Mutasem O. Taha

List of Publications by Year
in descending order

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149 papers	3,519 citations	136950 32 h-index	189892 50 g-index
151 all docs	151 docs citations	151 times ranked	3751 citing authors

#	Article	IF	Citations
1	Vitamin B12 binding to mutated human transcobalamin, in-silico study of TCN2 alanine scanning and ClinVar missense mutations/SNPs. Journal of Biomolecular Structure and Dynamics, 2023, 41, 3222-3233.	3.5	1
2	Discovery of new PKN2 inhibitory chemotypes via QSAR-guided selection of docking-based pharmacophores. Molecular Diversity, 2023, 27, 443-462.	3.9	21
3	Ligand-based Modeling of CXC Chemokine Receptor 4 and Identification of Inhibitors of Novel Chemotypes as Potential Leads towards New Anti- COVID-19 Treatments. Medicinal Chemistry, 2022, 18, 871-883.	1.5	11
4	Exploiting activity cliffs for building pharmacophore models and comparison with other pharmacophore generation methods: sphingosine kinase 1 as case study. Journal of Computer-Aided Molecular Design, 2022, 36, 39-62.	2.9	4
5	Discovery of new Cdc2-like kinase 4 (CLK4) inhibitors via pharmacophore exploration combined with flexible docking-based ligand/receptor contact fingerprints and machine learning. RSC Advances, 2022, 12, 10686-10700.	3.6	8
6	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. Vaccines, 2022, 10, 366.	4.4	39
7	Novel Ellipsoid Chitosan-Phthalate Lecithin Nanoparticles for siRNA Delivery. Frontiers in Bioengineering and Biotechnology, 2021, 9, 695371.	4.1	6
8	Inhibition of aggregation of amyloid-Î² through covalent modification with benzylpenicillin; potential relevance to Alzheimer's disease. Biochemistry and Biophysics Reports, 2021, 26, 100943.	1.3	3
9	Structure-based discovery of new polo-like kinase 1 (PLK1) inhibitors as potential anticancer agents via docking-based comparative intermolecular contacts analysis (dbCICA). Medicinal Chemistry Research, 2021, 30, 1747-1766.	2.4	3
10	Elaboration of Novel TTK1 Inhibitory Leads via QSAR-Guided Selection of Crystallographic Pharmacophores Followed By In Vitro Assay. Current Computer-Aided Drug Design, 2021, 17, 511-522.	1.2	9
11	Docking-generated multiple ligand poses for bootstrapping bioactivity classifying Machine Learning: Repurposing covalent inhibitors for COVID-19-related TMPRSS2 as case study. Computational and Structural Biotechnology Journal, 2021, 19, 4790-4824.	4.1	14
12	Inhibition of protein kinases by proton pump inhibitors: computational screening and in vitro evaluation. Medicinal Chemistry Research, 2021, 30, 2266-2276.	2.4	3
13	Design and Synthesis of New JAK1 Inhibitors based on Sulfonamide- Triazine Conjugates. Current Computer-Aided Drug Design, 2021, 17, 916-926.	1.2	3
14	Structure-Based Discovery and Bioactivity Evaluation of Novel Aurora-A Kinase Inhibitors as Anticancer Agents via Docking-Based Comparative Intermolecular Contacts Analysis (dbCICA). Molecules, 2020, 25, 6003.	3.8	12
15	Comprehensive Structural and Molecular Comparison of Spike Proteins of SARS-CoV-2, SARS-CoV and MERS-CoV, and Their Interactions with ACE2. Cells, 2020, 9, 2638.	4.1	138
16	Inhibition of monoglyceride lipase by proton pump inhibitors: investigation using docking and in vitro experiments. Pharmacological Reports, 2020, 72, 435-442.	3.3	4
17	Stable Chitosan-Based Nanoparticles Using Polyphosphoric Acid or Hexametaphosphate for Tandem Ionotropic/Covalent Crosslinking and Subsequent Investigation as Novel Vehicles for Drug Delivery. Frontiers in Bioengineering and Biotechnology, 2020, 8, 4.	4.1	87
18	Pharmacophore modeling of JAK1: A target infested with activity-cliffs. Journal of Molecular Graphics and Modelling, 2020, 99, 107615.	2.4	10

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19	Design and Synthesis of New Sulfonamides-Based Flt3 Inhibitors. Medicinal Chemistry, 2020, 16, 403-412.	1.5	2
20	Ligand Based Pharmacophore Modeling Followed by Biological Screening Lead to Discovery of Novel PDK1 Inhibitors as Anticancer Agents. Anti-Cancer Agents in Medicinal Chemistry, 2020, 20, 476-485.	1.7	3
21	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.	1.5	6
22	Discovery of novel Flt3 inhibitory chemotypes through extensive ligand-based and new structure-based pharmacophore modelling methods. Journal of Molecular Graphics and Modelling, 2019, 88, 128-151.	2.4	13
23	Discovery of new JNK3 inhibitory chemotypes via QSAR-Guided selection of docking-based pharmacophores and comparison with other structure-based pharmacophore modeling methods. Journal of Molecular Graphics and Modelling, 2019, 91, 30-51.	2.4	15
24	QSAR-guided pharmacophore modeling and subsequent virtual screening identify novel TYK2 inhibitor. Medicinal Chemistry Research, 2019, 28, 1368-1387.	2.4	6
25	Degradability of chitosan micro/nanoparticles for pulmonary drug delivery. Heliyon, 2019, 5, e01684.	3.2	163
26	The herbicide quinclorac as potent lipase inhibitor: Discovery via virtual screening and in vitro/in vivo validation. Chemical Biology and Drug Design, 2019, 93, 787-797.	3.2	10
27	Alginate Nanoparticles. , 2019, , 389-418.		1
28	Discovery of New Phosphoinositide 3-kinase Delta (PI3KÎ´) Inhibitors via Virtual Screening using Crystallography-derived Pharmacophore Modelling and QSAR Analysis. Medicinal Chemistry, 2019, 15, 588-601.	1.5	11
29	Inhibition of dipeptidyl peptidase IV by fexofenadine: Virtual screening study. Journal of Applied Pharmaceutical Science, 2019, 9, 28-32.	1.0	2
30	Ligand-based modeling of Akt3 lead to potent dual Akt1/Akt3 inhibitor. Journal of Molecular Graphics and Modelling, 2018, 83, 153-166.	2.4	10
31	Discovery of new Gyrase Î² inhibitors via structure based modeling. Computational Biology and Chemistry, 2018, 74, 263-272.	2.3	12
32	Exploring the influence of culture conditions on kefir's anticancer properties. Journal of Dairy Science, 2018, 101, 3771-3777.	3.4	24
33	Combining Stochastic Deformation/Relaxation and Intermolecular Contacts Analysis for Extracting Pharmacophores from Ligandâ€“Receptor Complexes. Journal of Chemical Information and Modeling, 2018, 58, 879-893.	5.4	11
34	Natural and semisynthetic polymers in pharmaceutical nanotechnology. , 2018, , 35-100.		22
35	Synthesis and Structure-Activity Relationship; Exploration of some Potent Anti-Cancer Phenyl Amidrazone Derivatives. Medicinal Chemistry, 2018, 14, 468-477.	1.5	3
36	Synthesis and Anticancer Properties of Methyl N1-(thien-4-yl)amidrazone- 3-carboxylates. Letters in Drug Design and Discovery, 2018, 15, 1268-1275.	0.7	1

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37	Inhibitory Effects of New Mercapto Xanthine Derivatives in Human mcf7 and k562 Cancer Cell Lines. Journal of Heterocyclic Chemistry, 2017, 54, 450-456.	2.6	7
38	Rosmarinic acid reverses the effects of metronidazole-induced infertility in male albino rats. Reproduction, Fertility and Development, 2017, 29, 1910.	0.4	4
39	Novel nanoparticles based on chitosan-dicarboxylate conjugates via tandem ionotropic/covalent crosslinking with tripolyphosphate and subsequent evaluation as drug delivery vehicles. International Journal of Pharmaceutics, 2017, 529, 15-31.	5.2	27
40	Unsupervised pharmacophore modeling combined with <scp>QSAR</scp> analyses revealed novel low micromolar <scp>SIRT2</scp> inhibitors. Journal of Molecular Recognition, 2017, 30, e2623.	2.1	4
41	Discovery of novel potent nuclear factor kappaâ€B inhibitors (IKKâ€Î²) via extensive ligandâ€based modeling and virtual screening. Journal of Molecular Recognition, 2017, 30, e2604.	2.1	3
42	Ligand-based computational modelling of platelet-derived growth factor beta receptor leading to new angiogenesis inhibitory leads. Computational Biology and Chemistry, 2017, 71, 170-179.	2.3	10
43	Simulated annealing molecular dynamics and ligandâ€“receptor contacts analysis for pharmacophore modeling. Future Medicinal Chemistry, 2017, 9, 1141-1159.	2.3	15
44	Computational modeling of the bat <scp>HKU4</scp> coronavirus <scp>3CL^{pro}</scp> inhibitors as a tool for the development of antivirals against the emerging <scp>M</scp>iddle <scp>E</scp>ast respiratory syndrome (<scp>MERS</scp>) coronavirus. Journal of Molecular Recognition, 2017, 30, e2644.	2.1	21
45	Docking-based comparative intermolecular contacts analysis and in silico screening reveal new potent acetylcholinesterase inhibitors. Medicinal Chemistry Research, 2017, 26, 2768-2784.	2.4	15
46	Discovery of Potent Bruton's Tyrosine Kinase Inhibitors Using Ligand Based Modeling. Anti-Cancer Agents in Medicinal Chemistry, 2017, 17, 265-275.	1.7	4
47	Discovery of potent adenosine A2a antagonists as potential anti-Parkinson disease agents. Non-linear QSAR analyses integrated with pharmacophore modeling. Chemico-Biological Interactions, 2016, 254, 93-101.	4.0	17
48	Innovative computer-aided methods for the discovery of new kinase ligands. Future Medicinal Chemistry, 2016, 8, 509-526.	2.3	16
49	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.	4.9	4
50	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. Journal of Computer-Aided Molecular Design, 2016, 30, 1149-1163.	2.9	22
51	Computer-aided discovery of new FGFR-1 inhibitors followed by in vitro validation. Future Medicinal Chemistry, 2016, 8, 1841-1869.	2.3	17
52	Ligand-based modeling of diverse aryalkylamines yields new potent P-glycoprotein inhibitors. European Journal of Medicinal Chemistry, 2016, 110, 204-223.	5.5	18
53	QSAR studies in the discovery of novel type-II diabetic therapies. Expert Opinion on Drug Discovery, 2016, 11, 197-214.	5.0	25
54	Novel anticancer compound [trifluoromethyl-substituted pyrazole N-nucleoside] inhibits FLT3 activity to induce differentiation in acute myeloid leukemia cells. Cancer Letters, 2016, 375, 199-208.	7.2	19

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55	Discovery of new selective cytotoxic agents against Bcl-2 expressing cancer cells using ligand-based modeling. Chemico-Biological Interactions, 2016, 250, 12-26.	4.0	13
56	Pharmacophore and QSAR Modeling of Neuronal Nitric Oxide Synthase Ligands and Subsequent Validation and In Silico Search for New Scaffolds. Medicinal Chemistry, 2016, 12, 371-393.	1.5	2
57	Enhanced drug encapsulation and extended release profiles of calciumâ€“alginate nanoparticles by using tannic acid as a bridging cross-linking agent. Journal of Microencapsulation, 2015, 32, 96-105.	2.8	57
58	Ligand-based modeling followed by in vitro bioassay yielded new potent glucokinase activators. Journal of Molecular Graphics and Modelling, 2015, 56, 91-102.	2.4	19
59	Oleuropein potently inhibits mammalian target of rapamycin: possible involvement of tandem anomeric hyperconjugationâ€“Michael reaction. Medicinal Chemistry Research, 2015, 24, 616-623.	2.4	2
60	Synthesis and evaluation of novel diphenylthiazole derivatives as potential anti-inflammatory agents. Medicinal Chemistry Research, 2015, 24, 3681-3695.	2.4	7
61	Antiproliferative activity of the isoindigo 5â€²-Br in HL-60 cells is mediated by apoptosis, dysregulation of mitochondrial functions and arresting cell cycle at G0/G1 phase. Cancer Letters, 2015, 361, 251-261.	7.2	20
62	Combining docking-based comparative intermolecular contacts analysis and k-nearest neighbor correlation for the discovery of new check point kinase 1 inhibitors. Journal of Computer-Aided Molecular Design, 2015, 29, 561-581.	2.9	23
63	The Anticancer Activity of the Substituted Pyridone-Annelated Isoindigo (5'-Cl) Involves G0/G1 Cell Cycle Arrest and Inactivation of CDKs in the Promyelocytic Leukemia Cell Line HL-60. Cellular Physiology and Biochemistry, 2015, 35, 1943-1957.	1.6	15
64	Î²-Caryophyllene as putative male contraceptive: enhances spermatogenesis but not spermiogenesis in albino rats. Medicinal Chemistry Research, 2015, 24, 3876-3884.	2.4	10
65	Synthesis and characterization of chitosan-lactateâ€“phthalate and evaluation of the corresponding zinc- and aluminum-crosslinked beads as potential controlled release matrices. European Polymer Journal, 2015, 73, 402-412.	5.4	11
66	Tryptophan and thiosemicarbazide derivatives: design, synthesis, and biological evaluation as potential Î²-d-galactosidase and Î²-d-glucosidase inhibitors. Medicinal Chemistry Research, 2015, 24, 2529-2550.	2.4	6
67	Identification of Small Molecule Memapsin Inhibitors via Computation-based Virtual Screening. Advances in Pharmacology and Pharmacy, 2015, 3, 53-63.	0.2	5
68	Synthesis and Antibacterial Activity of Some Novel N,N-Di-Oxalamide Derivatives. International Journal of Chemistry and Materials Research, 2015, 3, 165-175.	1.1	0
69	Haloperidol inhibits Memapsin 2: innovation by docking simulation and in vitro assay. Pakistan Journal of Pharmaceutical Sciences, 2015, 28, 139-46.	0.2	0
70	Ritodrine inhibits neuronal nitric oxide synthase, a potential link between tocolysis and autism. Medicinal Chemistry Research, 2014, 23, 5102-5109.	2.4	1
71	Synthesis and characterization of new derivatives of alginic acid and evaluation of their iron(III)-crosslinked beads as potential controlled release matrices. Pharmaceutical Development and Technology, 2014, 19, 856-867.	2.4	10
72	Evaluation of naproxen and cromolyn activities against cancer cells viability, proliferation, apoptosis, p53 and gene expression of survivin and caspase-3. Journal of Enzyme Inhibition and Medicinal Chemistry, 2014, 29, 153-161.	5.2	31

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73	Design, synthesis and structureâ€“activity relationship of new HSL inhibitors guided by pharmacophore models. Medicinal Chemistry Research, 2014, 23, 127-145.	2.4	8
74	Discovery of novel urokinase plasminogen activator (uPA) inhibitors using ligand-based modeling and virtual screening followed by in vitro analysis. Journal of Molecular Modeling, 2014, 20, 2080.	1.8	19
75	Synthesis and Antitumor Activities of Some New N1â€(Flavonâ€6â€yl)amidrazone Derivatives. Archiv Der Pharmazie, 2014, 347, 415-422.	4.1	15
76	Preparation andin vitrocharacterization 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.	2.4	8
77	Discovery of nanomolar phosphoinositide 3-kinase gamma (PI3KÎ³) inhibitors using ligand-based modeling and virtual screening followed by inÂvitro analysis. European Journal of Medicinal Chemistry, 2014, 84, 454-465.	5.5	27
78	The use of docking-based comparative intermolecular contacts analysis to identify optimal docking conditions within glucokinase and to discover of new GK activators. Journal of Computer-Aided Molecular Design, 2014, 28, 509-547.	2.9	33
79	Elaborate ligand-based modeling reveals new human neutrophil elastase inhibitors. Medicinal Chemistry Research, 2014, 23, 3876-3896.	2.4	13
80	Regression of endometrial implants treated with vitamin D3 in a rat model of endometriosis. European Journal of Pharmacology, 2013, 715, 72-75.	3.5	59
81	Famotidine inhibits glycogen synthase kinase-3Î²: An investigation by docking simulation and experimental validation. Journal of Enzyme Inhibition and Medicinal Chemistry, 2013, 28, 690-694.	5.2	6
82	Ligand-based pharmacophore exploration and QSAR analysis of transition state analogues followed by in silico screening guide the discovery of new sub-micromolar Î²-secreatase inhibitors. Medicinal Chemistry Research, 2013, 22, 1979-1997.	2.4	12
83	New leads for DPP IV inhibition: structure-based pharmacophore mapping and virtual screening study. Archives of Pharmacal Research, 2013, 36, 1326-1337.	6.3	8
84	Pharmacophore modeling, homology modeling, and in silico screening reveal mammalian target of rapamycin inhibitory activities for sotalol, glyburide, metipranolol, sulfamethizole, glipizide, and pioglitazone. Journal of Molecular Graphics and Modelling, 2013, 42, 39-49.	2.4	38
85	Elaborate ligand-based modeling reveal new migration inhibitory factor inhibitors. Journal of Molecular Graphics and Modelling, 2013, 42, 104-114.	2.4	18
86	Elaborate ligand-based modeling coupled with QSAR analysis and in silico screening reveal new potent acetylcholinesterase inhibitors. Journal of Computer-Aided Molecular Design, 2013, 27, 1075-1092.	2.9	31
87	Naproxen and Cromolyn as New Glycogen Synthase Kinase 3Î² Inhibitors for Amelioration of Diabetes and Obesity: An Investigation by Docking Simulation and Subsequent In Vitro/In Vivo Biochemical Evaluation. Journal of Biochemical and Molecular Toxicology, 2013, 27, 425-436.	3.0	23
88	Î²-Caryophyllene causes regression of endometrial implants in a rat model of endometriosis without affecting fertility. European Journal of Pharmacology, 2013, 702, 12-19.	3.5	42
89	Sunitinib as an anti-endometriotic agent. European Journal of Pharmaceutical Sciences, 2013, 49, 732-736.	4.0	19
90	Elaborate Ligand-Based Modeling Coupled with Multiple Linear Regression and k Nearest Neighbor QSAR Analyses Unveiled New Nanomolar mTOR Inhibitors. Journal of Chemical Information and Modeling, 2013, 53, 2587-2612.	5.4	50

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91	Design, Synthesis and Biological Evaluation of N4-Sulfonamido-Succinamic, Phthalamic, Acrylic and Benzoyl Acetic Acid Derivatives as Potential DPP IV Inhibitors. Open Medicinal Chemistry Journal, 2013, 7, 39-48.	2.4	9
92	Synthesis of a Novel Chitosan-Based Polymer and Application as a Matrix for Controlled Drug Delivery. Jordan Journal of Pharmaceutical Sciences, 2013, 6, 233-241.	1.1	0
93	Synthesis and biological activity assays of some new N1-(flavon-7-yl)amidrazone derivatives and related congeners. European Journal of Medicinal Chemistry, 2012, 54, 65-74.	5.5	20
94	Design, synthesis, and biological evaluation of sulfonic acid ester and benzenesulfonamide derivatives as potential CETP inhibitors. Medicinal Chemistry Research, 2012, 21, 3669-3680.	2.4	9
95	Application of docking-based comparative intermolecular contacts analysis to validate Hsp90Î± docking studies and subsequent in silico screening for inhibitors. Journal of Molecular Modeling, 2012, 18, 4843-4863.	1.8	30
96	Effect of particle morphology and pore size on the release kinetics of ephedrine from mesoporous MCM-41 materials. Journal of Porous Materials, 2012, 19, 825-833.	2.6	19
97	Rational exploration of new pyridinium-based HSP90Î± inhibitors tailored to thiamine structure. Medicinal Chemistry Research, 2012, 21, 487-510.	2.4	10
98	Ethosuximide and Phenobarbital Promote Wound Healing via Enhancing Collagenization. Chemical Biology and Drug Design, 2012, 79, 137-142.	3.2	7
99	Elaborate ligand-based modeling and subsequent synthetic exploration unveil new nanomolar Ca2+/calmodulin-dependent protein kinase II inhibitory leads. Bioorganic and Medicinal Chemistry, 2012, 20, 377-400.	3.0	23
100	Extensive ligand-based modeling and in silico screening reveal nanomolar inducible nitric oxide synthase (iNOS) inhibitors. Journal of Molecular Graphics and Modelling, 2012, 37, 1-26.	2.4	11
101	Elaborate ligand-based modeling reveal new submicromolar Rho kinase inhibitors. Journal of Computer-Aided Molecular Design, 2012, 26, 249-266.	2.9	33
102	Thujone corrects cholesterol and triglyceride profiles in diabetic rat model. Natural Product Research, 2011, 25, 1180-1184.	1.8	32
103	Preparation of Polyester-Based Metal-Cross Linked Polymeric Composites as Novel Materials Resistant to Bacterial Adhesion and Biofilm Formation. Molecules, 2011, 16, 933-950.	3.8	7
104	Preparation of Silver- and Zinc-Doped Mullite-Based Ceramics Showing Anti-Bacterial Biofilm Properties. Molecules, 2011, 16, 2862-2870.	3.8	14
105	Discovery of New Antifungal Leads via Pharmacophore Modeling and QSAR Analysis of Fungal Nâ€Myristoyl Transferase Inhibitors Followed by In Silico Screening. Chemical Biology and Drug Design, 2011, 78, 391-407.	3.2	23
106	Metal ion / Pyridinedicarboxylate Polymer composites as inhibitors of bacterial biofilm formation. Journal of Infection, 2011, 63, e8-e9.	3.3	0
107	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. Journal of Chemical Information and Modeling, 2011, 51, 647-669.	5.4	65
108	Discovery of new Î²-d-glucosidase inhibitors via pharmacophore modeling and QSAR analysis followed by in silico screening. Journal of Molecular Modeling, 2011, 17, 443-464.	1.8	12

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109	Discovery of new Î²â€<scp>D</scp>â€galactosidase inhibitors via pharmacophore modeling and QSAR analysis followed by in silico screening. Journal of Computational Chemistry, 2011, 32, 463-482.	3.3	12
110	Ligand-based modelling followed by synthetic exploration unveil novel glycogen phosphorylase inhibitory leads. Bioorganic and Medicinal Chemistry, 2011, 19, 4746-4771.	3.0	15
111	Discovery of new nanomolar peroxisome proliferator-activated receptor Î³ activators via elaborate ligand-based modeling. European Journal of Medicinal Chemistry, 2011, 46, 2513-2529.	5.5	30
112	Discovery of new renin inhibitory leads via sequential pharmacophore modeling, QSAR analysis, in silico screening and in vitro evaluation. Journal of Molecular Graphics and Modelling, 2011, 29, 843-864.	2.4	15
113	Some sulfonamide drugs inhibit ATPase activity of heat shock protein 90: investigation by docking simulation and experimental validation. Journal of Enzyme Inhibition and Medicinal Chemistry, 2011, 26, 603-609.	5.2	9
114	Discovery of new cholesteryl ester transfer protein inhibitors via ligand-based pharmacophore modeling and QSAR analysis followed by synthetic exploration. European Journal of Medicinal Chemistry, 2010, 45, 1598-1617.	5.5	51
115	Discovery of novel CDK1 inhibitors by combining pharmacophore modeling, QSAR analysis and in silico screening followed by in vitro bioassay. European Journal of Medicinal Chemistry, 2010, 45, 4316-4330.	5.5	40
116	Pharmacophore and QSAR modeling of estrogen receptor Î² ligands and subsequent validation and in silico search for new hits. Journal of Molecular Graphics and Modelling, 2010, 28, 383-400.	2.4	37
117	Elaborate ligand-based pharmacophore exploration and QSAR analysis guide the synthesis of novel pyridinium-based potent Î²-secretase inhibitory leads. Bioorganic and Medicinal Chemistry, 2010, 18, 3088-3115.	3.0	66
118	Elaborate Ligand-Based Modeling Reveals New Nanomolar Heat Shock Protein 90Î± Inhibitors. Journal of Chemical Information and Modeling, 2010, 50, 1706-1723.	5.4	42
119	In Silico Screening for Nonâ€nucleoside HIVâ€1 Reverse Transcriptase Inhibitors Using Physicochemical Filters and Highâ€Throughput Docking Followed by In Vitro Evaluation. Chemical Biology and Drug Design, 2009, 74, 258-265.	3.2	25
120	Homology modeling of MCH1 receptor and validation by docking/scoring and protein-aligned CoMFA. European Journal of Medicinal Chemistry, 2009, 44, 2583-2596.	5.5	13
121	Inhibition of dipeptidyl peptidase IV (DPP IV) is one of the mechanisms explaining the hypoglycemic effect of berberine. Journal of Enzyme Inhibition and Medicinal Chemistry, 2009, 24, 1061-1066.	5.2	117
122	Pharmacophore Modeling, Quantitative Structureâ^'Activity Relationship Analysis, and Shape-Complemented in Silico Screening Allow Access to Novel Influenza Neuraminidase Inhibitors. Journal of Chemical Information and Modeling, 2009, 49, 978-996.	5.4	58
123	Inhibition of glycogen synthase kinase by curcumin: Investigation by simulated molecular docking and subsequentin vitro/in vivoevaluation. Journal of Enzyme Inhibition and Medicinal Chemistry, 2009, 24, 771-778.	5.2	82
124	Docking Simulations and in Vitro Assay Unveil Potent Inhibitory Action of Papaverine against Protein Tyrosine Phosphatase 1B. Biological and Pharmaceutical Bulletin, 2009, 32, 640-645.	1.4	18
125	Discovery of DPP IV Inhibitors by Pharmacophore Modeling and QSAR Analysis followed by inâ€...silico Screening. ChemMedChem, 2008, 3, 1763-1779.	3.2	60
126	Development of predictive in silico model for cyclosporine- and aureobasidin-based P-glycoprotein inhibitors employing receptor surface analysis. Journal of Molecular Graphics and Modelling, 2008, 27, 439-451.	2.4	9

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127	Discovery of new MurF inhibitors via pharmacophore modeling and QSAR analysis followed by in-silico screening. Bioorganic and Medicinal Chemistry, 2008, 16, 1218-1235.	3.0	66
128	Sodium lauryl sulfate impedes drug release from zinc-crosslinked alginate beads: Switching from enteric coating release into biphasic profiles. International Journal of Pharmaceutics, 2008, 350, 291-300.	5.2	52
129	Olanzapine inhibits glycogen synthase kinase-3Î²: An investigation by docking simulation and experimental validation. European Journal of Pharmacology, 2008, 584, 185-191.	3.5	33
130	Pharmacophore Modeling, Quantitative Structureâ€“Activity Relationship Analysis, and in Silico Screening Reveal Potent Glycogen Synthase Kinase-3Î² Inhibitory Activities for Cimetidine, Hydroxychloroquine, and Gemifloxacin. Journal of Medicinal Chemistry, 2008, 51, 2062-2077.	6.4	90
131	Combining Ligand-Based Pharmacophore Modeling, Quantitative Structureâ^'Activity Relationship Analysis and in Silico Screening for the Discovery of New Potent Hormone Sensitive Lipase Inhibitors. Journal of Medicinal Chemistry, 2008, 51, 6478-6494.	6.4	78
132	Effect of Ionic Crosslinking on the Drug Release Properties ofChitosan Diacetate Matrices. Journal of Pharmaceutical Sciences, 2007, 96, 38-43.	3.3	23
133	Discovery of new potent human protein tyrosine phosphatase inhibitors via pharmacophore and QSAR analysis followed by in silico screening. Journal of Molecular Graphics and Modelling, 2007, 25, 870-884.	2.4	77
134	Combining docking, scoring and molecular field analyses to probe influenza neuraminidaseâ€“ligand interactions. Journal of Molecular Graphics and Modelling, 2007, 26, 443-456.	2.4	23
135	Berberine potently inhibits protein tyrosine phosphatase 1B: Investigation by docking simulation and experimental validation. Journal of Enzyme Inhibition and Medicinal Chemistry, 2006, 21, 163-171.	5.2	34
136	Discovery of potent inhibitors of pseudomonal quorum sensing via pharmacophore modeling and in silico screening. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 5902-5906.	2.2	51
137	Synthesis and in vitro behavior of iron-crosslinked N-methyl and N-benzyl hydroxamated derivatives of alginic acid as controlled release carriers. European Polymer Journal, 2006, 42, 2464-2474.	5.4	31
138	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.	5.2	7
139	Ligand-based assessment of factor Xa binding site flexibility via elaborate pharmacophore exploration and genetic algorithm-based QSAR modeling. European Journal of Medicinal Chemistry, 2005, 40, 701-727.	5.5	52
140	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. Journal of Medicinal Chemistry, 2005, 48, 8016-8034.	6.4	26
141	Investigation of the active constituents of Portulaca oleraceae L. (Portulacaceae) growing in Jordan. Pakistan Journal of Pharmaceutical Sciences, 2004, 17, 37-45.	0.2	14
142	Development of quantitative structureâ€“property relationship models for pseudoternary microemulsions formulated with nonionic surfactants and cosurfactants: application of data mining and molecular modeling. European Journal of Pharmaceutical Sciences, 2002, 15, 461-478.	4.0	9
143	Synthesis of iron-crosslinked chitosan succinate and iron-crosslinked hydroxamated chitosan succinate and their in vitro evaluation as potential matrix materials for oral theophylline sustained-release beads. European Journal of Pharmaceutical Sciences, 2001, 13, 159-168.	4.0	80
144	N-Acyliminium ion cyclisation versus rearrangement. The synthesis of 13,13-dimethylberberines and 3,4-dimethylisoquinolin-1-ones. Tetrahedron Letters, 2000, 41, 1993-1996.	1.4	13

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145	Spectrophotometric and Conductometric Study of the Complexation of Ranitidine to Fez+, Fe3+, Al*, Mg*+, Cu", Ni2+ and PtP+ Metal Ions: Pharmaceutical Implications. Scientia Pharmaceutica, 2000, 68, 357-367.	2.0	0
146	Synthesis of Chitosan Succinate and Chitosan Phthalate and Their Evaluation as Suggested Matrices in Orally Administered, Colon-Specific Drug Delivery Systems. Archiv Der Pharmazie, 1999, 332, 103-107.	4.1	92
147	The bis(homoallylic) stabilisation of an acyliminium ion and reactions with nucleophiles. Tetrahedron Letters, 1998, 39, 3341-3344.	1.4	12
148	The Oxidation of Homophthalimide Derivatives by Dioxygen in Alkaline Media and Cleavage-Cyclisation Reactions. Tetrahedron Letters, 1997, 38, 3051-3054.	1.4	10
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