Mahmoud E S Soliman

List of Publications by Year
in descending order

268	4,532	147801 31	182427 51
papers	citations	h-index	g-index

270	270	270	5679
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Deciphering the molecular mechanisms of selective non-covalency demonstrated differentially by 9-Allylnaphtho[1,8-ef]isoindole-7,8,10(9H)-trione (C11) against fibroblast growth factor receptors 1â€“4. Journal of Biomolecular Structure and Dynamics, 2023, 41, 2419-2430.	3.5	2
2	Impact of compound mutations I1171Nâ€‰+â€‰F1174I and I1171Nâ€‰+â€‰L1198H on the structure of ALK in NSCLC pathogenesis: atomistic insights. Journal of Biomolecular Structure and Dynamics, 2023, 41, 4735-4743.	3.5	6
3	Structural Insights into the Role of Pseudouridimycin Binding in Disruption of Bacterial RNA Polymerase Bridge Helix Conformational Arrangement. Current Pharmaceutical Biotechnology, 2023, 24, 562-569.	1.6	1
4	Comparative Dynamic Features of Apo and Bound MDM2 Protein Reveal the Mechanism of Inhibitor Recognition for Anti-Cancer Activity. Current Medicinal Chemistry, 2023, 30, 1193-1206.	2.4	0
5	Natural phyto, compounds as possible noncovalent inhibitors against SARS-CoV2 protease: computational approach. Journal of Biomolecular Structure and Dynamics, 2022, 40, 2284-2301.	3.5	19
6	In silico design and analysis of NS4B inhibitors against hepatitis C virus. Journal of Biomolecular Structure and Dynamics, 2022, 40, 1915-1929.	3.5	11
7	Weak spots inhibition in the Mycobacterium tuberculosis antigen 85C target for antitubercular drug design through selective irreversible covalent inhibitor-SER124. Journal of Biomolecular Structure and Dynamics, 2022, 40, 2934-2954.	3.5	12
8	In silico screening of phytopolyphenolics for the identification of bioactive compounds as novel protease inhibitors effective against SARS-CoV-2. Journal of Biomolecular Structure and Dynamics, 2022, 40, 10437-10453.	3.5	49
9	A meta-analysis of Cryptosporidium species in humans from southern Africa (2000â€“2020). Journal of Parasitic Diseases, 2022, 46, 304-316.	1.0	6
10	Ï€-hole interactions of group IIIâ€“VI elements with Ï€-systems and Lewis bases: a comparative study. Structural Chemistry, 2022, 33, 9-21.	2.0	9
11	Unusual chalcogenâ‹¯chalcogen interactions in likeâ‹¯like and unlike YîCîYâ‹¯YîCîY complexes (Y = O, S, and Se). Physical Chemistry Chemical Physics, 2022, 24, 3386-3399.	2.8	11
12	A synergistic multitargeted of BET and HDAC: an intra-molecular mechanism of communication in treatment of WaldenstrÃ¶m macroglobulinemia. Molecular Simulation, 2022, 48, 197-208.	2.0	3
13	Râ€¢-hole interactions of group IV-VII radical-containing molecules: A comparative study. Journal of Molecular Graphics and Modelling, 2022, 111, 108097.	2.4	5
14	Highlighting the mechanistic role of Olutasidenib (FT-2102) in the selective inhibition of mutated isocitrate dehydrogenase 1 (mIDH1) in cancer therapy. Informatics in Medicine Unlocked, 2022, 28, 100829.	3.4	8
15	Prioritizing the Catalytic Gatekeepers through Pan- Inhibitory Mechanism of Entrectinib against ALK, ROS1 and TRKA Tyrosine Kinases. Cell Biochemistry and Biophysics, 2022, 80, 11-21.	1.8	3
16	An Allosteric Inhibitory Potential of Triterpenes from Combretum racemosum on the Structural and Functional Dynamics of Plasmodium falciparum Lactate Dehydrogenase Binding Landscape. Chemistry and Biodiversity, 2022, 19, e202100646.	2.1	10
17	Dual enzymatic inhibitory mechanism of WM382 on plasmepsin IX and X: Atomistic perspectives from dynamic analysis. Informatics in Medicine Unlocked, 2022, 29, 100874.	3.4	1
18	Conjugated Dienones from Differently Substituted Cinnamaldehyde as Highly Potent Monoamine Oxidase-B Inhibitors: Synthesis, Biochemistry, and Computational Chemistry. ACS Omega, 2022, 7, 8184-8197.	3.5	10

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19	Simulation Models for Prediction of Bioavailability of Medicinal Drugsâ€"the Interface Between Experiment and Computation. AAPS PharmSciTech, 2022, 23, 86.	3.3	12
20	Multi-catalytic Sites Inhibition of Bcl2 Induces Expanding of Hydrophobic Groove: A New Avenue Towards WaldenstrÃ¶m Macroglobulinemia Therapy. Protein Journal, 2022, 41, 201-215.	1.6	2
21	Ïƒ-Hole and LP-Hole Interactions of PnicogenÂ·Â·Â·Pnicogen Homodimers under the External Electric Field Effect: A Quantum Mechanical Study. ACS Omega, 2022, 7, 11264-11275.	3.5	2
22	Nature-Inspired O-Benzyl Oxime-Based Derivatives as New Dual-Acting Agents Targeting Aldose Reductase and Oxidative Stress. Biomolecules, 2022, 12, 448.	4.0	11
23	Type Iâ€"IV Halogenâ‹¯Halogen Interactions: A Comparative Theoretical Study in Halobenzeneâ‹¯Halobenzene Homodimers. International Journal of Molecular Sciences, 2022, 23, 3114.	4.1	21
24	Lipid traits and type 2 diabetes risk in African ancestry individuals: A Mendelian Randomization study. EBioMedicine, 2022, 78, 103953.	6.1	23
25	Novel Sunifiram-carbamate hybrids as potential dual acetylcholinesterase inhibitor and NMDAR co-agonist: simulation-guided analogue design and pharmacological screening. Journal of Enzyme Inhibition and Medicinal Chemistry, 2022, 37, 1241-1256.	5.2	6
26	Inside the cracked kernel: establishing the molecular basis of AMG510 and MRTX849 in destabilising KRASG12C mutant switch I and II in cancer treatment. Journal of Biomolecular Structure and Dynamics, 2022, , 1-13.	3.5	4
27	External Electric Field Effect on the Strength of Ïƒ-Hole Interactions: A Theoretical Perspective in Likeâ‹¯Like Carbon-Containing Complexes. Molecules, 2022, 27, 2963.	3.8	4
28	Talazoparib Dual-targeting on Poly (ADP-ribose) Polymerase-1 and -16 Enzymes Offers a Promising Therapeutic Strategy in Small Cell Lung Cancer Therapy: Insight from Biophysical Computations. Cell Biochemistry and Biophysics, 2022, 80, 495-504.	1.8	2
29	From a Computational Perspective: Elucidating the Neurotherapeutic and Inhibitory properties of LRRK2 Kinase Domain by a benzothiazole-based compound. Current Pharmaceutical Biotechnology, 2022, 23, .	1.6	0
30	Revealing the role of fluorine pharmacophore in chalcone scaffold for shifting the MAO-B selectivity: investigation of a detailed molecular dynamics and quantum chemical study. Journal of Biomolecular Structure and Dynamics, 2021, 39, 6126-6139.	3.5	5
31	Molecular Basis of P131 Cryptosporidial-IMPDH Selectivityâ€"A Structural, Dynamical and Mechanistic Stance. Cell Biochemistry and Biophysics, 2021, 79, 11-24.	1.8	1
32	Investigating the Mechanistic Inhibitory Discrepancies of Novel Halogen and Alkyl Diâ€Substituted Oxadiazoleâ€Based Dibenzoâ€Azepineâ€Dione Derivatives on Poly (ADPâ€Ribose) Polymeraseâ€1. Chemistry and Biodiversity, 2021, 18, e2000802.	2.1	0
33	Could chroman-4-one derivative be a better inhibitor of PTR1? â€“ Reason for the identified disparity in its inhibitory potency in Trypanosoma brucei and Leishmania major. Computational Biology and Chemistry, 2021, 90, 107412.	2.3	4
34	Design, synthesis, and evaluation of â€œdual-siteâ€•binding diarylpyrimidines targeting both NNIBP and the NNRTI adjacent site of the HIV-1 reverse transcriptase. European Journal of Medicinal Chemistry, 2021, 211, 113063.	5.5	15
35	Functional Analysis of Single Nucleotide Polymorphism in ZUFSP Protein and Implication in Pathogenesis. Protein Journal, 2021, 40, 28-40.	1.6	1
36	A Mechanistic Probe into the Dual Inhibition of T. cruzi Glucokinase and Hexokinase in Chagas Disease Treatment â€“ A Stone Killing Two Birds?. Chemistry and Biodiversity, 2021, 18, e2000863.	2.1	1

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37	A probable means to an end: exploring P131 pharmacophoric scaffold to identify potential inhibitors of Cryptosporidium parvum inosine monophosphate dehydrogenase. Journal of Molecular Modeling, 2021, 27, 35.	1.8	2
38	Update and Potential Opportunities in CBP [Cyclic Adenosine Monophosphate (cAMP) Response Element-Binding Protein (CREB)-Binding Protein] Research Using Computational Techniques. Protein Journal, 2021, 40, 19-27.	1.6	4
39	Transcription-translation error: In-silico investigation of the structural and functional impact of deleterious single nucleotide polymorphisms in GULP1 gene. Informatics in Medicine Unlocked, 2021, 22, 100503.	3.4	0
40	Exploring the effect of ritonavir and TMC-310911 on SARS-CoV-2 and SARS-CoV main proteases: potential from a molecular perspective. Future Science OA, 2021, 7, FSO640.	1.9	3
41	East to West not North-West: Structure-Based Mechanistic Resolution of 8-Hydroxyl Replacement and Resulting Effects on the Activities of Imidazole-Based Heme Oxygenase-1 Inhibitors. Protein Journal, 2021, 40, 166-174.	1.6	1
42	Piecing the fragments together: Dynamical insights into the enhancement of BRD4-BD1 (BET protein) druggability in cancer chemotherapy using novel 8-methyl-pyrrolo[1,2-a]pyrazin-1(2H)-one derivatives. Current Pharmaceutical Biotechnology, 2021, 22, .	1.6	0
43	Targeting Protein Degradation in Cancer Treatment. Current Chemical Biology, 2021, 15, 5-18.	0.5	0
44	Piece of the puzzle: Remdesivir disassembles the multimeric SARS-CoV-2 RNA-dependent RNA polymerase complex. Cell Biochemistry and Biophysics, 2021, 79, 175-187.	1.8	6
45	Distinguishing the optimal binding mechanism through reversible and irreversible inhibition analysis of HSP72 protein in cancer therapy. Computers in Biology and Medicine, 2021, 132, 104301.	7.0	1
46	Development of Halogenated Pyrazolines as Selective Monoamine Oxidase-B Inhibitors: Deciphering via Molecular Dynamics Approach. Molecules, 2021, 26, 3264.	3.8	9
47	Immunoinformatics prediction of potential B-cell and T-cell epitopes as effective vaccine candidates for eliciting immunogenic responses against Epsteinâ€“Barr virus. Biomedical Journal, 2021, 44, 317-337.	3.1	11
48	Dualâ€Knockout of Mutant Isocitrate Dehydrogenase 1 and 2 Subtypes Towards Glioma Therapy: Structural Mechanistic Insights on the Role of Vorasidenib. Chemistry and Biodiversity, 2021, 18, e2100110.	2.1	7
49	Leveraging on Active Site Similarities; Identification of Potential Inhibitors of Zinc-Finger and UFSP domain Protein (ZUFSP). Current Pharmaceutical Biotechnology, 2021, 22, 995-1004.	1.6	0
50	On the Potentiality of X-T-X₃ Compounds (T = C, Si, and Ge, and X = F, Cl, and Br) as Tetrel- and Halogen-Bond Donors. ACS Omega, 2021, 6, 19330-19341.	3.5	11
51	Prospecting the therapeutic edge of a novel compound (B12) over berberine in the selective targeting of Retinoid X Receptor in colon cancer. Journal of Molecular Modeling, 2021, 27, 231.	1.8	6
52	Comparison of irreversible inhibition targeting HSP72 protein: the resurgence of covalent drug developments. Molecular Simulation, 2021, 47, 1093-1103.	2.0	2
53	Blue Biotechnology: Computational Screening of Sarcophyton Cembranoid Diterpenes for SARS-CoV-2 Main Protease Inhibition. Marine Drugs, 2021, 19, 391.	4.6	22
54	Insight into the Therapeutic Potential of a Bicyclic Hydroxypyridone Compound 2â€[(2,4â€Dichlorophenyl)methyl]â€7â€hydroxyâ€1,2,3,4â€tetrahydroâ€8 H â€pyrido[1,2â€•a]pyrazinâ€8â€one as COMT Inhibitor in the Treatment of Parkinson's Disease: A Molecular Dynamic Simulation Approach. Chemistry and Biodiversity, 2021, 18, e2100204.	2.1	2

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55	The Binding of Remdesivir to SARS-CoV-2 RNA-Dependent RNA Polymerase May Pave The Way Towards the Design of Potential Drugs for COVID-19 Treatment. Current Pharmaceutical Biotechnology, 2021, 22, 1520-1537.	1.6	4
56	Unveiling the mechanistic roles of chlorine substituted phthalazinone-based compounds containing chlorophenyl moiety towards the differential inhibition of poly (ADP-ribose) polymerase-1 in the treatment of lung cancer. Journal of Biomolecular Structure and Dynamics, 2021, , 1-9.	3.5	1
57	Closing the Gap: An Atomistic Structural and Functional Perspective of S. mansoni Universal Stress G4LZI3 Protein in Complex with Phenolic Compounds. Current Drug Discovery Technologies, 2021, 18, e01102020186453.	1.2	0
58	Effect of External Electric Field on Tetrel Bonding Interactions in (FTF₃Â·Â·Â·FH) Complexes (T) Tj ETQq0 0 0 rgBT /Overlock	3.5	9
59	Structure-based identification of novel scaffolds as potential HIV-1 entry inhibitors involving CCR5. Journal of Biomolecular Structure and Dynamics, 2021, , 1-12.	3.5	0
60	Diagnostic, Prognostic and Therapeutic Potential of Heat Shock Proteins in Schistosomiasis and Bladder Cancer: A Review. Letters in Drug Design and Discovery, 2021, 18, 650-665.	0.7	2
61	Glioma-Targeted Therapeutics: Computer-Aided Drug Design Prospective. Protein Journal, 2021, 40, 601-655.	1.6	9
62	Selective SIRT2 inhibitors as promising anticancer therapeutics: An update from 2016 to 2020. European Journal of Medicinal Chemistry, 2021, 224, 113709.	5.5	16
63	Structural alterations in the catalytic core of hSIRT2 enzyme predict therapeutic benefits of Garcinia mangostana derivatives in Alzheimer's disease: molecular dynamics simulation study. RSC Advances, 2021, 11, 8003-8018.	3.6	7
64	Atomistic insights into the selective therapeutic activity of 6-(2,4-difluorophenoxy)-5-((ethylmethyl)pyridine-3-yl)-8-methylpyrrolo[1,2-a]pyrazin-1(2H)-one towards bromodomain-containing proteins. Computational Biology and Chemistry, 2021, 95, 107592.	2.3	0
65	Mechanistic Insights into the Selective Dual BET and PLK1 Inhibitory Activity of a Novel Benzamide Compound in Castrationâ€Resistant Prostrate Cancer. Chemistry and Biodiversity, 2021, 18, e2100519.	2.1	1
66	Ïƒâ€Hole Interactions of Tetrahedral Group IVâ€“VIII Lewis Acid Centers with Lewis Bases: A Comparative Study. ChemistrySelect, 2021, 6, 11856-11864.	1.5	5
67	Genome-Wide Association and Mendelian Randomization Analysis Reveal the Causal Relationship Between White Blood Cell Subtypes and Asthma in Africans. Frontiers in Genetics, 2021, 12, 749415.	2.3	4
68	Dualâ€Inhibition of Human N â€Myristoyltransferase Subtypes Halts Common Cold Pathogenesis: Atomistic Perspectives from the Case of IMPâ€1088**. Chemistry and Biodiversity, 2021, , .	2.1	1
69	Dual targeting approach for Mycobacterium tuberculosis drug discovery: insights from DFT calculations and molecular dynamics simulations. Structural Chemistry, 2020, 31, 557-571.	2.0	12
70	An analogue of a kinase inhibitor exhibits subjective characteristics that contribute to its inhibitory activities as a potential anti-cancer candidate: insights through computational biomolecular modelling of UM-164 binding with lyn protein. RSC Advances, 2020, 10, 145-161.	3.6	11
71	Human Rhinovirus Inhibition Through Capsid â€œCanyonâ€•Perturbation: Structural Insights into The Role of a Novel Benzothiophene Derivative. Cell Biochemistry and Biophysics, 2020, 78, 3-13.	1.8	9
72	Leaving no stone unturned: Allosteric targeting of SARS-CoV-2 spike protein at putative druggable sites disrupts human angiotensin-converting enzyme interactions at the receptor binding domain. Informatics in Medicine Unlocked, 2020, 21, 100451.	3.4	17

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73	Probing the Highly Disparate Dual Inhibitory Mechanisms of Novel Quinazoline Derivatives against Mycobacterium tuberculosis Protein Kinases A and B. Molecules, 2020, 25, 4247.	3.8	1
74	A brief overview on recent advances in spiro[chromane-2,4â€²-piperidine]-4(3H)-one-functionalized compounds in medicinal chemistry research. Bioorganic and Medicinal Chemistry, 2020, 28, 115813.	3.0	16
75	Computational and drug target analysis of functional single nucleotide polymorphisms associated with Haemoglobin Subunit Beta (HBB) gene. Computers in Biology and Medicine, 2020, 125, 104018.	7.0	1
76	Identification of potential SARS-CoV-2 inhibitors from South African medicinal plant extracts using molecular modelling approaches. South African Journal of Botany, 2020, 133, 273-284.	2.5	24
77	Supramolecular self-assembled drug delivery system (SADDs) of vancomycin and tocopherol succinate as an antibacterial agent: inÂvitro, in silico and inÂvivo evaluations. Pharmaceutical Development and Technology, 2020, 25, 1090-1108.	2.4	7
78	Formulation of pH-Responsive Quatsomes from Quaternary Bicephalic Surfactants and Cholesterol for Enhanced Delivery of Vancomycin against Methicillin Resistant Staphylococcus aureus. Pharmaceutics, 2020, 12, 1093.	4.5	21
79	Natural Products Database Screening for the Discovery of Naturally Occurring SARSâ€Covâ€2 Spike Glycoprotein Blockers. ChemistrySelect, 2020, 5, 13309-13317.	1.5	24
80	Coupling of HSP72 Î±-Helix Subdomains by the Unexpected Irreversible Targeting of Lysine-56 over Cysteine-17; Coevolution of Covalent Bonding. Molecules, 2020, 25, 4239.	3.8	0
81	â€˜Polymorphism-aidedâ€™ Selective Targeting and Inhibition of Caspase-6 by a Novel Allosteric Inhibitor Towards Efficient Alzheimerâ€™s Disease Treatment. Cell Biochemistry and Biophysics, 2020, 78, 291-299.	1.8	1
82	Druggability and drug-likeness concepts in drug design: are biomodelling and predictive tools having their say?. Journal of Molecular Modeling, 2020, 26, 120.	1.8	45
83	Antibiotic resistance: bioinformatics-based understanding as a functional strategy for drug design. RSC Advances, 2020, 10, 18451-18468.	3.6	45
84	Thompson loop: opportunities for antitubercular drug design by targeting the weak spot in demethylmenaquinone methyltransferase protein. RSC Advances, 2020, 10, 23466-23483.	3.6	14
85	Delving into the Characteristic Features of â€œMenaceâ€•Mycobacterium tuberculosis Homologs: A Structural Dynamics and Proteomics Perspectives. Protein Journal, 2020, 39, 118-132.	1.6	7
86	Covalent Versus Non-covalent Enzyme Inhibition: Which Route Should We Take? A Justification of the Good and Bad from Molecular Modelling Perspective. Protein Journal, 2020, 39, 97-105.	1.6	36
87	Exploring the ring potential of 2,4-diaminopyrimidine derivatives towards the identification of novel caspase-1 inhibitors in Alzheimerâ€™s disease therapy. Journal of Molecular Modeling, 2020, 26, 68.	1.8	16
88	Lipidâ€Embedded Molecular Dynamics Simulation Model for Exploring the Reverse Prostaglandin D2 Agonism of CTâ€133 towards CRTH2 in the Treatment of Typeâ€2 Inflammation Dependent Diseases. Chemistry and Biodiversity, 2020, 17, e1900548.	2.1	4
89	The Dual-Targeting Activity of the Metabolite Substrate of Para-amino Salicyclic Acid in the Mycobacterial Folate Pathway: Atomistic and Structural Perspectives. Protein Journal, 2020, 39, 106-117.	1.6	2
90	Triple Mycobacterial ATP-synthase mutations impedes Bedaquiline binding: Atomistic and structural perspectives. Computational Biology and Chemistry, 2020, 85, 107204.	2.3	7

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91	InÂvitro, in silico studies of newly isolated tetrahydro-4-(7-hydroxy-10-methoxy-6,) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 747 boonei stem bark. Journal of Molecular Structure, 2020, 1216, 128225.	3.6	3
92	Exploring the Role of Asp1116 in Selective Drug Targeting of CREBcAMP- Responsive Element-binding Protein Implicated in Prostate Cancer. Combinatorial Chemistry and High Throughput Screening, 2020, 23, 178-184.	1.1	5
93	Integrating Bioinformatics Strategies in Cancer Immunotherapy: Current and Future Perspectives. Combinatorial Chemistry and High Throughput Screening, 2020, 23, 687-698.	1.1	7
94	Tweaking Î±-Galactoceramides: Probing the Dynamical Mechanisms of Improved Recognition for Invariant Natural Killer T-cell Receptor in Cancer Immunotherapeutics. Current Pharmaceutical Biotechnology, 2020, 21, 1354-1367.	1.6	2
95	Zoning in on Tankyrases: A Brief Review on the Past, Present and Prospective Studies. Anti-Cancer Agents in Medicinal Chemistry, 2020, 19, 1920-1934.	1.7	2
96	In Silico Repurposing of J147 for Neonatal Encephalopathy Treatment: Exploring Molecular Mechanisms of Mutant Mitochondrial ATP Synthase. Current Pharmaceutical Biotechnology, 2020, 21, 1551-1566.	1.6	5
97	Withdrawal Notice: Elucidating the Disparate Inhibitory Mechanisms of Novel 1-Heteroaryl-1,3-Propanediamine Derivatives and Maraviroc towards C-C Chemokine Receptor 5: Insights for Structural Modifications in HIV-1 Drug Discovery. Medicinal Chemistry, 2020, 17, .	1.5	1
98	DFT Study of the Structural and Electronic Properties of Selected Organogold(III) Compounds with Characteristic Anticancer Activity. Russian Journal of Physical Chemistry A, 2019, 93, 1543-1558.	0.6	15
99	Probing Binding Landscapes and Molecular Recognition Mechanisms of Atypical Antipsychotic Drugs towards the Selective Targeting of D₂ Dopamine Receptor. Molecular Informatics, 2019, 38, e1900044.	2.5	5
100	From genomic variation to protein aberration: Mutational analysis of single nucleotide polymorphism present in ULBP6 gene and implication in immune response. Computers in Biology and Medicine, 2019, 111, 103354.	7.0	7
101	â€˜Piperaziningâ€™ the catalytic gatekeepers: unraveling the pan-inhibition of SRC kinases; LYN, FYN and BLK by masitinib. Future Medicinal Chemistry, 2019, 11, 2365-2380.	2.3	2
102	CF3â€Pyridinyl Substitution on Antimalarial Therapeutics: Probing Differential Ligand Binding and Dynamical Inhibitory Effects of a Novel Triazolopyrimidineâ€Based Inhibitor onPlasmodium falciparumDihydroorotate Dehydrogenase. Chemistry and Biodiversity, 2019, 16, e1900365.	2.1	12
103	Selective Covalent Inhibition of â€œAllosteric Cys121â€•Distort the Binding of PTP1B Enzyme: A Novel Therapeutic Approach for Cancer Treatment. Cell Biochemistry and Biophysics, 2019, 77, 203-211.	1.8	13
104	Tracing Potential Covalent Inhibitors of an E3 Ubiquitin Ligase through Target-Focused Modelling. Molecules, 2019, 24, 3125.	3.8	4
105	Identification of highly potent and selective Cdc25 protein phosphatases inhibitors from miniaturization click-chemistry-based combinatorial libraries. European Journal of Medicinal Chemistry, 2019, 183, 111696.	5.5	26
106	Unveiling a New Era in Malaria Therapeutics: A Tailored Molecular Approach Towards the Design of Plasmepsin IX Inhibitors. Protein Journal, 2019, 38, 616-627.	1.6	11
107	The irony of chirality â€“ unveiling the distinct mechanistic binding and activities of 1-(3-(4-amino-5-(7-methoxy-5-methylbenzo[b]thiophen-2-yl)-7H-pyrrolo[2,3-d]pyrimidin-7-yl)pyrrolidin-1-yl)prop-2-e enantiomers as irreversible covalent FGFR4 inhibitors. Organic and Biomolecular Chemistry, 2019, 17, 1176-1190.	2.8	24
108	Molecular mechanism of resveratrol inhibition of Zika virus NS3 helicase: behind the scenes. Future Virology, 2019, 14, 73-84.	1.8	5

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109	Halting ionic shuttle to disrupt the synthetic machineryâ€"Structural and molecular insights into the inhibitory roles of Bedaquiline towards Mycobacterium tuberculosis ATP synthase in the treatment of tuberculosis. Journal of Cellular Biochemistry, 2019, 120, 16108-16119.	2.6	9
110	Revealing the distinct mechanistic binding and activity of 5-(1-(3,5-dichloropyridin-4-yl)ethoxy)-3-(5-(4-methylpiperazin-1-yl)-1H-benzo[d]imidazol-2-yl)-1H-indazole enantiomers against FGFR1. Physical Chemistry Chemical Physics, 2019, 21, 15120-15132.	2.8	6
111	Drug promiscuity: Exploring the polypharmacology potential of 1, 3, 6-trisubstituted 1, 4-diazepane-7-ones as an inhibitor of the â€˜god fatherâ€™ of immune checkpoint. Computational Biology and Chemistry, 2019, 80, 433-440.	2.3	14
112	Deciphering the canonical blockade of activated Hageman factor (FXIIa) by benzamidine in the coagulation cascade: A thorough dynamical perspective. Chemical Biology and Drug Design, 2019, 94, 1905-1918.	3.2	2
113	Broadening the horizon: Integrative pharmacophore-based and cheminformatics screening of novel chemical modulators of mitochondria ATP synthase towards interventive Alzheimerâ€™s disease therapy. Medical Hypotheses, 2019, 130, 109277.	1.5	12
114	Deciphering the â€˜Elixir of Lifeâ€™: Dynamic Perspectives into the Allosteric Modulation of Mitochondrial ATP Synthase by J147, a Novel Drug in the Treatment of Alzheimer's Disease. Chemistry and Biodiversity, 2019, 16, e1900085.	2.1	12
115	A Synergistic Combination Against Chronic Myeloid Leukemia: An Intra-molecular Mechanism of Communication in BCRâ€“ABL1 Resistance. Protein Journal, 2019, 38, 142-150.	1.6	3
116	Recruiting monomer for dimer formation: resolving the antagonistic mechanisms of novel immune check point inhibitors against Programmed Death Ligand-1 in cancer immunotherapy. Molecular Simulation, 2019, 45, 777-789.	2.0	17
117	Distinguishing the optimal binding mechanism of an E3 ubiquitin ligase: Covalent versus noncovalent inhibition. Journal of Cellular Biochemistry, 2019, 120, 12859-12869.	2.6	4
118	From a computational point of view: deciphering the molecular synergism between oxidative stress-induced lipid peroxidation products and metabolic dysfunctionality of human liver mitochondrial aldehyde dehydrogenase-2. Molecular Simulation, 2019, 45, 652-665.	2.0	1
119	Tracing Potential Covalent Inhibitors of an E3 Ubiquitin Ligase Through Target-Focused Modelling. Proceedings (mdpi), 2019, 22, 103.	0.2	0
120	Dynamic perspectives into the mechanisms of mutationâ€induced p53â€DNA binding loss and inactivation using active perturbation theory: Structural and molecular insights toward the design of potent reactivators in cancer therapy. Journal of Cellular Biochemistry, 2019, 120, 951-966.	2.6	18
121	Probing Gallate-Mediated Selectivity and High-Affinity Binding of Epigallocatechin Gallate: a Way-Forward in the Design of Selective Inhibitors for Anti-apoptotic Bcl-2 Proteins. Applied Biochemistry and Biotechnology, 2019, 187, 1061-1080.	2.9	24
122	Covalent vs. Nonâ€Covalent Inhibition: Tackling Drug Resistance in EGFR â€“ A Thorough Dynamic Perspective. Chemistry and Biodiversity, 2019, 16, e1800518.	2.1	8
123	Noteworthy effect of slight variation in aliphatic chain length of trisubstituted imidazole inhibitors against epidermal growth factor receptor L858R/T790M/C797S mutant in cancer therapy. Chemical Biology and Drug Design, 2019, 93, 798-810.	3.2	7
124	Probing the Dynamic Mechanism of Uncommon Allosteric Inhibitors Optimized to Enhance Drug Selectivity of SHP2 with Therapeutic Potential for Cancer Treatment. Applied Biochemistry and Biotechnology, 2019, 188, 260-281.	2.9	11
125	A dual target of Plasmepsin IX and X: Unveiling the atomistic superiority of a core chemical scaffold in malaria therapy. Journal of Cellular Biochemistry, 2019, 120, 7876-7887.	2.6	16
126	Domperidone nanocrystals with boosted oral bioavailability: fabrication, evaluation and molecular insight into the polymer-domperidone nanocrystal interaction. Drug Delivery and Translational Research, 2019, 9, 284-297.	5.8	32

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127	Microbes, not humans: exploring the molecular basis of Pseudouridimycin selectivity towards bacterial and not human RNA polymerase. Biotechnology Letters, 2019, 41, 115-128.	2.2	7
128	Navigating Research Toward the Re-emerging Nipah Virus- A New Piece to the Puzzle. Current Pharmaceutical Design, 2019, 25, 1392-1401.	1.9	1
129	Same Target, Different Therapeutic Outcomes: The Case of CAY10471 and Fevipiprant on CRTh2 Receptor in Treatment of Allergic Rhinitis and Asthma. Combinatorial Chemistry and High Throughput Screening, 2019, 22, 521-533.	1.1	7
130	Exploring the Lapse in Druggability: Sequence Analysis, Structural Dynamics and Binding Site Characterization of K-RasG12C Variant, a Feasible Oncotherapeutics Target. Anti-Cancer Agents in Medicinal Chemistry, 2019, 18, 1540-1550.	1.7	7
131	Turning to Computer-aided Drug Design in the Treatment of Diffuse Large B-cell Lymphoma: Has it been Helpful?. Anti-Cancer Agents in Medicinal Chemistry, 2019, 19, 1325-1339.	1.7	2
132	From the Explored to the Unexplored: Computer-Tailored Drug Design Attempts in the Discovery of Selective Caspase Inhibitors. Combinatorial Chemistry and High Throughput Screening, 2019, 22, 432-444.	1.1	4
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