Farhan A Pasha

List of Publications by Citations

41 papers	692 citations	16 h-index	23 g-index
43 ext. papers	736 ext. citations	3.9 avg, IF	3.62 L-index

#	Paper	IF	Citations
41	DFT-based QSAR study of testosterone and its derivatives. *Bioorganic and Medicinal Chemistry*, **2004**, 12, 171-7	3.4	56
40	Comparative QSAR study of phenol derivatives with the help of density functional theory. *Bioorganic and Medicinal Chemistry*, **2005**, 13, 6823-9	3.4	55
39	QSAR study of estrogens with the help of PM3-based descriptors. *International Journal of Quantum Chemistry*, **2005**, 104, 87-100	2.1	38
38	Pharmacophore and docking-based combined in-silico study of KDR inhibitors. *Journal of Molecular Graphics and Modelling*, **2009**, 28, 54-61	2.8	37
37	Atomic softness-based QSAR study of testosterone. *International Journal of Quantum Chemistry*, **2005**, 103, 237-245	2.1	33
36	Bipodal surface organometallic complexes with surface N-donor ligands and application to the catalytic cleavage of C-H and C-C bonds in n-butane. *Journal of the American Chemical Society*, **2013**, 135, 17943-51	16.4	31
35	Discovery of new inhibitors of resistant Streptococcus pneumoniae penicillin binding protein (PBP) 2x by structure-based virtual screening. *Journal of Medicinal Chemistry*, **2009**, 52, 5926-36	8.3	23
34	QSTR Study of Small Organic Molecules Against Tetrahymena pyriformis. *QSAR and Combinatorial Science*, **2007**, 26, 69-84		23
33	Quantum chemical QSAR study of flavones and their radical-scavenging activity. *Medicinal Chemistry Research*, **2007**, 16, 408-417	2.2	23
32	Mechanism of n-Butane Hydrogenolysis Promoted by Ta-Hydrides Supported on Silica. *ACS Catalysis*, **2014**, 4, 1868-1874	13.1	21
31	Hologram and 3D-quantitative structure toxicity relationship studies of azo dyes. *Journal of Molecular Modeling*, **2008**, 14, 293-302	2	21
30	DFT Based Atomic Softness and Its Application in Site Selectivity. *QSAR and Combinatorial Science*, **2003**, 22, 843-851		20
29	Semiempirical QSAR study and ligand receptor interaction of estrogens. *Molecular Diversity*, **2005**, 9, 215-20	3.1	20
28	Structure-function relationship of a plant NCS1 member--homology modeling and mutagenesis identified residues critical for substrate specificity of PLUTO, a nucleobase transporter from Arabidopsis. *PLoS ONE*, **2014**, 9, e91343	3.7	19
27	In silico QSAR studies of anilinoquinolines as EGFR inhibitors. *Journal of Molecular Modeling*, **2010**, 16, 263-77	2	17
26	CH and CC Activation of n-Butane with Zirconium Hydrides Supported on SBA15 Containing N-Donor Ligands: [(?SiNH)(?SiX)ZrH2], [(?SiNH)(?SiX)2ZrH], and[(?SiN?)(?SiX)ZrH] (X = NH OH). A DFT Study. *Organometallics*, **2014**, 33, 3320-3327	3.8	16
25	Pharmacophore identification and validation study of CK2 inhibitors using CoMFA/CoMSIA. *Chemical Biology and Drug Design*, **2009**, 74, 148-58	2.9	16

24	Structure–Activity Relationship To Screen Ni–Bisphosphine Complexes for the Oxidative Coupling of CO2 and Ethylene. *Organometallics*, **2017**, 36, 1107-1112	3.8	15
23	A novel role for pigment genes in the stress response in rainbow trout (Oncorhynchus mykiss). *Scientific Reports*, **2016**, 6, 28969	4.9	14
22	Efficient Hydrogenolysis of Alkanes at Low Temperature and Pressure Using Tantalum Hydride on MCM-41, and a Quantum Chemical Study. *ChemCatChem*, **2012**, 4, 363-369	5.2	13
21	Molecular docking and 3D QSAR studies of Chk2 inhibitors. *Chemical Biology and Drug Design*, **2009**, 73, 292-300	2.9	13
20	Quantitative structure activity relationship (QSAR) study of estrogen derivatives based on descriptors of energy and softness. *Chemical Biology and Drug Design*, **2007**, 70, 520-9	2.9	13
19	3D-quantitative structure activity analysis and quantum chemical analysis of pyrido-di-indoles. *International Journal of Quantum Chemistry*, **2008**, 108, 391-400	2.1	13
18	DFT-based de novo QSAR of Phenoloxidase Inhibitors. *Chemical Biology and Drug Design*, **2008**, 71, 483-493	2.9	13
17	DFT Study on the Impact of the Methylaluminoxane Cocatalyst in Ethylene Oligomerization Using a Titanium-Based Catalyst. *Organometallics*, **2015**, 34, 426-431	3.8	12
16	Mechanism based QSAR studies of N-phenylbenzamides as antimicrobial agents. *Environmental Toxicology and Pharmacology*, **2008**, 26, 128-35	5.8	12
15	CO2 activation through silylimido and silylamido zirconium hydrides supported on N-donor chelating SBA15 surface ligands. *Chemical Communications*, **2016**, 52, 2577-80	5.8	10
14	Pharmacophore based 3D-QSAR study of VEGFR-2 inhibitors. *Medicinal Chemistry Research*, **2009**, 18, 127-142	2.2	10
13	Elucidation of binding mode and three dimensional quantitative structure-activity relationship studies of a novel series of protein kinase B/Akt inhibitors. *Journal of Molecular Modeling*, **2009**, 15, 183-92	2	9
12	Novel applications of atomic softness and QSAR study of testosterone derivatives. *Medicinal Chemistry Research*, **2009**, 18, 455-466	2.2	9
11	SOMC grafting of vanadium oxytriisopropoxide (VO(O Pr)) on dehydroxylated silica; analysis of surface complexes and thermal restructuring mechanism.. *RSC Advances*, **2018**, 8, 20801-20808	3.7	8
10	Pharmacophore-based 3D-QSAR of HIF-1 inhibitors. *Archives of Pharmacal Research*, **2009**, 32, 317-23	6.1	8
9	Molecular dynamics and QM/MM-based 3D interaction analyses of cyclin-E inhibitors. *Journal of Molecular Modeling*, **2013**, 19, 879-91	2	7
8	Structural studies of B-type Aurora kinase inhibitors using computational methods. *Acta Pharmacologica Sinica*, **2010**, 31, 244-58	8	7
7	Receptor guided 3D-QSAR: a useful approach for designing of IGF-1R inhibitors. *Journal of Biomedicine and Biotechnology*, **2008**, 2008, 837653		7

6	QM and Pharmacophore based 3D-QSAR of MK886 Analogues against mPGES-1. *Bulletin of the Korean Chemical Society*, **2008**, 29, 647-655	1.2	7
5	3D and quantum QSAR of non-benzodiazepine compounds. *European Journal of Medicinal Chemistry* , **2008**, 43, 2361-72	6.8	6
4	2D-QSAR of non-benzodiazepines to benzodiazepines receptor (BZR). *Medicinal Chemistry Research*, **2009**, 18, 98-111	2.2	5
3	In silico quantitative structure-toxicity relationship study of aromatic nitro compounds. *Chemical Biology and Drug Design*, **2009**, 73, 537-44	2.9	5
2	Revisiting OD Bond Formation through Outer-Sphere Water Molecules versus Bimolecular Mechanisms in Water-Oxidation Catalysis (WOC) by Cp*Ir Based Complexes. *European Journal of Inorganic Chemistry*, **2019**, 2019, 2093-2100	2.3	4
1	Docking and Quantum Mechanics-Guided CoMFA Analysis of b-RAF Inhibitors. *Bulletin of the Korean Chemical Society*, **2008**, 29, 1499-1504	1.2	3