Generalized Chemical Block Systems on Chern-Simons φ[?] D[?] r2[?] S[?] r1 Topologies for the generation of the Roccustyrna Holomorphic Ligand.

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April 16, 2024

Abstract

SARS coronavirus 2 (SARS - CoV - 2) in the viral spike (S) encoding a SARS - COV - 2 SPIKE D614G mutation protein predominate over time in locales revealing the dynamic aspects of its key viral processes where it is found, implying that this change enhances viral transmission. In this paper, we strongly combine topology geometric methods for generalized formalisms of k - nearest neighbors as a Tipping–Ogilvie and Machine Learning application within the quantum computing context targeting the atomistic level of the protein apparatus of the SARS - COV - 2 viral characteristics. In this effort, we propose computer - aided rational drug design strategies efficient in computing docking usage, and powerful enough to achieve very high accuracy levels for this in - silico effort for the generation of AI - Quantum designed molecules of GisitorviffirnaTM, Roccustyrna_-gs1_TM, and Roccustyrna_fr1_TM ligands targeting the COVID - 19 - SARS - COV - 2 SPIKE D614G mutation by unifying Eigenvalue Statements into Shannon entropy quantities as composed on Tipping–Ogilvie driven Machine Learning potentials for nonzero Christoffel symbols for Schwarzschild (DFT) neuron (ι) : == == φ[?]D[?]r2[?]S[?]r102 (1+[?]) == == (A[?]A' (p)) * [?][?][?][?][?] *e- ρ (rr) –¯σ - ¯σσ¯o -i_+02 (1-) 2} ()) improver for Chern - Simons Topology Euclidean Geometrics. I also arrived at a new Zmatter derived finite - dimensional state integral with a symplectic ω == == (i˜)-1 (dx/x) [?] (dy/y) model for computing the analytically continued "holomorphic blocks" on an appropriate quantum Hilbert space H that compose physical Chern - Simons partition function to put pharmacophoric elements back together.

Γενεραλιζεδ ħεμισαλ Βλοςκ Σψστεμς ον ħερν-Σιμονς φ[;] Δ[;] ρ2[;] Σ[;] ρ1 Τοπολογιες φορ τηε γενερατιον οφ τηε Ροςςυστψρνα Ηολομορπηις Λιγανδ.

1. Δεπαρτμεντ οφ ΒιογενετολιγανδοροlΧΜΜΙΔΔΔ/ΧΠΡΠΠ˜Α/ΜΑ˜ΗΝΟΤ/ ΧΙΙ-˜ΔΝΝΔ˜Α ΑΔΜΕΤ/ΧΙΓ˜ΔΝΝΔ˜Α Στατιονς.

2. Αριστοτλε Υνιερσιτψ οφ Τηεσσαλονικι, Βιογενεα Πηαρμαςευτιςαλς Λτδ – Γρεεςε.

3. ℮λλ-Πηαρμαςψ Λτδ, Περσοναλιζεδ ΣψντηοςυρεΤΜ Στατιονς.

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Κєψωορδς: ˜Ο˜ΙΔ19, ΣΑΡΣ - ˜Ο˜ - 2 ΣΠΙΚΕ Δ614Γ, ħερν - Σιμονς

Τοπολογιςαλ, AI - Χυαντυμ ςομπυτινγ, Χυαντυμ - Ινσπιρєδ Εολυτιοναρψ Αλγοριτημ Πρєδιςτιє Τοξιςολογψ, ΧΣΑΡ χυαντυμ γατєς, ħєμινφομρατιςς αρτιφιςιαλ ιντελλιγєνςє, Πηασє Δατα Μινινγ, Μαςηινє Λєαρνινγ, ħєμι-ςαλ σπαςє єξπλορατιον,

ΑΒΣΤΡΑ˜Τ

ΣΑΡΣ ϲοροναιρυϲ 2 (ΣΑΡΣ - δ″ - 2) ιν τηε ιραλ σπικε(Σ) ενϲοδινγ α ΣΑΡΣ - Ὸ″ - 2 ΣΠΙΚΕ Δ614Γ μυτατιον προτειν πρεδομινατε οερ τιμε ιν λοϲαλες ρεεαλινγ τηε δψναμιϲ ασπεϲτϲ οφ ιτϲ κεψ ιραλ προϲεϲϲες ωηερε ιτ ιϲ φουνδ, ιμπλψινγ τηατ τηιϲ ϲηανγε ενηανϲες ιραλ τρανϲμιϲϲιον. Ιν τηιϲ παπερ, ωε στρονγλψ ϲομβινε τοπολογψ γεομετριϲ μετηοδϲ φορ γενεραλιζεδ φορμαλιϲμϲ οφ κ - νεαρεϲτ νειγηβορϲ ας α Τιππινγ–Ογιλιε ανδ Μαϲηινε Λεαρνινγ αππλιϲατιον ωιτηιν τηε χυαντυμ ϲομπυτινγ ϲοντεξτ ταργετινγ τηε ατομιϲτιϲ λεελ οφ τηε προτειν αππαρατυϲ οφ τηε ΣΑΡΣ - Ὸ″ - 2 ιραλ ϲηαραϲτεριϲτιϲϲ. Ιν τηιϲ εφφορτ, ωε προποϲε ϲομπυτερ - αιδεδ ρατιοναλ δρυγ δεϲιγν στρατεγιεϲ εφφιϲιεντ ιν ϲομπυτινγ δοϲκινγ υϲαγε, ανδ ποωερφυλ ενουγη το αϲηιεε ερψ ηιγη αϲϲυραϲψ λεελϲ φορ τηιϲ ιν - σιλιϲο εφφορτ φορ τηε γενερατιον οφ AI - Χυαντυμ δεϲιγνεδ μολεϲυλεϲ οφ ΓιϲιτοριφφιρναΤΜ, Ροϲϲυϲτψρνα_γϲ1_ΤΜ, ανδ Ροϲϲυϲτψρνα_φρ1_ΤΜ λιγανδϲ ταργετινγ τηε Ὸ″ΙΔ - 19 - ΣΑΡΣ - Ὸ″ - 2 ΣΠΙΚΕ Δ614Γ μυτατιον βψ υνιφψινγ Ειγεναλυε Στατεμεντϲ ιντο Σηαννον εντροπψ χυαντιτιεϲ ας ϲομποϲεδ ον Τιππινγ–Ογιλιε δριεν Μαϲηινε Λεαρνινγ ποτεντιαλϲ φορ νονζερο ℏριϲτοφφελ σψμβολϲ φορ Σϲηωαρζϲϲηιλδ(ΔΦΤ) νευρον (ι) : == == φ[?]D[?]r2[?]S[?]r1?0?2 (1+[?]?) == == (A[?]A’(p)) * [?][?][?][?][?] *e- ρ (rr)–¯σ - ¯σσ¯o -i_+?0?2 (1- ??) 2}?(?) ?) improver for Chern - Simons Topology Euclidean Geometrics. I also arrived at a new Zmatter derived finite - dimensional state integral with a symplectic ω == ==(i˜) -1 (dx/x) [?](dy/y) model for computing the analytically continued “holomorphic blocks” on an appropriate quantum Hilbert space H that compose physical Chern - Simons partition function to put pharmacophoric elements back together.

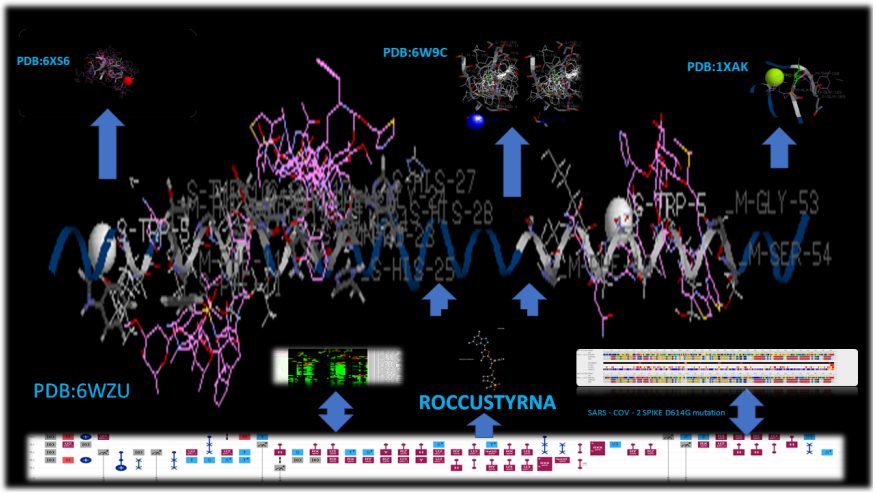

Illustration1. Roccustyrna_fr1_TM fragments when targeted onto the PDB:6wzu SARS - Cov - 2 protein targets.

SIGNIFICANT STATEMENTS

In this effort, we propose computer - aided rational drug design strategies efficient in computing docking usage, and powerful enough to achieve very high accuracy levels for this in - silico effort for the generation of AI - Quantum designed molecules of GisitorviffirnaTM, Roccustyrna_gs1_TM, and Roccustyrna_fr1_TM ligands targeting the COVID - 19 - SARS - COV - 2 SPIKE D614G mutation by unifying Molecular Pairs (MMP), Lindenbaum - Tarski logical spaces and Adaptive Weighted KNN Positioning for Matched Bemis and Murko (BM) driven eigenvalue statements into Shannon entropy quantities as composed by Tipping–Ogilvie driven Machine Learning potentials on a (DFT) neuron (ι) : == == φ[?]D[?]r2[?] S[?]r1 ?0?2 (1+[?]?) == == (A[?]A’ (p)) e * [?][?][?][?][?] (Group of Eqs.1-115) improver for Chern - Simons Topology Euclidean Geometrics.

INTRODUCTION

(1, 2, 3) The COVID - 19 viral infectious which emerged in China at the end of 2019 previously provisionally named 2019 - nCoV or 2019 novel coronavirus was officially declared in March 2020 a pandemic by the World

Health Organization (WHO) and is accountable for many fatal cases. (2, 4, 5) On January 202, the WHO committee declared a global health emergency (3, 4 - 6) based on the rate of the increasing spread of the infection (4, 5 - 7) in the range 2.0 - 6.0 with a reproductive number (rN) 5, 4 higher than SARS and Middle East respiratory Syndrome Coronavirus (MErS)respectively (8) with fatality rate of about 4%.(1 - 4) Collaborative efforts for Genomic characterization by using a simple DNA cryptography genetic code according to the main dogma of biology have been published that takes plaintext for communicating information through a process of DNA-rNA-Amino Acid coding. researchers in 2010 published a Cryptographic DNA - mobile based Code for Secure Networks Scheme in which binary plaintext is translated to text via a substitution wrapping code, introns are inserted into DNA hierarchal text structure on the general processes of gene expression by the transcription complex and a binary key is passed to the receiver over a secure channel to provide the details of the intron insertion. We cannot imagine a world without cryptography anymore. Whether it is to protect our banking information, e - mail, or phone calls, cryptography is a vital part of our digital infrastructure. Modern - day cryptography is usually split up into two phases. In the key exchange phase, an algorithm such as Elliptic Curve Diffie - Hellman key exchange (ECDH) or rSA is used to establish a shared secret key that can be used in an asymmetric encryption algorithm in the second phase. These algorithms have been and continue to be well - studied and have proven themselves to be secure if instantiated with proper parameters and implemented securely. Nowadays most people favor using cryptographic keys over sticks and more intricate cryptographic algorithms than wrapping at an angle. This opens the door to new types of cryptographic attacks. Attack avenues can roughly be divided into two categories: attacks on theoretic algorithm by trying to recover the key or message by using public information provided on the algorithm, and attacks on the implementation of the algorithm, which look at the soft - or hardware - specific properties.(5, 6, 7 - 9) Evolution, phylogeny, high contagion rates, molecular epidemiology, of SARS coronavirus, and epidemiology from scientists worldwide are underway to understand the rapid spread of the novel coronavirus (CoVs) , and to develop effective coding drug - protein - gene interactions of personalized intervention options for control, characterize, and prevention of viral outbreaks, and various devastating diseases. (1 - 10)Coronaviruses are positive - single stranded, and through transcription and ultimately translations enveloped large rNA viruses that infect humans and a wide range of animals. (4, 6, 7, 8, 9, 10) In Latin, Corona means –crow based on their shapes. As a comprehensive compendium and megadiverse country, Brazil accounts for 10–20% of known living species of available biogeochemical information in the world. However, a major part of the biological and chemical biodiversity in Brazil's natural products remains unexplored(2– 13, 14, 15, 16, 17) Molecular structures as a protein code (cipher - protein) were determined in heterodox interpretations (22) by solving the time - independent (21 - 22) Schrödinger equation: QM methods, vertex prizes, and edge costs including ab initio

Density Field Theories (DFT) (23) has become a common approach as a quantum - many body premium technique and semi - empirical computational scheme in place (24) of the quantum processor and docking energy used for studying molecule structure under QM simulated sampling error among other quantitative understanding observables. Density Field Theories (DFT) is continuously increasing for more systematic and less expensive methods(25) when compared to traditional drug development approaches to repositioning drugs and physical extracts and represent the similarities (26) and dissimilarities(27) between drugs and repurposed viral proteins, respectively. (28) However, the Schrödinger equations in Markovian and (27) non - Markovian scenarios cannot be solved for any but a one - data - driven (29)electron system method (the hydrogen atom) , to construct a family of solutions of (28, 30)equations and approximations need to be made. According to QM,(2 - 19, 23) and during the construction of stochastic Schrödinger (29) equations, an electron bound that converges quickly and reliably by acknowledging the conditional Bohmian wavefunction to an atom cannot possess any (2 - 17, 21, 22, 23, 24, 25, 26, 27, 28) arbitrary energy to produce the desired distribution or occupy any position in space using statistical and machine (23, 24 - 37, 38) learning concepts. Molecular Pairs (MMP) , Lindenbaum - Tarski logical spaces, Adaptive Weighted KNN Positioning Matched Bemis, and Murko(BM) driven eigenvalue statements were incorporated in this project when analyzing pharmacological data allowing a well - defined superposition for each fragmented pharmacophore. This shows that the application to quantum computing as orthogonally applied for the design of small molecules may allow pure mechanical computations both for re - generating Lipinski rules

and quantum inferences to bridge the gap between practical in vitro testing implementations and theoretical docking scalability predictions. (25, 27, 28) Since it has been shown that Path selection into a nonlinear riemann - Hilbert simple problem of any metal formula φ for quantum repeater networks towards the determination of the exact interpolating function of h(λ) can be geometrically represented by Chern - Simons logical spaces and subspaces I decided to cryptographically implement supersymmetric solutions and Borel Singularities for N == == 2 allowing a quantum repeater based vectorial Supersymmetric representation in this drug design project. (20, 26, 27, 28, 29, 30, 31) In general, the notions of Lindenbaum matrixand associated axiomatic formulations (AQFT) for Lindenbaum - Tarski guidedAdaptive Weighted KNN Positioning and its relative development to the product topology continuing to shape the field of algebraic logic introducing topology on a set to define the (31)cartesian product of topological spaces. As subbase supersymmetric solutions have paved the way until this day, to further algebraization of topology products, which had been begun by George Boole in the 19th century, as well as to an innovative language of logic, in a symmetric model theory containing no other constants but only one connective -. Philosophical interpretations of QM Molecular Pairs(MMP) as a core part of contemporary physics(Minkowski - type, wave - edge, etc) , (20, 27, 32 - 33) including von Neumann and Dirac formulation states as well as probabilistic transformations on Murko (BM)driven eigenvalue statements for algebraic multi - metrics(Triangle area, Bond - angle, etc) were incorporated in this project to treat Tipping–Ogilvie and Machine Learning observables as foundational according to the interaction information theory (QIT) reference frames. (20, 33, 34, 35) In this project, we show an original strategy and demonstrate the utility and the mechanics of this (32)unified molecular formalism as a Tipping–Ogilvie and Machine Learning QMMMP application within the quantum computing context as perturbed asymptotically through the example of coupled anti - de Sitter black harmonic black - hole oscillators and brane spacetimes. We expect this Lindenbaum - Tarski driven Chern - Simons representation to generate a valid QSAR modeling, and lead compound design formalism, in our molecular modeling and simulations in order to produce orthogonal coordinates as applied for the design of a novel multi - chemo - structure against the crystal structure of COVID - 19 protein targets.(29, 35, 36) A meta - server and a Kappa - Symmetry C++ algebra of local observables were incorporated for the docking of FDA - approved small molecules, peptide - mimetic, and humanized antibodies against potential targets of COVID - 19 via a generalized procedure of Quantization of classical fields which were fused together with QSAR automating modeling to lead the commutation and anticommutation relations. (37, 39, 41, 42) Dynamic niching and flexible heuristic genetic algorithmic states for automatic molecule re - coring and fragmentation were applied to fragment and re - core a database of molecules for use with the group contribution model Universal Quasihelical Functional Group Activity Coefficients(UNIFAC) against the structure and functions of SARS - CoV - 2 as linear functional on the algebra of free energy docking observables. Topological Chern - Simons theory in three dimensions(40, 41, 42) will be deployed as a pharmacophoric merging example of a rich QFT that depends on the topology of the 3 - manifold on linked fragments, and condensed chemical block systems where D - branes are wrapped on the Lagrangian M3 in X chemical spaces.(37, 38, 40, 43) Hybrid quantum repeater via a robust creation of entanglement between remote memory qubits was implemented for predicting drug targets and for multi - target and multi - site - based virtual screening against COVID - 19. To demonstrate its flexibility, we tackle a hugely different objective issued from a 5 - dimensional submanifold organic molecular domain (43, 44) as a transverse holomorphic structure, which means that there is a given 3 - dimensional foliation for each one tangent bundle modulo foliation. We show that our method can generate sets of optimized critical molecules as integrable structure complexes which having high energy or low energy, starting only from penicillamine derivatives. We can also set constraints on a synthesizability score and structural features when the 3 - brane is a chemical subspace of the 5 - brane, and the flux on the invariant 5 - brane vanishes when restricted to the 3 - brane, the 3 - brane refers to my transverse holomorphic chemical structure. (41, 42) Flexible Topology Euclidean Geometric was used to fragment molecules automatically in this molecular modeling and drug designing project on several parameters while keeping the definition of the groups as simple as possible. Maximum Common Substructure (MCS) topologies for generalized k - nearest neighbors on Tipping–Ogilvie and Machine Learning generated Molecular Pairs (MMP) , and an Adaptive Weighted KNN Positioning Matched Bemis and Murko (BM) approach employed for supercritical

entanglements introducing an advanced quantum mechanical inverse docking algorithm providing further insight to confirm the practicality of docking energy predictions. In this protocol, tools from conventional cryptography for wild type and selected mutations for Nsp3 (papain - like, PLpro domain) , Nsp5 Nsp15 (NendoU) , (Mpro, 3CLpro) , Nsp12 (RdRp) , N protein and Spike were combined as inputs and the key element functions of SARS - CoV - 2 protein pathways in understanding and designing possible novel antiviral agents, from both a quantum algebraic and a cheminformatic perspective along with the principles of the regulation of computer - aided drug discovery methodologies. Molecular scaffolds are generally used to describe the common core structures of the molecules (25, 33, 38, 39, and 44) . In this project the selected herbs classified into structural classes using the characteristic scaffolds of each group(14, 32, 33, 42) . In medicinal chemistry, a molecular scaffold is used to represent the core structure of a group of active compounds. Since the compounds with the same scaffold may influence a particular metabolic pathway, the molecular scaffolds can effectively contribute to the prediction of biological activities (8, 16, 40, 42, 43) . The scaffold of molecule groups is defined as a common sub - graph of the graphs of the molecule groups. Representatively, Maximum Common Substructure (MCS) , Matched Molecular Pairs (MMP) , and Bemis and Murko(BM) are the commonly used methods to produce molecular scaffolds (22–30, 39, 40, and 42, 44) . This paper concentrates on the unification of quantum mechanics fundamental theories into 3 - dimensional field wave equations for a N == == 2 supersymmetricgeneralized k - nearest molecular oscillator. By describing the second - order term for Tipping–Ogilvie 3 - manifolds which refer to our designed structure we expanded them into generalized chemical entities through Chern Simons connections over compact solutions when solving the Cluster of Eqs. of ? (?) ? == == ?? == == ??exp (-???) ? (?-?2 /??, 2?, 2???) ? (?, ?;?) == == [?]? == == 0[?]Γ(?+?) Γ (?) ??Γ(?+?) Γ (?) ?!?0?2 (1-?2(?+?) 2) ? == == 0, 1, 2. . . .? == == 1/2+?2+ 1/4?0?2 (1-??) 2}? (?) ?(k) * [?][?][?][?][?] *e- ρ (rr) == ==[?] k1mCQ 2t— (t) ?0?2 (1 +[?]?) == == (A[?]A' (p)) * [?][?][?][?][?] *e- ρ(rr) rc == == L 2 ± L 2 (1 - 6G2M2/L2) 2GM == == L 2 GM, 3GM!== ==[?] ([?]v[?]q * [?][?][?][?][?] * $e - r(rr)$ ==== $B + |a2'(t) > CQ2t|(t)$?0?2(1 + [?]?) ==== $(A[?]A'(p))$ (k) * [?][?][?][?][?] * $e - r(rr)$ ==== [?]$k1m$ * [?][?][?][?][?] * $e - r(rr)$ ==== [?]([?]v[?]q·[?]u[?]$p)^{CQ(a+)ta+\{1/12+(||a1'(t)>CQ1t|(t)>B+|a2'(t)>CQ2t|(t)?0?2(1+[?]?)====(A[?]A'(p))t|(t)}$ **(METHODS AND MATERI**

R**ESULTS**

In silico Prediction of the Roccustyrna ADMET Properties and Bioactivity Score

To predict important molecular properties such as logP, polar surface area, drug - likeness and bioactivity of our new prototype and small - sized Roccustyrna ligand 2 - ({ (fluoro ({((2E) - 5 - oxabicyclo (2.1.0)pentan - 2 - ylidene) cyano - lambda6 - sulfanyl})methyl) - phospho - rylidene} amino) - 4, 6 - dihydro - 1H - purin - 6 - one (1S, 2r, 3S) - 2 - ({((1S, 2S, 4S, 5r) - 4 - ethenyl - 4 - sulfonyl - bicyclo (1S, 2r, 3S) - 2 - ({ ((1S, 2S, 4S, 5r) - 4 - ethenyl - 4 - sulfonyl - bicyclo(3.2.0) heptan - 2 - yl) oxy} amino) - 3 - ((2r, 5r) - 5 - (2 - methyl - 6 - methylidene - 6, 9 - dihydro - 3H - purin - 9 - yl) - 3 - methylideneoxolan - 2 - yl) phosphirane - 1 - carbonitrile (3.2.0) heptan - 2 - yl) oxy} amino) - 3 - ((2r, 5r) - 5 - (2 - methyl - 6 - methylidene - 6, 9 - dihydro - 3H - purin - 9 - yl) - 3 - methyli deneoxolan - 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 (Table S1) , (Table S2) , (Table S3) , (Table S4) .

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

In this study, we have shown that the QMMM designed Roccustyrna small molecule which was designed in silico by using Topology Euclidean Geometric and Artificial Intelligence - Driven Predictive Neural Networks was engaged in the binding domains of the protein targets of of the (PDB:1xak) (Figure S2) with the docking energy values of (T.Energy, I.Energy, vdW, Coul, Numrotors, rMSD, Score) , (- 19.625, - 35.483, 7.633, - 43.116, 7, - 5.813) Kcal/mol, (Table S4) , (Table S5) The Roccustyrna chemical structure

interacted into the binding sites of the protein targets of (PDB:6w9c) ,(Figure S2) with the negative docking energies of the(T.Energy, I.Energy, vdW, Coul, Numrotors, rMSD, Score) , (- 36.678, - 55.648, - 7.519, - 48.129, 7, - 6.762) Kcal/Mol. The same combination of small molecules also generated hydrophobic interactions when docked onto the binding cavities of the amino acid of the 168 PrO, A1, 02J C with the docking energy values of (- 3.53, - 2369, - 1303, - 10.425, - 3.42, - 72.447, - 13.394, - 3.19, - 70.551) Kcal/mol. Our new QMMM designed cluster of quantum thinking small molecules additionally involved in the generation of the hydrogen bonding within the PJE: C:5 (PJE - 010) 010:C:6 Interacting chain (s) while generating hydrophobic interactions when docked into the binding domains of the amino acid of the 25THr, A6, 010 C with the docking energy values of (- 3.73, - 2415, 179, - 7.156, - 21.406, - 66.898 - 8.709, - 22.779) Kcal/mol. The combination of GisitorviffirnaTM, Roccustyrna_gs1_TM, and Roccustyrna_fr1_TM cluster of active pharmacophoric sites of the 2 - ({ (fluoro({ ((2E) - 5 - oxabicyclo(2.1.0) pentan - 2 - ylidene) cyano - lambda6 - sulfanyl}) methyl) phosphorylidene} amino) - 4, 6 - dihydro - 1H - purin - 6 - one(methylamino) - 1, 6 - diazabicyclo(3.2.0) heptan - 4 - yl) oxy} imino) interacted into the binding cavities of the amino acid of the 26 THr, A6 010C with the docking energy values of (- 3.81, - 2415, - 186, - 7.156, - 21.406, - 66.898, - 6.155, - 24.392, - 64.757) Kcal/mol. The combination of GisitorviffirnaTM, Roccustyrna_gs1_TM, and Roccustyrna_fr1_TM cluster of active pharmacophoric sites of the 2 - ({ (fluoro({ ((2E) - 5 - dimethyl - 7 - oxo - 4 - thia - 1 - azabicyclo (3.2.0) heptane - 2 - carbonyloxy) ({ ((2 - amino - 6 - oxo - 6,9 - dihydro - 3H - purin - 9 - yl) oxy) (hydroxy)phosphoryl} oxy) phosphinic acid - ylidene+,*cyano(2,6 - diazabicyclo*3.1.0+hex - 1 - oxabicyclo(2.1.0) pentan - 2 - ylidene) cyano - lambda6 - sulfanyl}) methyl) phosphor - rylidene} amino) - 4, 6 - dihydro - 1H - purin - 6 - onedihydro - 3H - purin - 9 - yl) - 3 - hydroxy - oxolan generated a docking effect which was involved in the generation of hydrogen bonds when docked into the binding cavities of the amino acid of 143 GLY A 6 010 C with the docking energy values of (- 62.905)Kcal/mol. In addition, the CoMFA contour map of electrostatic regions around Roccustyrna chemical structure indicated to us that contact residues from the Roccustyrna ligand when docked onto the SARS - COV - 2 protein targets of (PDB:2zu5) around the Roccustyrna chemical structure hit the entire sequence of the amino acid of the V - M - THr - 25, V - S - THr - 25, V - M - THr - 26, V - S - HIS - 41, V - M - LEU - 141, V - M - ASN - 142, V - S - ASN - 142, V - M - GLY - 143, V - S - CYS - 145, V - M - MET - 165 with the binding energy values of the - 97.2 and - 5.16512, - 4.15949, - 9.8487, - 4.77062, - 4.72901, - 6.7295, - 5.82428, - 5.35883, - 4.2588, - 5.37491 Kcal/mol respectively.(Figure S2d) The same prototype pharmacophoric elements named Roccustyrna when docked into the binding sites of the amino acid of the 164HIS, A5, PJE C2. generated hydrogen interactions with the binding energy values of the (- 16 3.07, - 153.73, - 2408) Kcal/mol/A, in the coupled atoms of the N3 and O2 with the docking energy values of (- 12.282, - 14.994, - 67.123 - 15.161, 15.336, 68.144) Kcal/Mol. The binding patterns of the 02J:C:1 (02J) active sites of the amino acid 168 PrO, A1, 02J C binding domains generated hydrophobic interactions with docking energy values of the (- 3.53, - 2369, - 1303, - 10.425, - 3.42, - 72.447, - 13.394, - 3.19, - 70.551)Kcal/mol/A inside the PJE:C:5 (PJE - 010) + 010:C:6 interacting chain (s) : A C of the amino acid of the 164HIS, A5, PJE C2. (Figure S3) D10 - C - 1099 DMS: A: 402(DMS) binding sites were also constructed when the combined pharmacophoric elements of the combination of GisitorviffirnaTM, Roccustyrna _gs1_TM, and Roccustyrna_fr1_TM ligands docked inside the (PDB: 6lu7) protein targets. Hydrogen Bonds were then identified when the RoccustyrnaTM's chemical coupled atoms interacted within the 298 ArG A amino acid 402 DMS A Ng+ 2377 O2 binding cavities with the docking energy values of (- 1.76, - 2.73, - 166.89, - 2331, - 6.971, - 0.756, - 7.541 - 9.7, - 0.883, - 7.581) Kcal/mol/A. Salt Bridges were also shown to be involved in the generation of the Sulfonium bonding when docked inside the DMS A 5.49 binding cavities within the 295 ASP A amino acid domains with the docking energy values of (- 402, - 2376, - 6.081, -6.367 -10.436, -2.231, -5.560) Kcal/mol/A. Pi - Cation Interactions of sulfonium bonding within our small molecule whole residue subsurface were also constructed within the amino acid 8 PHE A inside the 402 DMS A pharmacophoric sites with the docking energy values of (- 4.70, - 1.01, - 2376, - 6.081, - 6.367, - 8.339, - 4.556, - 4.264) Kcal/mo/A. (Figure S3), Hydrophobic Interactions were simultaneously generated by the Roccustyrna chemical residues when docked in the (PDB:6lu7) protein targets of inside the D10 - H - 1099. X77:A:401 (X77) side domains within the active sites of the amino acids of the 41 HIS A 401 X77 A, 165 MET A 401 X77 A, and 166 GLU A 401 X77 A with the docking

energy values of (- 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, - 18.9, - 3.90, - 4657, - 2881, - 21.763, - 15.894, - 23.429, - 24.934, - 13.635, - 23.312) Kcal/mol/A showing that my AI - quantum thinking chemical structure named Roccustyrna is capable of generating Hydrogen Bonds when docked onto the 41 HIS A 401 X77 A, 143 GLY A 401 X77 A, 144 SEr A 401 X77 A, and 166 GLU A 401 X77 A, sequence of amino acids while targeting the Npl 4680 N2, O3 4679 N2 Nam 4682 O2, and Nam 4683 O2 binding sites with the binding free energy values of the (- 3.46, - 3.79, - 106.13, - 611, - 20.860, - 19.573, - 32.52, - 19.394, - 16.086, - 32.767, - 2.17, - 2.94, - 148.03, - 2216 - 19.635, - 22.244, - 29.036 - 18.779, - 24.455, - 30.773, - 3.14, - 3.42, - 101.78, - 2228 - 16.096, - 21.679, - 26.816, - 14.503, - 23.707, - 29.056, - 1.98, - 2.80, - 158.32, - 2542 - 18.546, - 18.654, - 26.028 - 16.172, - 18.348, - 24.583) Kcal/molA respectively. (Figure S3) The 2 -({ (fluoro ({ ((2E) - 5 - oxabicyclo (2.1.0) pentan - 2 - ylidene)cyano - lambda6 - sulfanyl}) methyl)phosphorylidene} amino) - 4, 6 - dihydro - 1H - purin - 6 - one (1Z) - 2 - { ((2S, 3S, 5r) - 5 - (2 - amino - 6 - oxo - 6, 9 - dihydro - 1H - purin - 9 - yl) - 3 - hydroxyoxolan - 2 - yl) methylidene} - 2 - cyano - 1 - ({ ((2S, 4r, 5r) - 2 - methyl - 2 - (methylamino) - 1, 6 - diazabicyclo(3.2.0) heptan - 4 - yl) oxy} imino) - 1lambda5, 2lambda5 - azaphosphiridin - 1 - ylium druggable scaffold of the Roccustyrna small molecule therefore competes with endogenous SARS - CoV2 PLpro for binding to Lys711 and Arg355 targeting into the binding domains of the critical SARS - CoV2 PLpro residues onto the SARS - COV - 2 protein targets of(PDB:2zu5) within the binding sites of the amino acid of the V - M - THr - 25, V - S - THr - 25, V - M - THr - 26, V - S - HIS - 41, V - M - LEU - 141, V - M - ASN - 142, V - S - ASN - 142, V - M - GLY - 143, V - S - CYS - 145, V - M - MET - 165 with the binding energy values of the (- 97.2 and - 5.16512, - 4.15949, - 9.8487, - 4.77062, - 4.72901, - 6.7295, - 5.82428, - 5.35883, - 4.2588, - 5.37491) Kcal/mol respectively. CoMFA analysis of electrostatic regions around the Roccustyrna small molecule a chemical structure indicated to us that Hydrogen bonds, Salt bridges and Metal complexes containing Diphosphate, dihydrogen and ION binding sites were generated into the contact residues of the Roccustyrna's small molecule when docked onto the SARS - COV - 2 protein targets of the(PDB:2zu5) within the sequence of the amino acids of V - M - THr - 25, V - S - THr - 25, V - M - THr - 26, V - S - HIS - 41, V - M - LEU - 141, V - M - ASN - 142, V - S - ASN - 142, V - M - GLY - 143, V - S - CYS - 145, V - M - MET - 165 with the binding energy values of the negative docking values of the (- 97.2, and - 5.16512, - 4.15949, - 9.8487, - 4.77062, - 4.72901, - 6.7295, - 5.82428, - 5.35883, - 4.2588, - 5.37491) Kcal/mol/A respectively.(Figure S4a) , (Table S4), (Table S5) DMS:A:402 (DMS) binding sites into the 524 Nam 2578 O2 02J (5 - Methylisoxazole - 3 - carboxylic acid)domains were generated inside the 65 ASN A 402 DMS A cavities when RoccustyrnaTM drug deisgn interactred with the PDB:6lu7 protein targets with the docking energy values of (- 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 (- 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 interacted within the 403 DMS A contact residues of the binding sites of the 295 ASP amino acid with the docking energy values of (- 5.31, - 2581, - 6.227, - 1.042, - 6.293, - 10.460, - 2.019, - 5.344)Kcal/mol/A. (Figure S4) 999 ZN D 20947 Zn, ZN:A:998(ZN) , and 998 ZN A 20940 Zn 470 S Metal Complexes were also constructed into the 02J (5 - Methylisoxazole - 3 - carboxylic acid) PJE - C – 5 residues when the Roccustyrna's chemical fragment of (1Z) - 2 - { ((2S, 3S, 5r) - 5 - (2 - amino - 6 - oxo - 6, 9 - + - 6 - fluoro - 3, 4 - dihydropyrazine - 2 - carboxamide (7aR) - 5 - amino - N - * (S) - , 2 - * (3 - oxabicyclo(2.1.0) (1S, 4S) - 5 - oxabicyclo*2.1.0 +pentan - 2 ((2S, 5R, 6R) - 6 -((2S) - 2 - amino - 2 - phenylacetamido) - 3, 3 - dihydro - 1H - purin - 9 - yl - 4 - yl) oxy} - imino) - 1lambda5, 2lambda5 - azaphosphiridin - 1 - ylium generated tetrahedral side chains inside the 117 CYS D, 74 CYS A amino acids with the docking energy values of (- 1103.746, - 101.848, - 13.968, - 103.306, - 102.613, - 1118.874, - 104.964, - 32.313 - 118.938, - 103.573, - 30.6090Kcal/mol/A indicating that our multi - targeted drug design has the ability of generating a self - assembled monolayer inside the 1: Mg, NA (1) , 1, 10P, G Metal Complexes when docked onto the 1, 553A binding cavities of the amino acid of the ArG into the PDB:7bv2 protein targets. The combination of GisitorviffirnaTM, Roccustyrna_gs1_TM, and Roccustyrna_fr1_TM cluster of pharmacophoric (1Z) - 2

- { ((2S, 3S, 5r) - 5 - (2 - amino - 6 - 2 - yl)methylidene} - 2 - cyano - 12 - ({ (fluoro({ ((2E) - 5 - oxabicyclo(2.1.0) pentan - 2 - ylidene) cyano - lambda6 - sulfanyl}) methyl) phosphorylidene} amino) - 4, 6 - dihydro - 1H - purin - 6 - one - ({((2S, 4r, 5r) - 2 - methyl - 2 -(methylamino) - 1, 6 - dia - zabicyclo(3.2.0) heptan - 4 - yl) oxy} imino) - 1lambda5, 2lambda5 - azaphosphiridin - 1 - ylium active site of the 2 - lambda5 - azaphosphiridin - 1 - ylium was engaged in hydrogen bonding interactions with the formation of hydrogen bonds inside the N3 1266 O2 binding cavities within the amino acid sequence of V - S - HIS - 159, V - S - ARG - 160, V - S - ARG - 112 V - M - GLU - 148 V - M - PHE - 150, V - S - PHE - 150, V - S - HIS - 159, and V - M - TYR - 161 with the docking energy values of (- 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 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 (- 3.73, - 2415, - 179, - 7.156, - 21.406, - 66.898 - 8.709, - 22.779) Kcal/mol as illustrated in the (Figure S4). In this drug designing project the electrostatic regions around the combinationof GisitorviffirnaTM, Roccustyrna_gs1_TM, and Roccustyrna_fr1_ TM pharmacophoric elements of (7ar)- 5 - amino - N - ((S) - {2 - ((S)- ((E) - (amino - methylidene)amino) (cyano) methyl) hydrazin - 1 - yl}(aziridin - 1 - yl) phosphoryl) - 1 -((2E) - 2 - ((fluoro - methanimidoyl) imino) acetyl) - 7 - oxo - 1H, 7H, 7aH - pyrazolo (4, 3 - d) pyrimidine - 3 - carboxamide; N - { ((2 - amino - 6 - oxo - 6, 9 - dihydro - 1H - purin - 9 - yl) amino) ({1 - (5 -({ (cyano ({1 - ((diamino methylidene) amino) ethenyl})amino) oxy} methyl) - 3, 4 - dihydroxyoxolan - 2 - yl) - 1H - 1, 2, 4 - triazol - 3 - yl}(formamido) phosphoryl} - 6 - fluoro - 3, 4 - dihydropyrazine - 2 - carboxamide; (3 - (2 - amino - 5 - sulfanylidene - 1, 2, 4 - triazolidin - 3 - yl) oxaziridin - 2 - yl) ({3 - sulfanylidene - 1, 2, 4, 6 - tetraaza bicyclo(3.1.0) hexan - 6 - yl}) phosphoroso1 -(3, 4, 5 - trifluorooxolan - 2 - yl) - 1H - 1, 2, 4 - triazole - 3 - carboxylate 3 - hydroxyoxolan - 2 - yl)methylidene} - 2 - cyano - 1 - ({ ((2S, 4r, 5r) - 2 - methyl - 2 - (methylamino) - 1, 6 - diazabicyclo (3.2.0) heptan - 4 - yl) oxy} imino) - 1lambda5, 2 - lambda5 - azaphosphiridin - 1 - ylium(Figure S4a) , (Figure S4f) showing that the combination of GisitorviffirnaTM, Roccustyrna_gs1_TM, and Roccustyrna_fr1_TM binding site (s) inside the(PDB:6lu7) binding domains of the 02J:C:1(02J) regions while co - generating Hydrophobic Interactions and Hydrogen Bonds against the coupled atoms of the Nam 2411 O3 inside the cavities of the crucial entering amino acids of the 25 THr A 6 010 C and 143 GLY A 6 010 C with the docking energy values of(- 3.73, - 2415, - 179, - 7.156, - 21.406, - 66.898, - 8.709, - 22.779, - 70, - 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. Electrostatic CoMFA analysis of the contact residues of the best docking poses of the contact chemical residues indicated also that the entire Roccustyrna chemical structure when docked onto the SARS - COV - 2 protein targets of(PDB:3fqq) hits the positively charged SARS - CoV Mpro - N1 groups and SARS - CoV Mpro - N3 regions favored by negatively charged groups within the amino acid sequence 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 (- 101, - 14.0762, - 5.11094, - 7.98447, - 4.17314, - 4.43549, - 9.66939, - 9.42926, - 7.32)Kcal/mol/A. (Figure S2b) Other QSAR/CoMFA experiments have shown to us that the entire pharmacophoric residues of the Roccustyrna chemical design when docked onto the Mpro - N9 binding sites inside the SARS - COV - 2 protein targets of(PDB:6xs6) , interacted negatively with the Cys145 catalytic site of SARS - CoV - 2 Mpro charged groups within the sequence of the amino acid of V - M - LYS - 557, V - S - LYS - 557, V - M - ArG - 567, V - M - ASP - 568, V - S - ASP - 574, V - S - PHE - 43, V - M - ArG - 44, V - M - SEr - 45, and V - S - SEr - 45 with the docking energy values of (- 85.8, and - 5.56, - 8.38956, - 5.77168, - 6.13664, - 12.8661, - 5.37546, - 6.10391, - 5, 928) Kcal/mol respectively. (Figure S2c) Moreover, Cluster of the QSAR/QMMM/CoMFA map analysis of the electrostatic regions around the(rboximidoyl - 3 - fluoro - (1S, 4S) ((diaminomethylidene) amino) ethenyl})amino+oxy - methyl) - 3, 4 - dihydroxyoxolan - 2 - yl+ - 1, 2, 4 - triazol - 3 - yl - (formamido) phosphoryl + - 6 - fluoro - 3, 4 - dihydropyrazine - 2 - carboxamide(7ar) - 5 - amino - N - * (S) - , 2 - * (3 - oxabicyclo (2.1.0) (1S, 4S)- 5 - oxabicyclo*2.1.0 +pentan - 2 ((2S, 5r, 6r) - 6 -((2S) - 2 - amino - 2 - phenylacetamido) - 3, 3 -

dimethyl - 7 - oxo - 4 - thia - 1 - azabicyclo(3.2.0) heptane - 2 - carbonyloxy) ({((2 - amino - 6 - oxo - 6, 9 - dihydro - 3H - purin - 9 - yl) oxy) (hydroxy) phosphoryl} oxy)phosphinic acid - ylidene+, *cyano (2, 6 - diazabicyclo*3.1.0+hex - 1 - en - 6 - yl) (rboximidoyl - 3 - fluoro - (1S, 4S) ((diaminomethylidene)amino) ethenyl}) amino+oxy - methyl) - 3, 4 - dihydroxyoxolan - 2 - yl+ - 1, 2, 4 - triazol - 3 - yl -(formamido) phosphoryl + - 6 - fluoro - 3, 4 - dihydropyrazine - 2 - carboxamide (7ar) - 5 - amino - N - * (S) - , 2 - * (3 - { ((1S, 4S) - 5 - oxabicyclo (2.1.0) pentan - 2 - ylidene) { (cyano ({2, 6 - diazabicyclo(3.1.0) hex - 1 - en - 6 - yl}) phosphanyl -(fluoro) methyl} - lambda6 - sulfanyl}one pentan - 2 - ylidene) { (cyano ({2, 6 - diazabicyclo(3.1.0) hex - 1 - en - 6 - yl}) phosphanyl - lambda6 - (rboximidoyl - 3 - { ((1S,4S) - 5 - oxabicyclo (2.1.0) pentan - 2 - ylidene) {(cyano ({2,6 - diazabicyclo(3.1.0) hex - 1 - en - 6 - yl})phosphanyl) (fluoro) methyl} - lambda6 - su lfanyl}one (rboximidoyl - 3 - oxabicyclo(2.1.0) pentan - 2 - ylidene) {(cyano ({2,6 - diazabicyclo(3.1.0) hex - sulfanyl}oneboximidoyl - 3 - {((1S, 4S) - 5 - oxabicyclo (2.1.0)pentan - 2 - ylidene) contact residues of the Roccustyrna small molecule when docked onto the SARS - COV - 2 protein targets of(PDB:2ghv) after solving the (id[?][?][?][?][?] ε) * [?] == == [?]q?0 ¡ Ψ——T——Ψ ¿ (id[?][?][?][?][?] ε) * [?] == == (ε [?][?][?][?][?]id) e

$Z, z^{0:====[?][?]???rrH[?]M[?][?][?][?][?]H[?]N\ A[?](m0-xi)rA[?][?][?][?][?]???asparameterizedinputfor2/3[?]rrr^{0rr[?]rA[?]rA[?]rA?[?][?][?][?][?]ik4pZMA}$

DISCUSSIONS

We have shown in this note that the successful methods used in three dimensions to construct supersymetric chemical bridge extensions of general relativity can be generalized to any odd - dimensional spacetime when chemical reactions do not need to be considered in a simulation. We have restricted ourselves, however, to Poincar´e supergravity in terms of "bonded atoms", which have been distorted from some idealized geometry due to unbound van der Waals and Columbic interactions. The full antide Sitter extension remains an open problem when solving the Schrödinger equation for electron motions, since it requires an explicit description of chemical bonding and lots of information about the structures of molecules. In five dimensions, a Chern - Simons action for anti - de Sitter supergravity has been known for some time and since it can rely on force fields with fixed parameters, it is possible to provide better understanding of conformational analysis between conformers. That action reduces to the action considered here after a proper contraction is performed for mechanical deformation of DNA, RNA, and proteins, and changes in cellular structure, response, and function. There are good reasons to seek a full anti - de Sitter Chern - Simons formulation of supergravity. First, the bosonic Lagrangian in the Poincar´e case does not contain the Hilbert term thus making the contact with four dimensional theories rather obscure (6)**.**Secondly, the Poincar´e theory in odd dimensions does not possess black hole solutions while the anti - de Sitter theory does. In principle, a Chern - Simons anti - de Sitter supergravity can be constructed from the knowledge of the associated supergroup and an invariant tensor only(finding the invariant tensor, however, may prove to be a non - trivial task) . In five dimensions, the relevant supergroup is SU (2, 2|1) while in the important example of eleven dimensions the supergroup is OSp(32|1) . As the spacetime dimension increases, one faces a growing multiplicity of choices for the invariant tensor. The particular case of eleven dimensions seems to be particulary suited to admit an anti - de Sitter ChernSimons formulation. As shown, the super antide Sitter group is OSp (32|1) . A natural basis for the Lie algebra of Sp (32) is given by the Dirac matrices Γa, Γab, Γabcde, and this basis is easily extended to expand the superalgebra of OSp (32|1) .(42, 43, 47, 49) In this setup I have been discussing, I have managed to preserve the topological nature of CS theory while coupling to chemical space as infinitely massive sources at the expense of requiring the underlying 3 - manfiolds to generate my unique drug design with the highest docking energies of negative binding values when compared to other known SARS - CoV - 2 antivirals. In this context, the generalized fragments are viewed as external sources that have the ability to produce an effective description of quantum Hall effect, and can be coupled to the Chern - Simons theory. (44, 45, 48) It is probably true that the injudicious use involving the management of these quantum ideas or points can cause problems, it is also true that they do and should play an important role quantum mechanically in this drug discovery field (Figure S7),(Table S8), (Figure S8), (Table S9),(Figure S10), (Figure S11). **(METHODS AND MATERIALS)** (Scheme of Eqs.1 - 44) , (Group of Eqs.1 - 128) , (Cluster of Eqs.1 - 81) In this project, I implemented Inverse Docking Algorithms named EuTHTS Euclidean Topology Virtual Screening Algorithm with nonlinear electrodynamics for the designing of the combination

of GisitorviffirnaTM, Roccustyrna_gs1_TM, and Roccustyrna_fr1_TM ligands which generated the highest negative docking energies when compared to other FDA approved small molecules onto the SARS - COV - 2 protein targets. In this Schrödinger picture for the system minimum - energy of quantum mechanics the dynamics of quantum states for the ? (?0, ?) == == ? (?0) +? (?0, ?)and ? (?0, ?) == == ? (?0) +?(?0, ?) non - classical Shannon entropy is cryptografically governed by the system energy operator H : i[?]|? (?) ¿ /[?]? == == H |?(?) ¿ (42, 43, 44) which gives the following expression for the time derivative of the conditional probability ? (? (?) |?(?)) for nonzero Christoffel symbols for Schwarzschild in question: [?]? (? (?) | ?(?)) /[?]? == == {22? ?2?[?]?P ? (?)|[?]? (?) /[?]? ¿ (?) ?((??????, ??????) , ???????) == ==[?]?((??????, ??????) , ???????) ×log?(???????| (??????, ??????)) ?(???????) [?]? (??????, ??????) *?(???????| (??????, ??????)) xlog?(???????| (??????, ??????)) ?(???????) ?[?]?[?]?2[?]?[?]?1?

METHODS AND MATERIALS

Detailed methods are provided in the online version of this paper and include the following:

Lead contact

Data and code availability

EXPERIMENTAL MODEL AND SUBJECT DETAILS

P repa ration of the p rotein st ructu res

Sc reening NuBEE Phyto – lib ra ry, and COVID2019 ta rgets.

METHOD DETAILS

- **Biogenetoligandorol AI - heuristic (DFT) Generalized algorithm for Chern - Simons Weighted neuron () : [?] D[?] r2[?] S[?] r1 Topologies: A Quantum Hilbert space H attempt to put pharmacophoric elements back together.**
- **R occusty rna ligand: Docking Model, G rid points and P rotein ta rgets.**
- **In silico Bioactivity P rediction and ADMET Analysis of the** Roccustyrna **small molecule.**

ACKNOWLEDGMENTS

I would like to express my special thanks of gratitude to my teacher(George I Grigoriadis Pharmacist) who gave me the golden opportunity to do this wonderful project on the Quantum Chemistry topic, which also helped me in doing a lot of Research and I came to know about so many new things I am thankful to them.

AUTHOR CONTRIBUTIONS

Grigoriadis Ioannis's diverse contributions to the published work are accurate and agreed. Grigoriadis Ioannis has contributed to the below multiple roles:

- Conceptualization Ideas, formulation or evolution of overarching research goals and aims.
- Methodology, Development, or design of methodology; creation of models.
- Software, Programming, software development, designing computer programs, implementation of the computer code and supporting algorithms, and 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 otherfor mal techniques to analyze or synthesize study data.
- Investigation, conducting a research and investigation process, specifically perfor ming 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 necessaryfor interpreting the dataitself) 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 presentation of the published work by those from the original research group, specifically critical review, commentary, or revision including pre-or post-publication stages.
- Visualization, Preparation, creation, and presentation of the published work, specifically visualization/data presentation.
- Supervision, Oversight and leadership responsibility for the research activity planning and execution, including mentorship external to the core team.
- Project administration, Management, and coordination responsibility for the research activity planning, and execution.

DECLARATION OF INTERESTS

No potential competing interest was reported by the author.

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