289)
126.1025738 1.95890532 100 (1.9589)
134.0461215 5.996375544 9 (5.9964)
135.0301371 15.39694322 12 10 (10.757 4.6396)
136.0869237 1.902630549 33 (1.9026)
138.1025738 5.083500848 4 (5.0835)
140.1182239 5.729483613 3 (5.7295)
142.1338739 1.748821474 32 (1.7488)
150.0410362 1.320314853 22 (1.3203)
152.0566862 18.90373723 2 (18.904)
356.1720267 0.7907758483 25 (0.79078)
0 507.2214365 CNC1(C)CC(ONN2C(P)2(C#N)CC2OC(n3cnc4c3(nH)c((NH3+))nc4=O)CC2O)C2N CN 21
1 489.2108718 CNC1(C)C=C(ONN2C(P)2(C=C2CC=C(N3C=NC4=C(O)N=C((NH3+))N=C43)O2)C N) C2NCN21
2 152.0566862 (NH3+)C1=NC(=O)C2=NC=NC2N1
3 140.1182239 C(NH2+)C1(C)C=CC2NCN21
4 138.1025738 C(NH2+)C1(C)C=CC2=NCN21
5 472.1843227 CNC1(C)C=C(ONN2C(P)2(C)C=C2CC=C(N3C=NC4=C(O)N=C((NH3+))N=C43)O2)C 2=NCN21
6 158.1036364 (NH3+)C1NC2N=CNC2C(O)N1
7 156.0879864 (NH3+)C1NC2N=CN=C2C(O)N1
8 154.0723363 (NH3+)C1NC(=O)C2=NC=NC2N1
9 134.0461215 (NH2+)=C1N=CC2=NC=NC2=N1
10 135.0301371 (OH+)=C1N=CN=C2N=CN=C21
11 125.0457872 NC1=NC(=O)C(=NH2+)C=N1
12 135.0301371 (NH+)#CN=C1N=CN=C1C=O
13 45.04472458 NC=(NH2+)
14 43.02907452 (NH+)#CN
15 108.0192381 N=C1N=CN=C1C#(O+)
16 110.0348882 (NH2+)=C1N=CN=C1C=O

17	124.0617716	<chem>NC(=(NH2+))N=C1C=NC=N1</chem>
18	125.0457872	<chem>N=C1N=CN=C1C((NH3+))=O</chem>
19	109.0508726	<chem>(NH+)#CNC1C=NC=N1</chem>
20	107.0352225	<chem>(NH+)#CN=C1C=NC=N1</chem>
21	82.03997355	<chem>(NH2+)=C1C=NC=N1</chem>
22	150.0410362	<chem>(NH3+)C1=NC(=O)C2=NC=NC2=N1</chem>
23	133.0144871	<chem>N#CN=C1N=CN=C1C#(O+)</chem>
24	354.1563766	<chem>CNC1(C)C=C(O(NH2+))N2C(P)2(C=C2OC=CC2=O)CN)C2NCN21</chem>
25	356.1720267	<chem>CNC1(C)CC(O(NH2+))N2C(P)2(C=C2OC=CC2=O)CN)C2NCN21</chem>
26	489.2108718	<chem>CNC1(C)CC(ONN2C(P)2(C=C2OC(N3C=NC4=CN=C((NH3+))N=C43)=CC2=O)CN)C2NCN21</chem>
27	136.0617716	<chem>(NH2+)=C1N=CC2=NC=NC2N1</chem>
28	490.1948874	<chem>CNC1(C)CC(O(NH2+))N2C(P)2(C=C2OC(N3C=NC4=C(O)N=CN=C43)=CC2=O)CN)C2NCN21</chem>
29	274.1665474	<chem>CNC1(C)C=C(O(NH2+))N2C(P)2(C)CN)C2NCN21</chem>
30	272.1508973	<chem>CNC1(C)C=C(O(NH2+))N2C(P)2(C)CN)C2=NCN21</chem>
31	102.0341363	<chem>C(P)1(C=(NH2+))C=N1</chem>
32	142.1338739	<chem>C(NH2+)C1(C)CCC2NCN21</chem>
33	136.0869237	<chem>C=(NH+)C1(C)C=CC2=NCN21</chem>
34	256.1195972	<chem>CC1(N)C=C(O(NH2+))N2C(P)2(C)C=N)C2=NCN21</chem>
35	26.00252542	<chem>(C+)#N</chem>
36	241.1086982	<chem>C=(P)1CN1(NH2+)OC1=CC(C)(NC)N2CN=C12</chem>
37	243.1243482	<chem>C=(P)1CN1(NH2+)OC1=CC(C)(NC)N2CNC12</chem>
38	245.1399983	<chem>C=(P)1CN1(NH2+)OC1CC(C)(NC)N2CNC12</chem>
39	255.1243482	<chem>C=NC1(C)C=C(O(NH2+))N2C(P)2(C)C)C2=NCN21</chem>
40	270.1352473	<chem>C=NC1(C)C=C(O(NH2+))N2C(P)2(C)CN)C2=NCN21</chem>
41	253.1086982	<chem>C#(N+)C1(C)C=C(ONN2C(P)2(C)C)C2=NCN21</chem>
42	268.1195972	<chem>C=NC1(C)C=C(O(NH2+))N2C(P)2(C)C=N)C2=NCN21</chem>
43	266.1039472	<chem>C=NC1(C)C=C(O(NH2+))N2C(P)2(C)C#N)C2=NCN21</chem>
44	264.0882971	<chem>C#(N+)C1(C)C=C(ONN2C(P)2(C)C#N)C2=NCN21</chem>
45	234.0621655	<chem>(NH3+)C1=NC(O)=C2N=CN(C3=CC(=O)CO3)C2=N1</chem>
46	236.0778156	<chem>(NH3+)C1=NC(O)=C2N=CN(C3=CC(=O)CO3)C2N1</chem>
47	262.1665474	<chem>CNC1(C)CC(O(NH2+))N2C(PH)2CN)C2NCN21</chem>
48	258.1352473	<chem>CNC1(C)C=C(O(NH2+))N2C(PH)2CN)C2=NCN21</chem>
49	86.00283615	<chem>(NH+)#C(P)1=NC1</chem>
50	88.01848621	<chem>(NH2+)=C(P)1=NC1</chem>
51	242.1039472	<chem>CC1(N)C=C(O(NH2+))N2C(P)2=CN)C2=NCN21</chem>
52	227.0930481	<chem>C=NC1(C)C=C(O(NH2+))N2C(PH2)2)C2=NCN21</chem>
53	229.1086982	<chem>CNC1(C)C=C(O(NH2+))N2C(PH2)2)C2=NCN21</chem>
54	231.1243482	<chem>CNC1(C)C=C(O(NH2+))N2C(PH2)2)C2NCN21</chem>
55	256.1195972	<chem>C=NC1(C)C=C(O(NH2+))N2C(PH)2CN)C2=NCN21</chem>
56	171.1240375	<chem>CNC1(C)C=C(O(NH3+))C2NCN21</chem>
57	156.1131385	<chem>C(NH2+)C1(C)CC(=O)C2NCN21</chem>
58	101.0137352	<chem>N#C(P)1=CN1(NH3+)</chem>
59	134.0712737	<chem>C#(N+)C1(C)C=CC2=NCN21</chem>
60	225.0773981	<chem>C=C1C=C(O(NH2+))N2C(P)2=CN)C2=NCN21</chem>
61	239.0930481	<chem>C=NC1(C)C=C(O(NH2+))N2C(P)2=C)C2=NCN21</chem>
62	254.1039472	<chem>C=NC1(C)C=C(O(NH2+))N2C(P)2=CN)C2=NCN21</chem>
63	237.0773981	<chem>C#(N+)C1(C)C=C(ONN2C(P)2=C)C2=NCN21</chem>
64	252.0882971	<chem>C=NC1(C)C=C(O(NH2+))N2C(P)2=C=N)C2=NCN21</chem>
65	250.072647	<chem>C#(N+)C1(C)C=C(ONN2C(P)2=C=N)C2=NCN21</chem>
66	246.0621655	<chem>C=C1OC(N2C=NC3=C(O)N=C((NH3+))N=C32)=CC1=O</chem>
67	248.0778156	<chem>CC1OC(N2C=NC3=C(O)N=C((NH3+))N=C32)=CC1=O</chem>

68250.0934657	<chem>CC1OC(N2C=NC3=C(O)N=C((NH3+))NC32)=CC1=O</chem>
69232.082901	<chem>C=C1CC=C(N2C=NC3=C(O)N=C((NH3+))N=C32)O1</chem>
70252.1091157	<chem>CC1OC(N2C=NC3=C(O)NC((NH3+))NC32)=CC1=O</chem>
71254.1247658	<chem>CC1OC(N2C=NC3C2NC((NH3+))NC3O)=CC1=O</chem>
72256.1404159	<chem>CC1OC(N2CNC3C2NC((NH3+))NC3O)=CC1=O</chem>
73258.1560659	<chem>CC1OC(N2CNC3C2NC((NH3+))NC3O)=CC1O</chem>
74173.1396876	<chem>CNC1(C)CC(O(NH3+))C2NCN21</chem>
75140.0818384	<chem>CC1C=C(O(NH3+))C2=NCN21</chem>
76167.0927374	<chem>C=NC1(C)C=C(O(NH3+))C2=NCN21</chem>
77335.0890254	<chem>NC(P)1(C=C2OC(N3C=NC4=C(O)N=C((NH3+))N=C43)=CC2=O)CN1</chem>
78100.0184862	<chem>C(P)1(C#(NH+))C=N1</chem>
79318.0624763	<chem>C(P)1(C=C2OC(N3C=NC4=C(O)N=C((NH3+))N=C43)=CC2=O)C=N1</chem>
80337.1046754	<chem>NC(P)1(CC2OC(N3C=NC4=C(O)N=C((NH3+))N=C43)=CC2=O)CN1</chem>
81339.1203255	<chem>NC(P)1(CC2OC(N3C=NC4=C(O)N=C((NH3+))NC43)=CC2=O)CN1</chem>
82341.1359756	<chem>NC(P)1(CC2OC(N3C=NC4=C(O)NC((NH3+))NC43)=CC2=O)CN1</chem>
83343.1516256	<chem>NC(P)1(CC2OC(N3C=NC4C3NC((NH3+))NC4O)=CC2=O)CN1</chem>
84158.1287886	<chem>C(NH2+)C1(C)CC(O)C2NCN21</chem>
85142.0974884	<chem>CC1((NH3+))CC(=O)C2NCN21</chem>
86125.0709393	<chem>CC1=CC(=O)C2NCN12</chem>
87152.0818384	<chem>C=(NH+)C1(C)CC(=O)C2=NCN21</chem>
88150.0661883	<chem>C#(N+)C1(C)CC(=O)C2=NCN21</chem>
89350.0999244	<chem>NC(P)1(C=C2OC(N3C=NC4=C(O)N=C((NH3+))N=C43)=CC2=O)CN1N</chem>
90332.0893597	<chem>N#C(P)1(C=C2CC=C(N3C=NC4=C(O)N=C((NH3+))N=C43)O2)CN1N</chem>
91115.0293852	<chem>(CH2+)(P)1(C#N)CN1N</chem>
92333.0733753	<chem>C(P)1((C+)=C2OC(N3C=NC4=C(O)N=C(N)N=C43)=CC2=O)CN1N</chem>
93352.1155745	<chem>NC(P)1(CC2OC(N3C=NC4=C(O)N=C((NH3+))N=C43)=CC2=O)CN1N</chem>
94354.1312245	<chem>NC(P)1(CC2OC(N3C=NC4=C(O)N=C((NH3+))NC43)=CC2=O)CN1N</chem>
95356.1468746	<chem>NC(P)1(CC2OC(N3C=NC4=C(O)NC((NH3+))NC43)=CC2=O)CN1N</chem>
96358.1625246	<chem>NC(P)1(CC2OC(N3C=NC4C3NC((NH3+))NC4O)=CC2=O)CN1N</chem>
97111.0916748	<chem>(CH4+)C1C=CC2NCN21</chem>
98113.1073248	<chem>(CH4+)C1CCC2NCN21</chem>
9915.02292652	<chem>(CH3+)</chem>
100126.1025738	<chem>CC1((NH3+))C=CC2NCN21</chem>
10183.06037464	<chem>C#(CH+)C1NCN1</chem>
10285.07602471	<chem>C=(CH2+)C1NCN1</chem>
10384.08077574	<chem>C#CC(C)(NH2+)C</chem>
10486.0964258	<chem>C=CC(C)(NH2+)C</chem>
105109.0760247	<chem>(CH4+)C1C=CC2=NCN21</chem>
106124.0869237	<chem>C(NH2+)C1C=CC2=NCN21</chem>
10760.08077574	<chem>CC(NH2+)C</chem>
10856.04947561	<chem>C=C(NH+)C</chem>
10981.04472458	<chem>C#(CH+)C1=NCN1</chem>
11087.09167477	<chem>C(CH3+)C1NCN1</chem>
111112.0869237	<chem>C(NH+)=C(C)N1C=NC1</chem>
11259.06037464	<chem>C1NC(NH2+)1</chem>
11382.06512568	<chem>C#CC(C)=(NH+)C</chem>
114113.1073248	<chem>C(NH2+)C1(C)C=CCN1</chem>
115111.0916748	<chem>C(NH2+)C1(C)C=CC=N1</chem>
116107.0603746	<chem>(CH3+)=C1C=CC2=NCN21</chem>
117122.0712737	<chem>(CH2+)C1(N)C=CC2=NCN21</chem>
11879.02907452	<chem>C#(CH+)C1=NC=N1</chem>
11980.04947561	<chem>C#CC(C)=(N+)=C</chem>
120368.1104891	<chem>NC(P)1(CC2OC(N3C=NC4=C(O)N=C((NH3+))N=C43)=CC2=O)CN1NO</chem>

121 476.1792373

CC1CC(ONN2C(P)2(C=C2OC(N3C=NC4=C(O)N=C((NH3+))N=C43)=CC2=O)CN)C
2 NCN21

122 458.1686726

CC1C=C(ONN2C(P)2(C=C2CC=C(N3C=NC4=C(O)N=C((NH3+))N=C43)O2)CN)C2=
NCN21

123 241.1086982 C=C1C=C(O(NH2+))N2C(P)2(C)CN)C2=NCN21

124 459.1526882

CC1C=C(ONN2C(P)2(C)C=C2OC(N3C=NC4=C(O)N=C((NH3+))N=C43)=CC2=O)C2
NCN21

125 480.2105375

CC1CC(ONN2C(P)2(CN)CC2OC(N3C=NC4=C(O)N=C((NH3+))NC43)=CC2=O)C2
NC N21

126 491.1901364

CC1(N)CC(ONN2C(P)2(C=C2OC(N3C=NC4=C(O)N=C((NH3+))N=C43)=CC2=O)CN)
C2NCN21

127 491.1901364

CNC1CC(ONN2C(P)2(C=C2OC(N3C=NC4=C(O)N=C((NH3+))N=C43)=CC2=O)CN)C
2NCN21

128 32.04947561 C(NH3+)

129 30.03382555 C=(NH2+)

130 476.1792373

CNC1(C)CC(ONN2C(PH)2C=C2OC(N3C=NC4=C(O)N=C((NH3+))N=C43)=CC2=O)C
2NCN21

131 458.1686726

CNC1(C)C=C(ONN2C(P)2=C=C2CC=C(N3C=NC4=C(O)N=C((NH3+))N=C43)O2)
C2 NCN21

132 478.1948874

CNC1(C)CC(ONN2C(PH)2CC2OC(N3C=NC4=C(O)N=C((NH3+))N=C43)=CC2=O)C
2 NCN21

133 460.1843227

CNC1(C)CC(ONN2C(P)2=C=C2CC=C(N3C=NC4=C(O)N=C((NH3+))N=C43)O2)C
2N CN21

134 480.2105375

CNC1(C)CC(ONN2C(PH)2CC2OC(N3C=NC4=C(O)N=C((NH3+))NC43)=CC2=O)C2 N
CN21

135 462.1999728

CNC1(C)CC(ONN2C(PH)2C=C2CC=C(N3C=NC4=C(O)N=C((NH3+))N=C43)O2)C
2N CN21

136 247.1556484 CNC1(C)CC(O(NH2+))N2C(PH)2C)C2NCN21

137 233.1399983 CNC1(C)CC(O(NH2+))N2C(PH2)2)C2NCN21

138 308.0781263 (NH3+)C1=NC(O)=C2N=CN(C3=CC(=O)C(C(PH)4CN4)O3)C2=N1

139 310.0937764 (NH3+)C1=NC(O)=C2N=CN(C3=CC(=O)C(C(PH)4CN4)O3)C2N1

140 312.1094265 (NH3+)C1NC(O)=C2N=CN(C3=CC(=O)C(C(PH)4CN4)O3)C2N1

141 323.0890254 NN1C(PH)1CC1OC(N2C=NC3=C(O)N=C((NH3+))N=C32)=CC1=O

142 325.1046754 NN1C(PH)1CC1OC(N2C=NC3=C(O)N=C((NH3+))NC32)=CC1=O

143 327.1203255 NN1C(PH)1CC1OC(N2C=NC3=C(O)NC((NH3+))NC32)=CC1=O

144 449.1683383

CC1CC(ONN2C(PH)2CC2OC(N3C=NC4=C(O)N=C((NH3+))N=C43)=CC2=O)C2NC
N 21

145 186.1349366 CNC1(C)CC(ON=(NH2+))C2NCN21

146 281.0672273 (NH3+)C1=NC(O)=C2N=CN(C3=CC(=O)C(C(PH3))O3)C2=N1

147 490.1948874

CNC1(C)CC(ONN2C(P)2(C)C=C2OC(N3C=NC4=C(O)N=C((NH3+))N=C43)=CC2=O)
C2NCN21

148	257.1399983	CNC1(C)C=C(O(NH2+))N2C(P)2(C)C)C2=NCN21
149	461.1683383	CC1CC(ONN2C(P)2(C)C=C2OC(N3C=NC4=C(O)N=C((NH3+))N=C43)=CC2=O)C2N CN21
150	224.0778156	(NH3+)C1NC(O)=C2N=CN(C(=O)C=C=O)C2N1
151	280.1195972	C#C(P)1(CN)CN1(NH2+)OC1=CC(C)(N=C)N2CN=C12
152	186.098551	(NH3+)C1NC2C(N=CN2C=O)C(O)N1
153	184.082901	(NH3+)C1NC(O)=C2N=CN(C=O)C2N1
154	182.0672509	(NH3+)C1=NC(O)=C2N=CN(C=O)C2N1
155	180.0516009	(NH3+)C1=NC(O)=C2N=CN(C=O)C2=N1
156	178.0359508	NC1=NC(O)=C2N=CN(C#(O+))C2=N1
157	326.161462	C=C(O)C#C(P)1(CN)CN1(NH2+)OC1=CC(C)(NC)N2CNC12
158	204.0516009	(NH3+)C1=NC(O)=C2N=CN(C#CC=O)C2=N1
159	206.0672509	(NH3+)C1=NC(O)=C2N=CN(C#CC=O)C2N1
160	208.082901	(NH3+)C1NC(O)=C2N=CN(C#CC=O)C2N1
161	210.098551	(NH3+)C1NC2C(N=CN2C#CC=O)C(O)N1
162	330.1563766	CNC1(C)C=C(O(NH2+))N2C(P)2(CN)CC(=O)C=O)C2NCN21
163	174.0410362	(C+)#CN1C=NC2=C(O)N=C(N)N=C21
164	176.0566862	C#CN1C=NC2=C(O)N=C((NH3+))N=C21
165	180.0879864	C#CN1C=NC2=C(O)NC((NH3+))NC21
166	490.1948874	CNC1(C)CC(ONN2C(P)2(CN)CC2OC(N3C=NC(=C=O)C3=NC#(NH+))=CC2=O)C2NCN21
167	137.0457872	(NH+)#CNC1N=CN=C1C=O
168	463.1839884	CNC1(C)CC(ONN2C(P)2(C=C2OC(N3C=NC(=C=O)C3=(NH2+))=CC2=O)CN)C2NCN21
169	465.1996384	CNC1(C)CC(ONN2C(P)2(CN)CC2OC(N3C=NC(=C=O)C3=(NH2+))=CC2=O)C2NCN21
170	479.2265219	CNC1(C)CC(ONN2C(P)2(C=C2OC(N3C=NCC3=NC(N)=(NH2+))=CC2=O)CN)C2NCN21
171	464.2156228	CNC1(C)CC(ONN2C(P)2(CN)CC2OC(N3C=NCC3=NC#(NH+))=CC2=O)C2NCN21
172	462.1999728	CNC1(C)CC(ONN2C(P)2(C=C2OC(N3C=NCC3=NC#(NH+))=CC2=O)CN)C2NCN21
173	490.1948874	CNC1(C)C=C(ONN2C(P)2(C=C2OC(N3C=NC(=C(O)(NH+)=C=N)C3)=CC2=O)CN)C2NCN21
174	437.2047238	CNC1(C)CC(ONN2C(P)2(C=C2OC(N3C=NCC3=(NH2+))=CC2=O)CN)C2NCN21
175	86.03488817	N=C(N)(NH+)=C=O
176	322.0937764	C(PH)(C=C1OC(N2C=NC3=C(O)N=C((NH3+))N=C32)=CC1=O)CN
177	320.0781263	C(P)(=C=C1OC(N2C=NC3=C(O)N=C((NH3+))N=C32)=CC1=O)CN
178	184.1192865	CNC1(C)C=C(ON=(NH2+))C2NCN21
179	188.1505866	CNC1(C)CC(ON(NH3+))C2NCN21
180	200.1505866	C=(NH+)NOC1CC(C)(NC)N2CNC12
181	198.1349366	C=(NH+)NOC1=CC(C)(NC)N2CNC12
182	306.0624763	NC(PH)=C=C1OC(N2C=NC3=C(O)N=C((NH3+))N=C32)=CC1=O
183	308.0781263	NC(PH2)C=C1OC(N2C=NC3=C(O)N=C((NH3+))N=C32)=CC1=O
184	310.0937764	NC(PH2)CC1OC(N2C=NC3=C(O)N=C((NH3+))N=C32)=CC1=O
185	438.1635873	NC(P)1(CC2OC(N3C=NC4=C(O)N=C((NH3+))N=C43)=CC2=O)CN1NOCC1NCN1
186	451.1839884	


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-----+-----+-----+-----+-----+-----+-----+-----+
-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG | RESCHAIN_LIG |
| SIDECHAIN | DIST_H-A | DIST_D-A | DON_ANGLE | PROTISDON | DONORIDX |
DONORTYPE | ACCEPTORIDX | ACCEPTORTYPE | LIGCOO          | PROTCOO
|
=====+=====+=====+=====+=====+=====+=====+=====
==+=====+=====+=====+=====+=====+=====+=====
==+=====+=====+=====+=====+=====+=====+=====
==+=====+=====+=====+=====+=====+=====+=====
=+=====+=====+
| 208 | ARG | A | 506 | EDO | A | True | 2.79 | 3.54 | 133.91 |
True | 1613 | Ng+ | 5171 | O3 | 26.996, 92.071, 21.093 | 28.803, 94.111,
23.355 |
+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+
-----+
| 208 | ARG | A | 506 | EDO | A | True | 2.07 | 2.95 | 150.90 |
False | 5171 | O3 | 1610 | Ng+ | 26.996, 92.071, 21.093 | 26.528, 94.298,
22.974 |
+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+
-----+
| 212 | GLN | A | 506 | EDO | A | True | 2.33 | 3.25 | 155.36 |
True | 1650 | Nam | 5171 | O3 | 26.996, 92.071, 21.093 | 27.380, 90.549,
23.944 |
+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+
-----+
| 313 | THR | A | 506 | EDO | A | False | 3.19 | 3.93 | 133.41 |
True | 2429 | Nam | 5169 | O3 | 30.235, 90.751, 20.958 | 31.941, 93.285,
18.488 |
+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+
-----+
| 313 | THR | A | 506 | EDO | A | True | 3.04 | 3.89 | 146.22 |
False | 5169 | O3 | 2434 | O3 | 30.235, 90.751, 20.958 | 32.771, 90.620,
18.014 |
+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+
-----+

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****Water Bridges****

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+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG | RESCHAIN_LIG |
DIST_A-W | DIST_D-W | DON_ANGLE | WATER_ANGLE | PROTISDON | DONOR_IDX |
DONORTYPE | ACCEPTOR_IDX | ACCEPTORTYPE | WATER_IDX | LIGCOO
PROTCOO          | WATERCOO          |
=====+=====+=====+=====+=====+=====+=====+=====
==+=====+=====+=====+=====+=====+=====+=====
=====+=====+=====+=====+=====+=====+=====+=====
=====+=====+=====+=====+=====+=====+=====+=====
=+=====+=====+
| 313 | THR | A | 506 | EDO | A | 2.83 | 3.79 | 120.99 | 99.63 |
True | 2434 | O3 | 5169 | O3 | 5298 | 30.235, 90.751, 20.958 | 32.771,
90.620, 18.014 | 30.104, 88.349, 19.458 |
+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+

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EDO:B:405 (EDO) - SMALLMOLECULE

Interacting chain(s): B

Hydrogen Bonds

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+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
-----+
```

RESNR	RESTYPE	RESCHAIN	RESNR_LIG	RESTYPE_LIG	RESCHAIN_LIG		SIDECHAIN	DIST_H-A	DIST_D-A	DON_ANGLE	PROTISDON	DONORIDX		DONORTYPE	ACCEPTORIDX	ACCEPTORTYPE	LIGCOO		PROTCOO	
208	ARG	B	405	EDO	B		True	2.98	3.84	146.58				True	4186	Ng+	5191	O3		-1.831, 92.150, 31.712 -0.507, 90.101, 28.744
+-----+-----+-----+-----+-----+-----+-----+-----+																				
==+-----+-----+-----+-----+-----+-----+-----+-----+																				
==+-----+-----+-----+-----+-----+-----+-----+-----+																				
==+-----+-----+-----+-----+-----+-----+-----+-----+																				
208	ARG	B	405	EDO	B		True	2.98	3.84	146.58				True	4186	Ng+	5191	O3		-1.831, 92.150, 31.712 -0.507, 90.101, 28.744
+-----+-----+-----+-----+-----+-----+-----+-----+																				
-----+-----+-----+-----+-----+-----+-----+-----+																				
-----+																				
208	ARG	B	405	EDO	B		True	2.41	3.01	119.71				False	5189	O3	4183	Ng+		0.823, 93.141, 29.736 1.412, 90.919, 27.788
+-----+-----+-----+-----+-----+-----+-----+-----+																				
-----+-----+-----+-----+-----+-----+-----+-----+																				
-----+																				
212	GLN	B	405	EDO	B		True	2.11	3.08	169.77				True	4223	Nam	5189	O3		0.823, 93.141, 29.736 2.149, 91.127, 31.655
+-----+-----+-----+-----+-----+-----+-----+-----+																				
-----+-----+-----+-----+-----+-----+-----+-----+																				
-----+																				
313	THR	B	405	EDO	B		False	3.15	3.98	143.01				True	5002	Nam	5191	O3		-1.831, 92.150, 31.712 -4.848, 93.779, 29.689
+-----+-----+-----+-----+-----+-----+-----+-----+																				
-----+-----+-----+-----+-----+-----+-----+-----+																				
-----+																				

Water Bridges

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+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
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RESNR	RESTYPE	RESCHAIN	RESNR_LIG	RESTYPE_LIG	RESCHAIN_LIG		DIST_A-W	DIST_D-W	DON_ANGLE	WATER_ANGLE	PROTISDON	DONOR_IDX		DONORTYPE	ACCEPTOR_IDX	ACCEPTORTYPE	WATER_IDX	LIGCOO		PROTCOO		WATERCOO	
+-----+-----+-----+-----+-----+-----+-----+-----+																							
==+-----+-----+-----+-----+-----+-----+-----+-----+																							
==+-----+-----+-----+-----+-----+-----+-----+-----+																							
==+-----+-----+-----+-----+-----+-----+-----+-----+																							
==+-----+-----+-----+-----+-----+-----+-----+-----+																							

RESNR	RESTYPE	RESCHAIN	RESNR_LIG	RESTYPE_LIG	RESCHAIN_LIG	METAL_IDX	METAL_TYPE	TARGET_IDX	TARGET_TYPE	COORDINATION	DIST
LOCATION	RMS	GEOMETRY	COMPLEXNUM	METALCOO							

```

TARGETCOO      |
+=====+=====+=====+=====+=====+=====+=====
==+=====+=====+=====+=====+=====+=====+=====
==+=====+=====+=====+=====+=====+=====+=====
=====+=====+=====+=====+=====+=====+=====+
| 227 | GLU   | B   | 404 | MG      | B      | 5187 | Mg   | 4344 | O      |
2      | 2.24 | protein.sidechain | 98.07 | linear | 1      | 10.436, 108.864, 27.911 | 9.354,
107.168, 28.892 |
+-----+-----+-----+-----+-----+-----+-----+-----
+-----+-----+-----+-----+-----+-----+-----+-----
+-----+-----+-----+-----+-----+-----+-----+-----
+-----+-----+-----+-----+-----+-----+-----+-----
| 231 | GLU   | B   | 404 | MG      | B      | 5187 | Mg   | 4376 | O      |
2      | 2.99 | protein.sidechain | 98.07 | linear | 1      | 10.436, 108.864, 27.911 | 9.155,
107.715, 25.469 |
+-----+-----+-----+-----+-----+-----+-----+-----
+-----+-----+-----+-----+-----+-----+-----+-----
+-----+-----+-----+-----+-----+-----+-----+-----
+-----+-----+-----+-----+-----+-----+-----+-----

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SO4:A:501 (SO4) - SMALLMOLECULE

Interacting chain(s): A,B

Hydrogen Bonds

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+-----+-----+-----+-----+-----+-----+-----+-----
+-----+-----+-----+-----+-----+-----+-----+-----
+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG | RESCHAIN_LIG |
SIDECHAIN | DIST_H-A | DIST_D-A | DON_ANGLE | PROTISDON | DONORIDX |
DONORTYPE | ACCEPTORIDX | ACCEPTORTYPE | LIGCOO      | PROTCOO
|
+=====+=====+=====+=====+=====+=====+=====
==+=====+=====+=====+=====+=====+=====+=====
==+=====+=====+=====+=====+=====+=====+=====
+=====+=====+=====+=====+=====+=====+=====+
| 83  | ASP | B      | 501 | SO4      | A      | False | 1.94 | 2.87 | 158.06 | True
| 3212 | Nam  | 5148   | O2   | 4.307, 79.764, 8.458 | 4.378, 77.699, 6.460 |
+-----+-----+-----+-----+-----+-----+-----+-----
+-----+-----+-----+-----+-----+-----+-----+-----
+-----+
| 253 | ASP | A      | 501 | SO4      | A      | False | 1.75 | 2.69 | 158.09 |
True | 1963 | Nam    | 5151 | O3      | 2.293, 80.306, 9.882 | 2.680, 81.284, 12.359
|
+-----+-----+-----+-----+-----+-----+-----+-----
+-----+-----+-----+-----+-----+-----+-----+-----
+-----+
| 254 | THR | A      | 501 | SO4      | A      | False | 1.98 | 2.86 | 148.17 |
True | 1971 | Nam    | 5150 | O3      | 4.335, 78.849, 10.631 | 4.565, 79.523, 13.405
|
+-----+-----+-----+-----+-----+-----+-----+-----
+-----+-----+-----+-----+-----+-----+-----+-----
+-----+
| 254 | THR | A      | 501 | SO4      | A      | True  | 2.11 | 2.56 | 106.38 |
False | 5150 | O3     | 1976 | O3      | 4.335, 78.849, 10.631 | 6.204, 77.735, 11.976 |
+-----+-----+-----+-----+-----+-----+-----+-----
+-----+-----+-----+-----+-----+-----+-----+-----
+-----+

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Interacting chain(s): A

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+-----+-----+-----+-----+-----+-----+-----+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG | RESCHAIN_LIG |
SIDECHAIN | DIST_H-A | DIST_D-A | DON_ANGLE | PROTISDON | DONORIDX |
DONORTYPE | ACCEPTORIDX | ACCEPTORTYPE | LIGCOO          | PROTCOO
|
+=====+=====+=====+=====+=====+=====+=====+=====
==+=====+=====+=====+=====+=====+=====+=====
===+=====+=====+=====+=====+=====+=====+=====
==+=====+=====+=====+=====+=====+=====+=====
| 51 | GLY   | A      | 502 | SO4     | A      | False    | 3.66 | 4.05 | 106.38 |
True  | 381   | Nam    | 5156 | O3      |         | | 27.732, 124.421, 22.168 | 28.453, 127.892,
20.214 |
+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+
-----+
| 52 | ASN   | A      | 502 | SO4     | A      | False    | 3.31 | 3.90 | 120.35 |
True  | 385   | Nam    | 5156 | O3      |         | | 27.732, 124.421, 22.168 | 27.767, 124.941,
18.305 |
+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+
-----+
| 53 | SER   | A      | 502 | SO4     | A      | True     | 2.93 | 3.27 | 101.67 |
False | 5155  | O3     | 398  | O3      |         | | 25.866, 123.166, 23.003 | 23.364, 123.507,
20.924 |
+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+
-----+
| 53 | SER   | A      | 502 | SO4     | A      | False    | 1.72 | 2.66 | 158.29 | True
| 393 | Nam    | 5153   | O2    |         | 26.198, 123.393, 20.604 | 24.928, 124.616, 18.613 |
+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+
-----+

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+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG | RESCHAIN_LIG |
| DIST_A-W | DIST_D-W | DON_ANGLE | WATER_ANGLE | PROTISDON | DONOR_IDX |
| DONORTYPE | ACCEPTOR_IDX | ACCEPTORTYPE | WATER_IDX | LIGCOO
| PROTCOO | WATERCOO |
+=====+=====+=====+=====+=====+=====+=====+=====+
==+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+=====+
==+
| 49 | ARG | A | 502 | SO4 | A | 3.19 | 3.84 | 115.38 | 103.97 |

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True   | 370 | Ng+   | 5154   | O2     | 5194   | 27.729, 122.064, 21.789 | 27.192,
123.946, 26.322 | 29.651, 124.050, 23.379 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+
| 49 | ARG | A     | 502 | SO4   | A     | 3.91 | 3.84 | 115.38 | 136.91 |
True   | 370 | Ng+   | 5155   | O3     | 5194   | 25.866, 123.166, 23.003 | 27.192,
123.946, 26.322 | 29.651, 124.050, 23.379 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+
| 49 | ARG | A     | 502 | SO4   | A     | 3.79 | 3.66 | 100.34 | 124.13 |
True   | 370 | Ng+   | 5156   | O3     | 5360   | 27.732, 124.421, 22.168 | 27.192,
123.946, 26.322 | 25.238, 126.306, 24.311 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+
| 49 | ARG | A     | 502 | SO4   | A     | 3.46 | 3.66 | 100.34 | 133.24 |
True   | 370 | Ng+   | 5155   | O3     | 5360   | 25.866, 123.166, 23.003 | 27.192,
123.946, 26.322 | 25.238, 126.306, 24.311 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+
| 54 | TRP  | A     | 502 | SO4   | A     | 3.07 | 3.13 | 152.36 | 87.53   |
True   | 399 | Nam| 5153   | O2     | 5283   | 26.198, 123.393, 20.604 | 24.100,
127.181, 18.904 | 25.953, 126.375, 21.294 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+

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****Salt Bridges****

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+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG | RESCHAIN_LIG | DIST
| PROTISPOS | LIG_GROUP | LIG_IDX_LIST | LIGCOO          | PROTCOO          |
+=====+=====+=====+=====+=====+=====+=====+=====+=====+=====+
==+=====+=====+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+
| 49 | ARG | A     | 502 | SO4   | A     | 5.14 | True | Sulfate | 5152,5152 |
26.868, 123.261, 21.907 | 28.246, 124.697, 26.644 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+

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SO4:A:503 (SO4) - SMALLMOLECULE

Interacting chain(s): A

****Hydrogen Bonds****

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+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG | RESCHAIN_LIG
| SIDECHAIN | DIST_H-A | DIST_D-A | DON_ANGLE | PROTISDON | DONORIDX |

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DONORTYPE | ACCEPTORIDX | ACCEPTORTYPE | LIGCOO | PROTCOO |

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=====+=====+=====+=====+=====+=====+=====
==+=====+=====+=====+=====+=====+=====+=====
==+=====+=====+=====+=====+=====+=====+=====
==+=====+
| 183 | THR | A | 503 | SO4 | A | True | 3.32 | 4.07 | 135.45 |
False | 5160 | O3 | 1413 | O3 | 3.604, 114.161, 43.383 | 3.112, 112.365,
39.768 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+
| 183 | THR | A | 503 | SO4 | A | True | 3.65 | 3.94 | 100.39 |
True | 1413 | O3 | 5158 | O2 | 5.284, 114.898, 41.859 | 3.112, 112.365,
39.768 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+
| 184 | PHE | A | 503 | SO4 | A | False | 2.95 | 3.31 | 102.62 |
True | 1415 | Nam | 5158 | O2 | 5.284, 114.898, 41.859 | 5.002, 115.141,
38.575 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+
| 185 | LYS | A | 503 | SO4 | A | False | 1.82 | 2.69 | 146.36 |
True | 1426 | Nam | 5158 | O2 | 5.284, 114.898, 41.859 | 6.495, 113.312,
40.049 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+

```

Water Bridges

```

+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG | RESCHAIN_LIG |
DIST_A-W | DIST_D-W | DON_ANGLE | WATER_ANGLE | PROTISDON | DONOR_IDX |
DONORTYPE | ACCEPTOR_IDX | ACCEPTORTYPE | WATER_IDX | LIGCOO |
PROTCOO | WATERCOO |
=====+=====+=====+=====+=====+=====+=====
==+=====+=====+=====+=====+=====+=====+=====
=====+=====+=====+=====+=====+=====+=====+=====
=====+
| 186 | GLU | A | 503 | SO4 | A | 3.78 | 4.07 | 123.14 | 93.06 |
True | 1435 | Nam | 5160 | O3 | 5.210 | 3.604, 114.161, 43.383 | 5.533,
110.763, 39.160 | 2.443, 110.928, 41.805 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+

```

SO4:A:504 (SO4) - SMALLMOLECULE

Interacting chain(s): A

Hydrogen Bonds

```

+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+

```

```

-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG | RESCHAIN_LIG |
| SIDECHAIN | DIST_H-A | DIST_D-A | DON_ANGLE | PROTISDON | DONORIDX |
DONORTYPE | ACCEPTORIDX | ACCEPTORTYPE | LIGCOO          | PROTCOO
|
+=====+=====+=====+=====+=====+=====+=====+=====+
==+=====+=====+=====+=====+=====+=====+=====+
===+=====+=====+=====+=====+=====+=====+=====+
==+=====+=====+=====+=====+=====+=====+=====+
| 60  | ASP  | A    | 504  | SO4    | A      | True  | 3.25  | 3.82  | 119.18 |
False | 5166  | O3   | 459  | O2     |        |       | 13.818, 123.785, 10.585 | 16.644, 126.204,
11.437 |
+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+
-----+

```

****Salt Bridges****

```

+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG | RESCHAIN_LIG | DIST
| PROTISPOS | LIG_GROUP | LIG_IDX_LIST | LIGCOO          | PROTCOO          |
+=====+=====+=====+=====+=====+=====+=====+=====+
==+=====+=====+=====+=====+=====+=====+=====+
===+=====+=====+=====+=====+=====+=====+=====+
| 30  | ARG  | A    | 504  | SO4    | A      | 4.55 | True  | Sulfate | 5162,5162 |
12.961, 123.025, 9.630 | 16.284, 122.520, 12.696 |
+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+
| 138 | ARG  | A    | 504  | SO4    | A      | 5.34 | True  | Sulfate | 5162,5162 |
12.961, 123.025, 9.630 | 8.482, 124.188, 12.301 |
+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+
-----+

```

SO4:B:401 (SO4) - SMALLMOLECULE

Interacting chain(s): B

****Hydrogen Bonds****

```

+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+
-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG | RESCHAIN_LIG |
SIDECHAIN | DIST_H-A | DIST_D-A | DON_ANGLE | PROTISDON | DONORIDX |
DONORTYPE | ACCEPTORIDX | ACCEPTORTYPE | LIGCOO          | PROTCOO
|
+=====+=====+=====+=====+=====+=====+=====+=====+
==+=====+=====+=====+=====+=====+=====+=====+
===+=====+=====+=====+=====+=====+=====+=====+
==+=====+=====+=====+=====+=====+=====+=====+
| 52  | ASN  | B    | 401  | SO4    | B      | False | 3.09  | 3.90  | 140.37 | True
| 2958 | Nam  | 5176  | O3   |        |        |       | -8.323, 83.015, 2.251 | -10.293, 84.518, -0.757 |
+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+
-----+
| 53  | SER  | B    | 401  | SO4    | B      | False | 1.54  | 2.51  | 166.20 | True

```

2966	Nam	5174	O2	-7.792, 83.077, -0.099 -7.659, 85.248, -1.355
------	-----	------	----	---

```

+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+

```

****Water Bridges****

```

+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG | RESCHAIN_LIG |
| DIST_A-W | DIST_D-W | DON_ANGLE | WATER_ANGLE | PROTISDON | DONOR_IDX |
| DONORTYPE | ACCEPTOR_IDX | ACCEPTORTYPE | WATER_IDX | LIGCOO
| PROTCOO
| WATERCOO
+=====+=====+=====+=====+=====+=====+=====+=====+
==+=====+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+=====+=====+
+
| 49 | ARG | B | 401 | SO4 | B | 3.96 | 3.76 | 164.03 | 108.70 |
False | 5175 | O3 | 2941 | Ng+ | 5604 | -6.465, 81.744, 1.399 | -8.496,
77.945, 1.027 | -5.903, 79.471, -1.548 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| 49 | ARG | B | 401 | SO4 | B | 3.96 | 3.09 | 152.95 | 71.33 |
True | 2934 | Nam | 5173 | O2 | 5604 | -8.698, 81.080, 0.742 | -7.508,
77.361, -3.138 | -5.903, 79.471, -1.548 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| 51 | GLY | B | 401 | SO4 | B | 3.31 | 2.90 | 144.10 | 83.82 |
True | 2954 | Nam | 5173 | O2 | 5430 | -8.698, 81.080, 0.742 | -10.738,
81.737, -2.990 | -7.922, 81.987, -2.349 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| 54 | TRP | B | 401 | SO4 | B | 2.50 | 3.11 | 152.98 | 87.30 |
True | 2972 | Nam | 5174 | O2 | 5430 | -7.792, 83.077, -0.099 | -7.386,
84.555, -4.025 | -7.922, 81.987, -2.349 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+

```

****Salt Bridges****

```

+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG | RESCHAIN_LIG | DIST
| PROTISPOS | LIG_GROUP | LIG_IDX_LIST | LIGCOO
| PROTCOO
+=====+=====+=====+=====+=====+=====+=====+=====+
==+=====+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+-----+
| 49 | ARG | B | 401 | SO4 | B | 4.59 | True | Sulfate | 5172,5172 | -
7.832, 82.220, 1.094 | -7.183, 77.677, 1.214 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+

```

Interacting chain(s): A,B

-----+											
RESNR RESTYPE RESCHAIN RESNR_LIG RESTYPE_LIG RESCHAIN_LIG											
SIDECHAIN DIST_H-A DIST_D-A DON_ANGLE PROTISDON DONORIDX											
DONORTYPE ACCEPTORIDX ACCEPTORTYPE LIGCOO PROTCOO											
=====+											
==+=====+=====+=====+=====+=====+											
===+=====+=====+=====+=====+=====+											
==+=====+											
83	ASP	A	402	SO4	B	False	1.96	2.89	155.32	True	
639	Nam	5179	O2	19.914, 114.523, 30.262	19.623, 116.992, 31.726						
+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+											
-----+-----+-----+-----+-----+-----+-----+-----+-----+											
-----+											
252	SER	B	402	SO4	B	True	3.00	3.97	176.18		
False	5180	O3	4535	O3	21.169, 112.802, 31.511	18.851, 110.258,					
29.533											
+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+											
-----+-----+-----+-----+-----+-----+-----+-----+-----+											
-----+											
253	ASP	B	402	SO4	B	False	1.85	2.80	162.98		
True	4536	Nam	5178	O2	22.059, 113.747, 29.310	22.361, 110.967,					
29.100											
+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+											
-----+-----+-----+-----+-----+-----+-----+-----+-----+											
-----+											
254	THR	B	402	SO4	B	False	1.84	2.75	151.30		
True	4544	Nam	5180	O3	21.169, 112.802, 31.511	21.545, 110.084,					
31.608											
+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+											
-----+-----+-----+-----+-----+-----+-----+-----+-----+											
-----+											
254	THR	B	402	SO4	B	True	1.73	2.68	169.14		
True	4549	O3	5180	O3	21.169, 112.802, 31.511	20.099, 111.542,					
33.626											
+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+											
-----+-----+-----+-----+-----+-----+-----+-----+-----+											
-----+											
-----+											

```

+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG | RESCHAIN_LIG |
| DIST_A-W | DIST_D-W | DON_ANGLE | WATER_ANGLE | PROTISDON | DONOR_IDX |
| DONORTYPE | ACCEPTOR_IDX | ACCEPTORTYPE | WATER_IDX | LIGCOO
| PROTCOO
| WATERCOO
+=====+=====+=====+=====+=====+=====+=====+
+=====+=====+=====+=====+=====+=====+=====+

```

```

=====+=====+=====+=====+=====+=====
=====+=====+=====+=====+=====+=====
==+
| 253 | ASP | B | 402 | SO4 | B | 3.44 | 2.82 | 136.02 | 98.77 |
True | 4543 | O3 | 5178 | O2 | 5468 | 22.059, 113.747, 29.310 | 25.813,
112.960, 29.568 | 24.752, 115.246, 30.832 |
+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+

```

SO4:B:403 (SO4) - SMALLMOLECULE

Interacting chain(s): B

Hydrogen Bonds

```

+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+
+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG | RESCHAIN_LIG |
SIDECHAIN | DIST_H-A | DIST_D-A | DON_ANGLE | PROTISDON | DONORIDX |
DONORTYPE | ACCEPTORIDX | ACCEPTORTYPE | LIGCOO | PROTCOO |
|
+=====+=====+=====+=====+=====+=====
==+=====+=====+=====+=====+=====+=====
==+=====+=====+=====+=====+=====+=====
==+=====+=====+
| 10 | VAL | B | 403 | SO4 | B | False | 2.57 | 3.37 | 139.45 |
False | 5185 | O3 | 2643 | O2 | 20.136, 91.708, -14.929 | 22.507, 90.800, -
12.711 |
+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+
+
| 12 | LEU | B | 403 | SO4 | B | False | 2.10 | 3.03 | 156.50 | True
| 2653 | Nam | 5185 | O3 | 20.136, 91.708, -14.929 | 19.703, 88.713, -14.932 |
+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+
+
| 13 | ASP | B | 403 | SO4 | B | False | 3.51 | 4.02 | 114.76 | True
| 2661 | Nam | 5184 | O2 | 20.207, 90.798, -17.223 | 19.335, 86.874, -17.057 |
+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+
+

```

Water Bridges

```

+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+
+-----+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG | RESCHAIN_LIG |
DIST_A-W | DIST_D-W | DON_ANGLE | WATER_ANGLE | PROTISDON | DONOR_IDX |
DONORTYPE | ACCEPTOR_IDX | ACCEPTORTYPE | WATER_IDX | LIGCOO |
PROTCOO | WATERCOO |
+=====+=====+=====+=====+=====+=====
==+=====+=====+=====+=====+=====+=====
=====+=====+=====+=====+=====+=====
=====+=====+=====+=====+=====+=====

```

```

==+
| 170  | LYS  | B      | 403| SO4    | B      | 3.34  | 3.46  | 101.48 | 117.03  |
True   | 3900  | N3     | 5183  | O2      |        | 5608| 21.301, 92.888, -16.660 | 21.013,
93.185, -12.728 | 23.918, 92.902, -14.590 |
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+

```

****Salt Bridges****

```

+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG | RESCHAIN_LIG | DIST
| PROTISPOS | LIG_GROUP | LIG_IDX_LIST | LIGCOO      | PROTCOO      |
+=====+=====+=====+=====+=====+=====+=====+
==+=====+=====+=====+=====+=====+=====+
=====+=====+
| 170  | LYS  | B      | 403  | SO4    | B      | 3.94 | True      | Sulfate | 5182,5182 |
20.114, 92.023, -16.380 | 21.013, 93.185, -12.728 |
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+

```

File	Model	T.Energy	I.Energy	vdW	Coul	NumRotors	RMSD	Score
ligand_8b923b3ecd_1_run_2.log	1	-36.678	-55.648	-7.519	-48.129	7	0.000	-6.762
ligand_8b923b3ecd_1_run_16.log	1	-36.224	-53.111	-5.988	-47.123	7	2.941	-6.543
ligand_8b923b3ecd_1_run_4.log	1	-32.903	-52.904	-14.237	-38.667	7	3.940	-7.030

Figure4b. Shows the receptor binding domain and the CoMFA contour map of steric regions (blue, favored; yellow; disfavored) around Roccustyrna; Blue regions are favored by positively charged groups and red regions favored by negatively charged groups inside the SARS-COV-2 protein targets (pdb:6W9C). 02J:C:1 (02J) - SMALLMOLECULE

Interacting chain(s): A

****Hydrophobic Interactions****

```

+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG | RESCHAIN_LIG | DIST
| LIGCARBONIDX | PROTCARBONIDX | LIGCOO | PROTCOO |
+=====+=====+=====+=====+=====+=====+=====+=====+=====+
=+=====+=====+=====+=====+=====+=====+=====+=====+=====+
=====+
| 168 | PRO | A | 1 | 02J | C | 3.53 | 2369 | 1303 | -10.425,
3.420, 72.447 | -13.394, 3.190, 70.551 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+

```

PJE:C:5 (PJE-010) - SMALLMOLECULE

+ 010:C:6

Interacting chain(s): A

****Hydrophobic Interactions****

```
+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+
```

```
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG | RESCHAIN_LIG | DIST
| LIGCARBONIDX | PROTCARBONIDX | LIGCOO | PROTCOO |
```

```
+=====+=====+=====+=====+=====+=====+=====+=====
=+=====+=====+=====+=====+=====+=====+=====+=====
=====+
```

```
| 25 | THR | A | 6 | 010 | C | 3.73 | 2415 | 179 | -7.156,
21.406, 66.898 | -8.709, 22.779, 70.002 |
```

```
+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+
```

```
| 26 | THR | A | 6 | 010 | C | 3.81 | 2415 | 186 | -7.156,
21.406, 66.898 | -6.155, 24.392, 64.757 |
```

```
+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+
```

Hydrogen Bonds

```
+-----+-----+-----+-----+-----+-----+-----+-----+
- -----+-----+-----+-----+-----+-----+-----+-----+
-- -----+
```

```
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG | RESCHAIN_LIG |
SIDECHAIN | DIST_H-A | DIST_D-A | DON_ANGLE | PROTISDON | DONORIDX |
DONORTYPE | ACCEPTORIDX | ACCEPTORTYPE | LIGCOO | PROTCOO |
```

```
+=====+=====+=====+=====+=====+=====+=====+=====
=+=====+=====+=====+=====+=====+=====+=====+=====
=+=====+=====+=====+=====+=====+=====+=====+=====
=====+
```

```
| 143 | GLY | A | 6 | 010 | C | False | 1.93 | 2.80 | 145.29 | True
| 1105 | Nam | 2411 | O3 | -8.911, 17.849, 65.703 | -8.918, 17.918, 62.905 |
```

```
+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+
-----+
```

```
| 164 | HIS | A | 5 | PJE | C | False | 2.16 | 3.07 | 153.73 | False
| 2408 | N3 | 1266 | O2 | -12.282, 14.994, 67.123 | -15.161, 15.336, 68.144 |
```

```
+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+
-----+
```

Rocustyrna binding site(s) in 2CME (hypothetical protein 5).

SMALLMOLECULE

D10 (decane)

D10-B-1099

Interacting chains: A, B

Figure5a. Rocustyrna binding site(s) inside the (pdb:6lu7)binding domains. 02J:C:1 (02J) - SMALLMOLECULE

Interacting chain(s): A

****Hydrophobic Interactions****

```

+-----+-----+-----+-----+-----+-----+-----+-----+
--+-----+-----+-----+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG | RESCHAIN_LIG | DIST | LIGCARBONIDX |
| PROTCARBONIDX | LIGCOO | PROTCOO |
+=====+=====+=====+=====+=====+=====+=====+=====+
====+=====+=====+=====+=====+=====+=====+=====+
=+=====+=====+
| 168 | PRO | A | 1 | 02J | C | 3.53 | 2369 | 1303 | -10.425, 3.420, 72.447 | -13.394, 3.190,
70.551 |
+-----+-----+-----+-----+-----+-----+-----+-----+
--+-----+-----+-----+

```

PJE:C:5 (PJE-010) - SMALLMOLECULE

+ 010:C:6

Interacting chain(s): A

****Hydrophobic Interactions****

```

+-----+-----+-----+-----+-----+-----+-----+-----+
--+-----+-----+-----+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG | RESCHAIN_LIG | DIST | LIGCARBONIDX |
| PROTCARBONIDX | LIGCOO | PROTCOO |
+=====+=====+=====+=====+=====+=====+=====+=====+
====+=====+=====+=====+=====+=====+=====+=====+
=+=====+=====+
| 25 | THR | A | 6 | 010 | C | 3.73 | 2415 | 179 | -7.156, 21.406, 66.898 | -8.709, 22.779, 70.002
|

```


Index	Residue	AA	Metal	Target	Distance	Location
4	75A	HIS	9316	571	2.51	protein.sidechain

Hydrophobic Interactions

Index	Residue	AA	Distance	Ligand Atom	Protein Atom
1	53A	LEU	3.76	4787	254
2	53B	LEU	3.87	4793	869
3	53B	LEU	3.83	4795	866
4	77B	VAL	3.62	4795	1054

D10-C-1099

Interacting chains: C, D

Figure5b. Roccustyrna binding site(s) in (pdb:6lu7)D10-C-1099 DMS:A:402 (DMS) - SMALLMOLECULE

Interacting chain(s): A

****Hydrogen Bonds****

+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+

	RESNR	RESTYPE	RESCHAIN	RESNR_LIG	RESTYPE_LIG	RESCHAIN_LIG	SIDECHAIN	DIST_H-A	DIST_D-A	DON_ANGLE	PROTISDON	DONORIDX	DONORTYPE	ACCEPTORIDX	ACCEPTORTYPE	LIGCOO	PROTCOO
	298	ARG	A	402	DMS	A	True	1.76	2.73		166.89	True	2331				

+=====+=====+=====+=====+=====+=====+=====+=====+=====+=====+=====+=====+
==+=====+=====+=====+=====+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+=====+=====+=====+=====+=====+

	298	ARG	A	402	DMS	A	True	1.76	2.73		166.89	True	2331				

+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+

****Salt Bridges****

+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+

	RESNR	RESTYPE	RESCHAIN	RESNR_LIG	RESTYPE_LIG	RESCHAIN_LIG	DIST

+=====+=====+=====+=====+=====+=====+=====+=====+=====+=====+=====+=====+

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=====+=====+=====+=====+=====
====+

| 295 | ASP | A | 402 | DMS | A | 5.49 | False | Sulfonium | 2376 | 6.081, -1.005, -
6.367 | 10.436, 2.231, -5.560 |

+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+

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pi-Cation Interactions

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+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+

| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG | RESCHAIN_LIG | DIST | OFFSET
| PROTCARGED | LIG_GROUP | LIG_IDX_LIST | LIGCOO | PROTCOO |

+=====+=====+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+=====+=====+
=====+

| 8 | PHE | A | 402 | DMS | A | 4.70 | 1.01 | False | sulfonium | 2376 | 6.081, -
1.005, -6.367 | 8.339, -4.556, -4.264 |

+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+

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DMS:A:403 (DMS) - SMALLMOLECULE

Interacting chain(s):

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RZG:A:404 (RZG) - SMALLMOLECULE

Interacting chain(s): A

Hydrophobic Interactions

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+-----+-----+-----+-----+-----+-----+-----+-----+-----+

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--+-----+

| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG | RESCHAIN_LIG | DIST |
LIGCARBONIDX | PROTCARBONIDX | LIGCOO | PROTCOO |

+=====+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+=====+

| 165 | MET | A | 404 | RZG | A | 3.96 | 2384 | 1284 | 13.459, 2.162, 22.819 |
12.458, 1.105, 19.137 |

+-----+-----+-----+-----+-----+-----+-----+-----+
--+-----+-----+

| 189 | GLN | A | 404 | RZG | A | 3.68 | 2389 | 1469 | 11.044, 2.322, 24.179 |
12.243, 3.597, 27.411 |

+-----+-----+-----+-----+-----+-----+-----+-----+
--+-----+-----+

| 189 | GLN | A | 404 | RZG | A | 3.75 | 2388 | 1468 | 11.707, 1.106, 24.084 |
13.298, 2.520, 27.177 |

+-----+-----+-----+-----+-----+-----+-----+-----+
--+-----+-----+

****Hydrogen Bonds****

+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+

| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG | RESCHAIN_LIG | SIDECHAIN |
DIST_H-A | DIST_D-A | DON_ANGLE | PROTISDON | DONORIDX | DONORTYPE | ACCEPTORIDX |
ACCEPTORTYPE | LIGCOO | PROTCOO |

+=====+=====+=====+=====+=====+=====+=====+=====+
==+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+=====+

| 166 | GLU | A | 404 | RZG | A | False | 2.01 | 2.99 | 161.20 | False | 2392 |
N3 | 1291 | O2 | 9.311, 5.041, 22.782 | 10.444, 4.777, 20.029 |

+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+

| 189 | GLN | A | 404 | RZG | A | True | 3.08 | 3.67 | 120.00 | True | 1472 |
Nam | 2396 | O2 | 10.485, 5.379, 25.107 | 10.139, 4.011, 28.500 |

+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+

****Water Bridges****

+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+


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| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG | RESCHAIN_LIG | DIST_A-W |
| DIST_D-W | DON_ANGLE | WATER_ANGLE | PROTISDON | DONOR_IDX | DONORTYPE |
| ACCEPTOR_IDX | ACCEPTORTYPE | WATER_IDX | LIGCOO          | PROTCOO          |
| WATERCOO          |

+=====+=====+=====+=====+=====+=====+=====+=====+=====+
=+=====+=====+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+=====+=====+
==+=====+=====+

| 166 | GLU | A | 404 | RZG | A | 4.01 | 2.87 | 172.42 | 89.78 | True | 1288
| Nam | 2392 | N3 | 2573 | 9.311, 5.041, 22.782 | 9.967, 2.685, 18.385 | 9.274, 1.499, 20.904 |

+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
---+
```

****Salt Bridges****

```
+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+

| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG | RESCHAIN_LIG | DIST |
| PROTISPOS | LIG_GROUP | LIG_IDX_LIST | LIGCOO          | PROTCOO          |

+=====+=====+=====+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+=====+=====+=====+
=====+

| 41 | HIS | A | 404 | RZG | A | 5.18 | True | Carboxylate | 2393,2394 | 13.944, -
0.877, 23.349 | 11.774, -4.812, 20.770 |

+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
```

Index	Residue	AA	Distance	Ligand Atom	Protein Atom
1	25A	THR	3.73	2415	179
2	26A	THR	3.81	2415	186

Hydrogen Bonds

I	R	A	Dist	Dist	Don	Prote	Sid	Don	Acce
n		A	ance	ance	or	in	ech	or	ptor
d	s i d		H-A	D-A	Ang	dono	ain	Ato	Ato
e	u e				le	r?		m	m
x									
1	143A	GLY	1.93	2.80	145.29	✓	✗	1105 (Nam)	2411 (O3)

Hydrogen Bonds

Index	Residue	Atom	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Sidechain	Donor Atom	Acceptor Atom
1	160A	ARG	2.25	3.23	171.34	✓	✗	986 [Nam]	2475 [O3]
2	160B	ARG	2.15	3.13	176.63	✓	✗	2216 [Nam]	2471 [O3]
3	161A	TYR	2.32	3.19	148.19	✓	✗	997 [Nam]	2473 [O3]
4	161A	TYR	3.12	3.48	103.86	✗	✗	2473 [O3]	1000 [O2]

Water Bridges

Ind ex	Resi due	A A	Dist. A-W	Dist. D-W	Donor Angle	Water Angle	Protein donor?	Donor Atom	Acceptor Atom	Water Atom
1	99A	THR	3.08	3.19	134.41	71.38	✖	2475 [O3]	509 [O3]	2559
2	158B	LEU	2.76	2.87	122.75	88.92	✖	2471 [O3]	2201 [O2]	2668

Hydrophobic Interactions

Index	Residue	AA	Distance	Ligand Atom	Protein Atom
1	16C	VAL	4.00	4796	1271
2	45C	ILE	3.83	4796	1400
3	55D	LEU	3.89	4804	2067
4	77D	VAL	3.74	4805	2238

Hydrophobic Interactions

Index	Residue	AA	Distance	Ligand Atom	Protein Atom
1	22E	LEU	3.94	4811	2510
2	22F	LEU	3.98	4810	3102
3	55F	LEU	3.85	4815	3255
4	77F	VAL	3.70	4815	3429
5	95E	VAL	3.69	4809	2979

Hydrogen Bonds

RESNR RESTYPE RESCHAIN RESNR_LIG RESTYPE_LIG RESCHAIN_LIG SIDECHAIN												
DIST_H-A DIST_D-A DON_ANGLE PROTISDON DONORIDX DONORTYPE ACCEPTORIDX												
ACCEPTORTYPE LIGCOO PROTCOO												
41 HIS A 401 X77 A True 3.46 3.79 106.13 True 611 Npl												
4680 N2 -20.860, 19.573, -32.520 -19.394, 16.086, -32.767												
143 GLY A 401 X77 A False 2.17 2.94 148.03 True 2216												
Nam 4682 O2 -19.635, 22.244, -29.036 -18.779, 24.455, -30.773												
144 SER A 401 X77 A True 3.14 3.42 101.78 True 2228 O3												
4679 N2 -16.096, 21.679, -26.816 -14.503, 23.707, -29.056												
166 GLU A 401 X77 A False 1.98 2.80 158.32 True 2542												
Nam 4683 O2 -18.546, 18.654, -26.028 -16.172, 18.348, -24.583												

Hydrophobic Interactions

Index	Residue	AA	Distance	Ligand Atom	Protein Atom
1	53H	LEU	3.42	4825	4432
2	95H	VALL	3.89	4820	4762

Prediction of noncovalent interactions for PDB structure 2CME

Created on 2020/11/04 using PLIP v1.4.4

If you are using PLIP in your work, please cite:

Salentin, S. et al. PLIP: fully automated protein-ligand interaction profiler. Nucl. Acids Res. (1 July 2015) 43 (W1): W443-W447. doi: 10.1093/nar/gkv315

D10:B:1099 (D10) - SMALLMOLECULE

Interacting chain(s): A,B

Hydrophobic Interactions

```
+-----+-----+-----+-----+-----+-----+-----+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG | RESCHAIN_LIG |
| DIST | LIGCARBONIDX | PROTCARBONIDX | LIGCOO | PROTCOO |
+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+
| 53 | LEU | A | 1099 | D10 | B | 3.76 | 4787 | 254 | 48.955, 23.619, 16.401 | 47.080, 24.675,
13.313 |
+-----+-----+-----+-----+-----+-----+-----+-----+
| 53 | LEU | B | 1099 | D10 | B | 3.87 | 4793 | 869 | 52.046, 20.761, 11.577 | 49.032, 23.137,
11.111 |
```

+-----+

| 53 | LEU | B | 1099 | D10 | B | 3.83 | 4795 | 866 | 52.630, 20.477, 9.083 | 50.000, 23.248,

Metal Complexes

Index	Residue	AA	Metal	Target	Distance	Location
Complex 1: Zn, tetrahedral (4)						
1	39B	CYS	2498	1290	2.35	protein.sidechain
2	57B	CYS	2498	1432	2.45	protein.sidechain
3	59B	CYS	2498	1445	2.29	protein.sidechain
4	80B	CYS	2498	1595	2.18	protein.sidechain

[illegible]

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+	--	+

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D10:F:1099 (D10) - SMALLMOLECULE

Interacting chain(s): E,F

Hydrophobic Interactions

75	HIS	A	702	ZN	A	9316	Zn	571	N	4	2.51
protein.sidechain	22.12	tetrahedral	1			453.971, -0.809, 82.061	455.457, -2.777, 82.514				
+-----	+-----	+-----	+-----		+-----	+-----	+-----	+-----	+-----	+-----	+-----
+-----	+-----	+-----	+-----		+-----	+-----	+-----	+-----			+

ZN:A:703 (ZN) - ION

Interacting chain(s): A

****Metal Complexes****

+-----	+-----	+-----	+-----		+-----	+-----	+-----	+-----	+-----	+-----	+-----
+-----	+-----	+-----	+-----		+-----	+-----	+-----	+-----			+
RESNR	RESTYPE	RESCHAIN	RESNR_LIG	RESTYPE_LIG	RESCHAIN_LIG	METAL_IDX					
METAL_TYPE	TARGET_IDX	TARGET_TYPE	COORDINATION	DIST	LOCATION	RMS					
GEOMETRY	COMPLEXNUM	METALCOO		TARGETCOO							
+	+	+	+	+	+	+	+	+	+	+	+
+	+	+	+	+	+	+	+	+	+	+	+
+	+	+	+	+	+	+	+	+	+	+	+
16	CYS	A	703	ZN	A	9317	Zn	123	S	4	2.54
protein.sidechain	9.07	tetrahedral	1			435.828, 12.154, 80.716	438.343, 12.239, 81.054				
+-----	+-----	+-----	+-----		+-----	+-----	+-----	+-----	+-----	+-----	+-----
+-----	+-----	+-----	+-----		+-----	+-----	+-----	+-----			+
19	CYS	A	703	ZN	A	9317	Zn	138	S	4	2.28
protein.sidechain	9.07	tetrahedral	1			435.828, 12.154, 80.716	435.099, 14.147, 79.884				
+-----	+-----	+-----	+-----		+-----	+-----	+-----	+-----	+-----	+-----	+-----
+-----	+-----	+-----	+-----		+-----	+-----	+-----	+-----			+
33	HIS	A	703	ZN	A	9317	Zn	257	N	4	2.07
protein.sidechain	9.07	tetrahedral	1			435.828, 12.154, 80.716	434.938, 11.378, 82.420				
+-----	+-----	+-----	+-----		+-----	+-----	+-----	+-----	+-----	+-----	+-----
+-----	+-----	+-----	+-----		+-----	+-----	+-----	+-----			+
39	HIS	A	703	ZN	A	9317	Zn	298	N	4	2.05
protein.sidechain	9.07	tetrahedral	1			435.828, 12.154, 80.716	435.587, 10.663, 79.329				
+-----	+-----	+-----	+-----		+-----	+-----	+-----	+-----	+-----	+-----	+-----
+-----	+-----	+-----	+-----		+-----	+-----	+-----	+-----			+

ZN:B:701 (ZN) - ION

Interacting chain(s): B

****Metal Complexes****

+-----	+-----	+-----	+-----		+-----	+-----	+-----	+-----	+-----	+-----	+-----
+-----	+-----	+-----	+-----		+-----	+-----	+-----	+-----			+
RESNR	RESTYPE	RESCHAIN	RESNR_LIG	RESTYPE_LIG	RESCHAIN_LIG	METAL_IDX					
METAL_TYPE	TARGET_IDX	TARGET_TYPE	COORDINATION	DIST	LOCATION	RMS					
GEOMETRY	COMPLEXNUM	METALCOO		TARGETCOO							
+	+	+	+	+	+	+	+	+	+	+	+
+	+	+	+	+	+	+	+	+	+	+	+
+	+	+	+	+	+	+	+	+	+	+	+
5	CYS	B	701	ZN	B	9318	Zn	4694	S	4	2.53
protein.sidechain	22.85	tetrahedral	1			442.651, 0.750, 57.290	442.223, -0.879, 59.178				
+-----	+-----	+-----	+-----		+-----	+-----	+-----	+-----	+-----	+-----	+-----
+-----	+-----	+-----	+-----		+-----	+-----	+-----	+-----			+
8	CYS	B	701	ZN	B	9318	Zn	4715	S	4	2.41
protein.sidechain	22.85	tetrahedral	1			442.651, 0.750, 57.290	443.030, -1.102, 55.789				
+-----	+-----	+-----	+-----		+-----	+-----	+-----	+-----	+-----	+-----	+-----
+-----	+-----	+-----	+-----		+-----	+-----	+-----	+-----			+
26	CYS	B	701	ZN	B	9318	Zn	4853	S	4	2.38
protein.sidechain	22.85	tetrahedral	1			442.651, 0.750, 57.290	444.938, 1.418, 57.244				
+-----	+-----	+-----	+-----		+-----	+-----	+-----	+-----	+-----	+-----	+-----
+-----	+-----	+-----	+-----		+-----	+-----	+-----	+-----			+

Interacting chain(s): H

****Hydrophobic Interactions****

| DIST | LIGCARBONIDX | PROTCARBONIDX | LIGCOO | PROTCOO |

+=====+=====+=====+=====+=====+=====

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=====+=====+=====+=====+=====+=====

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=+=====+

| 53 | LEU | H | 1099 | D10 | H | 3.42 | 4825 | 4432 | 84.803, 13.060, -3.541 | 83.691, 12.515,

-

0.350 |

+-----+-----+-----+-----+-----+-----+-----

-

+-----

+-----

+

Diagram illustrating a sequence of 10 dashed lines with '+' signs at their left ends, arranged in three rows:

- Row 1: 4 dashed lines with '+' signs at their left ends.
- Row 2: 3 dashed lines with '+' signs at their left ends.
- Row 3: 3 dashed lines with '+' signs at their left ends.

The lines are connected by horizontal segments, with some segments being longer than others, creating a stepped appearance. The lines are labeled with '+' signs at their left ends, and some have additional '+' signs further to the right.

02J-C-1

Interacting chains: A

Interacting chain(s): A

****Hydrogen Bonds****

Handwriting practice lines consisting of three horizontal dashed lines. The top line has 11 plus signs (+) spaced evenly along it. The middle line has 10 plus signs (+) spaced evenly along it. The bottom line has 1 plus sign (+) at the beginning.

```
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG | RESCHAIN_LIG |
| SIDECHAIN | DIST_H-A | DIST_D-A | DON_ANGLE | PROTISDON | DONORIDX |
| DONORTYPE | ACCEPTORIDX | ACCEPTORTYPE | LIGCOO          | PROTCOO
|
```

[illegible]

65	ASN	A	402	DMS	A	True	2.05	2.94	148.03
True	524	Nam	2578	O2			8.211, -20.857, 29.787	11.058, -20.242,	

Hydrogen Bonds

Handwriting practice lines consisting of three rows of dashed lines with plus signs (+) placed at regular intervals for tracing and letter formation.

A handwriting practice sheet featuring four horizontal rows of dashed lines. Each row contains several plus signs (+) spaced evenly apart, intended for children to trace or copy as part of their writing practice. The first three rows are complete, while the fourth row ends with a plus sign followed by a dashed line segment.

Three horizontal dashed lines for handwriting practice. The top line has 11 plus signs, the middle line has 10 plus signs, and the bottom line has 1 plus sign.

Handwriting practice lines consisting of three rows of dashed lines with plus signs (+) for tracing. The first row has 6 plus signs, the second row has 7 plus signs, and the third row has 1 plus sign.

$\frac{1}{2} + \frac{1}{2} + \frac{1}{2} + \frac{1}{2}$

Handwriting practice lines for the letter 't'. The first row shows the letter 't' written on a three-line grid (top, middle, bottom). The second row shows the letter 't' written on a three-line grid. The third row shows the letter 't' written on a three-line grid.

-----+-----+-----+-----+-----+

DMS:A:404 (DMS) - SMALLMOLECULE

Interacting chain(s):

.
DMS:A:405 (DMS) - SMALLMOLECULE

Interacting chain(s): A

****Hydrogen Bonds****

-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG | RESCHAIN_LIG
| SIDECHAIN | DIST_H-A | DIST_D-A | DON_ANGLE | PROTISDON | DONORIDX |
DONORTYPE | ACCEPTORIDX | ACCEPTORTYPE | LIGCOO | PROTCOO
|
+=====+=====+=====+=====+=====+=====+=====+
====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+
=====+=====+
| 166 | GLU | A | 405 | DMS | A | False | 2.98 | 3.78 | 136.73 |
True | 1397 | N3 | 2590 | O2 | 6.826, 0.990, 17.467 | 9.995, 2.708, 18.620
|
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+

****Salt Bridges****

-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG | RESCHAIN_LIG |
DIST | PROTISPOS | LIG_GROUP | LIG_IDX_LIST | LIGCOO | PROTCOO
|
+=====+=====+=====+=====+=====+=====+=====+
====+=====+=====+=====+=====+=====+=====+
=====+=====+
| 166 | GLU | A | 405 | DMS | A | 4.61 | False | Sulfonium | 2589
| 5.647, 0.375, 18.090 | 5.179, 4.954, 18.233 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+

DMS:A:406 (DMS) - SMALLMOLECULE

Interacting chain(s):

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DMS:A:407 (DMS) - SMALLMOLECULE

Interacting chain(s): A

Hydrogen Bonds

```
+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+
-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG | RESCHAIN_LIG |
SIDECHAIN | DIST_H-A | DIST_D-A | DON_ANGLE | PROTISDON | DONORIDX |
DONORTYPE | ACCEPTORIDX | ACCEPTORTYPE | LIGCOO          | PROTCOO
|
|=====+=====+=====+=====+=====+=====+=====+=====+
===+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+=====+
=====+=====+
| 101 | TYR   | A     | 407   | DMS    | A      | False | 2.11 | 3.09 | 170.60 |
True  | 819   | Nam   | 2598  | O2     | 16.736, -18.622, -0.828 | 14.936, -16.113, -
0.791 |
+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+
-----+

```

pi-Cation Interactions

```
+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG | RESCHAIN_LIG |
DIST | OFFSET | PROTCHARGED | LIG_GROUP | LIG_IDX_LIST | LIGCOO          |
PROTCOO          |
|=====+=====+=====+=====+=====+=====+=====+=====+
===+=====+=====+=====+=====+=====+=====+=====+
=====+=====+
| 101   | TYR   | A     | 407   | DMS    | A      | 4.86 | 1.72 | False   | sulfonium |
2597   | 18.175, -18.367, -0.718 | 15.873, -16.767, 3.254 |
+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+

```

DMS:A:408 (DMS) - SMALLMOLECULE

Interacting chain(s): A

Water Bridges

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+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+
-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG | RESCHAIN_LIG |
DIST_A-W | DIST_D-W | DON_ANGLE | WATER_ANGLE | PROTISDON |
DONOR_IDX | DONORTYPE | ACCEPTOR_IDX | ACCEPTORTYPE | WATER_IDX |
LIGCOO          | PROTCOO          | WATERCOO          |
|=====+=====+=====+=====+=====+=====+=====+=====+
===+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+=====+
=====+=====+
=====+

```

40	ARG	A	408	DMS	A	3.21	3.68	124.56	90.94
True	310	Ng+	2602	O2	2817	24.144, -2.833, 19.394			
21.476, -4.849, 22.080 21.366, -1.584, 20.393									
+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+									
+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+									
+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+									
187	ASP	A	408	DMS	A	3.82	4.06	108.91	84.22
True	1560	O3	2602	O2	2983	24.144, -2.833, 19.394			
19.249, -2.941, 21.788 22.831, -1.210, 22.598									
+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+									
+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+									
+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+

Hydrophobic Interactions

Index	Residue	AA	Distance	Ligand Atom	Protein Atom
1	168A	PRO	3.53	2369	1303

PJE (composite ligand)

PJE-C-5

Composite ligand consists of PJE:C:5, 010:C:6.

Interacting chains: A

Figure6b. Roccustyrna binding sites into the 02J (5-Methylisoxazole-3-carboxylic acid) PJE-C-56LU7 protein targets. ZN:A:998 (ZN) - ION

Interacting chain(s): A

****Metal Complexes****

	RESNR		RESTYPE		RESCHAIN		RESNR_LIG		RESTYPE_LIG
	RESCHAIN_LIG		METAL_IDX		METAL_TYPE		TARGET_IDX		TARGET_TYPE
	COORDINATION		DIST		LOCATION		RMS		GEOMETRY
	COMPLEXNUM		METALCOO		TARGETCOO				
+=====+		+=====+		+=====+		+=====+		+=====+	
=====+		=====+		=====+		=====+		=====+	
=====+		=====+		=====+		=====+		=====+	
=====+		=====+		=====+		=====+		=====+	
	74		CYS		A		998		ZN
	4		2.20		protein.sidechain		14.02		tetrahedral
	32.313		118.938,		103.573,		30.609		
+-----+		+-----+		+-----+		+-----+		+-----+	
---+-----		---+-----		---+-----		---+-----		---+-----	
-----+		-----+		-----+		-----+		-----+	
	77		CYS		A		998		ZN
	4		2.27		protein.sidechain		14.02		tetrahedral
	32.313		120.386,		104.803,		33.996		
+-----+		+-----+		+-----+		+-----+		+-----+	
---+-----		---+-----		---+-----		---+-----		---+-----	
-----+		-----+		-----+		-----+		-----+	
	83		HIS		A		998		ZN
	4		2.04		protein.sidechain		14.02		tetrahedral
	32.313		119.028,		106.840,		31.527		
+-----+		+-----+		+-----+		+-----+		+-----+	
---+-----		---+-----		---+-----		---+-----		---+-----	
-----+		-----+		-----+		-----+		-----+	
	90		CYS		A		998		ZN
	4		2.38		protein.sidechain		14.02		tetrahedral
	32.313		116.584,		105.150,		32.928		
+-----+		+-----+		+-----+		+-----+		+-----+	
---+-----		---+-----		---+-----		---+-----		---+-----	
-----+		-----+		-----+		-----+		-----+	

ZN:A:999 (ZN) - ION

Interacting chain(s): A

****Metal Complexes****

```
+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+
.....+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG |
RESCHAIN_LIG | METAL_IDX | METAL_TYPE | TARGET_IDX |
TARGET_TYPE | COORDINATION | DIST | LOCATION          | RMS |
GEOMETRY | COMPLEXNUM | METALCOO           | TARGETCOO       |
+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+
```



```

=====+=====+=====+=====+=====+=====+=====+=====+=====+
| 117 | CYS | A | 999 | ZN | A | 20941 | Zn | 786 | S |
| 4 | 2.40 | protein.sidechain | 5.63 | tetrahedral | 1 | 98.622, 94.821, 25.390 |
99.262, 97.110, 25.093 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| 120 | CYS | A | 999 | ZN | A | 20941 | Zn | 806 | S |
| 4 | 2.29 | protein.sidechain | 5.63 | tetrahedral | 1 | 98.622, 94.821, 25.390 |
99.261, 94.205, 27.500 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| 128 | CYS | A | 999 | ZN | A | 20941 | Zn | 867 | S |
| 4 | 2.34 | protein.sidechain | 5.63 | tetrahedral | 1 | 98.622, 94.821, 25.390 |
99.794, 93.627, 23.753 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| 1068 | HOH | A | 999 | ZN | A | 20941 | Zn | 21056 | O |
| 4 | 2.47 | water | 5.63 | tetrahedral | 1 | 98.622, 94.821, 25.390 |
96.161, 94.761, 25.152 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+

```

ZN:B:998 (ZN) - ION

Interacting chain(s): B

****Metal Complexes****

```

+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG |
RESCHAIN_LIG | METAL_IDX | METAL_TYPE | TARGET_IDX |
TARGET_TYPE | COORDINATION | DIST | LOCATION | RMS |
GEOMETRY | COMPLEXNUM | METALCOO | TARGETCOO |
|
+=====+=====+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+=====+=====+
| 74 | CYS | B | 998 | ZN | B | 20942 | Zn | 1351 | S |
| 4 | 2.19 | protein.sidechain | 10.21 | tetrahedral | 1 | 117.333, 105.863,
51.917 | 117.150, 104.689, 53.755 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| 77 | CYS | B | 998 | ZN | B | 20942 | Zn | 1377 | S |
| 4 | 2.29 | protein.sidechain | 10.21 | tetrahedral | 1 | 117.333, 105.863,
51.917 | 115.819, 105.496, 50.243 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| 83 | HIS | B | 998 | ZN | B | 20942 | Zn | 1430 | N |

```

4	2.07	protein.sidechain	10.21	tetrahedral	1	117.333, 105.863, 51.917	116.930, 107.835, 52.389
---	------	-------------------	-------	-------------	---	--------------------------	--------------------------

90	CYS	B	998	ZN	B	20942	Zn	1462	S
4	2.36	protein.sidechain	10.21	tetrahedral	1	117.333, 105.863, 51.917	119.604, 105.866, 51.263		

ZN:B:999 (ZN) - ION

Interacting chain(s): B

****Metal Complexes****

RESNR	RESTYPE	RESCHAIN	RESNR_LIG	RESTYPE_LIG	RESCHAIN_LIG	METAL_IDX	METAL_TYPE	TARGET_IDX	TARGET_TYPE	COORDINATION	DIST	LOCATION	RMS	GEOMETRY	COMPLEXNUM	METALCOO	TARGETCOO
117	CYS	B	999	ZN	B	20943	Zn	1667	S	4	2.35	protein.sidechain	2.82	tetrahedral	1	137.197, 95.958, 60.083	136.561, 98.220, 60.179
120	CYS	B	999	ZN	B	20943	Zn	1687	S	4	2.48	protein.sidechain	2.82	tetrahedral	1	137.197, 95.958, 60.083	136.438, 95.012, 57.924
128	CYS	B	999	ZN	B	20943	Zn	1748	S	4	2.47	protein.sidechain	2.82	tetrahedral	1	137.197, 95.958, 60.083	136.060, 94.833, 61.960
1058	HOH	B	999	ZN	B	20943	Zn	21115	O	4	2.53	water	2.82	tetrahedral	1	137.197, 95.958, 60.083	139.712, 95.777, 60.243

ZN:C:998 (ZN) - ION


```

=====+=====+=====+=====+=====+=====+=====
=====+=====+=====+=====+=====+=====+=====
=====+=====+=====+=====+=====+=====+=====
| 117 | CYS | C | 999 | ZN | C | 20945 | Zn | 2541 | S
| 4 | 2.45 | protein.sidechain | 6.21 | tetrahedral | 1 | 137.050, 141.736, 13.631
| 137.160, 141.119, 15.996 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----
---+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----
.....+-----+
| 120 | CYS | C | 999 | ZN | C | 20945 | Zn | 2561 | S
| 4 | 2.35 | protein.sidechain | 6.21 | tetrahedral | 1 | 137.050, 141.736, 13.631
| 135.026, 140.836, 12.841 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----
---+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----
.....+-----+
| 128 | CYS | C | 999 | ZN | C | 20945 | Zn | 2622 | S
| 4 | 2.41 | protein.sidechain | 6.21 | tetrahedral | 1 | 137.050, 141.736, 13.631
| 138.921, 140.589, 12.629 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----
---+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----
.....+-----+
| 1065 | HOH | C | 999 | ZN | C | 20945 | Zn | 21181 | O
| 4 | 2.36 | water | 6.21 | tetrahedral | 1 | 137.050, 141.736, 13.631 |
137.249, 144.081, 13.413 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----
---+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----
.....+-----+

```

ZN:D:998 (ZN) - ION

Interacting chain(s): D

****Metal Complexes****

```

+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----
---+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----
.....+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG |
RESCHAIN_LIG | METAL_IDX | METAL_TYPE | TARGET_IDX |
TARGET_TYPE | COORDINATION | DIST | LOCATION | RMS |
GEOMETRY | COMPLEXNUM | METALCOO | TARGETCOO
|
+=====+=====+=====+=====+=====+=====+=====
=====+=====+=====+=====+=====+=====+=====
=====+=====+=====+=====+=====+=====+=====
=====+=====+=====+=====+=====+=====+=====
| 74 | CYS | D | 998 | ZN | D | 20946 | Zn | 3099 | S
| 4 | 2.35 | protein.sidechain | 12.76 | tetrahedral | 1 | 109.965, 122.817,
23.058 | 108.146, 122.844, 21.569 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----
---+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----
-----+-----+
| 77 | CYS | D | 998 | ZN | D | 20946 | Zn | 3125 | S
| 4 | 2.26 | protein.sidechain | 12.76 | tetrahedral | 1 | 109.965, 122.817,
23.058 | 111.591, 124.341, 22.668 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----
---+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----

```

```

-----+-----+
| 83 | HIS | D | 998 | ZN | D | 20946 | Zn | 3178 | N
| 4 | | 1.98 | protein.sidechain | 12.76 | tetrahedral | 1 | 109.965, 122.817,
23.058 | 109.117, 122.926, 24.848 |
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+
| 90 | CYS | D | 998 | ZN | D | 20946 | Zn | 3210 | S
| 4 | | 2.30 | protein.sidechain | 12.76 | tetrahedral | 1 | 109.965, 122.817,
23.058 | 110.751, 120.677, 23.359 |
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+

```

ZN:D:999 (ZN) - ION

Interacting chain(s): D

****Metal Complexes****

```

+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG |
RESCHAIN_LIG | METAL_IDX | METAL_TYPE | TARGET_IDX |
TARGET_TYPE | COORDINATION | DIST | LOCATION | RMS |
GEOMETRY | COMPLEXNUM | METALCOO | TARGETCOO
|
+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+
| 117 | CYS | D | 999 | ZN | D | 20947 | Zn | 3415 | S
| 4 | | 2.22 | protein.sidechain | 39.15 | tetrahedral | 1 | 103.746, 101.848,
13.968 | 103.306, 102.613, 16.001 |
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+
| 120 | CYS | D | 999 | ZN | D | 20947 | Zn | 3435 | S
| 4 | | 2.18 | protein.sidechain | 39.15 | tetrahedral | 1 | 103.746, 101.848,
13.968 | 105.355, 103.254, 13.535 |
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+
| 128 | CYS | D | 999 | ZN | D | 20947 | Zn | 3496 | S
| 4 | | 1.83 | protein.sidechain | 39.15 | tetrahedral | 1 | 103.746, 101.848,
13.968 | 103.541, 102.982, 12.547 |
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+
| 1062 | HOH | D | 999 | ZN | D | 20947 | Zn | 21244 | O
| 4 | | 2.42 | water | 39.15 | tetrahedral | 1 | 103.746, 101.848, 13.968 |
103.421, 99.451, 13.939 |
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+

```

ZN:E:998 (ZN) - ION

Interacting chain(s): E

****Metal Complexes****

RESNR	RESTYPE	RESCHAIN	RESNR_LIG	RESTYPE_LIG	RESCHAIN_LIG	METAL_IDX	METAL_TYPE	TARGET_IDX	TARGET_TYPE	COORDINATION	DIST	LOCATION	RMS	GEOMETRY	COMPLEXNUM	METALCOO	TARGETCOO
74	CYS	E	998	ZN	E	20948	Zn	3973	S	4	2.29	protein.sidechain	11.73	tetrahedral	1	136.302, 132.946, 42.028	137.708, 134.757, 42.103
77	CYS	E	998	ZN	E	20948	Zn	3999	S	4	2.17	protein.sidechain	11.73	tetrahedral	1	136.302, 132.946, 42.028	136.430, 131.447, 43.591
83	HIS	E	998	ZN	E	20948	Zn	4052	N	4	2.07	protein.sidechain	11.73	tetrahedral	1	136.302, 132.946, 42.028	134.333, 133.584, 42.079
90	CYS	E	998	ZN	E	20948	Zn	4084	S	4	2.34	protein.sidechain	11.73	tetrahedral	1	136.302, 132.946, 42.028	136.283, 132.061, 39.860

ZN:E:999 (ZN) - ION

Interacting chain(s): E

****Metal Complexes****

RESNR	RESTYPE	RESCHAIN	RESNR_LIG	RESTYPE_LIG	RESCHAIN_LIG	METAL_IDX	METAL_TYPE	TARGET_IDX	TARGET_TYPE	COORDINATION	DIST	LOCATION	RMS
-------	---------	----------	-----------	-------------	--------------	-----------	------------	------------	-------------	--------------	------	----------	-----

GEOMETRY		COMPLEXNUM	METAL	COORD	TARGET	
117	CYS	E	999	ZN	E	20949
4	2.40	protein.sidechain	7.54	tetrahedral	1	148.031, 137.597, 22.086
145.684, 137.947, 22.423						
120	CYS	E	999	ZN	E	20949
4	2.32	protein.sidechain	7.54	tetrahedral	1	148.031, 137.597, 22.086
148.587, 135.560, 23.058						
128	CYS	E	999	ZN	E	20949
4	2.36	protein.sidechain	7.54	tetrahedral	1	148.031, 137.597, 22.086
149.251, 139.414, 22.969						
1062	HOH	E	999	ZN	E	20949
4	2.50	water	7.54	tetrahedral	1	148.031, 137.597, 22.086
148.289, 137.758, 19.609						

ZN:F:998 (ZN) - ION

Interacting chain(s): F

Metal Complexes

GEOMETRY		COMPLEXNUM	METAL	COORD	TARGET	
74	CYS	F	998	ZN	F	20950
4	2.24	protein.sidechain	10.26	tetrahedral	1	136.049, 112.718, 43.005
137.361, 110.904, 43.087						
77	CYS	F	998	ZN	F	20950
4	2.21	protein.sidechain	10.26	tetrahedral	1	136.049, 112.718,

```

43.005 | 136.425, 114.165, 41.384 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| 83 | HIS | F | 998 | ZN | F | 20950 | Zn | 4916 | N
| 4 | 2.12 | protein.sidechain | 10.26 | tetrahedral | 1 | 136.049, 112.718,
43.005 | 134.050, 112.122, 42.628 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| 90 | CYS | F | 998 | ZN | F | 20950 | Zn | 4948 | S
| 4 | 2.36 | protein.sidechain | 10.26 | tetrahedral | 1 | 136.049, 112.718,
43.005 | 135.921, 113.589, 45.196 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+

```

ZN:F:999 (ZN) - ION

Interacting chain(s): F

Metal Complexes

```

+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG |
RESCHAIN_LIG | METAL_IDX | METAL_TYPE | TARGET_IDX |
TARGET_TYPE | COORDINATION | DIST | LOCATION | RMS |
GEOMETRY | COMPLEXNUM | METALCOO | TARGETCOO
|
+=====+=====+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+=====+=====+
| 117 | CYS | F | 999 | ZN | F | 20951 | Zn | 5153 | S
| 4 | 2.32 | protein.sidechain | 7.13 | tetrahedral | 1 | 144.749, 107.455, 64.104
| 142.581, 107.152, 63.330 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| 120 | CYS | F | 999 | ZN | F | 20951 | Zn | 5173 | S
| 4 | 2.31 | protein.sidechain | 7.13 | tetrahedral | 1 | 144.749, 107.455, 64.104
| 145.599, 109.413, 63.216 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| 128 | CYS | F | 999 | ZN | F | 20951 | Zn | 5234 | S
| 4 | 2.41 | protein.sidechain | 7.13 | tetrahedral | 1 | 144.749, 107.455, 64.104
| 146.003, 105.583, 63.236 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| 1057 | HOH | F | 999 | ZN | F | 20951 | Zn | 21365 | O
| 4 | 2.47 | water | 7.13 | tetrahedral | 1 | 144.749, 107.455, 64.104 |
144.533, 107.340, 66.557 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+

```



```
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
```

ZN:G:998 (ZN) - ION

Interacting chain(s): G

Metal Complexes

```
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
```

```
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG |
| RESCHAIN_LIG | METAL_IDX | METAL_TYPE | TARGET_IDX |
| TARGET_TYPE | COORDINATION | DIST | LOCATION | RMS |
| GEOMETRY | COMPLEXNUM | METALCOO | TARGETCOO |
```

```
|
|=====+=====+=====+=====+=====+=====+=====+=====+=====+=====+
|=====+=====+=====+=====+=====+=====+=====+=====+=====+=====+
|=====+=====+=====+=====+=====+=====+=====+=====+=====+=====+
|=====+=====+=====+=====+=====+=====+=====+=====+=====+=====+
|=====+=====+=====+=====+=====+=====+=====+=====+=====+=====+
```

```
| 74 | CYS | G | 998 | ZN | G | 20952 | Zn | 5711 | S
| 4 | 2.22 | protein.sidechain | 8.13 | tetrahedral | 1 | 101.772, 133.603, 39.336
| 100.475, 135.398, 39.149 |
```

```
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
```

```
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| 77 | CYS | G | 998 | ZN | G | 20952 | Zn | 5737 | S
| 4 | 2.21 | protein.sidechain | 8.13 | tetrahedral | 1 | 101.772, 133.603, 39.336
| 101.451, 132.007, 37.848 |
```

```
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
```

```
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| 83 | HIS | G | 998 | ZN | G | 20952 | Zn | 5790 | N
| 4 | 2.03 | protein.sidechain | 8.13 | tetrahedral | 1 | 101.772, 133.603, 39.336
| 103.711, 134.136, 39.084 |
```

```
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
```

```
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| 90 | CYS | G | 998 | ZN | G | 20952 | Zn | 5822 | S
| 4 | 2.37 | protein.sidechain | 8.13 | tetrahedral | 1 | 101.772, 133.603, 39.336
| 101.747, 132.794, 41.566 |
```

```
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
```

```
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
```

ZN:G:999 (ZN) - ION

Interacting chain(s): G

Metal Complexes

```
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----+
```

```

| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG | |
| RESCHAIN_LIG | METAL_IDX | METAL_TYPE | TARGET_IDX |
| TARGET_TYPE | COORDINATION | DIST | LOCATION | RMS | GEOMETRY |
| COMPLEXNUM | METALCOO | TARGETCOO |
=====+=====+=====+=====+=====+=====+=====
=====+=====+=====+=====+=====+=====+=====
=====+=====+=====+=====+=====+=====+=====
=====+=====+=====+=====+=====+=====+=====
| 117 | CYS | G | 999 | ZN | G | 20953 | Zn | 6027 | S
| 4 | 2.36 | protein.sidechain | 4.74 | tetrahedral | 1 | 90.358, 141.040, 58.747 |
92.674, 141.224, 58.353 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
---+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+
| 120 | CYS | G | 999 | ZN | G | 20953 | Zn | 6047 | S
| 4 | 2.39 | protein.sidechain | 4.74 | tetrahedral | 1 | 90.358, 141.040, 58.747 |
89.631, 138.849, 58.124 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
---+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+
| 128 | CYS | G | 999 | ZN | G | 20953 | Zn | 6108 | S
| 4 | 2.39 | protein.sidechain | 4.74 | tetrahedral | 1 | 90.358, 141.040, 58.747 |
89.253, 142.741, 57.484 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
---+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+
| 1064 | HOH | G | 999 | ZN | G | 20953 | Zn | 21430 | O
| 4 | 2.52 | water | 4.74 | tetrahedral | 1 | 90.358, 141.040, 58.747 |
90.100, 141.293, 61.241 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
---+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+

```

ZN:H:998 (ZN) - ION

Interacting chain(s): H

****Metal Complexes****

```

+-----+-----+-----+-----+-----+-----+-----+-----+-----+
---+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG |
| RESCHAIN_LIG | METAL_IDX | METAL_TYPE | TARGET_IDX |
| TARGET_TYPE | COORDINATION | DIST | LOCATION | RMS |
| GEOMETRY | COMPLEXNUM | METALCOO | TARGETCOO |
|
=====+=====+=====+=====+=====+=====+=====
=====+=====+=====+=====+=====+=====+=====
=====+=====+=====+=====+=====+=====+=====
=====+=====+=====+=====+=====+=====+=====
| 74 | CYS | H | 998 | ZN | H | 20954 | Zn | 6585 | S
| 4 | 2.21 | protein.sidechain | 11.43 | tetrahedral | 1 | 100.856, 113.346,
40.447 | 99.446, 111.645, 40.544 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
---+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+

```

77	CYS	H	998	ZN	H	20954	Zn	6611	S
4	2.26	protein.sidechain	11.43	tetrahedral	1	100.856, 113.346, 40.447	100.513, 115.048, 41.899		

83	HIS	H	998	ZN	H	20954	Zn	6664	N
4	2.07	protein.sidechain	11.43	tetrahedral	1	100.856, 113.346, 40.447	102.751, 112.566, 40.765		

90	CYS	H	998	ZN	H	20954	Zn	6696	S
4	2.34	protein.sidechain	11.43	tetrahedral	1	100.856, 113.346, 40.447	101.228, 114.001, 38.230		

ZN:H:999 (ZN) - ION

Interacting chain(s): H

Metal Complexes

	RESNR	RESTYPE	RESCHAIN	RESNR_LIG	RESTYPE_LIG	RESCHAIN_LIG	METAL_IDX	METAL_TYPE	TARGET_IDX	TARGET_TYPE	COORDINATION	DIST	LOCATION	RMS	GEOMETRY	COMPLEXNUM	METALCOO	TARGETCOO
117	CYS	H	999	ZN	H	20955	Zn	6901	S	4	2.32	protein.sidechain	6.69	tetrahedral	1	91.822, 106.447, 19.838	93.984, 106.182, 20.634	
120	CYS	H	999	ZN	H	20955	Zn	6921	S	4	2.35	protein.sidechain	6.69	tetrahedral	1	91.822, 106.447, 19.838	91.103, 108.567, 20.555	
128	CYS	H	999	ZN	H	20955	Zn	6982	S	4	2.35	protein.sidechain	6.69	tetrahedral	1	91.822, 106.447, 19.838	90.509, 104.769, 20.832	
1058	HOH	H	999	ZN	H	20955	Zn	21489	O	4	2.39	water	6.69	tetrahedral	1	91.822, 106.447, 19.838	92.043, 106.180, 17.476	

```
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
---+-----+-----+-----+-----+-----+-----+-----+-----+-----+
.....+-----+

```

ZN:I:998 (ZN) - ION

Interacting chain(s): I

Metal Complexes

```
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
---+-----+-----+-----+-----+-----+-----+-----+-----+-----+

```

```
.....+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG |
RESCHAIN_LIG | METAL_IDX | METAL_TYPE | TARGET_IDX |
TARGET_TYPE | COORDINATION | DIST | LOCATION | RMS |
GEOMETRY | COMPLEXNUM | METALCOO | TARGETCOO
|

```

```
+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+
```

```
| 74 | CYS | I | 998 | ZN | I | 20956 | Zn | 7459 | S
| 4 | 2.19 | protein.sidechain | 13.31 | tetrahedral | 1 | 118.443, 141.475,
50.406 | 118.358, 142.910, 52.055 |
```

```
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
---+-----+-----+-----+-----+-----+-----+-----+-----+-----+

```

```
.....+-----+
| 77 | CYS | I | 998 | ZN | I | 20956 | Zn | 7485 | S
| 4 | 2.24 | protein.sidechain | 13.31 | tetrahedral | 1 | 118.443, 141.475,
50.406 | 120.081, 141.603, 48.884 |
```

```
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
---+-----+-----+-----+-----+-----+-----+-----+-----+-----+

```

```
.....+-----+
| 83 | HIS | I | 998 | ZN | I | 20956 | Zn | 7538 | N
| 4 | 2.08 | protein.sidechain | 13.31 | tetrahedral | 1 | 118.443, 141.475,
50.406 | 118.714, 139.505, 51.028 |
```

```
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
---+-----+-----+-----+-----+-----+-----+-----+-----+-----+

```

```
.....+-----+
| 90 | CYS | I | 998 | ZN | I | 20956 | Zn | 7570 | S
| 4 | 2.38 | protein.sidechain | 13.31 | tetrahedral | 1 | 118.443, 141.475,
50.406 | 116.238, 141.356, 49.524 |
```

```
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
---+-----+-----+-----+-----+-----+-----+-----+-----+-----+

```

```
.....+-----+

```

ZN:I:999 (ZN) - ION

Interacting chain(s): I

Metal Complexes

```
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
---+-----+-----+-----+-----+-----+-----+-----+-----+-----+

```

```

-----+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG |
| RESCHAIN_LIG | METAL_IDX | METAL_TYPE | TARGET_IDX |
| TARGET_TYPE | COORDINATION | DIST | LOCATION | RMS |
| GEOMETRY | COMPLEXNUM | METALCOO | TARGETCOO |
+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+
| 117 | CYS | I | 999 | ZN | I | 20957 | Zn | 7775 | S
| 4 | 2.34 | protein.sidechain | 5.07 | tetrahedral | 1 | 98.117, 152.269, 54.603 |
98.583, 150.024, 55.074 |
+-----+-----+-----+-----+-----+-----+-----+
---+-----+-----+-----+-----+-----+-----+
+-----+-----+
| 120 | CYS | I | 999 | ZN | I | 20957 | Zn | 7795 | S
| 4 | 2.26 | protein.sidechain | 5.07 | tetrahedral | 1 | 98.117, 152.269, 54.603 |
98.982, 152.902, 52.616 |
+-----+-----+-----+-----+-----+-----+-----+
---+-----+-----+-----+-----+-----+-----+
+-----+-----+
| 128 | CYS | I | 999 | ZN | I | 20957 | Zn | 7856 | S
| 4 | 2.37 | protein.sidechain | 5.07 | tetrahedral | 1 | 98.117, 152.269, 54.603 |
99.036, 153.495, 56.409 |
+-----+-----+-----+-----+-----+-----+-----+
---+-----+-----+-----+-----+-----+-----+
+-----+-----+
| 1054 | HOH | I | 999 | ZN | I | 20957 | Zn | 21544 | O
| 4 | 2.41 | water | 5.07 | tetrahedral | 1 | 98.117, 152.269, 54.603 |
95.710, 152.438, 54.631 |
+-----+-----+-----+-----+-----+-----+-----+
---+-----+-----+-----+-----+-----+-----+
+-----+-----+

```

ZN:J:998 (ZN) - ION

Interacting chain(s): J

****Metal Complexes****

```

+-----+-----+-----+-----+-----+-----+-----+
---+-----+-----+-----+-----+-----+-----+
+-----+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG |
| RESCHAIN_LIG | METAL_IDX | METAL_TYPE | TARGET_IDX |
| TARGET_TYPE | COORDINATION | DIST | LOCATION | RMS |
| GEOMETRY | COMPLEXNUM | METALCOO | TARGETCOO |
|
+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+
| 74 | CYS | J | 998 | ZN | J | 20958 | Zn | 8333 | S
| 4 | 2.21 | protein.sidechain | 10.46 | tetrahedral | 1 | 119.837, 140.554,
30.186 | 119.929, 141.789, 28.358 |
+-----+-----+-----+-----+-----+-----+-----+
---+-----+-----+-----+-----+-----+-----+

```

```

-----+-----+
| 77 | CYS | J | 998 | ZN | J | 20958 | Zn | 8359 | S
| 4 | | 2.25 | protein.sidechain | 10.46 | tetrahedral | 1 | 119.837, 140.554,
30.186 | 118.180, 140.937, 31.664 |
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+
| 83 | HIS | J | 998 | ZN | J | 20958 | Zn | 8412 | N
| 4 | | 2.03 | protein.sidechain | 10.46 | tetrahedral | 1 | 119.837, 140.554,
30.186 | 119.610, 138.622, 29.596 |
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+
| 90 | CYS | J | 998 | ZN | J | 20958 | Zn | 8444 | S
| 4 | | 2.38 | protein.sidechain | 10.46 | tetrahedral | 1 | 119.837, 140.554,
30.186 | 121.989, 140.409, 31.186 |
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+

```

ZN:J:999 (ZN) - ION

Interacting chain(s): J

****Metal Complexes****

```

+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG |
RESCHAIN_LIG | METAL_IDX | METAL_TYPE | TARGET_IDX |
TARGET_TYPE | COORDINATION | DIST | LOCATION | RMS |
GEOMETRY | COMPLEXNUM | METALCOO | TARGETCOO
|
+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+
| 117 | CYS | J | 999 | ZN | J | 20959 | Zn | 8649 | S
| 4 | | 2.40 | protein.sidechain | 7.37 | tetrahedral | 1 | 140.665, 149.757, 25.126
| 140.055, 147.459, 24.789 |
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+
| 120 | CYS | J | 999 | ZN | J | 20959 | Zn | 8669 | S
| 4 | | 2.28 | protein.sidechain | 7.37 | tetrahedral | 1 | 140.665, 149.757, 25.126
| 139.801, 150.659, 27.028 |
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+
| 128 | CYS | J | 999 | ZN | J | 20959 | Zn | 8730 | S
| 4 | | 2.35 | protein.sidechain | 7.37 | tetrahedral | 1 | 140.665, 149.757, 25.126
| 139.852, 150.812, 23.195 |
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+
| 1072 | HOH | J | 999 | ZN | J | 20959 | Zn | 21617 | O

```

4	2.54	water	7.37	tetrahedral	1	140.665, 149.757, 25.126
143.202, 149.692, 25.219						

```

+-----+-----+-----+-----+-----+-----+
|-----|-----|-----|-----|-----|-----|
+-----+-----+-----+-----+-----+-----+
|-----+-----+-----+-----+-----+-----+
|-----+-----+-----+-----+-----+-----+
|-----+-----+-----+-----+-----+-----+

```

ZN:K:998 (ZN) - ION

Interacting chain(s): K

****Metal Complexes****

```

+-----+-----+-----+-----+-----+-----+
|-----|-----|-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+
|-----+-----+-----+-----+-----+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG |
| RESCHAIN_LIG | METAL_IDX | METAL_TYPE | TARGET_IDX |
| TARGET_TYPE | COORDINATION | DIST | LOCATION | RMS |
| GEOMETRY | COMPLEXNUM | METALCOO | TARGETCOO
|

```

```

+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+
| 74 | CYS | K | 998 | ZN | K | 20960 | Zn | 9207 | S
| 4 | 2.27 | protein.sidechain | 10.09 | tetrahedral | 1 | 107.588, 124.069,
58.141 | 105.700, 124.145, 59.403 |

```

```

+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+
| 77 | CYS | K | 998 | ZN | K | 20960 | Zn | 9233 | S
| 4 | 2.22 | protein.sidechain | 10.09 | tetrahedral | 1 | 107.588, 124.069,
58.141 | 109.070, 122.509, 58.676 |

```

```

+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+
| 83 | HIS | K | 998 | ZN | K | 20960 | Zn | 9286 | N
| 4 | 2.11 | protein.sidechain | 10.09 | tetrahedral | 1 | 107.588, 124.069,
58.141 | 107.166, 123.787, 56.090 |

```

```

+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+
| 90 | CYS | K | 998 | ZN | K | 20960 | Zn | 9318 | S
| 4 | 2.28 | protein.sidechain | 10.09 | tetrahedral | 1 | 107.588, 124.069,
58.141 | 108.459, 126.169, 58.018 |

```

```

+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+

```

ZN:K:999 (ZN) - ION

Interacting chain(s): K

****Metal Complexes****

```

+-----+-----+-----+-----+-----+-----+-----+-----+-----+
---+-----+-----+-----+-----+-----+-----+-----+-----+-----+
.....+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG |
RESCHAIN_LIG | METAL_IDX | METAL_TYPE | TARGET_IDX |
TARGET_TYPE | COORDINATION | DIST | LOCATION | RMS |
GEOMETRY | COMPLEXNUM | METALCOO | TARGETCOO
|
+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+
| 117 | CYS | K | 999 | ZN | K | 20961 | Zn | 9523 | S
| 4 | 2.32 | protein.sidechain | 9.65 | tetrahedral | 1 | 101.405, 145.210, 67.036
| 101.278, 144.500, 64.832 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
---+-----+-----+-----+-----+-----+-----+-----+-----+-----+
.....+-----+
| 120 | CYS | K | 999 | ZN | K | 20961 | Zn | 9543 | S
| 4 | 2.33 | protein.sidechain | 9.65 | tetrahedral | 1 | 101.405, 145.210, 67.036
| 103.348, 144.306, 67.954 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
---+-----+-----+-----+-----+-----+-----+-----+-----+-----+
.....+-----+
| 128 | CYS | K | 999 | ZN | K | 20961 | Zn | 9604 | S
| 4 | 2.34 | protein.sidechain | 9.65 | tetrahedral | 1 | 101.405, 145.210, 67.036
| 99.546, 144.318, 68.148 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
---+-----+-----+-----+-----+-----+-----+-----+-----+-----+
.....+-----+
| 1070 | HOH | K | 999 | ZN | K | 20961 | Zn | 21688 | O
| 4 | 2.47 | water | 9.65 | tetrahedral | 1 | 101.405, 145.210, 67.036 |
101.113, 147.645, 66.769 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
---+-----+-----+-----+-----+-----+-----+-----+-----+-----+
.....+-----+

```

ZN:L:998 (ZN) - ION

Interacting chain(s): L

****Metal Complexes****

```

+-----+-----+-----+-----+-----+-----+-----+-----+-----+
---+-----+-----+-----+-----+-----+-----+-----+-----+-----+
.....+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG |
RESCHAIN_LIG | METAL_IDX | METAL_TYPE | TARGET_IDX |
TARGET_TYPE | COORDINATION | DIST | LOCATION | RMS |
GEOMETRY | COMPLEXNUM | METALCOO | TARGETCOO
|
+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+
| 74 | CYS | L | 998 | ZN | L | 20962 | Zn | 10081 | S
| 4 | 2.29 | protein.sidechain | 8.45 | tetrahedral | 1 | 127.432, 124.018, 59.203

```



```

| 129.129, 124.107, 60.739 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| 77 | CYS | L | 998 | ZN | L | 20962 | Zn | 10107 | S
| 4 | 2.16 | protein.sidechain | 8.45 | tetrahedral | 1 | 127.432, 124.018, 59.203
| 125.976, 125.607, 59.359 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| 83 | HIS | L | 998 | ZN | L | 20962 | Zn | 10160 | N
| 4 | 2.02 | protein.sidechain | 8.45 | tetrahedral | 1 | 127.432, 124.018, 59.203
| 128.293, 124.280, 57.392 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| 90 | CYS | L | 998 | ZN | L | 20962 | Zn | 10192 | S
| 4 | 2.31 | protein.sidechain | 8.45 | tetrahedral | 1 | 127.432, 124.018, 59.203
| 126.568, 121.876, 59.059 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+

```

ZN:L:999 (ZN) - ION

Interacting chain(s): L

Metal Complexes

```

+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG |
| RESCHAIN_LIG | METAL_IDX | METAL_TYPE | TARGET_IDX |
| TARGET_TYPE | COORDINATION | DIST | LOCATION | RMS |
| GEOMETRY | COMPLEXNUM | METALCOO | TARGETCOO |
|
+=====+=====+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+=====+=====+
| 117 | CYS | L | 999 | ZN | L | 20963 | Zn | 10397 | S
| 4 | 2.32 | protein.sidechain | 5.15 | tetrahedral | 1 | 132.609, 103.967, 70.728
| 133.068, 104.466, 68.505 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| 120 | CYS | L | 999 | ZN | L | 20963 | Zn | 10417 | S
| 4 | 2.28 | protein.sidechain | 5.15 | tetrahedral | 1 | 132.609, 103.967, 70.728
| 130.572, 104.855, 71.226 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| 128 | CYS | L | 999 | ZN | L | 20963 | Zn | 10478 | S
| 4 | 2.22 | protein.sidechain | 5.15 | tetrahedral | 1 | 132.609, 103.967, 70.728
| 134.196, 104.988, 71.903 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+

```

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-----+-----+-----+-----+-----+-----+-----+-----
| 1070 | HOH   | L   | 999   | ZN     | L     | 20963 | Zn     | 21759 | O
| 4     | 2.42 | water   | 5.15 | tetrahedral | 1     | 132.609, 103.967, 70.728 |
132.749, 101.559, 70.977 |
+-----+-----+-----+-----+-----+-----+-----+-----
-----+-----+-----+-----+-----+-----+-----+-----
-----+-----+-----+-----+-----+-----+-----+-----

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ZN:M:998 (ZN) - ION

Interacting chain(s): M

****Metal Complexes****

```

+-----+-----+-----+-----+-----+-----+-----+-----
+-----+-----+-----+-----+-----+-----+-----+-----
+-----+-----+-----+-----+-----+-----+-----+-----
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG |
| RESCHAIN_LIG | METAL_IDX | METAL_TYPE | TARGET_IDX |
| TARGET_TYPE | COORDINATION | DIST | LOCATION | RMS |
| GEOMETRY | COMPLEXNUM | METALCOO | TARGETCOO
|
+=====+=====+=====+=====+=====+=====+=====+=====
=====+=====+=====+=====+=====+=====+=====+=====
=====+=====+=====+=====+=====+=====+=====+=====
=====+=====+=====+=====+=====+=====+=====+=====+
| 74 | CYS   | M   | 998   | ZN     | M     | 20964 | Zn     | 10955 | S
| 4   | 2.16 | protein.sidechain | 11.49 | tetrahedral | 1     | 122.417, 100.678,
112.594 | 122.622, 99.428, 110.842 |
+-----+-----+-----+-----+-----+-----+-----+-----
+-----+-----+-----+-----+-----+-----+-----+-----
+-----+-----+-----+-----+-----+-----+-----+-----
| 77 | CYS   | M   | 998   | ZN     | M     | 20964 | Zn     | 10981 | S
| 4   | 2.23 | protein.sidechain | 11.49 | tetrahedral | 1     | 122.417, 100.678,
112.594 | 124.047, 100.714, 114.117 |
+-----+-----+-----+-----+-----+-----+-----+-----
+-----+-----+-----+-----+-----+-----+-----+-----
+-----+-----+-----+-----+-----+-----+-----+-----
| 83 | HIS   | M   | 998   | ZN     | M     | 20964 | Zn     | 11034 | N
| 4   | 2.09 | protein.sidechain | 11.49 | tetrahedral | 1     | 122.417, 100.678,
112.594 | 122.219, 102.604, 111.816 |
+-----+-----+-----+-----+-----+-----+-----+-----
+-----+-----+-----+-----+-----+-----+-----+-----
+-----+-----+-----+-----+-----+-----+-----+-----
| 90 | CYS   | M   | 998   | ZN     | M     | 20964 | Zn     | 11066 | S
| 4   | 2.33 | protein.sidechain | 11.49 | tetrahedral | 1     | 122.417, 100.678,
112.594 | 120.265, 100.339, 113.422 |
+-----+-----+-----+-----+-----+-----+-----+-----
+-----+-----+-----+-----+-----+-----+-----+-----
+-----+-----+-----+-----+-----+-----+-----+-----

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ZN:M:999 (ZN) - ION

Interacting chain(s): M

[illegible]

Interacting chain(s): N

```
+-----+-----+-----+-----+-----+-----+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG |
| RESCHAIN_LIG | METAL_IDX | METAL_TYPE | TARGET_IDX |
| TARGET_TYPE | COORDINATION | DIST | LOCATION | RMS |
| GEOMETRY | COMPLEXNUM | METALCOO | TARGETCOO |
|
+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+
```

```

=====+=====+=====+=====+=====+=====+=====+=====+=====+
| 74 | CYS | N | 998 | ZN | N | 20966 | Zn | 11829 | S
| 4 | 2.27 | protein.sidechain | 11.60 | tetrahedral | 1 | 122.960, 100.769,
132.654 | 123.120, 99.438, 134.486 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| 77 | CYS | N | 998 | ZN | N | 20966 | Zn | 11855 | S
| 4 | 2.21 | protein.sidechain | 11.60 | tetrahedral | 1 | 122.960, 100.769,
132.654 | 121.416, 100.255, 131.155 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| 83 | HIS | N | 998 | ZN | N | 20966 | Zn | 11908 | N
| 4 | 2.13 | protein.sidechain | 11.60 | tetrahedral | 1 | 122.960, 100.769,
132.654 | 122.372, 102.695, 133.361 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| 90 | CYS | N | 998 | ZN | N | 20966 | Zn | 11940 | S
| 4 | 2.33 | protein.sidechain | 11.60 | tetrahedral | 1 | 122.960, 100.769,
132.654 | 125.164, 101.122, 131.978 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+

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ZN:N:999 (ZN) - ION

Interacting chain(s): N

Metal Complexes

```

+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG |
RESCHAIN_LIG | METAL_IDX | METAL_TYPE | TARGET_IDX |
TARGET_TYPE | COORDINATION | DIST | LOCATION | RMS |
GEOMETRY | COMPLEXNUM | METALCOO | TARGETCOO
|
+=====+=====+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+=====+=====+
| 117 | CYS | N | 999 | ZN | N | 20967 | Zn | 12145 | S
| 4 | 2.43 | protein.sidechain | 7.08 | tetrahedral | 1 | 144.742, 94.477, 138.335
| 143.627, 96.621, 138.603 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| 120 | CYS | N | 999 | ZN | N | 20967 | Zn | 12165 | S
| 4 | 2.44 | protein.sidechain | 7.08 | tetrahedral | 1 | 144.742, 94.477, 138.335
| 143.932, 93.459, 136.267 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| 128 | CYS | N | 999 | ZN | N | 20967 | Zn | 12226 | S

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| 4      | 2.30 | protein.sidechain | 7.08 | tetrahedral | 1      | 144.742, 94.477, 138.335
| 143.911, 93.158, 140.021 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| 1050 | HOH      | N      | 999      | ZN      | N      | 20967      | Zn      | 21884 | O
| 4      | 2.52 | water      | 7.08 | tetrahedral | 1      | 144.742, 94.477, 138.335 |
147.244, 94.715, 138.184 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+

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ZN:O:998 (ZN) - ION

Interacting chain(s): O

****Metal Complexes****

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+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG |
| RESCHAIN_LIG | METAL_IDX | METAL_TYPE | TARGET_IDX |
| TARGET_TYPE | COORDINATION | DIST | LOCATION | RMS |
| GEOMETRY | COMPLEXNUM | METALCOO | TARGETCOO |
|
+=====+=====+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+=====+=====+
| 74 | CYS      | O      | 998      | ZN      | O      | 20968      | Zn      | 12703 | S
| 4      | 2.27 | protein.sidechain | 8.91 | tetrahedral | 1      | 129.636, 120.541,
139.754 | 131.432, 120.804, 141.125 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| 77 | CYS      | O      | 998      | ZN      | O      | 20968      | Zn      | 12729 | S
| 4      | 2.30 | protein.sidechain | 8.91 | tetrahedral | 1      | 129.636, 120.541,
139.754 | 127.800, 121.868, 140.129 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| 83 | HIS      | O      | 998      | ZN      | O      | 20968      | Zn      | 12782 | N
| 4      | 2.03 | protein.sidechain | 8.91 | tetrahedral | 1      | 129.636, 120.541,
139.754 | 130.197, 121.005, 137.858 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| 90 | CYS      | O      | 998      | ZN      | O      | 20968      | Zn      | 12814 | S
| 4      | 2.35 | protein.sidechain | 8.91 | tetrahedral | 1      | 129.636, 120.541,
139.754 | 129.209, 118.235, 139.744 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+

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****Metal Complexes****

[illegible]

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****Metal Complexes****

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+-----+-----+-----+-----+-----+-----+-----+
+-+-----+-----+-----+-----+-----+-----+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG |
| RESCHAIN_LIG | METAL_IDX | METAL_TYPE | TARGET_IDX |
| TARGET_TYPE | COORDINATION | DIST | LOCATION      | RMS |
| GEOMETRY    | COMPLEXNUM | METALCOO          | TARGETCOO
|
```

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=====+=====+=====+=====+=====+=====+=====
=====+=====+=====+=====+=====+=====+=====
=====+=====+=====+=====+=====+=====+=====
=====+=====+=====+=====+=====+=====+=====+
| 74 | CYS | P | 998 | ZN | P | 20970 | Zn | 13577 | S
| 4 | 2.25 | protein.sidechain | 8.80 | tetrahedral | 1 | 110.199, 116.744,
140.268 | 108.485, 116.408, 141.691 |
+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+
| 77 | CYS | P | 998 | ZN | P | 20970 | Zn | 13603 | S
| 4 | 2.17 | protein.sidechain | 8.80 | tetrahedral | 1 | 110.199, 116.744,
140.268 | 111.984, 115.530, 140.503 |
+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+
| 83 | HIS | P | 998 | ZN | P | 20970 | Zn | 13656 | N
| 4 | 2.16 | protein.sidechain | 8.80 | tetrahedral | 1 | 110.199, 116.744,
140.268 | 109.414, 116.213, 138.332 |
+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+
| 90 | CYS | P | 998 | ZN | P | 20970 | Zn | 13688 | S
| 4 | 2.39 | protein.sidechain | 8.80 | tetrahedral | 1 | 110.199, 116.744,
140.268 | 110.673, 119.081, 140.093 |
+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+

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ZN:P:999 (ZN) - ION

Interacting chain(s): P

****Metal Complexes****

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+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG |
RESCHAIN_LIG | METAL_IDX | METAL_TYPE | TARGET_IDX |
TARGET_TYPE | COORDINATION | DIST | LOCATION | RMS |
GEOMETRY | COMPLEXNUM | METALCOO | TARGETCOO
|
=====+=====+=====+=====+=====+=====+=====
=====+=====+=====+=====+=====+=====+=====
=====+=====+=====+=====+=====+=====+=====
=====+=====+=====+=====+=====+=====+=====+
| 117 | CYS | P | 999 | ZN | P | 20971 | Zn | 13893 | S
| 4 | 2.35 | protein.sidechain | 5.77 | tetrahedral | 1 | 100.772, 135.856,
149.996 | 100.614, 135.152, 147.762 |
+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+
| 120 | CYS | P | 999 | ZN | P | 20971 | Zn | 13913 | S
| 4 | 2.42 | protein.sidechain | 5.77 | tetrahedral | 1 | 100.772, 135.856,
149.996 | 103.054, 135.433, 150.678 |
+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+

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-----+-----+-----+-----+-----+-----+-----+-----+-----
-----+-----+-----+-----+-----+-----+-----+-----+-----
| 128 | CYS | P | 999 | ZN | P | 20971 | Zn | 13974 | S
| 4 | 2.31 | protein.sidechain | 5.77 | tetrahedral | 1 | 100.772, 135.856,
149.996 | 99.272, 134.713, 151.324 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----
-----+-----+-----+-----+-----+-----+-----+-----+-----
-----+-----+-----+-----+-----+-----+-----+-----+-----
| 1057 | HOH | P | 999 | ZN | P | 20971 | Zn | 21987 | O
| 4 | 2.44 | water | 5.77 | tetrahedral | 1 | 100.772, 135.856, 149.996 |
100.179, 138.221, 149.893 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----
-----+-----+-----+-----+-----+-----+-----+-----+-----
-----+-----+-----+-----+-----+-----+-----+-----+-----

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ZN:Q:998 (ZN) - ION

Interacting chain(s): Q

Metal Complexes

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+-----+-----+-----+-----+-----+-----+-----+-----+-----
+-----+-----+-----+-----+-----+-----+-----+-----+-----
-----+-----+-----+-----+-----+-----+-----+-----+-----
-----+-----+-----+-----+-----+-----+-----+-----+-----
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG |
RESCHAIN_LIG | METAL_IDX | METAL_TYPE | TARGET_IDX |
TARGET_TYPE | COORDINATION | DIST | LOCATION | RMS |
GEOMETRY | COMPLEXNUM | METALCOO | TARGETCOO
|
+=====+=====+=====+=====+=====+=====+=====+=====+=====
=====+=====+=====+=====+=====+=====+=====+=====+=====
=====+=====+=====+=====+=====+=====+=====+=====+=====
=====+=====+=====+=====+=====+=====+=====+=====+=====+
| 74 | CYS | Q | 998 | ZN | Q | 20972 | Zn | 14451 | S
| 4 | 2.25 | protein.sidechain | 9.30 | tetrahedral | 1 | 109.028, 116.131,
105.044 | 107.224, 115.856, 103.725 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----
+-----+-----+-----+-----+-----+-----+-----+-----+-----
-----+-----+-----+-----+-----+-----+-----+-----+-----
-----+-----+-----+-----+-----+-----+-----+-----+-----
| 77 | CYS | Q | 998 | ZN | Q | 20972 | Zn | 14477 | S
| 4 | 2.15 | protein.sidechain | 9.30 | tetrahedral | 1 | 109.028, 116.131,
105.044 | 110.294, 117.827, 104.678 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----
+-----+-----+-----+-----+-----+-----+-----+-----+-----
-----+-----+-----+-----+-----+-----+-----+-----+-----
-----+-----+-----+-----+-----+-----+-----+-----+-----
| 83 | HIS | Q | 998 | ZN | Q | 20972 | Zn | 14530 | N
| 4 | 2.14 | protein.sidechain | 9.30 | tetrahedral | 1 | 109.028, 116.131,
105.044 | 108.402, 116.258, 107.084 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----
+-----+-----+-----+-----+-----+-----+-----+-----+-----
-----+-----+-----+-----+-----+-----+-----+-----+-----
-----+-----+-----+-----+-----+-----+-----+-----+-----
| 90 | CYS | Q | 998 | ZN | Q | 20972 | Zn | 14562 | S
| 4 | 2.37 | protein.sidechain | 9.30 | tetrahedral | 1 | 109.028, 116.131,
105.044 | 110.235, 114.096, 105.097 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----
+-----+-----+-----+-----+-----+-----+-----+-----+-----
-----+-----+-----+-----+-----+-----+-----+-----+-----
-----+-----+-----+-----+-----+-----+-----+-----+-----

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$$\dots + \dots + \dots$$

+++++ +++++ +++++ +++++ +++++ +++++

117	CVS	0	000	7N	0	20973	7n	14767	S
-----	-----	---	-----	----	---	-------	----	-------	---

105.957, 95.482, 97.423 |

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+.....+.....+.....

+.....

120	CYS	0	999	ZN	0	20973	Zn	14787	S
-----	-----	---	-----	----	---	-------	----	-------	---

108.130, 95.990, 94.422 |

128	CYS	0	999	ZN	0	20973	Zn	14848	S
-----	-----	---	-----	----	---	-------	----	-------	---

104.387, 95.509, 94.211 |

-----+-----+-----+-----+-----+-----+-----+-----

1080	HOH	0	999	ZN	0	20973	Zn	22068	0
------	-----	---	-----	----	---	-------	----	-------	---

106.543, 92.500, 95.341 |

-----+----- +----- +-----+----- +-----+-----+----- +-----

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RESNR | RESTYPE | RESCHAIN

TARGET	TYPE	COORDINATION	DIST	LOCATION	RMS
1	1	1	1	1	1
2	2	2	2	2	2
3	3	3	3	3	3
4	4	4	4	4	4
5	5	5	5	5	5
6	6	6	6	6	6
7	7	7	7	7	7
8	8	8	8	8	8
9	9	9	9	9	9
10	10	10	10	10	10
11	11	11	11	11	11
12	12	12	12	12	12
13	13	13	13	13	13
14	14	14	14	14	14
15	15	15	15	15	15
16	16	16	16	16	16
17	17	17	17	17	17
18	18	18	18	18	18
19	19	19	19	19	19
20	20	20	20	20	20
21	21	21	21	21	21
22	22	22	22	22	22
23	23	23	23	23	23
24	24	24	24	24	24
25	25	25	25	25	25
26	26	26	26	26	26
27	27	27	27	27	27
28	28	28	28	28	28
29	29	29	29	29	29
30	30	30	30	30	30
31	31	31	31	31	31
32	32	32	32	32	32
33	33	33	33	33	33
34	34	34	34	34	34
35	35	35	35	35	35
36	36	36	36	36	36
37	37	37	37	37	37
38	38	38	38	38	38
39	39	39	39	39	39
40	40	40	40	40	40
41	41	41	41	41	41
42	42	42	42	42	42
43	43	43	43	43	43
44	44	44	44	44	44
45	45	45	45	45	45
46	46	46	46	46	46
47	47	47	47	47	47
48	48	48	48	48	48
49	49	49	49	49	49
50	50	50	50	50	50
51	51	51	51	51	51
52	52	52	52	52	52
53	53	53	53	53	53
54	54	54	54	54	54
55	55	55	55	55	55
56	56	56	56	56	56
57	57	57	57	57	57
58	58	58	58	58	58
59	59	59	59	59	59
60	60	60	60	60	60
61	61	61	61	61	61
62	62	62	62	62	62
63	63	63	63	63	63
64	64	64	64	64	64
65	65	65	65	65	65
66	66	66	66	66	66
67	67	67	67	67	67
68	68	68	68	68	68
69	69	69	69	69	69
70	70	70	70	70	70
71	71	71	71	71	71
72	72	72	72	72	72
73	73	73	73	73	73
74	74	74	74	74	74
75	7				

GEOMETRY		COMPLEXNUM		METALCOO		TARGETCOO			
+=====+=====+=====+=====+=====+=====									
=====+=====+=====+=====+=====+=====									
=====+=====+=====+=====+=====+=====									
=====+=====+=====+=====+=====+=====									
74	CYS	R	998	ZN	R	20974	Zn	15325	S
4	2.23	protein.sidechain	12.36	tetrahedral	1	128.929, 119.490,			
104.510 130.660, 119.755, 103.136									
+-----+-----+-----+-----+-----+-----+-----+-----+-----									
---+-----+-----+-----+-----+-----+-----+-----+-----									
-----+-----+-----+-----+-----+-----+-----+-----+-----									
77	CYS	R	998	ZN	R	20974	Zn	15351	S
4	2.16	protein.sidechain	12.36	tetrahedral	1	128.929, 119.490,			
104.510 127.696, 117.736, 104.270									
+-----+-----+-----+-----+-----+-----+-----+-----+-----									
---+-----+-----+-----+-----+-----+-----+-----+-----									
-----+-----+-----+-----+-----+-----+-----+-----+-----									
83	HIS	R	998	ZN	R	20974	Zn	15404	N
4	2.05	protein.sidechain	12.36	tetrahedral	1	128.929, 119.490,			
104.510 129.708, 119.529, 106.403									
+-----+-----+-----+-----+-----+-----+-----+-----+-----									
---+-----+-----+-----+-----+-----+-----+-----+-----									
-----+-----+-----+-----+-----+-----+-----+-----+-----									
90	CYS	R	998	ZN	R	20974	Zn	15436	S
4	2.41	protein.sidechain	12.36	tetrahedral	1	128.929, 119.490,			
104.510 127.736, 121.579, 104.701									
+-----+-----+-----+-----+-----+-----+-----+-----+-----									
---+-----+-----+-----+-----+-----+-----+-----+-----									
-----+-----+-----+-----+-----+-----+-----+-----+-----									
-----+-----+-----+-----+-----+-----+-----+-----+-----									

ZN:R:999 (ZN) - ION

Interacting chain(s): R

Metal Complexes

RESNR	RESTYPE	RESCHAIN	RESNR_LIG	RESTYPE_LIG	RESCHAIN_LIG	METAL_IDX	METAL_TYPE	TARGET_IDX	TARGET_TYPE	COORDINATION	DIST	LOCATION	RMS	GEOMETRY	COMPLEXNUM	METALCOO	TARGETCOO
117	CYS	R	999	ZN	R	20975	Zn	15641	S	4	2.27	protein.sidechain	7.90	tetrahedral	1	131.222, 140.379, 93.770	131.639, 139.971, 95.963
120	CYS	R	999	ZN	R	20975	Zn	15661	S	4	2.34	protein.sidechain	7.90	tetrahedral	1	131.222, 140.379, 93.770	

```

| 129.354, 139.128, 93.109 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
---+-----+-----+-----+-----+-----+-----+-----+-----+
.....+-----+
| 128 | CYS | R | 999 | ZN | R | 20975 | Zn | 15722 | S
| 4 | 2.43 | protein.sidechain | 7.90 | tetrahedral | 1 | 131.222, 140.379, 93.770
| 133.161, 139.579, 92.548 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
---+-----+-----+-----+-----+-----+-----+-----+-----+
.....+-----+
| 1060 | HOH | R | 999 | ZN | R | 20975 | Zn | 22129 | O
| 4 | 2.50 | water | 7.90 | tetrahedral | 1 | 131.222, 140.379, 93.770 |
131.104, 142.874, 93.671 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
---+-----+-----+-----+-----+-----+-----+-----+-----+
.....+-----+

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ZN:S:998 (ZN) - ION

Interacting chain(s): S

****Metal Complexes****

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+-----+-----+-----+-----+-----+-----+-----+-----+-----+
---+-----+-----+-----+-----+-----+-----+-----+-----+
.....+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG |
RESCHAIN_LIG | METAL_IDX | METAL_TYPE | TARGET_IDX |
TARGET_TYPE | COORDINATION | DIST | LOCATION | RMS |
GEOMETRY | COMPLEXNUM | METALCOO | TARGETCOO
|
+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+
| 74 | CYS | S | 998 | ZN | S | 20976 | Zn | 16199 | S
| 4 | 2.22 | protein.sidechain | 8.53 | tetrahedral | 1 | 134.976, 131.177,
121.918 | 135.981, 133.156, 121.952 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
---+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+
| 77 | CYS | S | 998 | ZN | S | 20976 | Zn | 16225 | S
| 4 | 2.24 | protein.sidechain | 8.53 | tetrahedral | 1 | 134.976, 131.177,
121.918 | 135.663, 129.741, 123.500 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
---+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+
| 83 | HIS | S | 998 | ZN | S | 20976 | Zn | 16278 | N
| 4 | 2.13 | protein.sidechain | 8.53 | tetrahedral | 1 | 134.976, 131.177,
121.918 | 132.884, 131.459, 122.178 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
---+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+
| 90 | CYS | S | 998 | ZN | S | 20976 | Zn | 16310 | S
| 4 | 2.35 | protein.sidechain | 8.53 | tetrahedral | 1 | 134.976, 131.177,
121.918 | 134.979, 130.277, 119.747 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+

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-----+-----+-----+-----+-----+-----+-----+-----
-----+-----+-----+-----+-----+-----+-----+-----
-----+-----+-----+-----+-----+-----+-----+-----

ZN:S:999 (ZN) - ION

Interacting chain(s): S

Metal Complexes

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| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG |
RESCHAIN_LIG | METAL_IDX | METAL_TYPE | TARGET_IDX |
TARGET_TYPE | COORDINATION | DIST | LOCATION | RMS |
GEOMETRY | COMPLEXNUM | METALCOO | TARGETCOO
|

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=====+=====+=====+=====+=====+=====+=====+=====

=====+=====+=====+=====+=====+=====+=====+=====+
| 117 | CYS | S | 999 | ZN | S | 20977 | Zn | 16515 | S
| 4 | 2.38 | protein.sidechain | 4.61 | tetrahedral | 1 | 143.617, 138.404,
101.105 | 141.337, 138.263, 101.764 |

-----+-----+-----+-----+-----+-----+-----+-----
-----+-----+-----+-----+-----+-----+-----+-----
-----+-----+-----+-----+-----+-----+-----+-----

-----+-----+-----+-----+-----+-----+-----+-----
| 120 | CYS | S | 999 | ZN | S | 20977 | Zn | 16535 | S
| 4 | 2.28 | protein.sidechain | 4.61 | tetrahedral | 1 | 143.617, 138.404,
101.105 | 144.634, 136.496, 101.837 |

-----+-----+-----+-----+-----+-----+-----+-----
-----+-----+-----+-----+-----+-----+-----+-----
-----+-----+-----+-----+-----+-----+-----+-----

-----+-----+-----+-----+-----+-----+-----+-----
| 128 | CYS | S | 999 | ZN | S | 20977 | Zn | 16596 | S
| 4 | 2.31 | protein.sidechain | 4.61 | tetrahedral | 1 | 143.617, 138.404,
101.105 | 144.570, 140.293, 102.023 |

-----+-----+-----+-----+-----+-----+-----+-----
-----+-----+-----+-----+-----+-----+-----+-----
-----+-----+-----+-----+-----+-----+-----+-----

-----+-----+-----+-----+-----+-----+-----+-----
| 1066 | HOH | S | 999 | ZN | S | 20977 | Zn | 22196 | O
| 4 | 2.33 | water | 4.61 | tetrahedral | 1 | 143.617, 138.404, 101.105 |
143.560, 138.535, 98.778 |

-----+-----+-----+-----+-----+-----+-----+-----
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ZN:T:998 (ZN) - ION

Interacting chain(s): T

Metal Complexes

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	RESNR	RESTYPE	RESCHAIN	RESNR_LIG	RESTYPE_LIG	RESCHAIN_LIG	METAL_IDX	METAL_TYPE	TARGET_IDX	TARGET_TYPE	COORDINATION	DIST	LOCATION	RMS	GEOMETRY	COMPLEXNUM	METALCOO	TARGETCOO
74	CYS	T	998	ZN	T	20978	Zn	17073	S	4	2.30	protein.sidechain	10.44	tetrahedral	1	138.235, 111.330, 121.970	139.950, 109.793, 121.934	
77	CYS	T	998	ZN	T	20978	Zn	17099	S	4	2.19	protein.sidechain	10.44	tetrahedral	1	138.235, 111.330, 121.970	138.267, 112.866, 120.412	
83	HIS	T	998	ZN	T	20978	Zn	17152	N	4	2.11	protein.sidechain	10.44	tetrahedral	1	138.235, 111.330, 121.970	136.338, 110.441, 121.708	
90	CYS	T	998	ZN	T	20978	Zn	17184	S	4	2.28	protein.sidechain	10.44	tetrahedral	1	138.235, 111.330, 121.970	138.004, 112.132, 124.088	

ZN:T:999 (ZN) - ION

Interacting chain(s): T

****Metal Complexes****

	RESNR	RESTYPE	RESCHAIN	RESNR_LIG	RESTYPE_LIG	RESCHAIN_LIG	METAL_IDX	METAL_TYPE	TARGET_IDX	TARGET_TYPE	COORDINATION	DIST	LOCATION	RMS	GEOMETRY	COMPLEXNUM	METALCOO	TARGETCOO
117	CYS	T	999	ZN	T	20979	Zn	17389	S	4	2.90	protein.sidechain	40.43	tetrahedral	1	149.868, 107.463, 142.255	149.152, 105.577, 140.172	

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| 120 | CYS | T | 999 | ZN | T | 20979 | Zn | 17409 | S
| 4 | 2.51 | protein.sidechain | 40.43 | tetrahedral | 1 | 149.868, 107.463,
142.255 | 150.791, 109.676, 141.525 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+
| 128 | CYS | T | 999 | ZN | T | 20979 | Zn | 17470 | S
| 4 | 2.16 | protein.sidechain | 40.43 | tetrahedral | 1 | 149.868, 107.463,
142.255 | 150.971, 106.083, 141.014 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
-----+-----+-----+
| 1061 | HOH | T | 999 | ZN | T | 20979 | Zn | 22258 | O
| 4 | 2.42 | water | 40.43 | tetrahedral | 1 | 149.868, 107.463, 142.255 |
150.125, 106.995, 144.614 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
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ZN:U:998 (ZN) - ION

Interacting chain(s): U

Metal Complexes

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+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG |
| RESCHAIN_LIG | METAL_IDX | METAL_TYPE | TARGET_IDX |
| TARGET_TYPE | COORDINATION | DIST | LOCATION | RMS |
| GEOMETRY | COMPLEXNUM | METALCOO | TARGETCOO |
|
|=====+=====+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+=====+=====+
| 74 | CYS | U | 998 | ZN | U | 20980 | Zn | 17930 | S
| 4 | 2.30 | protein.sidechain | 10.30 | tetrahedral | 1 | 100.420, 124.979,
122.666 | 98.761, 126.573, 122.609 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+
| 77 | CYS | U | 998 | ZN | U | 20980 | Zn | 17956 | S
| 4 | 2.16 | protein.sidechain | 10.30 | tetrahedral | 1 | 100.420, 124.979,
122.666 | 100.290, 123.412, 121.192 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+
| 83 | HIS | U | 998 | ZN | U | 20980 | Zn | 18009 | N
| 4 | 2.11 | protein.sidechain | 10.30 | tetrahedral | 1 | 100.420, 124.979,
122.666 | 102.318, 125.840, 122.308 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+
| 90 | CYS | U | 998 | ZN | U | 20980 | Zn | 18041 | S

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4	2.33	protein.sidechain	10.30	tetrahedral	1	100.420, 124.979, 122.666	100.626, 124.324, 124.896
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ZN:U:999 (ZN) - ION

Interacting chain(s): U

****Metal Complexes****

RESNR	RESTYPE	RESCHAIN	RESNR_LIG	RESTYPE_LIG	RESCHAIN_LIG	METAL_IDX	METAL_TYPE	TARGET_IDX	TARGET_TYPE	COORDINATION	DIST	LOCATION	RMS	GEOMETRY	COMPLEXNUM	METALCOO	TARGETCOO
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117	CYS	U	999	ZN	U	20981	Zn	18246	S	4	2.35	protein.sidechain	6.31	tetrahedral	1	90.104, 129.765, 143.168	92.251, 130.347, 142.421
-----	-----	---	-----	----	---	-------	----	-------	---	---	------	-------------------	------	-------------	---	--------------------------	--------------------------

120	CYS	U	999	ZN	U	20981	Zn	18266	S	4	2.30	protein.sidechain	6.31	tetrahedral	1	90.104, 129.765, 143.168	89.646, 127.637, 142.437
-----	-----	---	-----	----	---	-------	----	-------	---	---	------	-------------------	------	-------------	---	--------------------------	--------------------------

128	CYS	U	999	ZN	U	20981	Zn	18327	S	4	2.39	protein.sidechain	6.31	tetrahedral	1	90.104, 129.765, 143.168	88.624, 131.340, 142.156
-----	-----	---	-----	----	---	-------	----	-------	---	---	------	-------------------	------	-------------	---	--------------------------	--------------------------

1076	HOH	U	999	ZN	U	20981	Zn	22335	O	4	2.45	water	6.31	tetrahedral	1	90.104, 129.765, 143.168	90.071, 130.143, 145.589
------	-----	---	-----	----	---	-------	----	-------	---	---	------	-------	------	-------------	---	--------------------------	--------------------------

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|-----|-----|-----|-----|-----|-----|
+-----+-----+-----+-----+-----+-----+
|-----|-----|-----|-----|-----|-----|
+-----+-----+-----+-----+-----+-----+

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ZN:V:998 (ZN) - ION

Interacting chain(s): V

****Metal Complexes****

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+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG |
| RESCHAIN_LIG | METAL_IDX | METAL_TYPE | TARGET_IDX |
| TARGET_TYPE | COORDINATION | DIST | LOCATION | RMS |
| GEOMETRY | COMPLEXNUM | METALCOO | TARGETCOO |
|
+=====+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+=====+
| 74 | CYS | V | 998 | ZN | V | 20982 | Zn | 18787 | S
| 4 | 2.23 | protein.sidechain | 12.12 | tetrahedral | 1 | 103.696, 105.231,
123.010 | 102.719, 103.222, 123.077 |
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
| 77 | CYS | V | 998 | ZN | V | 20982 | Zn | 18813 | S
| 4 | 2.17 | protein.sidechain | 12.12 | tetrahedral | 1 | 103.696, 105.231,
123.010 | 103.181, 106.725, 124.492 |
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
| 83 | HIS | V | 998 | ZN | V | 20982 | Zn | 18866 | N
| 4 | 2.05 | protein.sidechain | 12.12 | tetrahedral | 1 | 103.696, 105.231,
123.010 | 105.727, 105.025, 123.131 |
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
| 90 | CYS | V | 998 | ZN | V | 20982 | Zn | 18898 | S
| 4 | 2.43 | protein.sidechain | 12.12 | tetrahedral | 1 | 103.696, 105.231,
123.010 | 103.545, 105.952, 120.693 |
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+

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ZN:V:999 (ZN) - ION

Interacting chain(s): V

****Metal Complexes****

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+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG |
| RESCHAIN_LIG | METAL_IDX | METAL_TYPE | TARGET_IDX |
| TARGET_TYPE | COORDINATION | DIST | LOCATION | RMS |
| GEOMETRY | COMPLEXNUM | METALCOO | TARGETCOO |
|
+=====+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+=====+
| 120 | CYS | V | 999 | ZN | V | 20983 | Zn | 19123 | S
| 2 | 2.44 | protein.sidechain | 78.29 | linear | 1 | 94.028, 96.597, 100.772 |
94.153, 97.353, 103.087 |

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+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
| 1048 | HOH      | V      | 999      | ZN      | V      | 20983   | Zn      | 22384 | O
| 2      | 2.72 | water      | 78.29 | linear | 1      | 94.028, 96.597, 100.772 | 91.957,
94.843, 100.876 |
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+

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ZN:W:998 (ZN) - ION

Interacting chain(s): W

****Metal Complexes****

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+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG |
RESCHAIN_LIG | METAL_IDX | METAL_TYPE | TARGET_IDX |
TARGET_TYPE | COORDINATION | DIST | LOCATION      | RMS      |
GEOMETRY      | COMPLEXNUM | METALCOO      | TARGETCOO
|
+=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+
=====+=====+=====+=====+=====+=====+=====+
| 74  | CYS      | W      | 998      | ZN      | W      | 20984   | Zn      | 19661 | S
| 4      | 2.25 | protein.sidechain | 11.48 | tetrahedral | 1      | 116.892, 135.879,
132.151 | 116.772, 137.229, 133.942 |
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
| 77  | CYS      | W      | 998      | ZN      | W      | 20984   | Zn      | 19687 | S
| 4      | 2.23 | protein.sidechain | 11.48 | tetrahedral | 1      | 116.892, 135.879,
132.151 | 118.371, 136.362, 130.555 |
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
| 83  | HIS      | W      | 998      | ZN      | W      | 20984   | Zn      | 19740 | N
| 4      | 2.05 | protein.sidechain | 11.48 | tetrahedral | 1      | 116.892, 135.879,
132.151 | 117.342, 134.011, 132.879 |
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
| 90  | CYS      | W      | 998      | ZN      | W      | 20984   | Zn      | 19772 | S
| 4      | 2.41 | protein.sidechain | 11.48 | tetrahedral | 1      | 116.892, 135.879,
132.151 | 114.685, 135.366, 131.336 |
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+

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ZN:W:999 (ZN) - ION

Interacting chain(s): W

****Metal Complexes****

RESNR	RESTYPE	RESCHAIN	RESNR_LIG	RESTYPE_LIG	RESCHAIN_LIG	METAL_IDX	METAL_TYPE	TARGET_IDX	TARGET_TYPE	COORDINATION	DIST	LOCATION	RMS	GEOMETRY	COMPLEXNUM	METALCOO	TARGETCOO
117	CYS	W	999	ZN	W	20985	Zn	19977	S	4	2.33	protein.sidechain	5.86	tetrahedral	1	95.127, 142.425, 138.426	96.101, 140.347, 138.815
120	CYS	W	999	ZN	W	20985	Zn	19997	S	4	2.28	protein.sidechain	5.86	tetrahedral	1	95.127, 142.425, 138.426	95.711, 143.213, 136.367
128	CYS	W	999	ZN	W	20985	Zn	20058	S	4	2.28	protein.sidechain	5.86	tetrahedral	1	95.127, 142.425, 138.426	95.885, 143.804, 140.075
1044	HOH	W	999	ZN	W	20985	Zn	22429	O	4	2.43	water	5.86	tetrahedral	1	95.127, 142.425, 138.426	92.746, 142.071, 138.770

ZN:X:998 (ZN) - ION

Interacting chain(s): X

****Metal Complexes****

RESNR	RESTYPE	RESCHAIN	RESNR_LIG	RESTYPE_LIG	RESCHAIN_LIG	METAL_IDX	METAL_TYPE	TARGET_IDX	TARGET_TYPE	COORDINATION	DIST	LOCATION	RMS	GEOMETRY	COMPLEXNUM	METALCOO	TARGETCOO
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=====+=====+=====+=====+=====+=====+=====
| 74 | CYS | X | 998 | ZN | X | 20986 | Zn | 20535 | S
| 4 | 2.16 | protein.sidechain | 11.05 | tetrahedral | 1 | 116.196, 135.419,
112.137 | 115.850, 136.670, 110.415 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| 77 | CYS | X | 998 | ZN | X | 20986 | Zn | 20561 | S
| 4 | 2.27 | protein.sidechain | 11.05 | tetrahedral | 1 | 116.196, 135.419,
112.137 | 114.718, 135.449, 113.865 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| 83 | HIS | X | 998 | ZN | X | 20986 | Zn | 20614 | N
| 4 | 2.06 | protein.sidechain | 11.05 | tetrahedral | 1 | 116.196, 135.419,
112.137 | 116.172, 133.414, 111.659 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| 90 | CYS | X | 998 | ZN | X | 20986 | Zn | 20646 | S
| 4 | 2.35 | protein.sidechain | 11.05 | tetrahedral | 1 | 116.196, 135.419,
112.137 | 118.415, 135.739, 112.848 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+

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ZN:X:999 (ZN) - ION

Interacting chain(s): X

****Metal Complexes****

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+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| RESNR | RESTYPE | RESCHAIN | RESNR_LIG | RESTYPE_LIG |
RESCHAIN_LIG | METAL_IDX | METAL_TYPE | TARGET_IDX |
TARGET_TYPE | COORDINATION | DIST | LOCATION | RMS |
GEOMETRY | COMPLEXNUM | METALCOO | TARGETCOO
|
+=====+=====+=====+=====+=====+=====+=====
=====+=====+=====+=====+=====+=====+=====
=====+=====+=====+=====+=====+=====+=====
=====+=====+=====+=====+=====+=====+=====
| 117 | CYS | X | 999 | ZN | X | 20987 | Zn | 20851 | S
| 4 | 1.99 | protein.sidechain | 68.10 | tetrahedral | 1 | 134.607, 148.465,
105.131 | 133.246, 147.084, 104.692 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
| 120 | CYS | X | 999 | ZN | X | 20987 | Zn | 20871 | S
| 4 | 2.07 | protein.sidechain | 68.10 | tetrahedral | 1 | 134.607, 148.465,
105.131 | 132.824, 148.531, 106.174 |
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+
+-----+-----+-----+-----+-----+-----+-----+-----+-----+

```

| 128 | CYS | X | 999 | ZN | X | 20987 | Zn | 20932 | S
| 4 | 1.74 | protein.sidechain | 68.10 | tetrahedral | 1 | 134.607, 148.465,
105.131 | 133.246, 149.141, 104.288 |

+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----
---+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----

-----+-----+
| 1064 | HOH | X | 999 | ZN | X | 20987 | Zn | 22494 | O
| 4 | 2.30 | water | 68.10 | tetrahedral | 1 | 134.607, 148.465, 105.131 |
136.830, 148.832, 104.678 |

+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----
---+-----+-----+-----+-----+-----+-----+-----+-----+-----+-----

-----+-----+-----+-----+-----+
-----+-----+-----+-----+-----+-----+-----+-----+-----+-----

\$Leader_Info 2 {

Num_Members = 47
Total_Energy = 0.920
vdW = -2.068
Coulomb = -9.214
Internal = 12.203
rmsd = 10.703

}

\$Leader_Info 3 {

Num_Members = 47
Total_Energy = 1.118
vdW = -6.320
Coulomb = -4.765
Internal = 12.203
rmsd = 2.300

}

\$Leader_Info 4 {

Num_Members = 41
Total_Energy = 1.190
vdW = -6.775
Coulomb = -4.238
Internal = 12.203
rmsd = 3.039

}

\$Leader_Info 5 {

Num_Members = 44
Total_Energy = 1.613
vdW = -3.033
Coulomb = -7.556
Internal = 12.203
rmsd = 9.734

}

\$Leader_Info 6 {

Num_Members = 40
Total_Energy = 1.653
vdW = -3.268
Coulomb = -7.281
Internal = 12.203
rmsd = 9.324

}

\$Leader_Info 7 {

Num_Members = 46
Total_Energy = 1.675

```

        vdW = -6.062
        Coulomb = -4.466
        Internal = 12.203
        rmsd = 2.382
    }

$Leader_Info 8 {

        Num_Members = 42
        Total_Energy = 1.935
        vdW = -5.434
        Coulomb = -4.834
        Internal = 12.203
        rmsd = 1.449
    }

$Leader_Info 9 {

        Num_Members = 54
        Total_Energy = 2.091
        vdW = -3.880
        Coulomb = -6.231
        Internal = 12.203
        rmsd = 3.179
    }

$Leader_Info 10 {

        Num_Members = 37
        Total_Energy = 2.237
        vdW = -5.380
        Coulomb = -4.586
        Internal = 12.203
        rmsd = 3.188
    }

}


```

Figure6d. Comparative Docking Cluster Analysis between the Remdesivir and the Rocustyrna small molecules when docked onto the SARS-COV-2 protein targets, (pdb:7bv2). \$Number_of_Clusters = 10

\$Seed = -1985

```

$Leader_Info 1 {

        Num_Members = 77
        Total_Energy = -0.940
    }

```

```
vdW = -6.048
Coulomb = -7.095
Internal = 12.203
rmsd = 0.000

}

$Leader_Info 2 {

  Num_Members = 48
  Total_Energy = 0.889
  vdW = -1.962
  Coulomb = -9.351
  Internal = 12.203
  rmsd = 10.576

}

$Leader_Info 3 {

  Num_Members = 46
  Total_Energy = 1.079
  vdW = -6.312
  Coulomb = -4.811
  Internal = 12.203
  rmsd = 2.327

}

$Leader_Info 4 {

  Num_Members = 43
  Total_Energy = 1.251
  vdW = -6.762
  Coulomb = -4.189
  Internal = 12.203
  rmsd = 3.027

}

$Leader_Info 5 {

  Num_Members = 33
  Total_Energy = 1.326
```



```
vdW = -5.434
Coulomb = -5.442
Internal = 12.203
rmsd = 1.044

}

$Leader_Info 6 {

  Num_Members = 45
  Total_Energy = 1.546
  vdW = -2.813
  Coulomb = -7.844
  Internal = 12.203
  rmsd = 9.608

}

$Leader_Info 7 {

  Num_Members = 52
  Total_Energy = 1.660
  vdW = -3.285
  Coulomb = -7.258
  Internal = 12.203
  rmsd = 9.181

}

$Leader_Info 8 {

  Num_Members = 49
  Total_Energy = 1.673
  vdW = -5.928
  Coulomb = -4.601
  Internal = 12.203
  rmsd = 2.339

}

$Leader_Info 9 {

  Num_Members = 47
  Total_Energy = 2.034
```

```

vdW = -3.901
Coulomb = -6.267
Internal = 12.203
rmsd = 3.094

}

$Leader_Info 10 {

    Num_Members = 40
    Total_Energy = 2.103
    vdW = -5.122
    Coulomb = -4.977
    Internal = 12.203
    rmsd = 3.183

}

```

	Compound	Energy	V-M LYS 551	V-S LYS 551	V-S ARG 553	V-S ASP 618	V-M TYR 619	V-M PRO 620
1	☒ cav7bv2_POP-Rocustyrna-0.pdb	-66,7	☒ -4,7	☒ -10,5	☒ -4,8	☒ -6,7	☒ -5,1	☒ -6,3
2	☐ cav7bv2_POP-Remdesivir-0.pdb	42,1	☐ -0,1	☐ -0,2	25,1	0	0	0

Figure6e. Comparative Docking Enegy Analysis between the Remdesivir and the Roccustyrna small molecules when docked onto the SARS-COV-2 protein targets, (pdb:7bv2). \$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

}

\$Leader_Info 2 {

Num_Members = 50

Total_Energy = 0.906

vdW = -1.861

Coulomb = -9.436

Internal = 12.203

rmsd = 10.591

}

\$Leader_Info 3 {

Num_Members = 45

Total_Energy = 0.979

vdW = -6.333

Coulomb = -4.890

Internal = 12.203

rmsd = 2.336

}

\$Leader_Info 4 {

Num_Members = 44

Total_Energy = 1.216

vdW = -6.799

Coulomb = -4.187

Internal = 12.203

rmsd = 3.044

}

\$Leader_Info 5 {

Num_Members = 38

Total_Energy = 1.558

vdW = -2.867

Coulomb = -7.777

Internal = 12.203

rmsd = 9.638

}

\$Leader_Info 6 {

Num_Members = 51

Total_Energy = 1.667

vdW = -3.301

Coulomb = -7.235

Internal = 12.203

rmsd = 9.202

}

\$Leader_Info 7 {

Num_Members = 48

Total_Energy = 1.708

vdW = -5.906

Coulomb = -4.588

Internal = 12.203

rmsd = 2.351

}

\$Leader_Info 8 {

Num_Members = 28

Total_Energy = 2.054

vdW = -5.236

Coulomb = -4.912

Internal = 12.203

rmsd = 1.304

}

\$Leader_Info 9 {

Num_Members = 52

Total_Energy = 2.059

vdW = -4.013

Coulomb = -6.131

Internal = 12.203

rmsd = 3.035

}

\$Leader_Info 10 {

Num_Members = 43

Total_Energy = 2.242

vdW = -5.048

Coulomb = -4.913

Internal = 12.203

rmsd = 3.188

}

cav7bv2_POP. pd b:ClusterID	T op of cl us t er	Comp ou nd	E n e r g y	V- M- L YS - 55 1	V - S- L Y S - 55 1	V - S- A R G - 5 5 3	V - S- A S P - 61 8	V- M T Y R - 61 9	V- M P R O - 620
1	1	cav7bv 2 _POP- Roccust y rna - 0.p db	- 6 6. 7	- 4.7 15 16	- 1 0. 4 84 2	- 4. 7 9 99 53 8	- 6. 6 5 53 8	- 5. 1 33 9	- 6. 2 8 532
1	0.00 0 000	cav7bv 2 _POP- Remd esi vir- 0.pdb	42. 1	- 0.1 04 885	- 0. 1 9 98 6	25. 0 57 5	0 0 0	0 0 0	0 0 0

Table2b. Comparative Docking Energy Numerical Score Analysis between the Remdesivir and the Roccustyrna small molecules when docked onto the SARS-COV-2 protein targets, (pdb:7bv2).

This small molecule prototype was obtained directly from the solution of the $D[-(k^{(-4 - k^4 n^{33835} N^2) n^{33834} N^{213})/33834432, n] \text{ LocG}(S1) \text{ CSG}, k(S1) = \text{TrigToExp}[\text{ArcSin}[x[\tau] x'[22 \tau]^{\wedge} 244 y'[\tau]^{\wedge} \text{ArcSin}[242424222242424 \text{ Sin}[X] x[\tau]^{\wedge} 22]]] \text{ VectkG}[G] = \text{Rep}(\text{Dk}(C[G])) = \text{Z}(\text{Vectk}[G])$ equation (1) into the $(k^{(-8 - k^4 n^{33835} N^2) N^{211})/(1144788006720 \text{ Log}[3d N = 2 \text{ CS } k])$ (equation 2,3,4,14) by a procedure akin to geometric quantization as derived by a first phase solution was taken as the $13 (a+l) 3d N = 2 \text{ CS } ta+l-1A\Lambda[A\Lambda\Lambda] 2zEG k (\text{mod} 2\pi)$ equation (5) determined fragmentation. (36,37,39) and larger groups are prioritized over smaller chemical patterns with potential antiviral properties of the RoccustyrnaTM 's small molecule (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 PDB generated (Figure1b) patterns.

Roccustyrna ligand Protein targets

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

molecule's molecular force field parameterizations. (2,31-40) The preparations of the steps to be used for diagonal force field for modeling such as modifying the protonation state of all the keeping amino acid residues, to parameterize a simple group of knots and atoms by adding metal complexes, hydrogen atoms and freezing rotatable bonds was done interactively for a variety of all-Roccustyrna atoms in the publically available web servers and performed automatically by the programs cited without the need for intervention. (3,15,16,17) The search docking space to rapidly simulate the Roccustyrna's molecular systems and the configuration of the new molecule's grid box were interactively set in the KNIME designed BiogenetoligandoroITM pipeline which were represented as a grid box and the docking potentials are stored at the best grid points for the description of the Roccustyrna's molecular energetic and structures through the parameters of the center of coordinates, size of the grid and discretization (i.e., the spacing between the grid points). (5,13,29,31) The initial population for the rotational, and translational, was randomly generated within the conformational degrees and grid box using random values of freedom of the Roccustyrna ligand. (15,16,17,38) For each SARS-CoV-2 therapeutic target DockThor-VS default parameters were uploaded as a recommended set of parameters for the grid box (i.e., center and grid sizes) which can be used or modified according to the objectives of this docking experiment which was specially designed to deal with highly flexible ligands such as the Roccustyrna small molecule. (15,29,31) In this strategy, a replacement ligand based method was introduced by using a low mass phase phenotypic steady-state and crowding-based protocol and a multiple genetic parental algorithm 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 BiogenetoligandoroITM) is 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 SDumont 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 BiogenetoligandoroITM. The top docking energy-poses of each Roccustyrna-Protein complex were selected as top hit representatives of cluster energetic representatives to be made available in the homogeneity results analysis and Chern-Simons pharmacophoric fragmentation section (27,28). The binding affinity prediction and total energy ranking with the linear protein model and untailored for specific ligand interacted protein classes, of the Roccustyrna small molecule was generated by utilizing the DockTScoreGenLscoring function as a set of empirical scoring functions. BiogenetoligandoroITM 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, Roccustyrna's 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,3fqj, 2ghv,6yb7) (3,4,35,39) and the docking outputs were generated with NGL, a WebGL-based library for intra-molecular visualization.

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

The drug likeliness and bioactivity of the Roccustyrna small molecule were initially analyzed utilizing the Molinspiration server (<http://www.molinspiration.com>). (30,31) By using the Molinspiration web-tool, a cheminformatics multi-tasking software we calculated the Roccustyrna 's molecular modeling docking energy properties as well as drug likeness and bioactivity prediction of our prototype ligand (Mabkhot et al., 2016). (40,41) In this section, the Molinspiration-based drug-likeness analysis web platform was incorporated to predict the Roccustyrna 's two important factors, including the polar surface area (PSA), and lipophilicity level (log P) directly associated with the pharmacokinetic properties (PK) of the same lead structure (Beetge et al., 2000). (31,40) Then, by uploading the Roccustyrna 's smiles in the Molinspiration-based bioactivity analysis web server, we calculated the bioactivity score of this ligand through the systemic examinationion 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 Roccustyrna 's 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 Roccustyrna 's small molecule to penetrate the blood-brain barrier and its metabolism is of crucial importance to evaluate the risk of exposure to toxins and was evaluated by the MATE1, CYP, and OATP1B3 -OATP1B1 testing models. The Excretion of the Roccustyrna ligand was estimated by applying the advanced matched molecular pair analysis (MMPA), based on the renal OCT substrate and the toxicity which was then predicted accordingly on the Human Ether-a-go-go-related gene inhibition, mutagenic status, carcinogenic status, and acute oral toxicity default parameters (30,31,40,41).

Results

In silico Prediction of the Roccustyrna ADMET Properties and Bioactivity Score

To predict important molecular properties such as logP, polar surface area, drug-likeness and bioactivity of our new prototype and small sized Roccustyrna ligand (1S,2R,3S)- 2-([[(1S,2S,4S,5R)-4- ethenyl-4- sulfonylbicyclo (1S,2R,3S)-2-([[(1S,2S, 4S,5R)-4- ethenyl-4- sulfonylbicyclo[3.2.0]heptan-2-yl]oxy)amino)- 3-[(2R,5R)-5-(2-methyl-6-methylidene-6,9-dihydro-3H-purin-9-yl)-3-methylideneoxolan-2-yl]phosphirane-1-carbonitrile[3.2.0]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 (Table1c).

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 the (pdb:1xak) (Figure4a) 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, (Tables1a,1b,1c,2a,2b) The Roccustyrna chemical structure interacted into the binding sites of the protein targets (pdb:6w9c), (Figure4b),(Figure7e) 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. It 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, 70.551Kcal/mol . Our new QMMM designed small molecule named Roccustyrna 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 Roccustyrna 's active pharmacophoric site of the (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 Roccustyrna 's active pharmacophoric site of the dihydro-3H-purin-9-yl)-3- hydroxyoxolan generated a docking effect which was involved in the generation of hydrogen bonds when docked into the binding cavities of the amino acid of the 143 GLY A 6 010 C with the docking energy values of the 1.93, 2.8, 145.29, 1105, 2411, -8.911, 17.849, 65.703 -8.918, 17.918, 62.905 Kcal/mol. 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, 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 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. (Figure5b). D10-C-1099 DMS:A:402 (DMS) binding sites were also constructed when RoccustyrnaTM' s pharmacophoric elements 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' s 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 bondings when docked inside the DMS A 5.49 binding cavities of the amino acid of the 295 ASP A 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 bondings 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. (Figure5d). Hydrophobic Interactions were simultaneously generated by the Roccustyrna chemical residues when docked in the (pdb:6lu7)inside the D10-H-1099. X77:A:401 (X77) protein 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. (Figure7f). The (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-azaphosphoridin-1-yl)ium. 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 (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. (Figure7d). CoMFA contour map analysis of electrostatic regions around the Roccustyrna 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 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. (Figure6a)

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 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 bondings 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. (Figure6b). 999 ZN D 20947 Zn , ZN:A:998 (ZN) and 998 ZN A 20940 Zn 470 S Metal Complexes were constructed into the 02J (5-Methylisoxazole-3-carboxylic acid) PJE-C-56LU7 Roccustyrna's (1Z)-2-[(2S,3S,5R)-5-(2-amino-6-oxo-6,9-dihydro-1H-purin-9-yl-4-yl)oxy]imino)-1lambda5,2lambda5-azaphosphiridin-1-ylum. binding sites inside the 117 CYS D, 74 CYS A amino acids tetrahedral side chains with the docking energy values of the (-1103.746, -101.848, -13.968, -103.306, -102.613, -16.001 -1118.874, -104.964, -32.313 -118.938, -103.573, -30.6090Kcal/mol/A generated indicating to us 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 Roccustyrna's pharmacophoric (1Z)-2-[(2S,3S,5R)-5-(2-amino-6-2-yl)methylidene]-2-cyano-1-[(2S,4R,5R)-2-methyl-2-(methylamino)-1,6-diazabicyclo(3.2.0)heptan-4-yl)oxy]imino)-1lambda5,2lambda5-azaphosphiridin-1-ylum. 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 (Figure5c). (Figure6c). In this drug designing project the electrostatic regions around the RoccustyrnaTM's 3-hydroxyoxolan-2-yl)methylidene}-2-cyano-1-[(2S,4R,5R)-2-methyl-2-(methylamino)-1,6-diazabicyclo(3.2.0)heptan-4-yl)oxy]imino)-1lambda5,2lambda5-azaphosphiridin-1-ylum. substrate targets the SARS-COV-2 protein targets, (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, (Figure5a) showing that RoccustyrnaTM's binding site(s) inside the (pdb:6lu7) binding domains of the 02J:C:1 (02J) regions while co-generating Hydrophobic Interactions and Hydrogen Bonds against the coupled atoms of the Nam 2411 O3 inside the cavities of the crucial entering amino acids of the 25 THR A 6 010 C and 143 GLY A 6 010 C with the docking energy values of the (-3.73, -2415, -179, -7.156, 21.406, -66.898, -8.709, -22.779, -70.002, -26, -81, -2415, -186, -7.156, -21.406, -66.898, -6.155, -24.392, -64.757, -1.93, -2.80, -145, -29, -1105, -8.911, 17.849, -65.703, -8.918, -17.918, -62.905.)Kcal/mol/A respectively. 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 $= \gamma B \cdot (\hat{S}^1 + \hat{S}^2) + \hat{I}^1 \cdot A \cdot \hat{S}^2$, $\hat{S}^i = (\sigma_x, \sigma_y, \sigma_z) \hat{I}^i \rho_s(t) = \text{Tr}(\hat{U}(t) \rho_s(0) \hat{U}^\dagger(t))$, $\rho_s(0) = 1/2P(t') = d\Delta M(t') / \Delta M = f(t') dt'$, $\rho_s^- = \int_{-\infty}^0 f(t') \rho_s(t') dt' = \int_0^\infty f(t) \rho_s(t) dt$, $\int_{-\infty}^0 f(t') dt' = \int_0^\infty f(t) dt = 1$ $\rho_s^- s \rho_s^- s \rho_s^- s \rho_s^-$ equation (4)

$s(\pi/2) \rho_s^- s \rho_s(0) \rho_s^- s QFI \approx \sum_i=0^1 \text{Re}(\rho_{i12}) 2(1 \rho_{i11} + 1 \rho_{i22}) + (\rho_{i11} - \rho_{i22}) 2 \rho_{i11} + \rho_{i22}, \rho_{1ij} = \langle \phi_i | \langle 1 \rho_s(0) | \phi_j \rangle - 1 \rangle \rho_{0ij} = \langle \phi_i | \langle 0 \rho_s(0) | \phi_j \rangle - 0 \rangle - 1 \rangle H1 = \gamma B \cdot \hat{S}^1 \text{Re}(\rho_{i12}) \rho_{i12} \rho_s(0) \rho_s^- s S = 12(\langle \rangle - 01 \rangle) 30\% \rho_s(0) \rho_s^- s = H \otimes m 0 \rangle \otimes m = H \otimes H \otimes \dots \otimes H 00 \dots 0 = 12(0+1) \otimes 12(0+1) \otimes \dots \otimes 12(0+) = 12m(00 \dots 0 + 00 \dots 1 \rangle) + \dots + (11 \dots 1)$ equation (5).

Figure7a. CoMFA contour map of electrostatic regions around Roccustyrna chemical structure. Contact residues of the Roccustyrna small molecule when docked onto the SARS COV-2 protein targets, (pdb:3fqq). (green, favored; yellow; disfavored) around the Roccustyrna chemical structure. Blue regions are favored by positively charged groups and red regions favored by negatively charged groups within the sequence of the amino acid of the V-S-HIS-159, V-S-ARG-160, V-S-ARG-112 V-M-GLU-148 V-M-PHE-150, V-S-PHE-150, V-S-HIS-159, V-M-TYR-161 with the docking energy values of the -101, and binding free energies of the docking values of the 9-14.0762, - 5.11094, -7.98447, -4.17314, - 4.43549, -9.66939, -9.42926, -7.30085) $K\psi\alpha\lambda/\mu\text{ol}/\text{A}$.

\$Number_of_Clusters = 10
\$Seed = -1985

\$Leader_Info 1 {

Num_Members = 103
Total_Energy = -0.801
vdW = -6.010
Coulomb = -6.993
Internal = 12.203
rmsd = 0.000

}

\$Leader_Info 2 {

```
Num_Members = 45
Total_Energy = 0.879
vdW = -1.810
Coulomb = -9.514
Internal = 12.203
rmsd = 10.561

}
```

```
$Leader_Info 3 {

Num_Members = 48
Total_Energy = 1.109
vdW = -6.390
Coulomb = -4.703
Internal = 12.203
rmsd = 2.301

}
```

```
$Leader_Info 4 {

Num_Members = 38
Total_Energy = 1.389
vdW = -6.839
Coulomb = -3.975
Internal = 12.203
rmsd = 3.014

}
```

```
$Leader_Info 5 {

Num_Members = 18
Total_Energy = 1.508
vdW = -5.388
Coulomb = -5.306
Internal = 12.203
rmsd = 1.178

}
```

```
$Leader_Info 6 {

Num_Members = 38
Total_Energy = 1.584
vdW = -2.959
Coulomb = -7.659
Internal = 12.203

}
```

```
    rmsd = 9.553
}

$Leader_Info 7 {

    Num_Members = 48
    Total_Energy = 1.654
    vdW = -3.273
    Coulomb = -7.276
    Internal = 12.203
    rmsd = 9.126

}

$Leader_Info 8 {

    Num_Members = 46
    Total_Energy = 1.688
    vdW = -5.961
    Coulomb = -4.553
    Internal = 12.203
    rmsd = 2.366

}

$Leader_Info 9 {

    Num_Members = 17
    Total_Energy = 1.726
    vdW = -5.419
    Coulomb = -5.058
    Internal = 12.203
    rmsd = 1.243

}

$Leader_Info 10 {

    Num_Members = 46
    Total_Energy = 2.045
    vdW = -3.992
    Coulomb = -6.165
    Internal = 12.203
    rmsd = 3.005

}
```

(Figure7a) 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, (pdb:3fqg) hits the positively charged groups and red regions favored by negatively charged groups within the binding domains sequence 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. (Figure7b) 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 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, (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.

Figure7c. CoMFA contour map of electrostatic regions around Roccustyrna chemical structure. Contact residues of the Roccustyrna small molecule when docked onto the SARS-COV-2 protein targets, (pdb:2ghv). (green, favored; yellow; disfavored) around the Roccustyrna chemical structure. Blue regions are favored by positively charged groups and red regions favored by negatively charged groups within the sequence of the amino acid of the H-M-ASN-330, H-S-ASN-330, H-S-TYR-356, H-M-ASN-424, V-M-ASN-330, 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/A respectively.

\$Number_of_Clusters = 10

\$Seed = -1985

\$Leader_Info 1 {

Num_Members = 104
Total_Energy = -1.003
vdW = -6.070
Coulomb = -7.136
Internal = 12.203
rmsd = 0.000

}

\$Leader_Info 2 {

```
    Num_Members = 40
    Total_Energy = 1.099
    vdW = -6.281
    Coulomb = -4.822
    Internal = 12.203
    rmsd = 2.318
}
```

```
$Leader_Info 3 {

    Num_Members = 42
    Total_Energy = 1.181
    vdW = -6.789
    Coulomb = -4.233
    Internal = 12.203
    rmsd = 3.044

}
```

```
$Leader_Info 4 {

    Num_Members = 42
    Total_Energy = 1.564
    vdW = -5.419
    Coulomb = -5.220
    Internal = 12.203
    rmsd = 1.218

}
```

```
$Leader_Info 5 {

    Num_Members = 53
    Total_Energy = 1.673
    vdW = -6.045
    Coulomb = -4.484
    Internal = 12.203
    rmsd = 2.374

}
```

```
$Leader_Info 6 {

    Num_Members = 41
    Total_Energy = 2.046
    vdW = -3.774
    Coulomb = -6.382
    Internal = 12.203
    rmsd = 3.299

}
```

```
$Leader_Info 7 {
```



```

Num_Members = 12
Total_Energy = 2.186
vdW = -4.637
Coulomb = -5.380
Internal = 12.203
rmsd = 1.450

```

```

}

```

```

$Leader_Info 8 {

```

```

    Num_Members = 46
    Total_Energy = 2.231
    vdW = -5.016
    Coulomb = -4.955
    Internal = 12.203
    rmsd = 3.137

```

```

}

```

```

$Leader_Info 9 {

```

```

    Num_Members = 3
    Total_Energy = 2.273
    vdW = -5.032
    Coulomb = -4.898
    Internal = 12.203
    rmsd = 1.637

```

```

}

```

```

$Leader_Info 10 {

```

```

    Num_Members = 10
    Total_Energy = 2.469
    vdW = -4.273
    Coulomb = -5.461
    Internal = 12.203
    rmsd = 2.861

```

```

}

```

(Figure7c) 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, (pdb:2ghv). (green, favored; yellow; disfavored) around the entire Roccustyrna chemical structure regions has shown that our innovative drug design generated negatively charged groups within the sequence of the amino acid of the H-M-ASN-33, H-S-ASN-33, H-S-TYR-356, H-M-ASN-424, V-M-ASN-33, V-M-ALA-331, V-M-THR-332, V-S-THR-332, V-S-TYR-356, V-S-TRP-423, V-S-ILE-428, V-S-ARG-495 with the docking energy values of the -104.7 and -3.45708, -3.5, -3.97711, -3.5, -5.33228, -6.79753, -7.9376, -6.69969, -12.2528, -7.66989, -8.15072, -7.00332Kcal/mol respectively.

Figure7b. CoMFA contour map of electrostatic regions around Roccustyrna chemical structure. Contact residues of the Roccustyrna small molecule when docked onto the SARS-COV-2 protein targets, (pdb:6xs6). (green, favored; yellow; disfavored) around the Roccustyrna chemical structure. Blue regions are favored by positively charged groups and red regions favored by negatively charged groups within the sequence of the amino acid of 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/A respectively.

\$Number_of_Clusters = 10

\$Seed = -1985

\$Leader_Info 1 {

Num_Members = 107

Total_Energy = -0.917

vdW = -6.044

Coulomb = -7.075

Internal = 12.203

rmsd = 0.000

}

\$Leader_Info 2 {

Num_Members = 48
Total_Energy = 0.877
vdW = -1.827
Coulomb = -9.498
Internal = 12.203
rmsd = 10.632

}

\$Leader_Info 3 {

Num_Members = 47
Total_Energy = 1.090
vdW = -6.373
Coulomb = -4.739
Internal = 12.203
rmsd = 2.301

}

\$Leader_Info 4 {

Num_Members = 39
Total_Energy = 1.194
vdW = -6.823
Coulomb = -4.185
Internal = 12.203
rmsd = 3.048

}

\$Leader_Info 5 {

Num_Members = 42
Total_Energy = 1.550
vdW = -2.770
Coulomb = -7.882
Internal = 12.203
rmsd = 9.638

}

\$Leader_Info 6 {

```
    Num_Members = 47
    Total_Energy = 1.682
    vdW = -3.406
    Coulomb = -7.114
    Internal = 12.203
    rmsd = 9.190
}
```

```
$Leader_Info 7 {

    Num_Members = 51
    Total_Energy = 1.866
    vdW = -5.907
    Coulomb = -4.430
    Internal = 12.203
    rmsd = 2.383

}
```

```
$Leader_Info 8 {

    Num_Members = 42
    Total_Energy = 1.942
    vdW = -5.523
    Coulomb = -4.738
    Internal = 12.203
    rmsd = 1.422

}
```

```
$Leader_Info 9 {

    Num_Members = 48
    Total_Energy = 2.080
    vdW = -3.988
    Coulomb = -6.134
    Internal = 12.203
    rmsd = 3.060

}
```

```
$Leader_Info 10 {

    Num_Members = 35
    Total_Energy = 2.188
    vdW = -5.268
    Coulomb = -4.746
```

Internal = 12.203

rmsd = 3.183

}

Figure7d. CoMFA contour map of electrostatic regions around Roccustyrna chemical structure. Contact residues of the Roccustyrna small molecule when docked onto the SARS-COV-2 protein targets, (pdb:2zu5). (green, favored; yellow; disfavored) around the Roccustyrna chemical structure. Blue regions are favored by positively charged groups and red regions favored by negatively charged groups within the sequence of the amino acid of 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/A respectively.

\$Number_of_Clusters = 10

\$Seed = -1985

\$Leader_Info 1 {

Num_Members = 65

Total_Energy = -0.790
vdW = -5.994
Coulomb = -6.999
Internal = 12.203
rmsd = 0.000

}

\$Leader_Info 2 {

Num_Members = 51
Total_Energy = 1.009
vdW = -6.343
Coulomb = -4.851
Internal = 12.203
rmsd = 2.284

}

\$Leader_Info 3 {

Num_Members = 49
Total_Energy = 1.022
vdW = -0.908
Coulomb = -10.272
Internal = 12.203
rmsd = 10.740

}

\$Leader_Info 4 {

Num_Members = 57
Total_Energy = 1.212
vdW = -5.371
Coulomb = -5.620
Internal = 12.203
rmsd = 1.136

}

\$Leader_Info 5 {

Num_Members = 42
Total_Energy = 1.254
vdW = -6.875
Coulomb = -4.073
Internal = 12.203
rmsd = 3.047

}

\$Leader_Info 6 {

Num_Members = 43
Total_Energy = 1.544
vdW = -2.796
Coulomb = -7.862
Internal = 12.203
rmsd = 9.874

}

\$Leader_Info 7 {

Num_Members = 50
Total_Energy = 1.659
vdW = -3.314
Coulomb = -7.230
Internal = 12.203
rmsd = 9.438

}

\$Leader_Info 8 {

Num_Members = 54
Total_Energy = 1.666
vdW = -6.018
Coulomb = -4.518
Internal = 12.203
rmsd = 2.367

}

\$Leader_Info 9 {

Num_Members = 48
Total_Energy = 2.057
vdW = -3.931
Coulomb = -6.215
Internal = 12.203
rmsd = 3.183

}

\$Leader_Info 10 {

Num_Members = 38
Total_Energy = 2.195
vdW = -5.185
Coulomb = -4.823
Internal = 12.203
rmsd = 3.068

}

In addition, 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, (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. (Figure7d)

Figure7e. CoMFA contour map of electrostatic regions around Roccustyrna chemical structure. Contact residues of the Roccustyrna small molecule when docked onto the SARS- COV-2 protein targets, (pdb:6w9c). (green, favored; yellow; disfavored) around the Roccustyrna chemical structure. Blue regions are favored by positively charged groups and red regions favored by negatively charged groups within the sequence of the amino acid of 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 free energy values of the (-83.9, -4.21999, -12.6164, -7.60372,-6.69528, - 5.89416, -6.40663, -5.51621, -7.99273) Kcal/mol/A.

\$Number_of_Clusters = 10

\$Seed = -1985

\$Leader_Info 1 {

Num_Members = 95
Total_Energy = -0.933
vdW = -6.038
Coulomb = -7.098
Internal = 12.203
rmsd = 0.000

}

\$Leader_Info 2 {

Num_Members = 45
Total_Energy = 0.901
vdW = -1.638
Coulomb = -9.664
Internal = 12.203
rmsd = 10.829

}

\$Leader_Info 3 {

Num_Members = 46
Total_Energy = 0.906
vdW = -6.373
Coulomb = -4.923
Internal = 12.203
rmsd = 2.285

}

\$Leader_Info 4 {

Num_Members = 43
Total_Energy = 1.236
vdW = -6.729
Coulomb = -4.238
Internal = 12.203
rmsd = 3.039

}

\$Leader_Info 5 {

Num_Members = 43

Total_Energy = 1.544
vdW = -2.790
Coulomb = -7.869
Internal = 12.203
rmsd = 9.833

}

\$Leader_Info 6 {

Num_Members = 47
Total_Energy = 1.655
vdW = -3.285
Coulomb = -7.262
Internal = 12.203
rmsd = 9.412

}

\$Leader_Info 7 {

Num_Members = 44
Total_Energy = 1.678
vdW = -6.067
Coulomb = -4.457
Internal = 12.203
rmsd = 2.398

}

\$Leader_Info 8 {

Num_Members = 17
Total_Energy = 1.720
vdW = -5.478
Coulomb = -5.005
Internal = 12.203
rmsd = 1.388

}

\$Leader_Info 9 {

Num_Members = 39
Total_Energy = 2.144
vdW = -5.139
Coulomb = -4.919
Internal = 12.203

rmsd = 3.177

}

\$Leader_Info 10 {

Num_Members = 49

Total_Energy = 2.279

vdW = -4.029

Coulomb = -5.894

Internal = 12.203

rmsd = 3.106

}

The Roccustyrna small molecule hits also the entire binding domains of the SARS-COV-2 protein targets, (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. (Figure7e)

Figure7f. CoMFA contour map of electrostatic regions around Roccustyrna chemical structure. Contact residues of the Roccustyrna small molecule when docked onto the SARS- COV-2 protein targets, (pdb:2zu5). (green, favored; yellow; disfavored) around the Roccustyrna chemical structure. Blue regions are favored by positively charged groups and red regions favored by negatively charged groups within the sequence of the amino acid of 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/A respectively.

\$Number_of_Clusters = 10

\$Seed = -1985

\$Leader_Info 1 {

Num_Members = 120
Total_Energy = -1.005
vdW = -6.071
Coulomb = -7.137
Internal = 12.203
rmsd = 0.000

}

\$Leader_Info 2 {

Num_Members = 46
Total_Energy = 0.877
vdW = -1.802
Coulomb = -9.524
Internal = 12.203
rmsd = 10.737

}

\$Leader_Info 3 {

Num_Members = 46
Total_Energy = 1.168
vdW = -6.381
Coulomb = -4.654
Internal = 12.203
rmsd = 2.273

}

\$Leader_Info 4 {

Num_Members = 47
Total_Energy = 1.255
vdW = -6.860
Coulomb = -4.087
Internal = 12.203
rmsd = 3.035

}

\$Leader_Info 5 {

Num_Members = 51

Total_Energy = 1.588
vdW = -2.961
Coulomb = -7.654
Internal = 12.203
rmsd = 9.734

}

\$Leader_Info 6 {

Num_Members = 36
Total_Energy = 1.667
vdW = -3.350
Coulomb = -7.185
Internal = 12.203
rmsd = 9.307

}

\$Leader_Info 7 {

Num_Members = 27
Total_Energy = 1.822
vdW = -4.803
Coulomb = -5.577
Internal = 12.203
rmsd = 1.318

}

\$Leader_Info 8 {

Num_Members = 46
Total_Energy = 2.040
vdW = -5.682
Coulomb = -4.480
Internal = 12.203
rmsd = 2.333

}

\$Leader_Info 9 {

Num_Members = 48
Total_Energy = 2.074
vdW = -4.003
Coulomb = -6.125
Internal = 12.203
rmsd = 3.106

}

\$Leader_Info 10 {

Num_Members = 40

Total_Energy = 2.286

vdW = -4.858

Coulomb = -5.059

Internal = 12.203

rmsd = 3.149

}

Figure8. 3D Docking interactions of the Roccustyrna small molecule (1S,2R,3S)-2-([(1S,2S,4S,5R)-4-ethenyl-4-sulfonylbicyclo[3.2.0]heptan-2-yl]oxy)amino)-3-[(2R,5R)-5-(2-methyl-6-methylidene-6,9-dihydro-3H-purin-9-yl)-3-methylideneoxolan-2-yl]phosphirane-1-carbonitrile within the binding domains of the protein targets (PDB: 6YI3) of the N-terminal RNA-binding domain of the SARS-CoV-2 nucleocapsid phosphoprotein. The Roccustyrna ligand binds into the binding sites of the amino acids of the V-M-ILE-34, V-S-ILE-34, V-M-THR-36, V-S-THR-36, V-S-GLN-43, V-S-THR-95, V-M-GLU-96, V-S-GLU-96 with the total docking energies of the -96.6 Kcal/mol and the docking values of the (-4.76839, -9.02476, -9.66643, -6.43937, -8.09017, -13.9373, -9.26627, -7.55529) Kcal/mol respectively.

\$Number_of_Clusters = 10

\$Seed = -1985

\$Leader_Info 1 {

Num_Members = 95
 Total_Energy = -0.923
 vdW = -6.045
 Coulomb = -7.080
 Internal = 12.203
 rmsd = 0.000

}

\$Leader_Info 2 {

```
    Num_Members = 49
    Total_Energy = 0.925
    vdW = -1.415
    Coulomb = -9.863
    Internal = 12.203
    rmsd = 10.654
}
```

```
$Leader_Info 3 {

    Num_Members = 49
    Total_Energy = 1.017
    vdW = -6.368
    Coulomb = -4.818
    Internal = 12.203
    rmsd = 2.305

}
```

```
$Leader_Info 4 {

    Num_Members = 47
    Total_Energy = 1.168
    vdW = -6.825
    Coulomb = -4.209
    Internal = 12.203
    rmsd = 3.054

}
```

```
$Leader_Info 5 {

    Num_Members = 42
    Total_Energy = 1.561
    vdW = -2.838
    Coulomb = -7.804
    Internal = 12.203
    rmsd = 9.626

}
```

```
$Leader_Info 6 {

    Num_Members = 21
    Total_Energy = 1.680
    vdW = -5.334
    Coulomb = -5.188
    Internal = 12.203
    rmsd = 1.146

}
```

```
$Leader_Info 7 {
```

```

    Num_Members = 52
    Total_Energy = 1.768
    vdW = -5.833
    Coulomb = -4.602
    Internal = 12.203
    rmsd = 2.335

```

```

}

```

```

$Leader_Info 8 {

```

```

    Num_Members = 34
    Total_Energy = 1.857
    vdW = -2.799
    Coulomb = -7.547
    Internal = 12.203
    rmsd = 9.202

```

```

}

```

```

$Leader_Info 9 {

```

```

    Num_Members = 45
    Total_Energy = 2.117
    vdW = -3.761
    Coulomb = -6.325
    Internal = 12.203
    rmsd = 3.224

```

```

}

```

```

$Leader_Info 10 {

```

```

    Num_Members = 35
    Total_Energy = 2.141
    vdW = -5.115
    Coulomb = -4.947
    Internal = 12.203
    rmsd = 3.095

```

```

}

```

As illustrated in the (Figure8) 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 (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. (Figure6d)(Figure6e) In this project for the first time we generated a Comparative Docking Cluster Analysis between the Remdesivir and our prototype Roccustyrna small molecule when docked onto the SARS-COV-2 protein targets, (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. (Figure3). A quantum distribution correlation similarity analysis was implemented regarding the Roccustyrna active fragments of the: 20 107.0352225 (NH+)#CN=C1C=NC=N12182. 03997355(NH2+) =C1C=NC=N122150.

0410362(NH3+) C1=NC(=)C2=NC=NC2= N123133.014487 N#CN=C1N=CN=C1
 C#(O+)24354.1563766CNC1 (C)C=C(O(NH2) N2C(P)2(C=C2OC=CC2=O)CN)
 C2NCN2125356.1720267CNC1(C)CC(O(NH2+))N2C(P)2(C=C2OC=CC2=O)CN)C2NCN21
 (Figure2a). Geometrical descriptors of the Roccustyrna small molecule were calculated as
 follows, Dreiding energy = 287,17 kcal/mol MMFF94 energy = 234,59 kcal/mol, Minimal
 projection area = 63,36, Maximal projection area = 133,25, Minimal projection radius = 6,25,
 Maximal projection radius = 9,68, Length perpendicular to the max area = 8,32, Length
 perpendicular to the min area = 19,36, van der Waals volume = 440,91. 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,
 -6.28532Kcal/mol. On the other hand the Remdesivir drug when combined to the

Roccustyrna small molecule interacted at the same binding domains of the amino acids of the V-M-LYS-551, V-S-LYS-551, V-S-ARG-553, V-S-ASP-618, V-M-TYR-619, V-M-PRO-620 with positive and zero docking values of the +42.1, -0.104885, -0.19986, +25.0575, Kcal/mol. That means that the Remdesivir drug could induce the COVID19 disease.

Discussions

In this article, we are improving the speed and accuracy and proposing an alternative topological quantum computing optimization framework for the computation of topological invariants of knots, links and tangles through a discrete stochastic optimization multithreading procedure that uses nonlinear finite element analysis and a ground structure approach, for quantum repeater networks as applied to quantum homology inspired Chern-Simons topology evolutionary scalable and fast fragmentation algorithm in which the geometric concepts of proper time enter in the non-relativistic limit (20-38,39). (Figure2b), (Figure2c). In this computer-aided drug designing project we generated the RoccustyrnaTM PDB and MOL2 files which are consisting of the merged pharmacophoric elements of the small molecule 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)-1λ5,2λ5-azaphosphiridin-1-ylum. (Figure2d). (Figure1b) (Figure1c). The focus of this work is to develop a Quantum Heuristic Fragmentation driven Chern-Simons fragmentation algorithm that is as independent to allow for a faster multi-cut solutions as possible from the chosen pharmacophoric fragmentation scheme obtained by localization of the S3 partition function of $\{x \sin^{-1}(\sqrt{3}), x \sin^{-1}(\sqrt{779} \sqrt{\theta^3}), x \sin^{-1}(2 \sqrt{114109}), (\sqrt{1 - \sqrt{456457}} \sqrt{x}) x^{1/4} (2 \sqrt{456457} \sqrt{x} + 3)/(8 \sqrt{456457}^{3/4}) + (x - 3/3651656) \sin^{-1}(\sqrt{456457}^{1/4} x^{1/4}), 1/2 \sqrt{x/456456754 - x^2} + (x - 1/912913508) \sin^{-1}(\sqrt{456456754} \sqrt{x}), x \sin^{-1}(2^{3/4} \sqrt{57057}^{1/4}), x \sin^{-1}(\sqrt{\sum 444546 \theta}), \sin^{-1}(2^{3/4} \sqrt{431683182057}^{1/4} \sqrt{\sqrt{\theta}/(\sin^{-1}(44545545))})\} + \text{constant}$ 3d N = 2 CS{ $\theta \sin^{-1}(\sqrt{3}), \theta \sin^{-1}(\sqrt{779} \delta \phi = i \bar{q} \psi, \delta \bar{\phi} = i \bar{q} \bar{\psi}, \delta \psi = -\gamma \mu \bar{q} D \mu \phi - \bar{q} \sigma \phi - i f(\theta) \bar{q} \phi + i \bar{q} F, \delta \bar{\psi} = -\gamma \mu \bar{q} D \mu \bar{\phi} - \bar{\phi} \sigma \bar{q} - i f(\theta) \bar{\phi} \bar{q} + i \bar{F} \bar{q}, \delta F = \bar{q} (-\gamma \mu D \mu \psi + \sigma \psi + \lambda \phi) + i(2 - 1) 2 f(\theta) \bar{q} \psi, \delta \bar{F} = \bar{q} (-\gamma \mu D \mu \bar{\psi} + \bar{\psi} \sigma - \bar{\phi} \bar{\lambda}) + i(2 - 1) 2 f(\theta) \bar{q} \bar{\psi}, \sqrt{\theta^3}) - 3/5 \sqrt{779} \theta \sqrt{\theta^3} 2 F_1(1/2, 5/6, 11/6, 779 \theta^3), 1/6 \sqrt{1/49394 - 9 \theta} \sqrt{\theta} + (\theta - 1/889092) \sin^{-1}(3 \sqrt{49394} \sqrt{\theta}), \theta \sin^{-1}(\sqrt{\sin^{-1}(44545545)})\} + \text{constant}$ (equations4-11) 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 generated QSAR automating modeling lead compound design approach. In this hybrid drug designing approach, we have designed the RoccustyrnaTM 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 RoccustyrnaTM prototype rigid chemical

scaffold 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).

Conclusions

Here, for the first time we have generated drug repositioning In-Silico approaches against the COVID-19, not only for constructing, remerging and generating chemical and physical small molecule libraries available through publically available web servers, but also for the implementation of fragmentation and recoring in-silico quantum phase experiments introducing new fragment based machine-learning virtual screening experiments and employing in-house ligand libraries applied for the design of a quantum thinking novel multi-chemo-structure against the protein targets of COVID-19 main protease, the RoccustyrnaTM small molecule. By applying the Biogenetoligandorol accuracy (named EuTHTS Euclidean Topology Virtual Screening) algorithm, a Gravitational Topological (UFs) based Quantum-Parallel Particle Swarm Inspired framework was deployed by using 2D chemical features in which a generalized procedure of Quantization of classical heuristic fields was be fused together with QSAR automating modeling. I finally developed and implemented for the two algorithms using natural Euclidean Geometric Topologies and Artificial Intelligence-Driven Predictive Neural Networks, showing that it is possible to well-defined surjective atom mapping and to automate phase group and ligand-based fragmentations based on computed diagonal chemical descriptors. By identifying chemical patterns I made use of partial small fragment derivatives with the additional MM-PBSA-WSAS binding free energy calculation difficulties that the drug designs we deal with are not orthogonal. (30-42) Both Chern-Simons theories and knot theory algorithms applied in this project into merged pharmacophoric groups. Furthermore, the geometric topology driven heuristic algorithms which were used in this project are capable of fragmenting and remerging small molecules that could not be fragmented by the algorithm of the any of the known reference databases. (2,5-42) We have illustrated the power of such a Flexible heuristic algorithm approach interpreted as distinct quantum circuit, qubit preparations, and certain 1- and 2-qudit gates for automatic molecule fragmentation in a meaningful application to Molecular epidemiology, evolution and phylogeny of SARS coronavirus components, such as qubits. Our Biogenetoligandorol platform also offers utility to researchers simply wishing to interrogate and organize generalized Hadamard where $H \leftarrow [1 \ 1; 1 \ -1]/2$; $(-1)(i, j)|j \rangle \langle i|$ (2) and control-Z gates data, to create an inventory of available numerical docking $\in \{0,1,000,111\}$ and $b \in \{++++,-\}$ (3) data with particular clinical or genomic features, of the shaded tangle into two-dimensional $m \times m$ matrix $I2 \leftarrow E(m)$; m^2 -dimensional vector $|\Phi\rangle \leftarrow I2 \rightarrow$; (*maximally matrix $M1 \leftarrow I2 - M0$; (equation6) entangled state*) (* m -dimensional identity*) space such as available datasets or patients with particular mutations and calculate the fusion of the Roccustyrna's active fragments as it can be applied which may be used to draw independently of its drug identification Hilbert space $CSG,k(S1 \ S \leftarrow X \otimes |0\rangle \langle 0| + C \otimes |1 \rangle \langle 1| W \leftarrow S(I \otimes H)M1$; equation

(7) capabilities. (26,29-42) More specifically, in this project we implemented a Quantum principal applied and a Kappa-Symmetry inspired Inverse Docking Algorithmic analysis with nonlinear electrodynamics indicated to us that the RoccustyrnaTM small molecules generated the highest negative docking energies when compared to other FDA approved drugs against the SARS-COV-2 viruses protein targets and while it is probably true that the injudicious use involving the management of these 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.

Significant Statements

In this project I implemented Inverse Docking Algorithms with nonlinear electrodynamics for the designing of the RoccustyrnaTM small molecule that exerts the highest negative docking energies as compared to other FDA approved drugs when docked onto the SARS-

COV-2 viruses protein targets by solving the Chern-Simons Topology Euclidean Geometric in a Lindenbaum-Tarski equations (1-7) generated QSAR automating modeling and Artificial Intelligence-Driven Predictive Neural Networks.

☐ **Availability of data and materials**

The author confirms that the data supporting the findings of this study are available within its supplementary materials.

☐ **Competing interests**

No potential competing interest was reported by the author.

☐ **Funding**

The author received no financial support for the research, authorship, and/or publication of this article.

☐ **Authors' contributions**

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

Author has contributed in the below multiple roles:

- **Conceptualization 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, Provision 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 postpublication 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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Figures

Figure 1

Figure1a. 3D Docking interactions of the selected NuBEE physical elements inside the PDB:6XS6, SARS-CoV-2 Spike SARS-COV-2 SPIKE D614G variant, minus RBD, Figure1b. Quantum Circuit of the BiogenetoligandoirolTM Cluster for the Roccustyrna small molecule Merging and Hope-Re-coring

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algorithms. Gate nG0 ( param ) q { h q;}qreg q(3);creg c(3);reset q(0);reset q(1);reset
q(2);hq(0);u2(pi/2,pi/2) q(1);measure q(2) -> c(2);x q(0);reset q(1);resetq(2);u3(pi/2,pi/2,pi/2)
q(0);measure q(2) -> c(2);u2(pi/2,pi/2) q(2);cswap q(0),q(1),q(2);barrier q(0);u2(pi/2,pi/2) q(2);h q(0);t
q(2);t q(0);measure q(1) -> c(1);ch q(1),q(2); q(2);crx(pi/2) q(1),q(2);cu1(pi/2) q(1),q(2);tdg q(2);sdg q(2);cy
q(1),q(2);crz(pi/2) q(1),q(2);ch q(1),q(2);sdg q(1);u2(pi/2,pi/2) q(2);ry(pi/2) q(2);cu3(pi/2,pi/2,pi/2)
q(1),q(2);tdg q(1);nG0(pi/2) q(2);crx(pi/2) q(1),q(2);cu1(pi/2) q(1),q(2);cswap q(0),q(1),q(2);swap
q(1),q(2);cz q(1),q(2);rxx(pi/2) q(1),q(2);u1(pi/2) q(1);cry(pi/2) q(1),q(2);crz(pi/2) q(1),q(2);measure q(0) ->
c(0);z q(0);measure q(1) -> c(1);z q(0);rx(pi/2) q(1);rx(pi/2) q(0);u2(pi/2,pi/2) q(1);rx(pi/2) q(0);ch
q(1),q(2);ry(pi/2)q(0);ch q(1),q(2);u3(pi/2,pi/2,pi/2) q(0);cz q(1),q(2);ch q(0),q(1);u1 (pi/2) q(0);swap
q(1),q(2);sdg q(2);

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BBB permeant	No	
P-gp substrate	Yes	
CYP1A2 inhibitor	No	
CYP2C19 inhibitor	No	
CYP2C9 inhibitor	No	
CYP2D6 inhibitor	No	
CYP3A4 inhibitor	No	
Log <i>K_p</i> (skin permeation)	-10.55 cm/s	
Medicinal Chemistry		
PAINS	0 alert	
Brenk	3 alerts: Three-membered_heterocycle, oxy	gen-nitrogen_sinin
Leadlikeness	No; 1 violation: MW>350	
Synthetic accessibility	6.25

Figure 2

Figure2a. Geometrical descriptors of the Roccustyrna small molecule. Dreiding energy = 287,17 kcal/mol MMFF94 energy = 234,59 kcal/mol, Minimal projection area = 63,36, Maximal projection area = 133,25, Minimal projection radius = 6,25, Maximal projection radius = 9,68, Length perpendicular to the max area = 8,32, Length perpendicular to the min area = 19,36, van der Waals volume = 440,91 Figure2b. RoccustyrnaTM small molecule's PDB file Figure2c. RoccustyrnaTM_Prefered_IUPACName=(1Z)⌘⌘

(((2S,3S,5R)-5-(2-amino-6-oxo-6,9-dihydro-1H-purin-9-yl)-3-hydroxyoxolan-2-yl)methylidene)-2-cyano-1-((((2S,4R,5R)-2-methyl-2-(methylamino)-1,6-diazabicyclo(3.2.0)heptan-4-yl)oxy}imino)-1lambda5,2lambda5-azaphosphiridin-1-yl)ium. Figure 2d. RoccustyrnaTM_Preferred_IUPACName=(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-azaphosphiridin-1-yl)ium. For instance, a generalized coordinate is commonly used in the study of tunnelling effects and may be a bond length, a bond angle, or a dihedral angle in solid state systems. 2d Structure Map of the RoccustyrnaTM Atoms Geometrical Descriptors of the RoccustyrnaTM small molecule: Dreiding energy = 305,20 kcal/mol, MMFF94 energy = 35,06 kcal/mol, Minimal projection area = 66,49, Maximal projection area = 123,65 Minimal projection radius = 5,71 Maximal projection radius = 9,24 Length perpendicular to the max area = 10,29 Length perpendicular to the min area = 19,04 van der Waals volume = 409,41 Donor count = 5 Donor sites = 6 Acceptor count 11 Acceptor sites = 14 127.9718331 C#CC#P1C=S1#(NH+)33 93.98748321(NH+)#S1=PC134 59.99024648C#S#(NH+)35

Figure 3

Figure3. Roccustyrna active fragments smiles distribution analysis.

Figure 4

Figure4a. Binding patterns, CoMFA contour map and aminoacid interactions of the steric regions (blue, favored; yellow; disfavored) around Rocustyrna scaffold (Ser682, Thy456, and Arg624 with a distance of 1.224, 2.445, and 2.159 Å, respectively); Blue regions are favored by positively charged groups and red regions favored by negatively charged groups inside the SARS-COV-2 protein targets (pdb:1xak). EDO:A:506 (EDO) - SMALLMOLECULE Figure4b. Shows the receptor binding domain and the CoMFA contour map of steric regions (blue, favored; yellow; disfavored) around Rocustyrna; Blue regions are favored by positively charged groups and red regions favored by negatively charged groups inside the SARS-COV-2 protein targets (pdb:6W9C). 02J:C:1 (02J) - SMALLMOLECULE

Figure 5

Figure5a. Rocustyrna binding site(s) inside the 2CME (hypothetical protein 5) binding domains. 02J:C:1 (02J) - SMALLMOLECULE Figure5b. Rocustyrna binding site(s) in 2CME (hypothetical protein 5) D10-C-1099 DMS:A:402 (DMS) - SMALLMOLECULE Figure5c. Rocustyrna binding site(s) in 2CME (hypothetical protein 5) D10-F-1099. 2J:C:1 (02J) - SMALLMOLECULE Figure5d. Rocustyrna binding site(s) in 2CME (hypothetical protein 5) D10-H-1099. X77:A:401 (X77) - SMALLMOLECULE

Figure 6

Figure6a. Roccustyrna binding sites into the 02J (5-Methylisoxazole-3-carboxylic acid) 6LU7 protein targets. DMS:A:402 (DMS) - SMALLMOLECULE Figure6b. Roccustyrna binding sites into the 02J (5-Methylisoxazole-3-carboxylic acid) PJE-C-56LU7 protein targets. ZN:A:998 (ZN) - ION Figure6c. CoMFA contour map of electrostatic regions around Roccustyrna chemical structure. Contact residues of the Roccustyrna small molecule when docked onto the SARS-COV-2 protein targets, (pdb:7bv2). (green,

favored; yellow; disfavored) around the Roccustyrna chemical structure. Blue regions are favored by positively charged groups and red regions favored by negatively charged groups. Figure6d. Comparative Docking Cluster Analysis between the Remdesivir and the Roccustyrna small molecules when docked onto the SARS-COV-2 protein targets, (pdb:7bv2). Figure6e. Comparative Docking Energy Analysis between the Remdesivir and the Roccustyrna small molecules when docked onto the SARS-COV-2 protein targets, (pdb:7bv2). \$Number_of_Clusters = 10

Figure 7

Figure7a. CoMFA contour map of electrostatic regions around Roccustyrna chemical structure. Contact residues of the Roccustyrna small molecule when docked onto the SARS COV-2 protein targets, (pdb:3fqj). (green, favored; yellow; disfavored) around the Roccustyrna chemical structure. Blue regions are favored by positively charged groups and red regions favored by negatively charged groups within the sequence of the amino acid of the V-S-HIS-159, V-S-ARG-160, V-S-ARG-112 V-M-GLU-148 V-M-PHE-150, V-S-PHE-150, V-S-HIS-159, V-M-TYR-161 with the docking energy values of the -101, -14.0762, -5.11094, -7.98447, -4.17314, -4.43549, -9.66939, -9.42926, -7.30085

Figure7b. CoMFA contour map of electrostatic regions around Roccustyrna chemical structure. Contact residues of the Roccustyrna small molecule when docked onto the SARS- COV-2 protein targets, (pdb:6xs6). (green, favored; yellow; disfavored) around the Roccustyrna chemical structure. Blue regions are favored by positively charged groups and red regions favored by negatively charged groups within the sequence of the amino acid of 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 respectively.

Figure7c. CoMFA contour map of electrostatic regions around Roccustyrna chemical structure. Contact residues of the Roccustyrna small molecule when docked onto the SARS- COV-2 protein targets, (pdb:2ghv). (green, favored; yellow; disfavored) around the Roccustyrna chemical structure. Blue regions are favored by positively charged groups and red regions favored by negatively charged groups within the sequence of the amino acid of the H-M-ASN-330, H-S-ASN-330, H-S-TYR-356, H-M-ASN-424, V-M-ASN-330, 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 respectively.

Figure7d. CoMFA contour map of electrostatic regions around Roccustyrna chemical structure. Contact residues of the Roccustyrna small molecule when docked onto the SARS- COV-2 protein targets, (pdb:2zu5). (green, favored; yellow; disfavored) around the Roccustyrna chemical structure. Blue regions are favored by positively charged groups and red regions favored by negatively charged groups within the sequence of the amino acid of 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.

Figure7e. CoMFA contour map of electrostatic regions around Roccustyrna chemical structure. Contact residues of the Roccustyrna small molecule when docked onto the SARS- COV-2 protein targets, (pdb:6w9c). (green, favored; yellow; disfavored) around the Roccustyrna chemical structure. Blue regions are favored by positively charged groups and red regions favored by negatively charged groups within the sequence of the amino acid of the V-S-PRO-59, V-S-ARG-65, V-M-THR-75, V-S-THR-75, V-M-PRO-77, V-S-PRO-77, V-M-HIS-47, V-S-HIS-47 with the docking energies of the -83.9, -4.21999, -12.6164, -7.60372, -6.69528, -5.89416, -6.40663, -5.51621, -7.99273.

Figure 8

3D Docking interactions of the Roccustyrna small molecule (1S,2R,3S)-2-(((1S,2S,4S,5R)-4-ethenyl-4-sulfonylbicyclo[3.2.0]heptan-2-yl)oxy)amino-3-((2R,5R)-5-(2-methyl-6-methylidene-6,9-dihydro-3H-purin-9-yl)-3-methylideneoxolan-2-yl)phosphirane-1-carbonitrile within the binding domains of the protein targets (PDB: 6YI3) of the N-terminal RNA-binding domain of the SARS-CoV-2 nucleocapsid phosphoprotein. The Roccustyrna ligand binds into the binding sites of the amino acids of the V-M-ILE-34, V-S-ILE-34, V-M-THR-36, V-S-THR-36, V-S-GLN-43, V-S-THR-95, V-M-GLU-96, V-S-GLU-96 with the total docking energies of the -96.6 Kcal/mol and the docking values of the -4.76839, -9.02476, -9.66643, -6.43937, -8.09017, -13.9373, -9.26627, -7.55529 Kcal/mol respectively.