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	Metal complexes in cancer therapy – an update from drug design perspective. Drug Design, Development and Therapy, 2017, Volume11, 599-616.	4.3	668
2	Theory and Applications of Covalent Docking in Drug Discovery: Merits and Pitfalls. Molecules, 2015, 20, 1984-2000.	3.8	112
3	Integrated Approach to Structure-Based Enzymatic Drug Design: Molecular Modeling, Spectroscopy, and Experimental Bioactivity. Chemical Reviews, 2014, 114, 493-537.	47.7	100
4	Recent advancements in the development of anti-tuberculosis drugs. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 370-386.	2.2	97
5	Exploration of chlorinated thienyl chalcones: A new class of monoamine oxidase-B inhibitors. International Journal of Biological Macromolecules, 2016, 91, 680-695.	7.5	69
6	Co-encapsulation of multi-lipids and polymers enhances the performance of vancomycin in lipidâ€“polymer hybrid nanoparticles: In vitro and in silico studies. Materials Science and Engineering C, 2016, 61, 616-630.	7.3	64
7	Zika virus NS5 protein potential inhibitors: an enhanced in silico approach in drug discovery. Journal of Biomolecular Structure and Dynamics, 2018, 36, 1118-1133.	3.5	61
8	Ultra-small lipid-dendrimer hybrid nanoparticles as a promising strategy for antibiotic delivery: In vitro and in silico studies. International Journal of Pharmaceutics, 2016, 504, 1-10.	5.2	55
9	An integrated molecular dynamics, principal component analysis and residue interaction network approach reveals the impact of M184V mutation on HIV reverse transcriptase resistance to lamivudine. Molecular BioSystems, 2014, 10, 2215-2228.	2.9	52
10	Across the blood-brain barrier: Neurotherapeutic screening and characterization of naringenin as a novel CRMP-2 inhibitor in the treatment of Alzheimer's disease using bioinformatics and computational tools. Computers in Biology and Medicine, 2018, 98, 168-177.	7.0	49
11	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
12	The impact of Thr91 mutation on c-Src resistance to UM-164: molecular dynamics study revealed a new opportunity for drug design. Molecular BioSystems, 2017, 13, 1157-1171.	2.9	48
13	Can We Rely on Computational Predictions To Correctly Identify Ligand Binding Sites on Novel Protein Drug Targets? Assessment of Binding Site Prediction Methods and a Protocol for Validation of Predicted Binding Sites. Cell Biochemistry and Biophysics, 2017, 75, 15-23.	1.8	46
14	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
15	Antibiotic resistance: bioinformatics-based understanding as a functional strategy for drug design. RSC Advances, 2020, 10, 18451-18468.	3.6	45
16	Monoamine oxidase inhibitory activity of 2-aryl-4H-chromen-4-ones. Bioorganic Chemistry, 2015, 58, 72-80.	4.1	41
17	Pharmacophore-Based 3D-QSAR Analysis of Thienyl Chalcones as a New Class of Human MAO-B Inhibitors: Investigation of Combined Quantum Chemical and Molecular Dynamics Approach. Journal of Physical Chemistry B, 2017, 121, 1186-1203.	2.6	40
18	Î³-Cyclodextrin capped silver nanoparticles for molecular recognition and enhancement of antibacterial activity of chloramphenicol. Journal of Inorganic Biochemistry, 2016, 157, 15-24.	3.5	39

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19	Quantum mechanics implementation in drug-design workflows: does it really help?. Drug Design, Development and Therapy, 2017, Volume 11, 2551-2564.	4.3	39
20	From mutational inactivation to aberrant gainâ€ofâ€function: Unraveling the structural basis of mutant p53 oncogenic transition. Journal of Cellular Biochemistry, 2018, 119, 2646-2652.	2.6	39
21	Synthesis and structural studies of pentacycloundecane-based HIV-1 PR inhibitors: A hybrid 2D NMR and docking/QM/MM/MD approach. European Journal of Medicinal Chemistry, 2011, 46, 3976-3985.	5.5	38
22	Reversible versus irreversible inhibition modes of ERK2: a comparative analysis for ERK2 protein kinase in cancer therapy. Future Medicinal Chemistry, 2018, 10, 1003-1015.	2.3	38
23	Per-Residue Energy Footprints-Based Pharmacophore Modeling as an Enhanced In Silico Approach in Drug Discovery: A Case Study on the Identification of Novel Î²-Secretase1 (BACE1) Inhibitors as Anti-Alzheimer Agents. Cellular and Molecular Bioengineering, 2016, 9, 175-189.	2.1	37
24	Computational mutagenesis reveals the role of active-site tyrosine in stabilising a boat conformation for the substrate: QM/MM molecular dynamics studies of wild-type and mutant xylanases. Organic and Biomolecular Chemistry, 2009, 7, 460-468.	2.8	36
25	Structural insights into the South African HIV-1 subtype C protease: impact of hinge region dynamics and flap flexibility in drug resistance. Journal of Biomolecular Structure and Dynamics, 2013, 31, 1370-1380.	3.5	36
26	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
27	Implementing QM in docking calculations: is it a waste of computational time?. Drug Discovery Today, 2017, 22, 1216-1223.	6.4	35
28	A perspective on targeting non-structural proteins to combat neglected tropical diseases: Dengue, West Nile and Chikungunya viruses. European Journal of Medicinal Chemistry, 2014, 87, 677-702.	5.5	34
29	New drug design with covalent modifiers. Expert Opinion on Drug Discovery, 2016, 11, 79-90.	5.0	33
30	Investigation of flap flexibility of Î²-secretase using molecular dynamic simulations. Journal of Biomolecular Structure and Dynamics, 2016, 34, 1008-1019.	3.5	33
31	An unexplored remarkable PNIPAM-osmolyte interaction study: An integrated experimental and simulation approach. Journal of Colloid and Interface Science, 2017, 504, 417-428.	9.4	33
32	Pentacycloundecane-based inhibitors of wild-type C-South African HIV-protease. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 2274-2277.	2.2	32
33	Comparison of the Molecular Dynamics and Calculated Binding Free Energies for Nine FDAâ€Approved HIVâ€1 PR Drugs Against Subtype B and Câ€SA HIV PR. Chemical Biology and Drug Design, 2013, 81, 208-218.	3.2	32
34	Induced Mutation Proves a Potential Target for TB Therapy: A Molecular Dynamics Study on LprG. Cell Biochemistry and Biophysics, 2018, 76, 345-356.	1.8	32
35	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
36	Flap dynamics of plasmepsin proteases: insight into proposed parameters and molecular dynamics. Molecular BioSystems, 2015, 11, 1061-1066.	2.9	31

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37	Anti-oxidant behavior of functionalized chalcone-a combined quantum chemical and crystallographic structural investigation. Journal of Molecular Structure, 2017, 1146, 301-308.	3.6	31
38	Mechanism of glycoside hydrolysis: A comparative QM/MM molecular dynamics analysis for wild type and Y69F mutant retaining xylanases. Organic and Biomolecular Chemistry, 2009, 7, 5236.	2.8	28
39	Possible allosteric binding site on Gyrase B, a key target for novel anti-TB drugs: homology modelling and binding site identification using molecular dynamics simulation and binding free energy calculations. Medicinal Chemistry Research, 2015, 24, 2055-2074.	2.4	28
40	Delving into Zika virus structural dynamics â€“ a closer look at NS3 helicase loop flexibility and its role in drug discovery. RSC Advances, 2017, 7, 22133-22144.	3.6	28
41	Co-inhibition as a strategic therapeutic approach to overcome rifampin resistance in tuberculosis therapy: atomistic insights. Future Medicinal Chemistry, 2018, 10, 1665-1675.	2.3	27
42	Multi-drug resistance profile of PR20 HIV-1 protease is attributed to distorted conformational and drug binding landscape: molecular dynamics insights. Journal of Biomolecular Structure and Dynamics, 2016, 34, 135-151.	3.5	26
43	Polyelectrolyte complex of vancomycin as a nanoantibiotic: Preparation, in vitro and in silico studies. Materials Science and Engineering C, 2016, 63, 489-498.	7.3	26
44	A comparative molecular dynamics study on BACE1 and BACE2 flap flexibility. Journal of Receptor and Signal Transduction Research, 2016, 36, 505-514.	2.5	26
45	Allosteric inhibition abrogates dysregulated LFA-1 activation: Structural insight into mechanisms of diminished immunologic disease. Computational Biology and Chemistry, 2018, 73, 49-56.	2.3	26
46	Ligand- and structure-basedin silicostudies to identify kinesin spindle protein (KSP) inhibitors as potential anticancer agents. Journal of Biomolecular Structure and Dynamics, 2018, 36, 3687-3704.	3.5	26
47	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
48	Chikungunya virus (CHIKV) inhibitors from natural sources: a medicinal chemistry perspective. Journal of Natural Medicines, 2015, 69, 451-462.	2.3	25
49	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- enantiomers as irreversible covalent FGFR4 inhibitors. Organic and Biomolecular Chemistry, 2019, 17, 1176-1190.	2.8	24
50	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
51	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
52	Natural Products Database Screening for the Discovery of Naturally Occurring SARSâ€Covâ€2 Spike Glycoprotein Blockers. ChemistrySelect, 2020, 5, 13309-13317.	1.5	24
53	Dynamics of the thumb-finger regions in a GH11 xylanase Bacillus circulans: comparison between the Michaelis and covalent intermediate. RSC Advances, 2015, 5, 82381-82394.	3.6	23
54	Characterization of Thienylchalcones as hMAOâ€B Inhibitors: Synthesis, Biochemistry and Molecular Dynamics Studies. ChemistrySelect, 2017, 2, 11113-11119.	1.5	23

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55	Lipid traits and type 2 diabetes risk in African ancestry individuals: A Mendelian Randomization study. EBioMedicine, 2022, 78, 103953.	6.1	23
56	Pentacycloundecane derived hydroxy acid peptides: A new class of irreversible non-scissile ether bridged type isoster as potential HIV-1 wild type C-SA protease inhibitors. Bioorganic Chemistry, 2012, 40, 19-29.	4.1	22
57	Zika virus drug targets: a missing link in drug design and discovery â€“ a route map to fill the gap. RSC Advances, 2016, 6, 68719-68731.	3.6	22
58	Blue Biotechnology: Computational Screening of Sarcophyton Cembranoid Diterpenes for SARS-CoV-2 Main Protease Inhibition. Marine Drugs, 2021, 19, 391.	4.6	22
59	Flap flexibility amongst plasmepsins I, II, III, IV, and V: Sequence, structural, and molecular dynamics analyses. Proteins: Structure, Function and Bioinformatics, 2015, 83, 1693-1705.	2.6	21
60	Per-residue energy decomposition pharmacophore model to enhance virtual screening in drug discovery: a study for identification of reverse transcriptase inhibitors as potential anti-HIV agents. Drug Design, Development and Therapy, 2016, 10, 1365.	4.3	21
61	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
62	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
63	Allosteric inhibition induces an open WPD-loop: a new avenue towards glioblastoma therapy. RSC Advances, 2018, 8, 40187-40197.	3.6	20
64	Synthesis, 2D-NMR and molecular modelling studies of pentacycloundecane lactam-peptides and peptoids as potential HIV-1 wild type C-SA protease inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2013, 28, 78-88.	5.2	19
65	A critical survey of average distances between catalytic carboxyl groups in glycoside hydrolases. Proteins: Structure, Function and Bioinformatics, 2014, 82, 1747-1755.	2.6	19
66	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
67	Potential Ebola drug targets â€" filling the gap: a critical step forward towards the design and discovery of potential drugs. Biologia (Poland), 2017, 72, 1-13.	1.5	18
68	Preparation and Optimization of Meropenem-Loaded Solid Lipid Nanoparticles: In Vitro Evaluation and Molecular Modeling. AAPS PharmSciTech, 2017, 18, 2011-2025.	3.3	18
69	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
70	Comprehensive Computational and Experimental Analysis of Biomaterial toward the Behavior of Imidazolium-Based Ionic Liquids: An Interplay between Hydrophilic and Hydrophobic Interactions. Journal of Physical Chemistry B, 2017, 121, 4909-4922.	2.6	17
71	Characterizing the ligand-binding landscape of Zika NS3 helicase-promising lead compounds as potential inhibitors. Future Virology, 2017, 12, 261-273.	1.8	17
72	Ebola virus: A gap in drug design and discovery â€•experimental and computational perspective. Chemical Biology and Drug Design, 2017, 89, 297-308.	3.2	17

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73	Does Size Really Matter? Probing the Efficacy of Structural Reduction in the Optimization of Bioderived Compounds â€“ A Computational â€œProof-of-Conceptâ€• Computational and Structural Biotechnology Journal, 2018, 16, 573-586.	4.1	17
74	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
75	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
76	Synthesis and molecular modelling studies of novel carbapeptide analogs for inhibition of HIV-1 protease. European Journal of Medicinal Chemistry, 2012, 53, 13-21.	5.5	16
77	A Hybrid Structure/Pharmacophoreâ€Based Virtual Screening Approach to Design Potential Leads: A Computerâ€Aided Design of <scp>S</scp>outh <scp>A</scp>frican <scp>HIV</scp>â€1 Subtype <scp>C</scp> Protease Inhibitors. Drug Development Research, 2013, 74, 283-295.	2.9	16
78	Identification of Novel <scp>G</scp>yrase <scp>B</scp> Inhibitors as Potential Antiâ€TB drugs: Homology Modelling, Hybrid Virtual Screening and Molecular Dynamics Simulations. Chemical Biology and Drug Design, 2013, 82, 205-215.	3.2	16
79	Identification of irreversible protein splicing inhibitors as potential anti-TB drugs: insight from hybrid non-covalent/covalent docking virtual screening and molecular dynamics simulations. Medicinal Chemistry Research, 2014, 23, 2312-2323.	2.4	16
80	Sliding Clamp of DNA Polymerase III as a Drug Target for TB Therapy: Comprehensive Conformational and Binding Analysis from Molecular Dynamic Simulations. Cell Biochemistry and Biophysics, 2016, 74, 473-481.	1.8	16
81	Non-active site mutations disturb the loop dynamics, dimerization, viral budding and egress of VP40 of the Ebola virus. Molecular BioSystems, 2017, 13, 585-597.	2.9	16
82	An update on the discovery and development of selective heat shock protein inhibitors as anti-cancer therapy. Expert Opinion on Drug Discovery, 2018, 13, 903-918.	5.0	16
83	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
84	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
85	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
86	Selective SIRT2 inhibitors as promising anticancer therapeutics: An update from 2016 to 2020. European Journal of Medicinal Chemistry, 2021, 224, 113709.	5.5	16
87	Synthesis, screening and computational investigation of pentacycloundecane-peptoids as potent CSA-HIV PR inhibitors. European Journal of Medicinal Chemistry, 2012, 57, 459-467.	5.5	15
88	Pentacycloundecaneâ€diolâ€Based HIVâ€1 Protease Inhibitors: Biological Screening, 2<scp>Dâ€…</scp>NMR, and Molecular Simulation Studies. ChemMedChem, 2012, 7, 1009-1019.	3.2	15
89	Compensatory Role of Double Mutation N348I/M184V on Nevirapine Binding Landscape: Insight from Molecular Dynamics Simulation. Protein Journal, 2014, 33, 432-446.	1.6	15
90	Single H5N1 influenza A neuraminidase mutation develops resistance to oseltamivir due to distorted conformational and drug binding landscape: multiple molecular dynamics analyses. RSC Advances, 2015, 5, 10849-10861.	3.6	15

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91	Egress and invasion machinery of malaria: an in-depth look into the structural and functional features of the flap dynamics of plasmepsin IX and X. RSC Advances, 2018, 8, 21829-21840.	3.6	15
92	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
93	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
94	Synergistic Interplay of The Co-administration of Rifampin And Newly Developed Anti-TB Drug: Could It Be a Promising New Line of TB Therapy?. Combinatorial Chemistry and High Throughput Screening, 2018, 21, 453-460.	1.1	15
95	Heatâ€Shock Protein 90 (Hsp90) as Anticancer Target for Drug Discovery: An Ample Computational Perspective. Chemical Biology and Drug Design, 2015, 86, 1131-1160.	3.2	14
96	Adenosine Monophosphate-Activated Protein Kinase (AMPK) as a Diverse Therapeutic Target: A Computational Perspective. Applied Biochemistry and Biotechnology, 2016, 178, 810-830.	2.9	14
97	Novel quinazolinone-based 2,4-thiazolidinedione-3-acetic acid derivatives as potent aldose reductase inhibitors. Future Medicinal Chemistry, 2017, 9, 2147-2166.	2.3	14
98	Targeting HCV polymerase: a structural and dynamic perspective into the mechanism of selective covalent inhibition. RSC Advances, 2018, 8, 42210-42222.	3.6	14
99	Exploring the Câ€Terminal Tail Dynamics: Structural and Molecular Perspectives into the Therapeutic Activities of Novel CRMPâ€2 Inhibitors, Naringenin and Naringeninâ€7â€Oâ€glucuronide, in the Treatment of Alzheimer's Disease. Chemistry and Biodiversity, 2018, 15, e1800437.	2.1	14
100	Bioinformatics-based tools in drug discovery: the cartography from single gene to integrative biological networks. Drug Discovery Today, 2018, 23, 1658-1665.	6.4	14
101	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
102	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
103	Integrated Computational Tools for Identification of CCR5 Antagonists as Potential HIV-1 Entry Inhibitors: Homology Modeling, Virtual Screening, Molecular Dynamics Simulations and 3D QSAR Analysis. Molecules, 2014, 19, 5243-5265.	3.8	13
104	Antipyrineâ€“gamma cyclodextrin inclusion complex: Molecular modeling, preparation, characterization and cytotoxicity studies. Journal of Molecular Structure, 2015, 1089, 38-47.	3.6	13
105	Molecular Dynamics Simulations of Ligandâ€Induced Flap Conformational Changes in Cathepsinâ€Dâ€”A Comparative Study. Journal of Cellular Biochemistry, 2016, 117, 2643-2657.	2.6	13
106	Synthesis, characterization and molecular modelling of a novel dipyridamole supramolecule â€“ X-ray structure, quantum mechanics and molecular dynamics study to comprehend the hydrogen bond structureâ€“activity relationship. Journal of Molecular Structure, 2016, 1105, 194-204.	3.6	13
107	Diabetes mellitus caused by mutations in human insulin: analysis of impaired receptor binding of insulinsWakayama,Los AngelesandChicagousing pharmacoinformatics. Journal of Biomolecular Structure and Dynamics, 2017, 35, 724-737.	3.5	13
108	Sequence, Structural Analysis and Metrics to Define the Unique Dynamic Features of the Flap Regions Among Aspartic Proteases. Protein Journal, 2017, 36, 385-396.	1.6	13

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109	In Silico SAR Studies of HIV-1 Inhibitors. Pharmaceuticals, 2018, 11, 69.	3.8	13
110	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
111	Therapeutic, Molecular and Computational Aspects of Novel Monoamine Oxidase (MAO) Inhibitors. Combinatorial Chemistry and High Throughput Screening, 2017, 20, 492-509.	1.1	13
112	Homology Modeling in Drug Discovery-an Update on the Last Decade. Letters in Drug Design and Discovery, 2017, 14, .	0.7	13
113	Target-Bound Generated Pharmacophore Model to Improve the Pharmacophore-Based Virtual Screening: Identification of G-Protein Coupled Human CCR2 Receptors Inhibitors as Anti-Inflammatory Drugs. Cellular and Molecular Bioengineering, 2014, 7, 45-57.	2.1	12
114	The binding landscape of plasmepsin V and the implications for flap dynamics. Molecular BioSystems, 2016, 12, 1457-1467.	2.9	12
115	Alcohol Metabolic Inefficiency: Structural Characterization of Polymorphism-Induced ALDH2 Dysfunctionality and Allosteric Site Identification for Design of Potential Wildtype Reactivators. Protein Journal, 2018, 37, 216-222.	1.6	12
116	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
117	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
118	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
119	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
120	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
121	Covalent Inhibition in Drug Discovery: Filling the Void in Literature. Current Topics in Medicinal Chemistry, 2018, 18, 1135-1145.	2.1	12
122	Simulation Models for Prediction of Bioavailability of Medicinal Drugsâ€”the Interface Between Experiment and Computation. AAPS PharmSciTech, 2022, 23, 86.	3.3	12
123	Understanding the cross-resistance of oseltamivir to H1N1 and H5N1 influenza A neuraminidase mutations using multidimensional computational analyses. Drug Design, Development and Therapy, 2015, 9, 4137.	4.3	11
124	Hybrid Receptor-Bound/MM-GBSA-Per-residue Energy-Based Pharmacophore Modelling: Enhanced Approach for Identification of Selective LTA4H Inhibitors as Potential Anti-inflammatory Drugs. Cell Biochemistry and Biophysics, 2017, 75, 35-48.	1.8	11
125	Dynamics of allosteric modulation ofÂlymphocyte function associated antigen-1 closure-open switch: unveiling the structural mechanisms associated with outside-in signaling activation. Biotechnology Letters, 2017, 39, 1843-1851.	2.2	11
126	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

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127	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
128	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
129	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
130	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
131	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
132	Unusual chalcogenâ‹¯chalcogen interactions in likeâ‹¯like and unlike Yî€Cî€¥â‹¯Yî€Cî€¥ complexes (Y = O, S, and Se). Physical Chemistry Chemical Physics, 2022, 24, 3386-3399.	2.8	11
133	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
134	Emergence of a Promising Lead Compound in the Treatment of Triple Negative Breast Cancer: An Insight into Conformational Features and Ligand Binding Landscape of c-Src Protein with UM-164. Applied Biochemistry and Biotechnology, 2018, 185, 655-675.	2.9	10
135	Dual Drug Targeting of Mutant Bcrâ€Abl Induces Inactive Conformation: New Strategy for the Treatment of Chronic Myeloid Leukemia and Overcoming Monotherapy Resistance. Chemistry and Biodiversity, 2018, 15, e1700533.	2.1	10
136	Discovery of new class of methoxy carrying isoxazole derivatives as COX-II inhibitors: Investigation of a detailed molecular dynamics study. Journal of Molecular Structure, 2018, 1157, 19-28.	3.6	10
137	Anti-cancer Glycosidase Inhibitors from Natural Products: A Computational and Molecular Modelling Perspective. Anti-Cancer Agents in Medicinal Chemistry, 2015, 15, 933-946.	1.7	10
138	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
139	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
140	Linear and cyclic glycopeptide as HIV protease inhibitors. European Journal of Medicinal Chemistry, 2013, 60, 144-154.	5.5	9
141	VP40 of the Ebola Virus as a Target for EboV Therapy: Comprehensive Conformational and Inhibitor Binding Landscape from Accelerated Molecular Dynamics. Cell Biochemistry and Biophysics, 2017, 75, 65-78.	1.8	9
142	Identification of Binding Mode and Prospective Structural Features of Novel Nef Protein Inhibitors as Potential Anti-HIV Drugs. Cell Biochemistry and Biophysics, 2017, 75, 49-64.	1.8	9
143	Covalent simulations of covalent/irreversible enzyme inhibition in drug discovery: a reliable technical protocol. Future Medicinal Chemistry, 2018, 10, 2265-2275.	2.3	9
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