Sk. Abdul Amin

List of Publications by Year in Descending Order

90 papers	1,319 citations	21 h-index	31 g-index
93 ext. papers	1,736 ext. citations	3.8 avg, IF	5.82 L-index

#	Paper	IF	Citations
90	A critical analysis of urea transporter B inhibitors: molecular fingerprints, pharmacophore features for the development of next-generation diuretics.. *Molecular Diversity*, **2022**, 1	3.1	
89	Synthesis, biological activity, structure activity relationship study and liposomal formulation development of some arylsulfonyl pyroglutamic acid derivatives. *Journal of Molecular Structure*, **2022**, 1248, 131512	3.4	1
88	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	3.5	1
87	A fragment-based structural analysis of MMP-2 inhibitors in search of meaningful structural fragments.. *Computers in Biology and Medicine*, **2022**, 144, 105360	7	
86	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	3.4	0
85	Chemical-informatics approach to COVID-19 drug discovery: Monte Carlo based QSAR, virtual screening and molecular docking study of some molecules as papain-like protease (PLpro) inhibitors. *Journal of Biomolecular Structure and Dynamics*, **2021**, 39, 4764-4773	3.6	49
84	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, 917-939	3.5	1
83	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*, **2021**, 53, 116534	3.4	0
82	Exploring sodium glucose cotransporter (SGLT2) inhibitors with machine learning approach: A novel hope in anti-diabetes drug discovery.. *Journal of Molecular Graphics and Modelling*, **2021**, 111, 108106	2.8	1
81	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	5.1	1
80	Ligand-based design of anticancer MMP2 inhibitors: a review. *Future Medicinal Chemistry*, **2021**, 13, 1987-2013	4	2
79	Exploring naphthyl derivatives as SARS-CoV papain-like protease (PLpro) inhibitors and its implications in COVID-19 drug discovery. *Molecular Diversity*, **2021**, 1	3.1	4
78	Protease targeted COVID-19 drug discovery: What we have learned from the past SARS-CoV inhibitors?. *European Journal of Medicinal Chemistry*, **2021**, 215, 113294	6.8	12
77	Therapies of Hematological Malignancies: An Overview of the Potential Targets and Their Inhibitors. *Current Chemical Biology*, **2021**, 15, 19-49	0.4	1
76	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	3.4	32
75	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	1.8	5
74	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	3.4	58

73	HDAC6 as privileged target in drug discovery: A perspective. *Pharmacological Research*, **2021**, 163, 105274	10.2	34
72	Outline of gelatinase inhibitors as anti-cancer agents: A patent mini-review for 2010-present. *European Journal of Medicinal Chemistry*, **2021**, 213, 113044	6.8	5
71	Development of decision trees to discriminate HDAC8 inhibitors and non-inhibitors using recursive partitioning. *Journal of Biomolecular Structure and Dynamics*, **2021**, 39, 1-8	3.6	15
70	Small molecule drug conjugates (SMDCs): an emerging strategy for anticancer drug design and discovery. *New Journal of Chemistry*, **2021**, 45, 5291-5321	3.6	11
69	First structure-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	3.1	18
68	Unmasking of crucial structural fragments for coronavirus protease inhibitors and its implications in COVID-19 drug discovery. *Journal of Molecular Structure*, **2021**, 1237, 130366	3.4	2
67	Insight into the structural requirement of aryl sulphonamide based gelatinases (MMP-2 and MMP-9) inhibitors - Part I: 2D-QSAR, 3D-QSAR topomer CoMFA and Naïve Bayes studies - 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	3.5	2
66	Synthesis, biological evaluation, and molecular docking analysis of novel linker-less benzamide based potent and selective HDAC3 inhibitors. *Bioorganic Chemistry*, **2021**, 114, 105050	5.1	5
65	Urea transporter and its specific and nonspecific inhibitors: State of the art and pharmacological perspective. *European Journal of Pharmacology*, **2021**, 911, 174508	5.3	1
64	Inhibitors of gelatinases (MMP-2 and MMP-9) for the management of hematological malignancies. *European Journal of Medicinal Chemistry*, **2021**, 223, 113623	6.8	12
63	Quantitative activity–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	3.6	1
62	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, 1683-1696	3.6	4
61	Fight against novel coronavirus: A perspective of medicinal chemists. *European Journal of Medicinal Chemistry*, **2020**, 201, 112559	6.8	44
60	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	3.5	5
59	Matrix metalloproteinase-9 (MMP-9) and its inhibitors in cancer: A minireview. *European Journal of Medicinal Chemistry*, **2020**, 194, 112260	6.8	84
58	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	3.5	5
57	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	3.5	3
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	3.6	8

55	Histone deacetylase 3 (HDAC3) inhibitors as anticancer agents: A review. *European Journal of Medicinal Chemistry*, **2020**, 192, 112171	6.8	22
54	Collagenases and gelatinases and their inhibitors as anticancer agents **2020**, 265-294		4
53	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	3.6	5
52	Exploration of histone deacetylase 8 inhibitors through classification QSAR study: Part II. *Journal of Molecular Structure*, **2020**, 1204, 127529	3.4	8
51	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	3.6	4
50	Dissecting the Drug Development Strategies Against SARS-CoV-2 Through Diverse Computational Modeling Techniques. *Methods in Pharmacology and Toxicology*, **2020**, 329	1.1	4
49	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	3.6	27
48	Structural exploration of tetrahydroisoquinoline derivatives as HDAC8 inhibitors through multi-QSAR modeling study. *Journal of Biomolecular Structure and Dynamics*, **2020**, 38, 1551-1564	3.6	8
47	Histone deacetylase 3 inhibitors in learning and memory processes with special emphasis on benzamides. *European Journal of Medicinal Chemistry*, **2019**, 166, 369-380	6.8	18
46	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	3.5	10
45	QSAR modelling on a series of arylsulfonamide-based hydroxamates as potent MMP-2 inhibitors. *SAR and QSAR in Environmental Research*, **2019**, 30, 247-263	3.5	9
44	Structural exploration of arylsulfonamide-based ADAM17 inhibitors through validated comparative multi-QSAR modelling studies. *Journal of Molecular Structure*, **2019**, 1185, 128-142	3.4	8
43	Designing potential HDAC3 inhibitors to improve memory and learning. *Journal of Biomolecular Structure and Dynamics*, **2019**, 37, 2133-2142	3.6	18
42	Synthesis, anticancer activity, structure-activity relationship and binding mode of interaction studies of substituted pentanoic acids. *Future Medicinal Chemistry*, **2019**, 11, 1679-1702	4.1	9
41	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	5.1	19
40	Histone deacetylase 8 (HDAC8) and its inhibitors with selectivity to other isoforms: An overview. *European Journal of Medicinal Chemistry*, **2019**, 164, 214-240	6.8	46
39	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	3.6	8
38	Structural refinement and prediction of potential CCR2 antagonists through validated multi-QSAR modeling studies. *Journal of Biomolecular Structure and Dynamics*, **2019**, 37, 75-94	3.6	9

37	Structure-activity relationships of HDAC8 inhibitors: Non-hydroxamates as anticancer agents. *Pharmacological Research*, **2018**, 131, 128-142	10.2	24
36	Identification of molecular fingerprints of phenylindole derivatives as cytotoxic agents: a multi-QSAR approach. *Structural Chemistry*, **2018**, 29, 1095-1107	1.8	9
35	Structural exploration of hydroxyethylamines as HIV-1 protease inhibitors: new features identified. *SAR and QSAR in Environmental Research*, **2018**, 29, 385-408	3.5	15
34	Design of Aminopeptidase N Inhibitors as Anti-cancer Agents. *Journal of Medicinal Chemistry*, **2018**, 61, 6468-6490	8.3	50
33	Exploring in house glutamate inhibitors of matrix metalloproteinase-2 through validated robust chemico-biological quantitative approaches. *Structural Chemistry*, **2018**, 29, 285-297	1.8	14
32	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	3.5	11
31	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	3.6	43
30	Shedding light on designing potential meprin inhibitors through ligand-based robust validated computational approaches: A proposal to chemists!. *Journal of Biomolecular Structure and Dynamics* , **2018**, 36, 3003-3022	3.6	4
29	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	3.6	18
28	Application of Computation in the Biosynthesis of Phytochemicals **2018**, 255-276		
27	A Review on Camptothecin Analogs with Promising Cytotoxic Profile. *Anti-Cancer Agents in Medicinal Chemistry*, **2018**, 18, 1796-1814	2.2	12
26	Integrin Antagonists: A Special Emphasis on Structural Requirements of N-benzoyl-L-biphenylalanines as 47 and 41 Antagonists. *Current Signal Transduction Therapy*, **2018**, 13, 105-118	0.8	1
25	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	3.4	10
24	An integrated QSAR modeling approach to explore the structure-property and selectivity relationships of N-benzoyl-L-biphenylalanines as integrin antagonists. *Molecular Diversity*, **2018**, 22, 129-158	3.1	9
23	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	1.2	1
22	Selective and nonselective HDAC8 inhibitors: a therapeutic patent review. *Pharmaceutical Patent Analyst*, **2018**, 7, 259-276	0.6	10
21	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	6.8	33
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	5.1	30

19	Diverse classes of HDAC8 inhibitors: in search of molecular fingerprints that regulate activity. *Future Medicinal Chemistry*, **2018**, 10, 1589-1602	4.1	25
18	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	3.6	17
17	First report on the structural exploration and prediction of new BPTES analogs as glutaminase inhibitors. *Journal of Molecular Structure*, **2017**, 1143, 49-64	3.4	31
16	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	6.8	44
15	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	3.5	21
14	An integrated ligand-based modelling approach to explore the structure-property relationships of influenza endonuclease inhibitors. *Structural Chemistry*, **2017**, 28, 1663-1678	1.8	12
13	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	3.5	22
12	Homoisoflavonoids as potential antiangiogenic agents for retinal neovascularization. *Biomedicine and Pharmacotherapy*, **2017**, 95, 818-827	7.5	8
11	Understanding Chemico-Biological Interactions of Glutamate MMP-2 Inhibitors through Rigorous Alignment-Dependent 3D-QSAR Analyses. *ChemistrySelect*, **2017**, 2, 7888-7898	1.8	7
10	Structure-activity relationships of hydroxamate-based histone deacetylase-8 inhibitors: reality behind anticancer drug discovery. *Future Medicinal Chemistry*, **2017**, 9, 2211-2237	4.1	22
9	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	0.9	6
8	Designing Potential Antitrypanosomal Thiazol-2-ethylamines through Predictive Regression Based and Classification Based QSAR Analyses. *Current Drug Discovery Technologies*, **2017**, 14, 39-52	1.5	15
7	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	0.8	4
6	An Integrated Multi-QSAR Modeling Approach for Designing Knoevenagel- Type Indoles with Enhancing Cytotoxic Profiles. *Current Computer-Aided Drug Design*, **2017**, 13, 336-345	1.4	6
5	Is dual inhibition of metalloenzymes HDAC-8 and MMP-2 a potential pharmacological target to combat hematological malignancies?. *Pharmacological Research*, **2017**, 122, 8-19	10.2	40
4	First molecular modeling report on novel arylpyrimidine kynurenine monooxygenase inhibitors through multi-QSAR analysis against Huntington's disease: A proposal to chemists!. *Bioorganic and Medicinal Chemistry Letters*, **2016**, 26, 5712-5718	2.9	36
3	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	0.9	17
2	Modelling the cytotoxic activity of pyrazolo-triazole hybrids using descriptors calculated from the open source tool PaDEL-descriptorPeer review under responsibility of Taibah University.View all notes. *Journal of Taibah University for Science*, **2016**, 10, 896-905	3	14

1	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	1.5	14