Tarun Jha

List of Publications by Year
in descending order

187 papers	3,849 citations	147726 31 h-index	214721 47 g-index
190 all docs	190 docs citations	190 times ranked	3377 citing authors

#	Article	IF	Citations
1	Matrix metalloproteinase-9 (MMP-9) and its inhibitors in cancer: A minireview. European Journal of Medicinal Chemistry, 2020, 194, 112260.	2.6	270
2	Protease targeted COVID-19 drug discovery and its challenges: Insight into viral main protease (Mpro) and papain-like protease (PLpro) inhibitors. Bioorganic and Medicinal Chemistry, 2021, 29, 115860.	1.4	126
3	HDAC6 as privileged target in drug discovery: A perspective. Pharmacological Research, 2021, 163, 105274.	3.1	115
4	Design of Aminopeptidase N Inhibitors as Anti-cancer Agents. Journal of Medicinal Chemistry, 2018, 61, 6468-6490.	2.9	83
5	Chemical-informatics approach to COVID-19 drug discovery: Monte Carlo based QSAR, virtual screening and molecular docking study of some in-house molecules as papain-like protease (PLpro) inhibitors. Journal of Biomolecular Structure and Dynamics, 2021, 39, 4764-4773.	2.0	77
6	Histone deacetylase 8 (HDAC8) and its inhibitors with selectivity to other isoforms: An overview. European Journal of Medicinal Chemistry, 2019, 164, 214-240.	2.6	72
7	Histone deacetylase 3 (HDAC3) inhibitors as anticancer agents: A review. European Journal of Medicinal Chemistry, 2020, 192, 112171.	2.6	69
8	Fight against novel coronavirus: A perspective of medicinal chemists. European Journal of Medicinal Chemistry, 2020, 201, 112559.	2.6	58
9	Is dual inhibition of metalloenzymes HDAC-8 and MMP-2 a potential pharmacological target to combat hematological malignancies?. Pharmacological Research, 2017, 122, 8-19.	3.1	57
10	Arylsulfonamides and selectivity of matrix metalloproteinase-2: An overview. European Journal of Medicinal Chemistry, 2017, 129, 72-109.	2.6	55
11	Design of dual MMP-2/HDAC-8 inhibitors by pharmacophore mapping, molecular docking, synthesis and biological activity. RSC Advances, 2015, 5, 72373-72386.	1.7	53
12	Chemical-informatics approach to COVID-19 drug discovery: Exploration of important fragments and data mining based prediction of some hits from natural origins as main protease (Mpro) inhibitors. Journal of Molecular Structure, 2021, 1224, 129026.	1.8	53
13	Exploring pyrazolo[3,4-d]pyrimidine phosphodiesterase 1 (PDE1) inhibitors: a predictive approach combining comparative validated multiple molecular modelling techniques. Journal of Biomolecular Structure and Dynamics, 2018, 36, 590-608.	2.0	52
14	Combating breast cancer with non-steroidal aromatase inhibitors (NSAIs): Understanding the chemico-biological interactions through comparative SAR/QSAR study. European Journal of Medicinal Chemistry, 2017, 137, 365-438.	2.6	51
15	Robust design of some selective matrix metalloproteinase-2 inhibitors over matrix metalloproteinase-9 through in silico/fragment-based lead identification and de novo lead modification: Syntheses and biological assays. Bioorganic and Medicinal Chemistry, 2016, 24, 4291-4309.	1.4	48
16	HDAC3 is a potential validated target for cancer: An overview on the benzamide-based selective HDAC3 inhibitors through comparative SAR/QSAR/QAAR approaches. European Journal of Medicinal Chemistry, 2018, 157, 1127-1142.	2.6	48
17	Inhibitors of gelatinases (MMP-2 and MMP-9) for the management of hematological malignancies. European Journal of Medicinal Chemistry, 2021, 223, 113623.	2.6	47
18	QSAR study on some pyridoacridine ascididemin analogues as anti-tumor agents. Bioorganic and Medicinal Chemistry, 2003, 11, 5493-5499.	1.4	41

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19	First molecular modeling report on novel arylpyrimidine kynurenine monooxygenase inhibitors through multi-QSAR analysis against Huntingtonâ€™s disease: A proposal to chemists!. Bioorganic and Medicinal Chemistry Letters, 2016, 26, 5712-5718.	1.0	41
20	Design, synthesis and biological screening of 2-aminobenzamides as selective HDAC3 inhibitors with promising anticancer effects. European Journal of Pharmaceutical Sciences, 2018, 124, 165-181.	1.9	41
21	Small molecule drug conjugates (SMDCs): an emerging strategy for anticancer drug design and discovery. New Journal of Chemistry, 2021, 45, 5291-5321.	1.4	39
22	5-N-Substituted-2-(substituted benzenesulphonyl) glutamines as antitumor agents. Part II: Synthesis, biological activity and QSAR study. Bioorganic and Medicinal Chemistry, 2004, 12, 1413-1423.	1.4	37
23	First report on the structural exploration and prediction of new BPTES analogs as glutaminase inhibitors. Journal of Molecular Structure, 2017, 1143, 49-64.	1.8	37
24	Studies on the production and purification of an antimicrobial compound and taxonomy of the producer isolated from the marine environment of the Sundarbans. Applied Microbiology and Biotechnology, 2005, 66, 497-505.	1.7	35
25	Folate decorated epigallocatechin-3-gallate (EGCG) loaded PLGA nanoparticles; in-vitro and in-vivo targeting efficacy against MDA-MB-231 tumor xenograft. International Journal of Pharmaceutics, 2020, 585, 119449.	2.6	35
26	QSAR study on some anti-HIV HEPT analogues using physicochemical and topological parameters. Bioorganic and Medicinal Chemistry, 2004, 12, 1493-1503.	1.4	34
27	Good and bad molecular fingerprints for human rhinovirus 3C protease inhibition: identification, validation, and application in designing of new inhibitors through Monte Carlo-based QSAR study. Journal of Biomolecular Structure and Dynamics, 2020, 38, 66-77.	2.0	34
28	First structureâ€“activity relationship analysis of SARS-CoV-2 virus main protease (Mpro) inhibitors: an endeavor on COVID-19 drug discovery. Molecular Diversity, 2021, 25, 1827-1838.	2.1	33
29	Structural findings of phenylindoles as cytotoxic antimitotic agents in human breast cancer cell lines through multiple validated QSAR studies. Toxicology in Vitro, 2015, 29, 1392-1404.	1.1	32
30	Structure-activity relationships of HDAC8 inhibitors: Non-hydroxamates as anticancer agents. Pharmacological Research, 2018, 131, 128-142.	3.1	32
31	Design, synthesis, biological evaluation and molecular docking study of arylcarboxamido piperidine and piperazine-based hydroxamates as potential HDAC8 inhibitors with promising anticancer activity. European Journal of Pharmaceutical Sciences, 2019, 138, 105046.	1.9	32
32	Synthesis, screening and quantitative structureâ€“activity relationship (QSAR) studies of some glutamine analogues for possible anticancer activity. Bioorganic and Medicinal Chemistry, 2002, 10, 2119-2131.	1.4	31
33	Exploring QSAR and pharmacophore mapping of structurally diverse selective matrix metalloproteinase-2 inhibitors. Journal of Pharmacy and Pharmacology, 2013, 65, 1541-1554.	1.2	31
34	Structureâ€“activity relationships of hydroxamate-based histone deacetylase-8 inhibitors: reality behind anticancer drug discovery. Future Medicinal Chemistry, 2017, 9, 2211-2237.	1.1	31
35	QSAR study on adenosine kinase inhibition of pyrrolo[2,3- d]pyrimidine nucleoside analogues using the hansch approach. Bioorganic and Medicinal Chemistry Letters, 2002, 12, 899-902.	1.0	30
36	A new bisbenzylisoquinoline alkaloid isolated from Thalictrum foliolosum, as a potent inhibitor of DNA topoisomerase IB of Leishmania donovani. FÃ¬toterapÃ¬Ã¢, 2016, 109, 25-30.	1.1	30

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37	Diverse classes of HDAC8 inhibitors: in search of molecular fingerprints that regulate activity. Future Medicinal Chemistry, 2018, 10, 1589-1602.	1.1	30
38	Development of decision trees to discriminate HDAC8 inhibitors and non-inhibitors using recursive partitioning. Journal of Biomolecular Structure and Dynamics, 2021, 39, 1-8.	2.0	30
39	Dual activity of amphiphilic Zn(II) nitroporphyrin derivatives as HIV-1 entry inhibitors and in cancer photodynamic therapy. European Journal of Medicinal Chemistry, 2019, 174, 66-75.	2.6	29
40	Dissecting Histone Deacetylase 3 in Multiple Disease Conditions: Selective Inhibition as a Promising Therapeutic Strategy. Journal of Medicinal Chemistry, 2021, 64, 8827-8869.	2.9	29
41	QSAR Study on Some p-Arylthio Cinnamides as Antagonists of Biochemical ICAM-1/LFA-1 Interaction and ICAM-1/JY-8 Cell Adhesion in Relation to Anti-inflammatory Activity. Bioorganic and Medicinal Chemistry, 2003, 11, 1615-1619.	1.4	28
42	Hot nuclear matter in asymmetry chiral sigma model. Nuclear Physics A, 2004, 733, 169-184.	0.6	28
43	Exploring QSAR onÂ3-aminopyrazoles asÂantitumor agents forÂtheirÂinhibitory activity ofÂCDK2/cyclin A. European Journal of Medicinal Chemistry, 2006, 41, 1190-1195.	2.6	28
44	Cytotoxic potential of dispirooxindolo/acenaphthoquino andrographolide derivatives against MCF-7 cell line. MedChemComm, 2015, 6, 702-707.	3.5	27
45	A pentanoic acid derivative targeting matrix metalloproteinase-2 (MMP-2) induces apoptosis in a chronic myeloid leukemia cell line. European Journal of Medicinal Chemistry, 2017, 141, 37-50.	2.6	26
46	Histone deacetylase 3 inhibitors in learning and memory processes with special emphasis on benzamides. European Journal of Medicinal Chemistry, 2019, 166, 369-380.	2.6	26
47	Protease targeted COVID-19 drug discovery: What we have learned from the past SARS-CoV inhibitors?. European Journal of Medicinal Chemistry, 2021, 215, 113294.	2.6	26
48	Syntheses, biological evaluation and QSAR study on antitumor activity of 1,5-N,Nâ€²-disubstituted-2-(substituted benzenesulphonyl) glutamamides. Bioorganic and Medicinal Chemistry, 2002, 10, 1841-1854.	1.4	24
49	Comparative validated molecular modeling of p53-HDM2 inhibitors as antiproliferative agents. European Journal of Medicinal Chemistry, 2015, 90, 860-875.	2.6	24
50	QSAR Study on the Affinity of Some Arylpiperazines towards the 5-HT1A/Î±1-Adrenergic Receptor Using the E-State Index. Bioorganic and Medicinal Chemistry Letters, 2003, 13, 2837-2842.	1.0	23
51	Synergistic effect of methanol extract of Abies webbiana leaves on sleeping time induced by standard sedatives in mice and anti-inflammatory activity of extracts in rats. Journal of Ethnopharmacology, 2004, 93, 397-402.	2.0	23
52	Comparative QSAR modelling of 2-phenylindole-3-carbaldehyde derivatives as potential antimitotic agents. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 1737-1739.	1.0	23
53	Validated predictive QSAR modeling of N-aryl-oxazolidinone-5-carboxamides for anti-HIV protease activity. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 6082-6087.	1.0	23
54	Synthesis, pharmacological activity and comparative QSAR modeling of 1,5-N,Nâ€²-substituted-2-(substituted naphthalenesulphonyl) glutamamides as possible anticancer agents. European Journal of Medicinal Chemistry, 2010, 45, 1760-1771.	2.6	23

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55	Anthocephaline, a New Indole Alkaloid and Cadambine, a Potent Inhibitor of DNA Topoisomerase IB of Leishmania donovani (LdTOP1LS), Isolated from Anthocephalus cadamba. Natural Product Communications, 2015, 10, 1934578X1501000.	0.2	23
56	Hydroxyethylamine derivatives as HIV-1 protease inhibitors: a predictive QSAR modelling study based on Monte Carlo optimization. SAR and QSAR in Environmental Research, 2017, 28, 973-990.	1.0	23
57	Exploring structural requirements of aurone derivatives as antimalarials by validated DFT-based QSAR, HQSAR, and COMFAâ€“COMSIA approach. Medicinal Chemistry Research, 2013, 22, 6029-6045.	1.1	22
58	Insight into the structural requirements of pyrimidine-based phosphodiesterase 10A (PDE10A) inhibitors by multiple validated 3D QSAR approaches. SAR and QSAR in Environmental Research, 2017, 28, 253-273.	1.0	22
59	Exploring structural requirements of 1-N-substituted thiocarbamoyl-3-phenyl-2-pyrazolines as antiamoebic agents using comparative QSAR modelling. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 4021-4026.	1.0	21
60	Monte Carlo based modelling approach for designing and predicting cytotoxicity of 2-phenylindole derivatives against breast cancer cell line MCF7. Toxicology in Vitro, 2018, 52, 23-32.	1.1	21
61	Designing potential HDAC3 inhibitors to improve memory and learning. Journal of Biomolecular Structure and Dynamics, 2019, 37, 2133-2142.	2.0	21
62	Structural exploration for the refinement of anticancer matrix metalloproteinase-2 inhibitor designing approaches through robust validated multi-QSARs. Journal of Molecular Structure, 2018, 1156, 501-515.	1.8	20
63	A Review on Camptothecin Analogs with Promising Cytotoxic Profile. Anti-Cancer Agents in Medicinal Chemistry, 2019, 18, 1796-1814.	0.9	20
64	Constraints on nuclear matter parameters of an effective chiral model. Physical Review C, 2008, 78, .	1.1	19
65	Predictive comparative QSAR modelling of (phenylpiperazinyl-alkyl) oxindoles as selective 5-HT1A antagonists by stepwise regression, PCRA, FA-MLR and PLS techniques. European Journal of Medicinal Chemistry, 2010, 45, 1119-1127.	2.6	19
66	Stepwise development of structureâ€“activity relationship of diverse PARP-1 inhibitors through comparative and validatedin silico modeling techniques and molecular dynamics simulation. Journal of Biomolecular Structure and Dynamics, 2015, 33, 1756-1779.	2.0	19
67	Exploring structural requirements of unconventional Knoevenagel-type indole derivatives as anticancer agents through comparative QSAR modeling approaches. Canadian Journal of Chemistry, 2016, 94, 637-644.	0.6	19
68	Insight into structural features of phenyltetrazole derivatives as ABCG2 inhibitors for the treatment of multidrug resistance in cancer. SAR and QSAR in Environmental Research, 2019, 30, 457-475.	1.0	19
69	Design of 5-fluorouracil (5-FU) loaded, folate conjugated peptide linked nanoparticles, a potential new drug carrier for selective targeting of tumor cells. MedChemComm, 2019, 10, 559-572.	3.5	19
70	Attributes of a rotating neutron star with a hyperon core. Physical Review C, 2008, 77, .	1.1	18
71	Exploration of structural and physicochemical requirements and search of virtual hits for aminopeptidase N inhibitors. Molecular Diversity, 2013, 17, 123-137.	2.1	18
72	Structural findings of quinolone carboxylic acids in cytotoxic, antiviral, and anti-HIV-1 integrase activity through validated comparative molecular modeling studies. Medicinal Chemistry Research, 2014, 23, 3096-3127.	1.1	18

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73	Spermicidal and Contraceptive Potential of Desgalactotigonin: A Prospective Alternative of Nonoxynol-9. PLoS ONE, 2014, 9, e107164.	1.1	17
74	A New Ellagic Acid Glycoside and DNA Topoisomerase IB Inhibitory Activity of Saponins from Putranjiva roxburghii. Natural Product Communications, 2014, 9, 1934578X1400900.	0.2	17
75	Selective and nonselective HDAC8 inhibitors: a therapeutic patent review. Pharmaceutical Patent Analyst, 2018, 7, 259-276.	0.4	17
76	In silico modelling, identification of crucial molecular fingerprints, and prediction of new possible substrates of human organic cationic transporters 1 and 2. New Journal of Chemistry, 2020, 44, 4129-4143.	1.4	17
77	Chrysin-loaded PLGA attenuates OVA-induced allergic asthma by modulating TLR/NF-Î°B/NLRP3 axis. Nanomedicine: Nanotechnology, Biology, and Medicine, 2020, 30, 102292.	1.7	17
78	Quantitative structureâ€“activity relationship study on some benzodiazepine derivatives as anti-Alzheimer agents. Journal of Molecular Modeling, 2004, 10, 328-334.	0.8	16
79	QSAR modeling on dopamine D2 receptor binding affinity of 6-methoxy benzamides. Il Farmaco, 2005, 60, 818-825.	0.9	16
80	Neutron star matter in an effective model. Physical Review C, 2006, 74, .	1.1	16
81	Exploring in house glutamate inhibitors of matrix metalloproteinase-2 through validated robust chemico-biological quantitative approaches. Structural Chemistry, 2018, 29, 285-297.	1.0	16
82	Leishmanial lipid affords protection against oxidative stress induced hepatic injury by regulating inflammatory mediators and confining apoptosis progress. Toxicology Letters, 2015, 232, 499-512.	0.4	15
83	Structural exploration of hydroxyethylamines as HIV-1 protease inhibitors: new features identified. SAR and QSAR in Environmental Research, 2018, 29, 385-408.	1.0	15
84	Multiple molecular modelling studies on some derivatives and analogues of glutamic acid as matrix metalloproteinase-2 inhibitors. SAR and QSAR in Environmental Research, 2018, 29, 43-68.	1.0	15
85	Molecular dynamics analysis of phytochemicals from Ageratina adenophora against COVID-19 main protease (Mpro) and human angiotensin-converting enzyme 2 (ACE2). Biocatalysis and Agricultural Biotechnology, 2021, 32, 101924.	1.5	15
86	Insight into the Structural Requirements of Theophylline-Based Aldehyde Dehydrogenase IAl (ALDHIAl) Inhibitors Through Multi-QSAR Modeling and Molecular Docking Approaches. Current Drug Discovery Technologies, 2016, 13, 84-100.	0.6	15
87	Designing Potential Antitrypanosomal Thiazol-2-ethylamines through Predictive Regression Based and Classification Based QSAR Analyses. Current Drug Discovery Technologies, 2017, 14, 39-52.	0.6	15
88	Quantitative structureâ€“activity relationship study using refractotopological state atom index on some neonicotinoid insecticides. Bioorganic and Medicinal Chemistry, 2004, 12, 6137-6145.	1.4	14
89	QSAR modelling on a series of arylsulfonamide-based hydroxamates as potent MMP-2 inhibitors. SAR and QSAR in Environmental Research, 2019, 30, 247-263.	1.0	14
90	Synthesis, biological evaluation, and molecular docking analysis of novel linker-less benzamide based potent and selective HDAC3 inhibitors. Bioorganic Chemistry, 2021, 114, 105050.	2.0	14

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91	Quantitative Structure-Activity Relationship Study on Some Azidopyridinyl Neonicotinoid Insecticides for Their Selective Affinity Towards the Drosophila Nicotinic Receptor Over Mammalian ?4?2 Receptor Using Electrotopological State Atom Index. Drug Design and Discovery, 2003, 18, 81-89.	0.3	14
92	Antitussive activity ofAbies webbiana Lindl. leaf extract against sulphur dioxide-induced cough re?ex in mice. Phytotherapy Research, 2003, 17, 930-932.	2.8	13
93	Antibacterial activity of Abies webbiana. FÃ¬toterapÃ¬Ã¢, 2007, 78, 153-155.	1.1	13
94	Chenopodium album metabolites act as dual topoisomerase inhibitors and induce apoptosis in the MCF7 cell line. MedChemComm, 2016, 7, 837-844.	3.5	13
95	Benzamide porphyrins with directly conjugated and distal pyridyl or pyridinium groups substituted to the porphyrin macrocycles: Study of the photosensitising abilities as inducers of apoptosis in cancer cells under photodynamic conditions. Journal of Photochemistry and Photobiology B: Biology, 2018, 178, 228-236.	1.7	13
96	Synthesis, anticancer activity, structureâ€“activity relationship and binding mode of interaction studies of substituted pentanoic acids. Future Medicinal Chemistry, 2019, 11, 1679-1702.	1.1	13
97	meso-Thiophenium Porphyrins and Their Zn(II) Complexes: A New Category of Cationic Photosensitizers. ACS Medicinal Chemistry Letters, 2020, 11, 2041-2047.	1.3	13
98	Outline of gelatinase inhibitors as anti-cancer agents: A patent mini-review for 2010-present. European Journal of Medicinal Chemistry, 2021, 213, 113044.	2.6	13
99	Design, synthesis and binding mode of interaction of novel small molecule o-hydroxy benzamides as HDAC3-selective inhibitors with promising antitumor effects in 4T1-Luc breast cancer xenograft model. Bioorganic Chemistry, 2021, 117, 105446.	2.0	13
100	Bulk viscosity in a hyperonic star andr-mode instability. Physical Review C, 2010, 82, .	1.1	12
101	The Role of 3D Pharmacophore Mapping Based Virtual Screening for Identification of Novel Anticancer Agents: An Overview. Current Topics in Medicinal Chemistry, 2013, 13, 1098-1126.	1.0	12
102	Leishmanial lipid suppresses the bacterial endotoxin-induced inflammatory response with attenuation of tissue injury in sepsis. Journal of Leukocyte Biology, 2014, 96, 325-336.	1.5	12
103	Structural findings of cinnolines as anti-schizophrenic PDE10A inhibitors through comparative chemometric modeling. Molecular Diversity, 2014, 18, 655-671.	2.1	12
104	Lipid from Infective L. donovani Regulates Acute Myeloid Cell Growth via Mitochondria Dependent MAPK Pathway. PLoS ONE, 2015, 10, e0120509.	1.1	12
105	An integrated ligand-based modelling approach to explore the structure-property relationships of influenza endonuclease inhibitors. Structural Chemistry, 2017, 28, 1663-1678.	1.0	12
106	Understanding Chemicoâ€Biological Interactions of Glutamate MMPâ€2 Inhibitors through Rigorous Alignmentâ€Dependent 3Dâ€QSAR Analyses. ChemistrySelect, 2017, 2, 7888-7898.	0.7	12
107	Reliable structural information for rational design of benzoxazole type potential cholesteryl ester transfer protein (CETP) inhibitors through multiple validated modeling techniques. Journal of Biomolecular Structure and Dynamics, 2019, 37, 4528-4541.	2.0	12
108	Towards the Development of Anticancer Drugs from Andrographolide: Semisynthesis, Bioevaluation, QSAR Analysis and Pharmacokinetic Studies. Current Topics in Medicinal Chemistry, 2015, 15, 1013-1026.	1.0	12

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109	Ligand-based quantitative structural assessments of SARS-CoV-2 3CLpro inhibitors: An analysis in light of structure-based multi-molecular modeling evidences. Journal of Molecular Structure, 2022, 1251, 132041.	1.8	12
110	QSAR modeling of neonicotinoid insecticides for their selective affinity towards Drosophila nicotinic receptors over mammalian Î±4Î²2 receptors. Canadian Journal of Chemistry, 2006, 84, 458-463.	0.6	11
111	Structural Findings of 2â€Phenylindoleâ€3â€Carbaldehyde Derivatives for Antimitotic Activity by FAâ€sMLR QSAR Analysis. Chemical Biology and Drug Design, 2010, 75, 204-213.	1.5	11
112	Chemometric modeling and pharmacophore mapping in coronary heart disease: 2-arylbenzoxazoles as cholesteryl ester transfer protein inhibitors. MedChemComm, 2011, 2, 840.	3.5	11
113	Homoisoflavonoids as potential antiangiogenic agents for retinal neovascularization. Biomedicine and Pharmacotherapy, 2017, 95, 818-827.	2.5	11
114	Structural refinement and prediction of potential CCR2 antagonists through validated multi-QSAR modeling studies. Journal of Biomolecular Structure and Dynamics, 2019, 37, 75-94.	2.0	11
115	Structural exploration of tetrahydroisoquinoline derivatives as HDAC8 inhibitors through multi-QSAR modeling study. Journal of Biomolecular Structure and Dynamics, 2020, 38, 1551-1564.	2.0	11
116	Ligand Based Validated Comparative Chemometric Modeling and Pharmacophore Mapping of Aurone Derivatives as Antimalarial Agents. Current Computer-Aided Drug Design, 2013, 9, 417-432.	0.8	11
117	Possible anticancer agents: QSAR analogs of glutamamide: Synthesis and pharmacological activity of 1,5-N,Nâ€²-disubstituted-2-(substituted benzenesulphonyl) glutamamides. European Journal of Medicinal Chemistry, 2009, 44, 70-82.	2.6	10
118	Chemometric Modeling of 5-Phenylthiophenecarboxylic Acid Derivatives as Anti-Rheumatic Agents. Current Computer-Aided Drug Design, 2012, 8, 182-195.	0.8	10
119	An integrated QSAR modeling approach to explore the structureâ€“property and selectivity relationships of N-benzoyl-l-biphenylalanines as integrin antagonists. Molecular Diversity, 2018, 22, 129-158.	2.1	10
120	Properties of Neutron stars with hyperon cores in parametrized hydrostatic conditions. International Journal of Modern Physics E, 2018, 27, 1850097.	0.4	10
121	Exploration of histone deacetylase 8 inhibitors through classification QSAR study: Part II. Journal of Molecular Structure, 2020, 1204, 127529.	1.8	10
122	Identification of structural fingerprints for ABCG2 inhibition by using Monte Carlo optimization, Bayesian classification, and structural and physicochemical interpretation (SPCI) analysis. SAR and QSAR in Environmental Research, 2020, 31, 439-455.	1.0	10
123	Evaluation of Efficacy of Curcumin along with Lycopene and Piperine in the Management of Oral Submucous Fibrosis. Contemporary Clinical Dentistry, 2019, 10, 531-541.	0.2	10
124	Anthocephaline, a new indole alkaloid and cadambine, a potent inhibitor of DNA topoisomerase IB of Leishmania donovani (LdTOP1LS), isolated from Anthocephalus cadamba. Natural Product Communications, 2015, 10, 297-9.	0.2	10
125	Quantitative Structure-Activity Relationship Study on Some Azidopyridinyl Neonicotinoid Insecticides for Their Selective Affinity Towards the Drosophila Nicotinic Receptor Over Mammalian a4ÃŸ2 Receptor Using Electrotopological State Atom Index. Drug Design and Discovery, 2003, 18, 81-89.	0.3	9
126	QSAR modelling of pancreatic Î²-cell KATP channel openers R/S-3,4-dihydro-2,2-dimethyl-6-halo-4-(substituted phenylaminocarbonylamino)-2H-1-benzopyrans using MLRâ€“FA techniques. European Journal of Medicinal Chemistry, 2009, 44, 359-364.	2.6	9

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127	Leishmanial sphingolipid induces apoptosis in Sarcoma 180 cancer cells through regulation of tumour growth via angiogenic switchover. Tumor Biology, 2015, 36, 3109-3118.	0.8	9
128	Integrating regression and classification-based QSARs with molecular docking analyses to explore the structure-antiaromatase activity relationships of letrozole-based analogs. Canadian Journal of Chemistry, 2017, 95, 1285-1295.	0.6	9
129	Identification of molecular fingerprints of phenylindole derivatives as cytotoxic agents: a multi-QSAR approach. Structural Chemistry, 2018, 29, 1095-1107.	1.0	9
130	Structural exploration of arylsulfonamide-based ADAM17 inhibitors through validated comparative multi-QSAR modelling studies. Journal of Molecular Structure, 2019, 1185, 128-142.	1.8	9
131	Deconfinement of nonstrange hadronic matter with nucleons and Î” baryons to quark matter in neutron stars. International Journal of Modern Physics D, 2019, 28, 1950040.	0.9	9
132	Effective anti-aromatase therapy to battle against estrogen-mediated breast cancer: Comparative SAR/QSAR assessment on steroidal aromatase inhibitors. European Journal of Medicinal Chemistry, 2020, 208, 112845.	2.6	9
133	Robust classification-based molecular modelling of diverse chemical entities as potential SARS-CoV-2 3CL^{pro} inhibitors: theoretical justification in light of experimental evidences. SAR and QSAR in Environmental Research, 2021, 32, 473-493.	1.0	9
134	Ligand-based design of anticancer MMP2Âinhibitors: aÂreview. Future Medicinal Chemistry, 2021, 13, 1987-2013.	1.1	9
135	The first report on predictive comparative ligand-based multi-QSAR modeling analysis of 4-pyrimidinone and 2-pyridinone based APJ inhibitors. New Journal of Chemistry, 2022, 46, 11591-11607.	1.4	9
136	Lipid Isolated from aLeishmania donovaniStrain ReducesEscherichia coliInduced Sepsis in Mice through Inhibition of Inflammatory Responses. Mediators of Inflammation, 2014, 2014, 1-15.	1.4	8
137	Structural Insight Into the Viral 3C-Like Protease Inhibitors: Comparative SAR/QSAR Approaches. , 2017, , 317-409.		8
138	Structural analysis of arylsulfonamide-based carboxylic acid derivatives: a QSAR study to identify the structural contributors toward their MMP-9 inhibition. Structural Chemistry, 2021, 32, 417-430.	1.0	8
139	Exploring naphthyl derivatives as SARS-CoV papain-like protease (PLpro) inhibitors and its implications in COVID-19 drug discovery. Molecular Diversity, 2022, 26, 215-228.	2.1	8
140	Applying comparative molecular modelling techniques on diverse hydroxamate-based HDAC2 inhibitors: an attempt to identify promising structural features for potent HDAC2 inhibition. SAR and QSAR in Environmental Research, 2022, 33, 1-22.	1.0	8
141	Selective inhibition of histone deacetylase 3 by novel hydrazide based small molecules as therapeutic intervention for the treatment of cancer. European Journal of Medicinal Chemistry, 2022, 238, 114470.	2.6	8
142	Antineoplastic impact of leishmanial sphingolipid in tumour growth with regulation of angiogenic event and inflammatory response. Apoptosis: an International Journal on Programmed Cell Death, 2015, 20, 869-882.	2.2	7
143	Shedding light on designing potential meprin Î² inhibitors through ligand-based robust validated computational approaches: A proposal to chemists!. Journal of Biomolecular Structure and Dynamics, 2018, 36, 3003-3022.	2.0	7
144	Exploration of good and bad structural fingerprints for inhibition of indoleamine-2,3-dioxygenase enzyme in cancer immunotherapy using Monte Carlo optimization and Bayesian classification QSAR modeling. Journal of Biomolecular Structure and Dynamics, 2020, 38, 1-14.	2.0	7

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145	Essential elements regulating HDAC8 inhibition: a classification based structural analysis and enzyme-inhibitor interaction study of hydroxamate based HDAC8 inhibitors. Journal of Biomolecular Structure and Dynamics, 2020, 38, 5513-5525.	2.0	7
146	Quantitative activityâ€“activity relationship (QAAR) driven design to develop hydroxamate derivatives of pentanoic acids as selective HDAC8 inhibitors: synthesis, biological evaluation and binding mode of interaction studies. New Journal of Chemistry, 2021, 45, 17149-17162.	1.4	7
147	How the structural properties of the indole derivatives are important in kinase targeted drug design?: A case study on tyrosine kinase inhibitors. Bioorganic and Medicinal Chemistry, 2022, 53, 116534.	1.4	7
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