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	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
2	Synthesis, biological activity, structure activity relationship study and liposomal formulation development of some arylsulfonyl pyroglutamic acid derivatives. Journal of Molecular Structure, 2022, 1248, 131512.	1.8	3
3	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
4	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
5	Synthesis, anticancer activity, SAR and binding mode of interaction studies of substituted pentanoic acids: part II. Future Medicinal Chemistry, 2022, 14, 17-34.	1.1	3
6	A critical analysis of urea transporter B inhibitors: molecular fingerprints, pharmacophore features for the development of next-generation diuretics. Molecular Diversity, 2022, 26, 2549-2559.	2.1	1
7	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
8	Exploring sodium glucose cotransporter (SGLT2) inhibitors with machine learning approach: A novel hope in anti-diabetes drug discovery. Journal of Molecular Graphics and Modelling, 2022, 111, 108106.	1.3	7
9	Insight into the structural requirements of gelatinases (MMP-2 and MMP-9) inhibitors by multiple validated molecular modelling approaches: Part II. SAR and QSAR in Environmental Research, 2022, 33, 167-192.	1.0	3
10	A fragment-based structural analysis of MMP-2 inhibitors in search of meaningful structural fragments. Computers in Biology and Medicine, 2022, 144, 105360.	3.9	3
11	Binary quantitative activity-activity relationship (QAAR) studies to explore selective HDAC8 inhibitors: In light of mathematical models, DFT-based calculation and molecular dynamic simulation studies. Journal of Molecular Structure, 2022, 1260, 132833.	1.8	4
12	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
13	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
14	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
15	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
16	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
17	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
18	HDAC6 as privileged target in drug discovery: A perspective. Pharmacological Research, 2021, 163, 105274.	3.1	115

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19	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
20	Cancer photocytotoxicity and anti-inflammatory response of cis-A₂B₂ type meso-p-nitrophenyl and p-hydroxyphenyl porphyrin and its zinc(<scp>ii</scp>) complex: a synthetic alternative to the THPP synthon. New Journal of Chemistry, 2021, 45, 2060-2068.	1.4	6
21	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
22	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
23	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
24	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
25	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
26	Therapies of Hematological Malignancies: An Overview of the Potential Targets and Their Inhibitors. Current Chemical Biology, 2021, 15, 19-49.	0.2	2
27	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
28	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
29	Unmasking of crucial structural fragments for coronavirus protease inhibitors and its implications in COVID-19 drug discovery. Journal of Molecular Structure, 2021, 1237, 130366.	1.8	6
30	Insight into the structural requirement of aryl sulphonamide based gelatinases (MMP-2 and MMP-9) inhibitors â€“ Part I: 2D-QSAR, 3D-QSAR topomer CoMFA and NaÃ¯ve Bayes studies â€“ First report of 3D-QSAR Topomer CoMFA analysis for MMP-9 inhibitors and jointly inhibitors of gelatinases together. SAR and QSAR in Environmental Research, 2021, 32, 655-687.	1.0	4
31	A robust classification-dependent multi-molecular modelling study on some biphenyl sulphonamide based MMP-8 inhibitors. SAR and QSAR in Environmental Research, 2021, 32, 835-861.	1.0	5
32	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
33	Urea transporter and its specific and nonspecific inhibitors: State of the art and pharmacological perspective. European Journal of Pharmacology, 2021, 911, 174508.	1.7	4
34	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
35	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
36	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

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37	Ligand-based design of anticancer MMP2Âinhibitors: aÂreview. Future Medicinal Chemistry, 2021, 13, 1987-2013.	1.1	9
38	First molecular modelling report on tri-substituted pyrazolines as phosphodiesterase 5 (PDE5) inhibitors through classical and machine learning based multi-QSAR analysis. SAR and QSAR in Environmental Research, 2021, 32, 1-23.	1.0	3
39	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
40	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
41	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
42	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
43	Exploration of histone deacetylase 8 inhibitors through classification QSAR study: Part II. Journal of Molecular Structure, 2020, 1204, 127529.	1.8	10
44	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
45	Exploring indole derivatives as myeloid cell leukaemia-1 (Mcl-1) inhibitors with multi-QSAR approach: a novel hope in anti-cancer drug discovery. New Journal of Chemistry, 2020, 44, 17494-17506.	1.4	6
46	Dissecting the Drug Development Strategies Against SARS-CoV-2 Through Diverse Computational Modeling Techniques. Methods in Pharmacology and Toxicology, 2020, , 329-431.	0.1	4
47	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
48	Photodynamic activity attained through the ruptured Ï€-conjugation of pyridyl groups with a porphyrin macrocycle: synthesis and the photophysical and photobiological evaluation of 5-mono-(4-nitrophenyl)-10,15,20-tris-[4-(phenoxymethyl)pyridine]-porphyrin and its Zn(ii) complex. Photochemical and Photobiological Sciences, 2020, 19, 1776-1789.	1.6	3
49	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
50	Fight against novel coronavirus: A perspective of medicinal chemists. European Journal of Medicinal Chemistry, 2020, 201, 112559.	2.6	58
51	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
52	Matrix metalloproteinase-9 (MMP-9) and its inhibitors in cancer: A minireview. European Journal of Medicinal Chemistry, 2020, 194, 112260.	2.6	270
53	Exploring the structural aspects of ureido-amino acid-based APN inhibitors: a validated comparative multi-QSAR modelling study. SAR and QSAR in Environmental Research, 2020, 31, 325-345.	1.0	5
54	Discriminations of active from inactive HDAC8 inhibitors Part II: Bayesian classification study to find molecular fingerprints. SAR and QSAR in Environmental Research, 2020, 31, 245-260.	1.0	4

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55	Effect of Î› coupling on liquid gas phase transition in warm asymmetric nuclear matter. Nuclear Physics A, 2020, 1002, 121974.	0.6	1
56	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
57	Histone deacetylase 3 (HDAC3) inhibitors as anticancer agents: A review. European Journal of Medicinal Chemistry, 2020, 192, 112171.	2.6	69
58	Collagenases and gelatinases and their inhibitors as anticancer agents. , 2020, , 265-294.		6
59	Chrysin-loaded PLGA attenuates OVA-induced allergic asthma by modulating TLR/NF-ÎºB/NLRP3 axis. Nanomedicine: Nanotechnology, Biology, and Medicine, 2020, 30, 102292.	1.7	17
60	An Equation of State for Magnetized Neutron Star Matter and Tidal Deformation in Neutron Star Mergers. Astrophysical Journal, 2020, 900, 49.	1.6	6
61	Designing potential HDAC3 inhibitors to improve memory and learning. Journal of Biomolecular Structure and Dynamics, 2019, 37, 2133-2142.	2.0	21
62	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
63	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
64	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
65	Intermolecular association of some selected melanin monomers and their optical absorption. Computational and Theoretical Chemistry, 2019, 1151, 43-49.	1.1	6
66	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
67	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
68	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
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	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
71	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
72	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

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73	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
74	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
75	A Review on Camptothecin Analogs with Promising Cytotoxic Profile. Anti-Cancer Agents in Medicinal Chemistry, 2019, 18, 1796-1814.	0.9	20
76	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
77	Structure-activity relationships of HDAC8 inhibitors: Non-hydroxamates as anticancer agents. Pharmacological Research, 2018, 131, 128-142.	3.1	32
78	Identification of molecular fingerprints of phenylindole derivatives as cytotoxic agents: a multi-QSAR approach. Structural Chemistry, 2018, 29, 1095-1107.	1.0	9
79	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
80	Design of Aminopeptidase N Inhibitors as Anti-cancer Agents. Journal of Medicinal Chemistry, 2018, 61, 6468-6490.	2.9	83
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	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
83	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
84	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
85	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
86	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
87	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
88	First Report on the Validated Classification-Based Chemometric Modeling of Human Rhinovirus 3C Protease (HRV 3Cpro) Inhibitors. International Journal of Quantitative Structure-Property Relationships, 2018, 3, 1-20.	1.1	1
89	Selective and nonselective HDAC8 inhibitors: a therapeutic patent review. Pharmaceutical Patent Analyst, 2018, 7, 259-276.	0.4	17
90	Properties of Neutron stars with hyperon cores in parametrized hydrostatic conditions. International Journal of Modern Physics E, 2018, 27, 1850097.	0.4	10

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91	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
92	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
93	Diverse classes of HDAC8 inhibitors: in search of molecular fingerprints that regulate activity. Future Medicinal Chemistry, 2018, 10, 1589-1602.	1.1	30
94	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
95	Integrin Antagonists: A Special Emphasis on Structural Requirements of N-benzoyl-L-biphenylalanines as Î±4Î²7 and Î±4Î²1 Antagonists. Current Signal Transduction Therapy, 2018, 13, 105-118.	0.3	1
96	Arylsulfonamides and selectivity of matrix metalloproteinase-2: An overview. European Journal of Medicinal Chemistry, 2017, 129, 72-109.	2.6	55
97	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
98	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
99	Possible anticancer agents: synthesis, pharmacological activity, and molecular modeling studies on some 5-N -Substituted-2-N-(substituted benzenesulphonyl)-L(+)Glutamines. Medicinal Chemistry Research, 2017, 26, 1437-1458.	1.1	1
100	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
101	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
102	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
103	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
104	Homoisoflavonoids as potential antiangiogenic agents for retinal neovascularization. Biomedicine and Pharmacotherapy, 2017, 95, 818-827.	2.5	11
105	Understanding Chemicoâ€Biological Interactions of Glutamate MMPâ€2 Inhibitors through Rigorous Alignmentâ€Dependent 3Dâ€QSAR Analyses. ChemistrySelect, 2017, 2, 7888-7898.	0.7	12
106	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
107	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
108	Structural Insight Into the Viral 3C-Like Protease Inhibitors: Comparative SAR/QSAR Approaches. , 2017, , 317-409.		8

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109	Predictive Quantitative Structure Toxicity Relationship Study on Avian Toxicity of Some Diverse Agrochemical Pesticides by Monte Carlo Method. International Journal of Quantitative Structure-Property Relationships, 2017, 2, 19-34.	1.1	1
110	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
111	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
112	Possible Binding Mode Analysis of Pyrazolo-triazole Hybrids as Potential Anticancer Agents through Validated Molecular Docking and 3D-QSAR Modeling Approaches. Letters in Drug Design and Discovery, 2017, 14, 515-527.	0.4	6
113	An Integrated Multi-QSAR Modeling Approach for Designing Knoevenagel- Type Indoles with Enhancing Cytotoxic Profiles. Current Computer-Aided Drug Design, 2017, 13, 336-345.	0.8	6
114	Ligand- and Structure-Based Drug Design of Non-Steroidal Aromatase Inhibitors (NSAIs) in Breast Cancer. , 2017, , 118-186.		0
115	Nitric Oxide Synthase (NOS) Inhibitors in Cancer Angiogenesis. Current Enzyme Inhibition, 2016, 12, 49-66.	0.3	2
116	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
117	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
118	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
119	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
120	Chenopodium album metabolites act as dual topoisomerase inhibitors and induce apoptosis in the MCF7 cell line. MedChemComm, 2016, 7, 837-844.	3.5	13
121	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
122	Lipid from Infective L. donovani Regulates Acute Myeloid Cell Growth via Mitochondria Dependent MAPK Pathway. PLoS ONE, 2015, 10, e0120509.	1.1	12
123	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
124	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
125	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
126	Cytotoxic potential of dispirooxindolo/acenaphthoquino andrographolide derivatives against MCF-7 cell line. MedChemComm, 2015, 6, 702-707.	3.5	27

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127	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
128	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
129	Comparative validated molecular modeling of p53-HDM2 inhibitors as antiproliferative agents. European Journal of Medicinal Chemistry, 2015, 90, 860-875.	2.6	24
130	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
131	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
132	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
133	Ligand- and Structure-Based Drug Design of Non-Steroidal Aromatase Inhibitors (NSAIs) in Breast Cancer. Advances in Chemical and Materials Engineering Book Series, 2015, , 400-470.	0.2	5
134	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
135	Spermicidal and Contraceptive Potential of Desgalactotigonin: A Prospective Alternative of Nonoxynol-9. PLoS ONE, 2014, 9, e107164.	1.1	17
136	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
137	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
138	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
139	Structural findings of cinnolines as anti-schizophrenic PDE10A inhibitors through comparative chemometric modeling. Molecular Diversity, 2014, 18, 655-671.	2.1	12
140	Massive neutron stars and their implications. Pramana - Journal of Physics, 2014, 82, 831-839.	0.9	0
141	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
142	A new ellagic acid glycoside and DNA topoisomerase IB inhibitory activity of saponins from Putranjiva roxburghii. Natural Product Communications, 2014, 9, 675-7.	0.2	3
143	Exploration of structural and physicochemical requirements and search of virtual hits for aminopeptidase N inhibitors. Molecular Diversity, 2013, 17, 123-137.	2.1	18
144	Cholesteryl ester transfer protein inhibitors in coronary heart disease: Validated comparative QSAR modeling of N, N-disubstituted trifluoro-3-amino-2-propanols. Computers in Biology and Medicine, 2013, 43, 1545-1555.	3.9	6

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145	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
146	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
147	TSALLIS STATISTICS AND THE ROLE OF A STABILIZED RADION IN THE SUPERNOVAE SN1987A COOLING. International Journal of Modern Physics A, 2013, 28, 1350152.	0.5	3
148	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
149	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
150	Chemometric Modeling of 5-Phenylthiophenecarboxylic Acid Derivatives as Anti-Rheumatic Agents. Current Computer-Aided Drug Design, 2012, 8, 182-195.	0.8	10
151	Chemometric modeling and pharmacophore mapping in coronary heart disease: 2-arylbenzoxazoles as cholesteryl ester transfer protein inhibitors. MedChemComm, 2011, 2, 840.	3.5	11
152	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
153	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
154	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
155	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
156	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
157	Bulk viscosity in a hyperonic star andr-mode instability. Physical Review C, 2010, 82, .	1.1	12
158	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
159	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
160	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
161	Attributes of a rotating neutron star with a hyperon core. Physical Review C, 2008, 77, .	1.1	18
162	Constraints on nuclear matter parameters of an effective chiral model. Physical Review C, 2008, 78, .	1.1	19

#	Article	IF	Citations
163	Chemoimmunotherapeutic Approach to Prolonged Survival Time in Combination with Immunization and Glutamic Acid Derivatives with Antitumor Activity in Tumor-Bearing Mice. Biological and Pharmaceutical Bulletin, 2007, 30, 2334-2339.	0.6	5
164	Structural finding of R/S-3,4-dihydro-2,2-dimethyl-6-halo-4-(substituted) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 707 Td (phenylaminocarbo Canadian Journal of Chemistry, 2007, 85, 1053-1063.	0.6	6
165	Antibacterial activity of Abies webbiana. FÃ¬toterapÃ¬Ã¢, 2007, 78, 153-155.	1.1	13
166	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
167	Exploring QSAR onÂ3-aminopyrazoles asÂantitumor agents forÂtheirÂinhibitory activity ofÂCDK2/cyclin A. European Journal of Medicinal Chemistry, 2006, 41, 1190-1195.	2.6	28
168	Neutron star matter in an effective model. Physical Review C, 2006, 74, .	1.1	16
169	QSAR modeling on dopamine D2 receptor binding affinity of 6-methoxy benzamides. Il Farmaco, 2005, 60, 818-825.	0.9	16
170	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
171	Quantitative structureâ€“activity relationship study on some benzodiazepine derivatives as anti-Alzheimer agents. Journal of Molecular Modeling, 2004, 10, 328-334.	0.8	16
172	Hot nuclear matter in asymmetry chiral sigma model. Nuclear Physics A, 2004, 733, 169-184.	0.6	28
173	QSAR study on some anti-HIV HEPT analogues using physicochemical and topological parameters. Bioorganic and Medicinal Chemistry, 2004, 12, 1493-1503.	1.4	34
174	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
175	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
176	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
177	QSAR study on some pyridoacridine ascididemin analogues as anti-tumor agents. Bioorganic and Medicinal Chemistry, 2003, 11, 5493-5499.	1.4	41
178	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
179	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
180	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

#	Article	IF	Citations
181	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
182	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
183	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
184	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
185	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
186	Quantitative structure activity relationship (QSAR) studies of some substituted benzenesulphonyl glutamines as tumour suppressors. Indian Journal of Biochemistry and Biophysics, 2001, 38, 120-3.	0.2	7
187	Possible antineoplastic agents: Part XIII. Synthesis, biological evaluation and QSAR studies of some 1-(substituted benzenesulphonyl)-5-oxopyrrolidine-2-carboxylic acid derivatives. Anti-cancer Drug Design, 1993, 8, 95-100.	0.3	0