

# Mutasem O. Taha

## List of Publications by Year in descending order

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149  
papers

3,519  
citations

156536

32  
h-index

214428

50  
g-index

151  
all docs

151  
docs citations

151  
times ranked

4142  
citing authors

#	ARTICLE	IF	CITATIONS
1	Degradability of chitosan micro/nanoparticles for pulmonary drug delivery. <i>Heliyon</i> , 2019, 5, e01684.	1.4	163
2	Comprehensive Structural and Molecular Comparison of Spike Proteins of SARS-CoV-2, SARS-CoV and MERS-CoV, and Their Interactions with ACE2. <i>Cells</i> , 2020, 9, 2638.	1.8	138
3	Inhibition of dipeptidyl peptidase IV (DPP IV) is one of the mechanisms explaining the hypoglycemic effect of berberine. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2009, 24, 1061-1066.	2.5	117
4	Synthesis of Chitosan Succinate and Chitosan Phthalate and Their Evaluation as Suggested Matrices in Orally Administered, Colon-Specific Drug Delivery Systems. <i>Archiv Der Pharmazie</i> , 1999, 332, 103-107.	2.1	92
5	Pharmacophore Modeling, Quantitative Structure-Activity Relationship Analysis, and in Silico Screening Reveal Potent Glycogen Synthase Kinase-3 $\beta$ Inhibitory Activities for Cimetidine, Hydroxychloroquine, and Gemifloxacin. <i>Journal of Medicinal Chemistry</i> , 2008, 51, 2062-2077.	2.9	90
6	Stable Chitosan-Based Nanoparticles Using Polyphosphoric Acid or Hexametaphosphate for Tandem Ionotropic/Covalent Crosslinking and Subsequent Investigation as Novel Vehicles for Drug Delivery. <i>Frontiers in Bioengineering and Biotechnology</i> , 2020, 8, 4.	2.0	87
7	Inhibition of glycogen synthase kinase by curcumin: Investigation by simulated molecular docking and subsequent <i>in vitro</i> / <i>in vivo</i> evaluation. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2009, 24, 771-778.	2.5	82
8	Synthesis of iron-crosslinked chitosan succinate and iron-crosslinked hydroxamated chitosan succinate and their <i>in vitro</i> evaluation as potential matrix materials for oral theophylline sustained-release beads. <i>European Journal of Pharmaceutical Sciences</i> , 2001, 13, 159-168.	1.9	80
9	Combining Ligand-Based Pharmacophore Modeling, Quantitative Structure-Activity Relationship Analysis and in Silico Screening for the Discovery of New Potent Hormone Sensitive Lipase Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2008, 51, 6478-6494.	2.9	78
10	Discovery of new potent human protein tyrosine phosphatase inhibitors via pharmacophore and QSAR analysis followed by <i>in silico</i> screening. <i>Journal of Molecular Graphics and Modelling</i> , 2007, 25, 870-884.	1.3	77
11	Discovery of new MurF inhibitors via pharmacophore modeling and QSAR analysis followed by <i>in-silico</i> screening. <i>Bioorganic and Medicinal Chemistry</i> , 2008, 16, 1218-1235.	1.4	66
12	Elaborate ligand-based pharmacophore exploration and QSAR analysis guide the synthesis of novel pyridinium-based potent $\beta$ -secretase inhibitory leads. <i>Bioorganic and Medicinal Chemistry</i> , 2010, 18, 3088-3115.	1.4	66
13	Docking-Based Comparative Intermolecular Contacts Analysis as New 3-D QSAR Concept for Validating Docking Studies and in Silico Screening: NMT and GP Inhibitors as Case Studies. <i>Journal of Chemical Information and Modeling</i> , 2011, 51, 647-669.	2.5	65
14	Discovery of DPP IV Inhibitors by Pharmacophore Modeling and QSAR Analysis followed by <i>in-silico</i> Screening. <i>ChemMedChem</i> , 2008, 3, 1763-1779.	1.6	60
15	Regression of endometrial implants treated with vitamin D3 in a rat model of endometriosis. <i>European Journal of Pharmacology</i> , 2013, 715, 72-75.	1.7	59
16	Pharmacophore Modeling, Quantitative Structure-Activity Relationship Analysis, and Shape-Complemented in Silico Screening Allow Access to Novel Influenza Neuraminidase Inhibitors. <i>Journal of Chemical Information and Modeling</i> , 2009, 49, 978-996.	2.5	58
17	Enhanced drug encapsulation and extended release profiles of calcium alginate nanoparticles by using tannic acid as a bridging cross-linking agent. <i>Journal of Microencapsulation</i> , 2015, 32, 96-105.	1.2	57
18	Ligand-based assessment of factor Xa binding site flexibility via elaborate pharmacophore exploration and genetic algorithm-based QSAR modeling. <i>European Journal of Medicinal Chemistry</i> , 2005, 40, 701-727.	2.6	52

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19	Sodium lauryl sulfate impedes drug release from zinc-crosslinked alginate beads: Switching from enteric coating release into biphasic profiles. <i>International Journal of Pharmaceutics</i> , 2008, 350, 291-300.	2.6	52
20	Discovery of potent inhibitors of pseudomonal quorum sensing via pharmacophore modeling and in silico screening. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2006, 16, 5902-5906.	1.0	51
21	Discovery of new cholesteryl ester transfer protein inhibitors via ligand-based pharmacophore modeling and QSAR analysis followed by synthetic exploration. <i>European Journal of Medicinal Chemistry</i> , 2010, 45, 1598-1617.	2.6	51
22	Elaborate Ligand-Based Modeling Coupled with Multiple Linear Regression and k Nearest Neighbor QSAR Analyses Unveiled New Nanomolar mTOR Inhibitors. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 2587-2612.	2.5	50
23	Elaborate Ligand-Based Modeling Reveals New Nanomolar Heat Shock Protein 90 $\pm$ Inhibitors. <i>Journal of Chemical Information and Modeling</i> , 2010, 50, 1706-1723.	2.5	42
24	$\hat{1}^2$ -Caryophyllene causes regression of endometrial implants in a rat model of endometriosis without affecting fertility. <i>European Journal of Pharmacology</i> , 2013, 702, 12-19.	1.7	42
25	Discovery of novel CDK1 inhibitors by combining pharmacophore modeling, QSAR analysis and in silico screening followed by in vitro bioassay. <i>European Journal of Medicinal Chemistry</i> , 2010, 45, 4316-4330.	2.6	40
26	Reported Adverse Effects and Attitudes among Arab Populations Following COVID-19 Vaccination: A Large-Scale Multinational Study Implementing Machine Learning Tools in Predicting Post-Vaccination Adverse Effects Based on Predisposing Factors. <i>Vaccines</i> , 2022, 10, 366.	2.1	39
27	Pharmacophore modeling, homology modeling, and in silico screening reveal mammalian target of rapamycin inhibitory activities for sotalol, glyburide, metipranolol, sulfamethizole, glipizide, and pioglitazone. <i>Journal of Molecular Graphics and Modelling</i> , 2013, 42, 39-49.	1.3	38
28	Pharmacophore and QSAR modeling of estrogen receptor $\hat{1}^2$ ligands and subsequent validation and in silico search for new hits. <i>Journal of Molecular Graphics and Modelling</i> , 2010, 28, 383-400.	1.3	37
29	Berberine potently inhibits protein tyrosine phosphatase 1B: Investigation by docking simulation and experimental validation. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2006, 21, 163-171.	2.5	34
30	Olanzapine inhibits glycogen synthase kinase-3 $\hat{1}^2$ : An investigation by docking simulation and experimental validation. <i>European Journal of Pharmacology</i> , 2008, 584, 185-191.	1.7	33
31	Elaborate ligand-based modeling reveal new submicromolar Rho kinase inhibitors. <i>Journal of Computer-Aided Molecular Design</i> , 2012, 26, 249-266.	1.3	33
32	The use of docking-based comparative intermolecular contacts analysis to identify optimal docking conditions within glucokinase and to discover of new GK activators. <i>Journal of Computer-Aided Molecular Design</i> , 2014, 28, 509-547.	1.3	33
33	Thujone corrects cholesterol and triglyceride profiles in diabetic rat model. <i>Natural Product Research</i> , 2011, 25, 1180-1184.	1.0	32
34	Synthesis and in vitro behavior of iron-crosslinked N-methyl and N-benzyl hydroxamated derivatives of alginate as controlled release carriers. <i>European Polymer Journal</i> , 2006, 42, 2464-2474.	2.6	31
35	Elaborate ligand-based modeling coupled with QSAR analysis and in silico screening reveal new potent acetylcholinesterase inhibitors. <i>Journal of Computer-Aided Molecular Design</i> , 2013, 27, 1075-1092.	1.3	31
36	Evaluation of naproxen and cromolyn activities against cancer cells viability, proliferation, apoptosis, p53 and gene expression of survivin and caspase-3. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2014, 29, 153-161.	2.5	31

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37	Discovery of new nanomolar peroxisome proliferator-activated receptor $\gamma$ activators via elaborate ligand-based modeling. <i>European Journal of Medicinal Chemistry</i> , 2011, 46, 2513-2529.	2.6	30
38	Application of docking-based comparative intermolecular contacts analysis to validate Hsp90 docking studies and subsequent in silico screening for inhibitors. <i>Journal of Molecular Modeling</i> , 2012, 18, 4843-4863.	0.8	30
39	Discovery of nanomolar phosphoinositide 3-kinase gamma (PI3K $\gamma$ ) inhibitors using ligand-based modeling and virtual screening followed by in vitro analysis. <i>European Journal of Medicinal Chemistry</i> , 2014, 84, 454-465.	2.6	27
40	Novel nanoparticles based on chitosan-dicarboxylate conjugates via tandem ionotropic/covalent crosslinking with tripolyphosphate and subsequent evaluation as drug delivery vehicles. <i>International Journal of Pharmaceutics</i> , 2017, 529, 15-31.	2.6	27
41	Effects of Variable Docking Conditions and Scoring Functions on Corresponding Protein-Aligned Comparative Molecular Field Analysis Models Constructed from Diverse Human Protein Tyrosine Phosphatase 1B Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2005, 48, 8016-8034.	2.9	26
42	In Silico Screening for Non-nucleoside HIV-1 Reverse Transcriptase Inhibitors Using Physicochemical Filters and High-throughput Docking Followed by In Vitro Evaluation. <i>Chemical Biology and Drug Design</i> , 2009, 74, 258-265.	1.5	25
43	QSAR studies in the discovery of novel type-II diabetic therapies. <i>Expert Opinion on Drug Discovery</i> , 2016, 11, 197-214.	2.5	25
44	Exploring the influence of culture conditions on kefir's anticancer properties. <i>Journal of Dairy Science</i> , 2018, 101, 3771-3777.	1.4	24
45	Effect of Ionic Crosslinking on the Drug Release Properties of Chitosan Diacetate Matrices. <i>Journal of Pharmaceutical Sciences</i> , 2007, 96, 38-43.	1.6	23
46	Combining docking, scoring and molecular field analyses to probe influenza neuraminidase ligand interactions. <i>Journal of Molecular Graphics and Modelling</i> , 2007, 26, 443-456.	1.3	23
47	Discovery of New Antifungal Leads via Pharmacophore Modeling and QSAR Analysis of Fungal Myristoyl Transferase Inhibitors Followed by In Silico Screening. <i>Chemical Biology and Drug Design</i> , 2011, 78, 391-407.	1.5	23
48	Elaborate ligand-based modeling and subsequent synthetic exploration unveil new nanomolar Ca <sup>2+</sup> /calmodulin-dependent protein kinase II inhibitory leads. <i>Bioorganic and Medicinal Chemistry</i> , 2012, 20, 377-400.	1.4	23
49	Naproxen and Cromolyn as New Glycogen Synthase Kinase $\beta$ Inhibitors for Amelioration of Diabetes and Obesity: An Investigation by Docking Simulation and Subsequent In Vitro/In Vivo Biochemical Evaluation. <i>Journal of Biochemical and Molecular Toxicology</i> , 2013, 27, 425-436.	1.4	23
50	Combining docking-based comparative intermolecular contacts analysis and k-nearest neighbor correlation for the discovery of new check point kinase 1 inhibitors. <i>Journal of Computer-Aided Molecular Design</i> , 2015, 29, 561-581.	1.3	23
51	Combining molecular dynamics simulation and ligand-receptor contacts analysis as a new approach for pharmacophore modeling: beta-secretase 1 and check point kinase 1 as case studies. <i>Journal of Computer-Aided Molecular Design</i> , 2016, 30, 1149-1163.	1.3	22
52	Natural and semisynthetic polymers in pharmaceutical nanotechnology. , 2018, , 35-100.		22
53	Computational modeling of the bat HKU4 coronavirus 3CL <sup>pro</sup> inhibitors as a tool for the development of antivirals against the emerging Middle East respiratory syndrome (MERS) coronavirus. <i>Journal of Molecular Recognition</i> , 2017, 30, e2644.	1.1	21
54	Discovery of new PKN2 inhibitory chemotypes via QSAR-guided selection of docking-based pharmacophores. <i>Molecular Diversity</i> , 2023, 27, 443-462.	2.1	21

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55	Synthesis and biological activity assays of some new N1-(flavon-7-yl)amidrazone derivatives and related congeners. <i>European Journal of Medicinal Chemistry</i> , 2012, 54, 65-74.	2.6	20
56	Antiproliferative activity of the isoindigo 5-Br in HL-60 cells is mediated by apoptosis, dysregulation of mitochondrial functions and arresting cell cycle at G0/G1 phase. <i>Cancer Letters</i> , 2015, 361, 251-261.	3.2	20
57	Effect of particle morphology and pore size on the release kinetics of ephedrine from mesoporous MCM-41 materials. <i>Journal of Porous Materials</i> , 2012, 19, 825-833.	1.3	19
58	Sunitinib as an anti-endometriotic agent. <i>European Journal of Pharmaceutical Sciences</i> , 2013, 49, 732-736.	1.9	19
59	Discovery of novel urokinase plasminogen activator (uPA) inhibitors using ligand-based modeling and virtual screening followed by in vitro analysis. <i>Journal of Molecular Modeling</i> , 2014, 20, 2080.	0.8	19
60	Ligand-based modeling followed by in vitro bioassay yielded new potent glucokinase activators. <i>Journal of Molecular Graphics and Modelling</i> , 2015, 56, 91-102.	1.3	19
61	Novel anticancer compound [trifluoromethyl-substituted pyrazole N-nucleoside] inhibits FLT3 activity to induce differentiation in acute myeloid leukemia cells. <i>Cancer Letters</i> , 2016, 375, 199-208.	3.2	19
62	Docking Simulations and in Vitro Assay Unveil Potent Inhibitory Action of Papaverine against Protein Tyrosine Phosphatase 1B. <i>Biological and Pharmaceutical Bulletin</i> , 2009, 32, 640-645.	0.6	18
63	Elaborate ligand-based modeling reveal new migration inhibitory factor inhibitors. <i>Journal of Molecular Graphics and Modelling</i> , 2013, 42, 104-114.	1.3	18
64	Ligand-based modeling of diverse aralkylamines yields new potent P-glycoprotein inhibitors. <i>European Journal of Medicinal Chemistry</i> , 2016, 110, 204-223.	2.6	18
65	Discovery of potent adenosine A2a antagonists as potential anti-Parkinson disease agents. Non-linear QSAR analyses integrated with pharmacophore modeling. <i>Chemico-Biological Interactions</i> , 2016, 254, 93-101.	1.7	17
66	Computer-aided discovery of new FGFR-1 inhibitors followed by in vitro validation. <i>Future Medicinal Chemistry</i> , 2016, 8, 1841-1869.	1.1	17
67	Innovative computer-aided methods for the discovery of new kinase ligands. <i>Future Medicinal Chemistry</i> , 2016, 8, 509-526.	1.1	16
68	Ligand-based modelling followed by synthetic exploration unveil novel glycogen phosphorylase inhibitory leads. <i>Bioorganic and Medicinal Chemistry</i> , 2011, 19, 4746-4771.	1.4	15
69	Discovery of new renin inhibitory leads via sequential pharmacophore modeling, QSAR analysis, in silico screening and in vitro evaluation. <i>Journal of Molecular Graphics and Modelling</i> , 2011, 29, 843-864.	1.3	15
70	Synthesis and Antitumor Activities of Some New N1-(Flavon-7-yl)amidrazone Derivatives. <i>Archiv Der Pharmazie</i> , 2014, 347, 415-422.	2.1	15
71	The Anticancer Activity of the Substituted Pyridone-Annulated Isoindigo (5'-Cl) Involves G0/G1 Cell Cycle Arrest and Inactivation of CDKs in the Promyelocytic Leukemia Cell Line HL-60. <i>Cellular Physiology and Biochemistry</i> , 2015, 35, 1943-1957.	1.1	15
72	Simulated annealing molecular dynamics and ligand-receptor contacts analysis for pharmacophore modeling. <i>Future Medicinal Chemistry</i> , 2017, 9, 1141-1159.	1.1	15

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73	Docking-based comparative intermolecular contacts analysis and in silico screening reveal new potent acetylcholinesterase inhibitors. <i>Medicinal Chemistry Research</i> , 2017, 26, 2768-2784.	1.1	15
74	Discovery of new JNK3 inhibitory chemotypes via QSAR-Guided selection of docking-based pharmacophores and comparison with other structure-based pharmacophore modeling methods. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 91, 30-51.	1.3	15
75	Preparation of Silver- and Zinc-Doped Mullite-Based Ceramics Showing Anti-Bacterial Biofilm Properties. <i>Molecules</i> , 2011, 16, 2862-2870.	1.7	14
76	Docking-generated multiple ligand poses for bootstrapping bioactivity classifying Machine Learning: Repurposing covalent inhibitors for COVID-19-related TMPRSS2 as case study. <i>Computational and Structural Biotechnology Journal</i> , 2021, 19, 4790-4824.	1.9	14
77	Investigation of the active constituents of <i>Portulaca oleraceae</i> L. (Portulacaceae) growing in Jordan. <i>Pakistan Journal of Pharmaceutical Sciences</i> , 2004, 17, 37-45.	0.2	14
78	N-Acyliminium ion cyclisation versus rearrangement. The synthesis of 13,13-dimethylberberines and 3,4-dimethylisoquinolin-1-ones. <i>Tetrahedron Letters</i> , 2000, 41, 1993-1996.	0.7	13
79	Homology modeling of MCH1 receptor and validation by docking/scoring and protein-aligned CoMFA. <i>European Journal of Medicinal Chemistry</i> , 2009, 44, 2583-2596.	2.6	13
80	Elaborate ligand-based modeling reveals new human neutrophil elastase inhibitors. <i>Medicinal Chemistry Research</i> , 2014, 23, 3876-3896.	1.1	13
81	Discovery of new selective cytotoxic agents against Bcl-2 expressing cancer cells using ligand-based modeling. <i>Chemico-Biological Interactions</i> , 2016, 250, 12-26.	1.7	13
82	Discovery of novel Flt3 inhibitory chemotypes through extensive ligand-based and new structure-based pharmacophore modelling methods. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 88, 128-151.	1.3	13
83	The bis(homoallylic) stabilisation of an acyliminium ion and reactions with nucleophiles. <i>Tetrahedron Letters</i> , 1998, 39, 3341-3344.	0.7	12
84	Discovery of new Î²-d-glucosidase inhibitors via pharmacophore modeling and QSAR analysis followed by in silico screening. <i>Journal of Molecular Modeling</i> , 2011, 17, 443-464.	0.8	12
85	Discovery of new Î²-galactosidase inhibitors via pharmacophore modeling and QSAR analysis followed by in silico screening. <i>Journal of Computational Chemistry</i> , 2011, 32, 463-482.	1.5	12
86	Ligand-based pharmacophore exploration and QSAR analysis of transition state analogues followed by in silico screening guide the discovery of new sub-micromolar Î²-secretase inhibitors. <i>Medicinal Chemistry Research</i> , 2013, 22, 1979-1997.	1.1	12
87	Discovery of new Gyrase Î² inhibitors via structure based modeling. <i>Computational Biology and Chemistry</i> , 2018, 74, 263-272.	1.1	12
88	Structure-Based Discovery and Bioactivity Evaluation of Novel Aurora-A Kinase Inhibitors as Anticancer Agents via Docking-Based Comparative Intermolecular Contacts Analysis (dbCICA). <i>Molecules</i> , 2020, 25, 6003.	1.7	12
89	A Concise Route to Tetrahydrophenanthridinones and Functionalised Isoquinolones. <i>Synlett</i> , 1996, 1996, 820-822.	1.0	11
90	Extensive ligand-based modeling and in silico screening reveal nanomolar inducible nitric oxide synthase (iNOS) inhibitors. <i>Journal of Molecular Graphics and Modelling</i> , 2012, 37, 1-26.	1.3	11

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91	Synthesis and characterization of chitosan-lactate-phthalate and evaluation of the corresponding zinc- and aluminum-crosslinked beads as potential controlled release matrices. <i>European Polymer Journal</i> , 2015, 73, 402-412.	2.6	11
92	Combining Stochastic Deformation/Relaxation and Intermolecular Contacts Analysis for Extracting Pharmacophores from Ligand-Receptor Complexes. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 879-893.	2.5	11
93	Discovery of New Phosphoinositide 3-kinase Delta (PI3K $\delta$ ) Inhibitors via Virtual Screening using Crystallography-derived Pharmacophore Modelling and QSAR Analysis. <i>Medicinal Chemistry</i> , 2019, 15, 588-601.	0.7	11
94	Ligand-based Modeling of CXC Chemokine Receptor 4 and Identification of Inhibitors of Novel Chemotypes as Potential Leads towards New Anti- COVID-19 Treatments. <i>Medicinal Chemistry</i> , 2022, 18, 871-883.	0.7	11
95	The Oxidation of Homophthalimide Derivatives by Dioxygen in Alkaline Media and Cleavage-Cyclisation Reactions. <i>Tetrahedron Letters</i> , 1997, 38, 3051-3054.	0.7	10
96	Rational exploration of new pyridinium-based HSP90 $\alpha$ inhibitors tailored to thiamine structure. <i>Medicinal Chemistry Research</i> , 2012, 21, 487-510.	1.1	10
97	Synthesis and characterization of new derivatives of alginic acid and evaluation of their iron(III)-crosslinked beads as potential controlled release matrices. <i>Pharmaceutical Development and Technology</i> , 2014, 19, 856-867.	1.1	10
98	$\hat{1}^2$ -Caryophyllene as putative male contraceptive: enhances spermatogenesis but not spermiogenesis in albino rats. <i>Medicinal Chemistry Research</i> , 2015, 24, 3876-3884.	1.1	10
99	Ligand-based computational modelling of platelet-derived growth factor beta receptor leading to new angiogenesis inhibitory leads. <i>Computational Biology and Chemistry</i> , 2017, 71, 170-179.	1.1	10
100	Ligand-based modeling of Akt3 lead to potent dual Akt1/Akt3 inhibitor. <i>Journal of Molecular Graphics and Modelling</i> , 2018, 83, 153-166.	1.3	10
101	The herbicide quinclorac as potent lipase inhibitor: Discovery via virtual screening and in vitro/in vivo validation. <i>Chemical Biology and Drug Design</i> , 2019, 93, 787-797.	1.5	10
102	Pharmacophore modeling of JAK1: A target infested with activity-cliffs. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 99, 107615.	1.3	10
103	Development of quantitative structure-property relationship models for pseudoternary microemulsions formulated with nonionic surfactants and cosurfactants: application of data mining and molecular modeling. <i>European Journal of Pharmaceutical Sciences</i> , 2002, 15, 461-478.	1.9	9
104	Development of predictive in silico model for cyclosporine- and aureobasidin-based P-glycoprotein inhibitors employing receptor surface analysis. <i>Journal of Molecular Graphics and Modelling</i> , 2008, 27, 439-451.	1.3	9
105	Some sulfonamide drugs inhibit ATPase activity of heat shock protein 90: investigation by docking simulation and experimental validation. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2011, 26, 603-609.	2.5	9
106	Design, synthesis, and biological evaluation of sulfonic acid ester and benzenesulfonamide derivatives as potential CETP inhibitors. <i>Medicinal Chemistry Research</i> , 2012, 21, 3669-3680.	1.1	9
107	Elaboration of Novel TTK1 Inhibitory Leads via QSAR-Guided Selection of Crystallographic Pharmacophores Followed By In Vitro Assay. <i>Current Computer-Aided Drug Design</i> , 2021, 17, 511-522.	0.8	9
108	Design, Synthesis and Biological Evaluation of N4-Sulfonamido-Succinamic, Phthalamic, Acrylic and Benzoyl Acetic Acid Derivatives as Potential DPP IV Inhibitors. <i>Open Medicinal Chemistry Journal</i> , 2013, 7, 39-48.	0.9	9

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109	New leads for DPP IV inhibition: structure-based pharmacophore mapping and virtual screening study. Archives of Pharmacal Research, 2013, 36, 1326-1337.	2.7	8
110	Design, synthesis and structure-activity relationship of new HSL inhibitors guided by pharmacophore models. Medicinal Chemistry Research, 2014, 23, 127-145.	1.1	8
111	Preparation and <i>in vitro</i> characterization of glibenclamide-loaded alginate hexyl-amide beads: a novel drug delivery system to improve the dissolution rate. Pharmaceutical Development and Technology, 2014, 19, 881-890.	1.1	8
112	Discovery of new Cdc2-like kinase 4 (CLK4) inhibitors <i>via</i> pharmacophore exploration combined with flexible docking-based ligand/receptor contact fingerprints and machine learning. RSC Advances, 2022, 12, 10686-10700.	1.7	8
113	QSPR modeling of pseudoternary microemulsions formulated employing lecithin surfactants: Application of data mining, molecular and statistical modeling. International Journal of Pharmaceutics, 2005, 295, 135-155.	2.6	7
114	Preparation of Polyester-Based Metal-Cross Linked Polymeric Composites as Novel Materials Resistant to Bacterial Adhesion and Biofilm Formation. Molecules, 2011, 16, 933-950.	1.7	7
115	Ethosuximide and Phenobarbital Promote Wound Healing via Enhancing Collagenization. Chemical Biology and Drug Design, 2012, 79, 137-142.	1.5	7
116	Synthesis and evaluation of novel diphenylthiazole derivatives as potential anti-inflammatory agents. Medicinal Chemistry Research, 2015, 24, 3681-3695.	1.1	7
117	Inhibitory Effects of New Mercapto Xanthine Derivatives in Human mcf7 and k562 Cancer Cell Lines. Journal of Heterocyclic Chemistry, 2017, 54, 450-456.	1.4	7
118	Famotidine inhibits glycogen synthase kinase-3 $\beta$ : An investigation by docking simulation and experimental validation. Journal of Enzyme Inhibition and Medicinal Chemistry, 2013, 28, 690-694.	2.5	6
119	Tryptophan and thiosemicarbazide derivatives: design, synthesis, and biological evaluation as potential $\beta$ -d-galactosidase and $\beta$ -d-glucosidase inhibitors. Medicinal Chemistry Research, 2015, 24, 2529-2550.	1.1	6
120	QSAR-guided pharmacophore modeling and subsequent virtual screening identify novel TYK2 inhibitor. Medicinal Chemistry Research, 2019, 28, 1368-1387.	1.1	6
121	Novel Ellipsoid Chitosan-Phthalate Lecithin Nanoparticles for siRNA Delivery. Frontiers in Bioengineering and Biotechnology, 2021, 9, 695371.	2.0	6
122	Investigation of Binding Characteristics of Phosphoinositide-dependent Kinase-1 (PDK1) Co-crystallized Ligands Through Virtual Pharmacophore Modeling Leading to Novel Anti-PDK1 Hits. Medicinal Chemistry, 2020, 16, 860-880.	0.7	6
123	Identification of Small Molecule Memapsin Inhibitors via Computation-based Virtual Screening. Advances in Pharmacology and Pharmacy, 2015, 3, 53-63.	0.1	5
124	Cytotoxic activity of the novel heterocyclic compound G-11 is primarily mediated through intrinsic apoptotic pathway. Apoptosis: an International Journal on Programmed Cell Death, 2016, 21, 873-886.	2.2	4
125	Rosmarinic acid reverses the effects of metronidazole-induced infertility in male albino rats. Reproduction, Fertility and Development, 2017, 29, 1910.	0.1	4
126	Unsupervised pharmacophore modeling combined with <i>QSAR</i> analyses revealed novel low micromolar <i>SIRT2</i> inhibitors. Journal of Molecular Recognition, 2017, 30, e2623.	1.1	4



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127	Inhibition of monoglyceride lipase by proton pump inhibitors: investigation using docking and in vitro experiments. <i>Pharmacological Reports</i> , 2020, 72, 435-442.	1.5	4
128	Discovery of Potent Bruton's Tyrosine Kinase Inhibitors Using Ligand Based Modeling. <i>Anti-Cancer Agents in Medicinal Chemistry</i> , 2017, 17, 265-275.	0.9	4
129	Exploiting activity cliffs for building pharmacophore models and comparison with other pharmacophore generation methods: sphingosine kinase 1 as case study. <i>Journal of Computer-Aided Molecular Design</i> , 2022, 36, 39-62.	1.3	4
130	Discovery of novel potent nuclear factor kappa $\beta$ inhibitors (IKK $\beta$ ) via extensive ligand-based modeling and virtual screening. <i>Journal of Molecular Recognition</i> , 2017, 30, e2604.	1.1	3
131	Inhibition of aggregation of amyloid $\beta$ through covalent modification with benzylpenicillin; potential relevance to Alzheimer's disease. <i>Biochemistry and Biophysics Reports</i> , 2021, 26, 100943.	0.7	3
132	Structure-based discovery of new polo-like kinase 1 (PLK1) inhibitors as potential anticancer agents via docking-based comparative intermolecular contacts analysis (dbCICA). <i>Medicinal Chemistry Research</i> , 2021, 30, 1747-1766.	1.1	3
133	Inhibition of protein kinases by proton pump inhibitors: computational screening and in vitro evaluation. <i>Medicinal Chemistry Research</i> , 2021, 30, 2266-2276.	1.1	3
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