Nilanjan Adhikari

List of Publications by Year
in descending order

110 papers	2,631 citations	201575 27 h-index	243529 44 g-index
111 all docs	111 docs citations	111 times ranked	2412 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	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
9	Arylsulfonamides and selectivity of matrix metalloproteinase-2: An overview. European Journal of Medicinal Chemistry, 2017, 129, 72-109.	2.6	55
10	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
11	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
12	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
13	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
14	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
15	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
16	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
17	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
18	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

#	Article	IF	Citations
19	QSAR study on some anti-HIV HEPT analogues using physicochemical and topological parameters. Bioorganic and Medicinal Chemistry, 2004, 12, 1493-1503.	1.4	34
20	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
21	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
22	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
23	Structure-activity relationships of HDAC8 inhibitors: Non-hydroxamates as anticancer agents. Pharmacological Research, 2018, 131, 128-142.	3.1	32
24	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
25	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
26	Diverse classes of HDAC8 inhibitors: in search of molecular fingerprints that regulate activity. Future Medicinal Chemistry, 2018, 10, 1589-1602.	1.1	30
27	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
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	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
30	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
31	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
32	Identification of structural requirements and prediction of inhibitory activity of natural flavonoids against Zika virus through molecular docking and Monte Carlo based QSAR Simulation. Natural Product Research, 2019, 33, 851-857.	1.0	25
33	Comparative validated molecular modeling of p53-HDM2 inhibitors as antiproliferative agents. European Journal of Medicinal Chemistry, 2015, 90, 860-875.	2.6	24
34	Pharmacoinformatics study of Piperolactam A from Piper betle root as new lead for non steroidal anti fertility drug development. Computational Biology and Chemistry, 2017, 67, 213-224.	1.1	24
35	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
36	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

#	Article	IF	Citations
37	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
38	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
39	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
40	Designing potential HDAC3 inhibitors to improve memory and learning. Journal of Biomolecular Structure and Dynamics, 2019, 37, 2133-2142.	2.0	21
41	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
42	A Review on Camptothecin Analogs with Promising Cytotoxic Profile. Anti-Cancer Agents in Medicinal Chemistry, 2019, 18, 1796-1814.	0.9	20
43	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
44	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
45	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
46	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
47	Selective and nonselective HDAC8 inhibitors: a therapeutic patent review. Pharmaceutical Patent Analyst, 2018, 7, 259-276.	0.4	17
48	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
49	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
50	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
51	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
52	Recent Developments on Synthesis of Indole Derivatives Through Green Approaches and Their Pharmaceutical Applications. Current Organic Chemistry, 2020, 24, 2665-2693.	0.9	15
53	Insight into the Structural Requirements of Theophylline-Based Aldehyde Dehydrogenase lAl (ALDHlAl) Inhibitors Through Multi-QSAR Modeling and Molecular Docking Approaches. Current Drug Discovery Technologies, 2016, 13, 84-100.	0.6	15
54	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

#	Article	IF	Citations
55	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
56	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
57	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
58	First Report on 3â€(3â€oxoaryl) Indole Derivatives as Anticancer Agents: Microwave Assisted Synthesis, In Vitro Screening and Molecular Docking Studies. ChemistrySelect, 2019, 4, 4478-4482.	0.7	13
59	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
60	Structural findings of cinnolines as anti-schizophrenic PDE10A inhibitors through comparative chemometric modeling. Molecular Diversity, 2014, 18, 655-671.	2.1	12
61	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
62	Understanding Chemicoâ€Biological Interactions of Glutamate MMPâ€2 Inhibitors through Rigorous Alignmentâ€Dependent 3Dâ€QSAR Analyses. ChemistrySelect, 2017, 2, 7888-7898.	0.7	12
63	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
64	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
65	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
66	Chemometric modeling and pharmacophore mapping in coronary heart disease: 2-arylbenzoxazoles as cholesteryl ester transfer protein inhibitors. MedChemComm, 2011, 2, 840.	3.5	11
67	Homoisoflavonoids as potential antiangiogenic agents for retinal neovascularization. Biomedicine and Pharmacotherapy, 2017, 95, 818-827.	2.5	11
68	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
69	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
70	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
71	Chemometric Modeling of 5-Phenylthiophenecarboxylic Acid Derivatives as Anti-Rheumatic Agents. Current Computer-Aided Drug Design, 2012, 8, 182-195.	0.8	10
72	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

#	Article	IF	Citations
73	Exploration of histone deacetylase 8 inhibitors through classification QSAR study: Part II. Journal of Molecular Structure, 2020, 1204, 127529.	1.8	10
74	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
75	Identification of molecular fingerprints of phenylindole derivatives as cytotoxic agents: a multi-QSAR approach. Structural Chemistry, 2018, 29, 1095-1107.	1.0	9
76	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
77	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
78	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
79	Identification of molecular fingerprints of natural products for the inhibition of breast cancer resistance protein (BCRP). Phytomedicine, 2021, 85, 153523.	2.3	9
80	Ligand-based design of anticancer MMP2Âinhibitors: aÂreview. Future Medicinal Chemistry, 2021, 13, 1987-2013.	1.1	9
81	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
82	Structural Insight Into the Viral 3C-Like Protease Inhibitors: Comparative SAR/QSAR Approaches. , 2017, , 317-409.		8
83	2-Phenylindole derivatives as anticancer agents: synthesis and screening against murine melanoma, human lung and breast cancer cell lines. Synthetic Communications, 2019, 49, 2258-2269.	1.1	8
84	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
85	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
86	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
87	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
88	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
89	Identification of structural fingerprints for inÂvivo toxicity by using Monte Carlo based QSTR modeling of nitroaromatics. Toxicology Mechanisms and Methods, 2020, 30, 257-265.	1.3	7
90	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

#	Article	IF	Citations
91	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
92	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
93	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
94	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
95	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
96	Collagenases and gelatinases and their inhibitors as anticancer agents. , 2020, , 265-294.		6
97	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
98	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
99	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
100	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
101	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
102	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
103	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
104	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
105	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
106	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
107	Nitric Oxide Synthase (NOS) Inhibitors in Cancer Angiogenesis. Current Enzyme Inhibition, 2016, 12, 49-66.	0.3	2
108	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

#	Article	IF	Citations
109	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
110	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