Serdar Durdagi

List of Publications by Citations

161 papers	2,955 citations	31 h-index	46 g-index
184 ext. papers	3,431 ext. citations	4 avg, IF	5.54 L-index

#	Paper	IF	Citations
161	Discovery of potent carbonic anhydrase and acetylcholine esterase inhibitors: novel sulfamoylcarbamates and sulfamides derived from acetophenones. *Bioorganic and Medicinal Chemistry*, **2015**, 23, 3592-602	3.4	119
160	Acetylcholinesterase and carbonic anhydrase inhibitory properties of novel urea and sulfamide derivatives incorporating dopaminergic 2-aminotetralin scaffolds. *Bioorganic and Medicinal Chemistry*, **2016**, 24, 2318-29	3.4	103
159	Carbonic anhydrase inhibitory properties of novel benzylsulfamides using molecular modeling and experimental studies. *Bioorganic Chemistry*, **2014**, 56, 75-82	5.1	99
158	Kinetic and docking studies of phenol-based inhibitors of carbonic anhydrase isoforms I, II, IX and XII evidence a new binding mode within the enzyme active site. *Bioorganic and Medicinal Chemistry*, **2011**, 19, 1381-9	3.4	89
157	Identification of novel cholesterol-binding regions in Kir2 channels. *Journal of Biological Chemistry*, **2013**, 288, 31154-64	5.4	77
156	Combined receptor and ligand-based approach to the universal pharmacophore model development for studies of drug blockade to the hERG1 pore domain. *Journal of Chemical Information and Modeling*, **2011**, 51, 463-74	6.1	77
155	Computational design of novel fullerene analogues as potential HIV-1 PR inhibitors: Analysis of the binding interactions between fullerene inhibitors and HIV-1 PR residues using 3D QSAR, molecular docking and molecular dynamics simulations. *Bioorganic and Medicinal Chemistry*, **2008**, 16, 9957-74	3.4	77
154	Nanoscale enzyme inhibitors: fullerenes inhibit carbonic anhydrase by occluding the active site entrance. *Bioorganic and Medicinal Chemistry*, **2010**, 18, 2822-8	3.4	63
153	Modeling of open, closed, and open-inactivated states of the hERG1 channel: structural mechanisms of the state-dependent drug binding. *Journal of Chemical Information and Modeling*, **2012**, 52, 2760-74	6.1	60
152	3D QSAR CoMFA/CoMSIA, molecular docking and molecular dynamics studies of fullerene-based HIV-1 PR inhibitors. *Bioorganic and Medicinal Chemistry Letters*, **2008**, 18, 6283-9	2.9	56
151	The synthesis of novel sulfamides derived from benzylphenethylamines as acetylcholinesterase, butyrylcholinesterase and carbonic anhydrase enzymes inhibitors. *Bioorganic Chemistry*, **2017**, 74, 238-250	5.1	55
150	Development of accurate binding affinity predictions of novel renin inhibitors through molecular docking studies. *Journal of Molecular Graphics and Modelling*, **2010**, 29, 425-35	2.8	53
149	In silico drug screening approach for the design of magic bullets: a successful example with anti-HIV fullerene derivatized amino acids. *Journal of Chemical Information and Modeling*, **2009**, 49, 1139-43	6.1	50
148	Structure-activity relationships for the interaction of 5,10-dihydroindeno[1,2-b]indole derivatives with human and bovine carbonic anhydrase isoforms I, II, III, IV and VI. *European Journal of Medicinal Chemistry*, **2012**, 49, 68-73	6.8	49
147	Combinatorial peptide library screening for discovery of diverse glucosidase inhibitors using molecular dynamics simulations and binary QSAR models. *Journal of Biomolecular Structure and Dynamics*, **2019**, 37, 726-740	3.6	49
146	Does the donor-acceptor concept work for designing synthetic metals? III. Theoretical investigation of copolymers between quinoid acceptors and aromatic donors. *Journal of Molecular Modeling*, **2006**, 12, 687-701	2	48
145	Structural refinement of the hERG1 pore and voltage-sensing domains with ROSETTA-membrane and molecular dynamics simulations. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 2922-34	4.2	44

144	The application of 3D-QSAR studies for novel cannabinoid ligands substituted at the C1Sposition of the alkyl side chain on the structural requirements for binding to cannabinoid receptors CB1 and CB2. *Journal of Medicinal Chemistry*, **2007**, 50, 2875-85	8.3	42
143	Inhibition of acetylcholinesterase and butyrylcholinesterase with uracil derivatives: kinetic and computational studies. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2019**, 34, 429-437	5.6	41
142	Design, synthesis and biological evaluation of novel nitroaromatic compounds as potent glutathione reductase inhibitors. *Bioorganic and Medicinal Chemistry Letters*, **2011**, 21, 5398-402	2.9	41
141	Binding of novel fullerene inhibitors to HIV-1 protease: insight through molecular dynamics and molecular mechanics Poisson-Boltzmann surface area calculations. *Journal of Computer-Aided Molecular Design*, **2011**, 25, 959-76	4.2	41
140	Application of 3D QSAR CoMFA/CoMSIA and in silico docking studies on novel renin inhibitors against cardiovascular diseases. *European Journal of Medicinal Chemistry*, **2009**, 44, 3703-11	6.8	40
139	Antihypertensive drug valsartan in solution and at the AT1 receptor: conformational analysis, dynamic NMR spectroscopy, in silico docking, and molecular dynamics simulations. *Journal of Chemical Information and Modeling*, **2009**, 49, 726-39	6.1	39
138	Interaction of carbonic anhydrase isozymes I, II, and IX with some pyridine and phenol hydrazinecarbothioamide derivatives. *Bioorganic and Medicinal Chemistry Letters*, **2015**, 25, 5636-41	2.9	34
137	Synthesis of Some Novel Norbornene-Fused Pyridazines as Potent Inhibitors of Carbonic Anhydrase and Acetylcholinesterase. *Journal of Heterocyclic Chemistry*, **2016**, 53, 2049-2056	1.9	34
136	Binding Interactions of Dopamine and Apomorphine in D2High and D2Low States of Human Dopamine D2 Receptor Using Computational and Experimental Techniques. *ACS Chemical Neuroscience*, **2016**, 7, 185-95	5.7	34
135	Carbonic anhydrase inhibitors: Design, synthesis, kinetic, docking and molecular dynamics analysis of novel glycine and phenylalanine sulfonamide derivatives. *Bioorganic and Medicinal Chemistry*, **2015**, 23, 7353-8	3.4	33
134	Investigation of Inhibition Mechanism of Chemokine Receptor CCR5 by Micro-second Molecular Dynamics Simulations. *Scientific Reports*, **2015**, 5, 13180	4.9	33
133	Synthesis, biological activity and multiscale molecular modeling studies of bis-coumarins as selective carbonic anhydrase IX and XII inhibitors with effective cytotoxicity against hepatocellular carcinoma. *Bioorganic Chemistry*, **2019**, 87, 838-850	5.1	32
132	Inhibition of human carbonic anhydrase isozymes I, II and VI with a series of bisphenol, methoxy and bromophenol compounds. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2012**, 27, 467-75	5.6	32
131	Cholesterol up-regulates neuronal G protein-gated inwardly rectifying potassium (GIRK) channel activity in the hippocampus. *Journal of Biological Chemistry*, **2017**, 292, 6135-6147	5.4	31
130	Synthesis, anticholinesterase activity and molecular modeling study of novel carbamate-substituted thymol/carvacrol derivatives. *Bioorganic and Medicinal Chemistry*, **2017**, 25, 1352-1363	3.4	31
129	Inhibition of mammalian carbonic anhydrases I-XIV with grayanotoxin III: solution and in silico studies. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2014**, 29, 469-75	5.6	31
128	Insights into the molecular basis of action of the AT1 antagonist losartan using a combined NMR spectroscopy and computational approach. *Biochimica Et Biophysica Acta - Biomembranes*, **2014**, 1838, 1031-46	3.8	29
127	A computational study on cannabinoid receptors and potent bioactive cannabinoid ligands: homology modeling, docking, de novo drug design and molecular dynamics analysis. *Molecular Diversity*, **2010**, 14, 257-76	3.1	29

126	Combined 3D QSAR and molecular docking studies to reveal novel cannabinoid ligands with optimum binding activity. *Bioorganic and Medicinal Chemistry Letters*, **2007**, 17, 6754-63	2.9	29
125	Virtual screening of eighteen million compounds against dengue virus: Combined molecular docking and molecular dynamics simulations study. *Journal of Molecular Graphics and Modelling*, **2016**, 66, 99-107	2.8	29
124	Characterization, in Vivo Evaluation, and Molecular Modeling of Different Propofol-Cyclodextrin Complexes To Assess Their Drug Delivery Potential at the Blood-Brain Barrier Level. *Journal of Chemical Information and Modeling*, **2016**, 56, 1914-1922	6.1	27
123	Elucidation of conformational states, dynamics, and mechanism of binding in human δ-opioid receptor complexes. *Journal of Chemical Information and Modeling*, **2014**, 54, 2294-308	6.1	25
122	Fullerene-based inhibitors of HIV-1 protease. *Journal of Peptide Science*, **2015**, 21, 862-70	2.1	25
121	Modeling and protein engineering studies of active and inactive states of human dopamine D2 receptor (D2R) and investigation of drug/receptor interactions. *Molecular Diversity*, **2015**, 19, 321-32	3.1	25
120	Structure-guided topographic mapping and mutagenesis to elucidate binding sites for the human ether-a-go-go-related gene 1 potassium channel (KCNH2) activator NS1643. *Journal of Pharmacology and Experimental Therapeutics*, **2012**, 342, 441-52	4.7	25
119	Protein-protein interactions: inhibition of mammalian carbonic anhydrases I-XV by the murine inhibitor of carbonic anhydrase and other members of the transferrin family. *Journal of Medicinal Chemistry*, **2012**, 55, 5529-35	8.3	25
118	AT1 antagonists: a patent review (2008 - 2012). *Expert Opinion on Therapeutic Patents*, **2013**, 23, 1483-94	6.8	24
117	Effects of propolis, caffeic acid phenethyl ester, and pollen on renal injury in hypertensive rat: An experimental and theoretical approach. *Cell Biochemistry and Function*, **2017**, 35, 304-314	4.2	24
116	NS1643 interacts around L529 of hERG to alter voltage sensor movement on the path to activation. *Biophysical Journal*, **2015**, 108, 1400-1413	2.9	23
115	Molecular modeling and in vitro approaches towards cholinesterase inhibitory effect of some natural xanthohumol, naringenin, and acyl phloroglucinol derivatives. *Phytomedicine*, **2018**, 42, 25-33	6.5	23
114	Synthesis, biological activity and multiscale molecular modeling studies for coumaryl-carboxamide derivatives as selective carbonic anhydrase IX inhibitors. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2017**, 32, 1042-1052	5.6	23
113	The discovery of new potent non-peptide Angiotensin II AT1 receptor blockers: a concise synthesis, molecular docking studies and biological evaluation of N-substituted 5-butylimidazole derivatives. *European Journal of Medicinal Chemistry*, **2012**, 55, 358-74	6.8	23
112	Investigating the molecular mechanism of staphylococcal DNA gyrase inhibitors: A combined ligand-based and structure-based resources pipeline. *Journal of Molecular Graphics and Modelling*, **2018**, 85, 122-129	2.8	21
111	Investigation of PDE5/PDE6 and PDE5/PDE11 selective potent tadalafil-like PDE5 inhibitors using combination of molecular modeling approaches, molecular fingerprint-based virtual screening protocols and structure-based pharmacophore development. *Journal of Enzyme Inhibition and*	5.6	20
110	Proposing Novel MAO-B Hit Inhibitors Using Multidimensional Molecular Modeling Approaches and Application of Binary QSAR Models for Prediction of Their Therapeutic Activity, Pharmacokinetic and Toxicity Properties. *ACS Chemical Neuroscience*, **2018**, 9, 1768-1782	5.7	20
109	Role of the pH in state-dependent blockade of hERG currents. *Scientific Reports*, **2016**, 6, 32536	4.9	20

108	Targeting the NF-B/IB complex via fragment-based E-Pharmacophore virtual screening and binary QSAR models. *Journal of Molecular Graphics and Modelling*, **2019**, 86, 264-277	2.8	20
107	Virtual drug repurposing study against SARS-CoV-2 TMPRSS2 target. *Turkish Journal of Biology*, **2020**, 44, 185-191	3.1	19
106	Comparison of thermal effects of stilbenoid analogs in lipid bilayers using differential scanning calorimetry and molecular dynamics: correlation of thermal effects and topographical position with antioxidant activity. *European Biophysics Journal*, **2011**, 40, 865-75	1.9	19
105	Partial interdigitation of lipid bilayers. *International Journal of Quantum Chemistry*, **2011**, 111, 1172-1183	2.1	19
104	Leveraging NMR and X-ray Data of the Free Ligands to Build Better Drugs Targeting Angiotensin II Type 1 G-Protein Coupled Receptor. *Current Medicinal Chemistry*, **2016**, 23, 36-59	4.3	18
103	Solubility profiles, hydration and desolvation of curcumin complexed with cyclodextrin and hydroxypropyl-cyclodextrin. *Journal of Molecular Structure*, **2017**, 1134, 91-98	3.4	17
102	Effects of Cholesterol on GPCR Function: Insights from Computational and Experimental Studies. *Advances in Experimental Medicine and Biology*, **2019**, 1135, 89-103	3.6	17
101	Structural and dynamical properties of Bi3+ in water. *Chemical Physics Letters*, **2005**, 406, 20-23	2.5	16
100	In vitro and in silico approaches to appraise Polygonum maritimum L. as a source of innovative products with anti-ageing potential. *Industrial Crops and Products*, **2018**, 111, 391-399	5.9	16
99	In silico investigation of PARP-1 catalytic domains in holo and apo states for the design of high-affinity PARP-1 inhibitors. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2016**, 31, 112-20	5.6	15
98	Analysis of the Glutamate Agonist LY404,039 Binding to Nonstatic Dopamine Receptor D2 Dimer Structures and Consensus Docking. *ACS Chemical Neuroscience*, **2017**, 8, 1404-1415	5.7	15
97	An efficient synthesis of a rationally designed 1,5 disubstituted imidazole AT(1) angiotensin II receptor antagonist: reorientation of imidazole pharmacophore groups in losartan reserves high receptor affinity and confirms docking studies. *Journal of Computer-Aided Molecular Design*, **2010**,	4.2	15
96	Atomistic molecular dynamics simulations of typical and atypical antipsychotic drugs at the dopamine D2 receptor (D2R) elucidates their inhibition mechanism. *Journal of Biomolecular Structure and Dynamics*, **2017**, 35, 738-754	3.6	14
95	Biological Insights of the Dopaminergic Stabilizer ACR16 at the Binding Pocket of Dopamine D2 Receptor. *ACS Chemical Neuroscience*, **2017**, 8, 826-836	5.7	14
94	Rehabilitating drug-induced long-QT promoters: in-silico design of hERG-neutral cisapride analogues with retained pharmacological activity. *BMC Pharmacology & Toxicology*, **2014**, 15, 14	2.6	14
93	Structure driven design of novel human ether-a-go-go-related-gene channel (hERG1) activators. *PLoS ONE*, **2014**, 9, e105553	3.7	14
92	Host-Guest Interactions between Candesartan and Its Prodrug Candesartan Cilexetil in Complex with 2-Hydroxypropyl-cyclodextrin: On the Biological Potency for Angiotensin II Antagonism. *Molecular Pharmaceutics*, **2019**, 16, 1255-1271	5.6	13
91	Molecular Simulations of Solved Co-crystallized X-Ray Structures Identify Action Mechanisms of PDE Inhibitors. *Biophysical Journal*, **2015**, 109, 1163-8	2.9	13

90	Integration of multi-scale molecular modeling approaches with experiments for the in silico guided design and discovery of novel hERG-Neutral antihypertensive oxazalone and imidazolone derivatives and analysis of their potential restrictive effects on cell proliferation. *European Journal of Medicinal Chemistry*, **2018**, 145, 273-290	6.8	13
89	Discovery of selective dengue virus inhibitors using combination of molecular fingerprint-based virtual screening protocols, structure-based pharmacophore model development, molecular dynamics simulations and in vitro studies. *Journal of Molecular Graphics and Modelling*, **2018**, 79, 88-102	2.8	13
88	Development of Small Molecule MEIS Inhibitors that modulate HSC activity. *Scientific Reports*, **2020**, 10, 7994	4.9	12
87	Structure-based design of hERG-neutral antihypertensive oxazalone and imidazolone derivatives. *Journal of Molecular Graphics and Modelling*, **2018**, 79, 103-117	2.8	12
86	Comparative molecular dynamics simulations of the potent synthetic classical cannabinoid ligand AMG3 in solution and at binding site of the CB1 and CB2 receptors. *Bioorganic and Medicinal Chemistry*, **2008**, 16, 7377-87	3.4	12
85	Screening of Clinically Approved and Investigation Drugs as Potential Inhibitors of SARS-CoV-2 Main Protease and Spike Receptor-Binding Domain Bound with ACE2 COVID19 Target Proteins: A Virtual Drug Repurposing Study		12
84	Drug repurposing studies of PARP inhibitors as a new therapy for inherited retinal degeneration. *Cellular and Molecular Life Sciences*, **2020**, 77, 2199-2216	10.3	12
83	Integrating Ligand and Target-Driven Based Virtual Screening Approaches With Human Cell Line Models and Time-Resolved Fluorescence Resonance Energy Transfer Assay to Identify Novel Hit Compounds Against BCL-2. *Frontiers in Chemistry*, **2020**, 8, 167	5	12
82	Virtual screening of small molecules databases for discovery of novel PARP-1 inhibitors: combination of in silico and in vitro studies. *Journal of Biomolecular Structure and Dynamics*, **2017**, 35, 1899-1915	3.6	11
81	Design, Synthesis, and Molecular Modeling Studies of Novel Coumarin Carboxamide Derivatives as eEF-2K Inhibitors. *Journal of Chemical Information and Modeling*, **2020**, 60, 1766-1778	6.1	11
80	Kinetic and in silico analysis of thiazolidin-based inhibitors of carbonic anhydrase isoenzymes. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2013**, 28, 370-4	5.6	11
79	Oligomerization and cooperativity in GPCRs from the perspective of the angiotensin AT1 and dopamine D2 receptors. *Neuroscience Letters*, **2019**, 700, 30-37	3.3	11
78	Discovering novel carbonic anhydrase type IX (CA IX) inhibitors from seven million compounds using virtual screening and in vitro analysis. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2016**, 31, 425-33	5.6	10
77	Kinetic and in silico studies of hydroxy-based inhibitors of carbonic anhydrase isoforms I and II. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2016**, 31, 31-7	5.6	10
76	Synthesis of 1,4-bis(indolin-1-ylmethyl)benzene derivatives and their structure-activity relationships for the interaction of human carbonic anhydrase isoforms I and II. *Bioorganic and Medicinal Chemistry*, **2013**, 21, 1477-82	3.4	10
75	The signaling pathway of dopamine D2 receptor (D2R) activation using normal mode analysis (NMA) and the construction of pharmacophore models for D2R ligands. *Journal of Biomolecular Structure and Dynamics*, **2017**, 35, 2040-2048	3.6	9
74	Novel tumor necrosis factor-α (TNF-α) inhibitors from small molecule library screening for their therapeutic activity profiles against rheumatoid arthritis using target-driven approaches and binary QSAR models. *Journal of Biomolecular Structure and Dynamics*, **2019**, 37, 2464-2476	3.6	9
73	3D QSAR/CoMFA and CoMSIA studies on antileukemic steroidal esters coupled with conformationally flexible nitrogen mustards. *Journal of Chemical Information and Modeling*, **2008**, 48, 2254-64	6.1	9

72	Combined molecular modeling and cholinesterase inhibition studies on some natural and semisynthetic O-alkylcoumarin derivatives. *Bioorganic Chemistry*, **2019**, 84, 355-362	5.1	9
71	Formation of the inclusion complex of water soluble fluorescent calix[4]arene and naringenin: solubility, cytotoxic effect and molecular modeling studies. *Journal of Biomolecular Structure and Dynamics*, **2020**, 38, 3801-3813	3.6	9
70	Screening of FDA approved drugs for finding potential inhibitors against Granzyme B as a potent drug-repurposing target. *Journal of Molecular Graphics and Modelling*, **2020**, 95, 107462	2.8	9
69	Current status of multiscale simulations on GPCRs. *Current Opinion in Structural Biology*, **2019**, 55, 93-103	8.1	8
68	The effects of pollen, propolis, and caffeic acid phenethyl ester on tyrosine hydroxylase activity and total RNA levels in hypertensive rats caused by nitric oxide synthase inhibition: experimental, docking and molecular dynamic studies. *Journal of Biomolecular Structure and Dynamics*, **2018**, 36, 609-620	3.6	8
67	Molecular insights into the AT1 antagonism based on biophysical and in silico studies of telmisartan. *Medicinal Chemistry Research*, **2013**, 22, 4842-4857	2.2	8
66	The neutralization effect of montelukaston SARS-CoV-2 is shown by multiscale in silicosimulations and combined in□vitro studies. *Molecular Therapy*, **2021**,	11.7	8
65	Novel AChE and BChE inhibitors using combined virtual screening, text mining and in vitro binding assays. *Journal of Biomolecular Structure and Dynamics*, **2020**, 38, 3342-3358	3.6	8
64	Discovery of Klotho peptide antagonists against Wnt3 and Wnt3a target proteins using combination of protein engineering, protein-protein docking, peptide docking and molecular dynamics simulations. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2017**, 32, 84-98	5.6	7
63	Toward Understanding the Impact of Dimerization Interfaces in Angiotensin II Type 1 Receptor. *Journal of Chemical Information and Modeling*, **2019**, 59, 4314-4327	6.1	6
62	Investigation of inhibition of human glucose 6-phosphate dehydrogenase by some 99mTc chelators by in silico and in vitro methods. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2016**, 31, 141-147	5.6	6
61	Identifying new piperazine-based PARP1 inhibitors using text mining and integrated molecular modeling approaches. *Journal of Biomolecular Structure and Dynamics*, **2021**, 39, 681-690	3.6	6
60	A QM protein-ligand investigation of antipsychotic drugs with the dopamine D2 Receptor (D2R). *Journal of Biomolecular Structure and Dynamics*, **2018**, 36, 2668-2677	3.6	6
59	Near-physiological-temperature serial crystallography reveals conformations of SARS-CoV-2 main protease active site for improved drug repurposing. *Structure*, **2021**, 29, 1382-1396.e6	5.2	6
58	Identification of novel serotonin reuptake inhibitors targeting central and allosteric binding sites: A virtual screening and molecular dynamics simulations study. *Journal of Molecular Graphics and Modelling*, **2017**, 74, 193-202	2.8	5
57	Structural modeling of the N-terminal signal-receiving domain of IB□*Frontiers in Molecular Biosciences*, **2015**, 2, 32	5.6	5
56	Mechanism of K+/Na+ selectivity in potassium channels from the perspective of the non-selective bacterial channel NaK. *Channels*, **2011**, 5, 198-200	3	5
55	Screening of Clinically Approved and Investigation Drugs as Potential Inhibitors of COVID-19 Main Protease: A Virtual Drug Repurposing Study		5

54	Synthesis, anticholinesterase activity and molecular modeling studies of novel carvacrol-substituted amide derivatives. *Journal of Biomolecular Structure and Dynamics*, **2020**, 38, 841-859	3.6	5
53	Synthesis, molecular docking and molecular dynamics studies of novel tacrine-carbamate derivatives as potent cholinesterase inhibitors. *Bioorganic Chemistry*, **2021**, 115, 105225	5.1	5
52	Transcription factor NF-B as target for SARS-CoV-2 drug discovery efforts using inflammation-based QSAR screening model. *Journal of Molecular Graphics and Modelling*, **2021**, 108, 107968	2.8	5
51	First universal pharmacophore model for hERG1 K channel activators: acthER. *Journal of Molecular Graphics and Modelling*, **2017**, 74, 153-170	2.8	4
50	Mutated form (G52E) of inactive diphtheria toxin CRM197: molecular simulations clearly display effect of the mutation to NAD binding. *Journal of Biomolecular Structure and Dynamics*, **2016**, 34, 2462-8	3.6	4
49	Proposing novel TNF direct inhibitor Scaffolds using fragment-docking based e-pharmacophore modeling and binary QSAR-based virtual screening protocols pipeline. *Journal of Molecular Graphics and Modelling*, **2018**, 85, 111-121	2.8	4
48	Drug Re-positioning Studies for Novel HIV-1 Inhibitors Using Binary QSAR Models and Multi-target-driven In Silico Studies. *Molecular Informatics*, **2021**, 40, e2000012	3.8	4
47	New nimesulide derivatives with amide/sulfonamide moieties: Selective COX-2 inhibition and antitumor effects. *European Journal of Medicinal Chemistry*, **2021**, 221, 113566	6.8	4
46	Structural Investigation of the Dopamine-2 Receptor Agonist Bromocriptine Binding to Dimeric D2R and D2R States. *Journal of Chemical Information and Modeling*, **2018**, 58, 826-836	6.1	3
45	Biochemical changes induced by grape seed extract and low level laser therapy administration during intraoral wound healing in rat liver: an experimental and in silico study. *Journal of Biomolecular Structure and Dynamics*, **2018**, 36, 993-1008	3.6	3
44	Designing of multi-targeted molecules using combination of molecular screening and in silico drug cardiotoxicity prediction approaches. *Journal of Molecular Graphics and Modelling*, **2014**, 50, 16-34	2.8	3
43	An effort to discover the preferred conformation of the potent AMG3 cannabinoid analog when reaching the active sites of the cannabinoid receptors. *European Journal of Medicinal Chemistry*, **2012**, 47, 44-51	6.8	3
42	Structural investigation of vesnarinone at the pore domains of open and open-inactivated states of hERG1 K channel. *Journal of Molecular Graphics and Modelling*, **2017**, 77, 399-412	2.8	3
41	Structural modification of ellipticine derivatives with alkyl groups of varying length is influential on their effects on human DNA topoisomerase II: a combined experimental and computational study. *Medicinal Chemistry Research*, **2020**, 29, 189-198	2.2	3
40	Proposing novel MDM2 inhibitors: Combined physics-driven high-throughput virtual screening and in vitro studies. *Chemical Biology and Drug Design*, **2020**, 96, 684-700	2.9	3
39	Integrated Binary QSAR-Driven Virtual Screening and In Vitro Studies for Finding Novel hMAO-B-Selective Inhibitors. *Journal of Chemical Information and Modeling*, **2020**, 60, 4047-4055	6.1	3
38	An Integrated in silico Approach and in vitro Study for the Discovery of Small-Molecule USP7 Inhibitors as Potential Cancer Therapies. *ChemMedChem*, **2021**, 16, 555-567	3.7	3
37	Screening of Clinically Approved and Investigation Drugs as Potential Inhibitors of SARS-CoV-2: A Combined in silico and in vitro Study. *Molecular Informatics*, **2021**, e2100062	3.8	3

36	Instant determination of the artemisinin from various Artemisia annua L. extracts by LC-ESI-MS/MS and their in-silico modelling and in vitro antiviral activity studies against SARS-CoV-2. *Phytochemical Analysis*, **2021**,	3.4	3
35	In silico characterization of adipokinetic hormone receptor and screening for pesticide candidates against stick insect, Carausius morosus. *Journal of Molecular Graphics and Modelling*, **2020**, 101, 107720	2.8	2
34	Kinetic and docking studies of cytosolic/tumor-associated carbonic anhydrase isozymes I, II and IX with some hydroxylic compounds. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2016**, 31, 1214-20	5.6	2
33	Rehabilitation Studies for withdrawn Drugs from the Market: Derivation of Non-hERG1 Channel Blocker Cisapride Analogues using Multi-Faceted Approaches. *Biophysical Journal*, **2013**, 104, 266a	2.9	2
32	Development of Atomistic Models for Closed, Open and Open-Inactivated States of hERG1 Channel using Rosetta Protein Modeling Suite and Molecular Dynamics Simulations. *Biophysical Journal*, **2012**, 102, 679a	2.9	2
31	Mechanistic insight into the impact of a bivalent ligand on the structure and dynamics of a GPCR oligomer.. *Computational and Structural Biotechnology Journal*, **2022**, 20, 925-936	6.8	2
30	Bis benzothiophene Schiff bases: synthesis and in silico-guided biological activity studies. *Turkish Journal of Chemistry*, **2020**, 44, 1164-1176	1	2
29	Physics-driven identification of clinically approved and investigation drugs against human neutrophil serine protease 4 (NSP4): A virtual drug repurposing study. *Journal of Molecular Graphics and Modelling*, **2020**, 101, 107744	2.8	2
28	Near-Physiological-Temperature Serial Femtosecond X-ray Crystallography Reveals Novel Conformations of SARS-CoV-2 Main Protease Active Site for Improved Drug Repurposing		2
27	Potent novel inhibitors against hepatitis C virus NS3 (HCV NS3 GT-3a) protease domain. *Journal of Molecular Graphics and Modelling*, **2020**, 101, 107727	2.8	2
26	Hybrid and TR-FRET-Guided Discovery of Novel BCL-2 Inhibitors. *ACS Pharmacology and Translational Science*, **2021**, 4, 1111-1123	5.9	2
25	In vitro and in silico studies of nitrobenzamide derivatives as potential anti-neuroinflammatory agents. *Journal of Biomolecular Structure and Dynamics*, **2020**, 38, 4655-4668	3.6	2
24	Investigation of supramolecular interaction of quercetin with N,N-dimethylamine-functionalized p-sulfonated calix[4,8]arenes using molecular modeling and their in vitro cytotoxic response towards selected cancer cells. *New Journal of Chemistry*,	3.6	2
23	Novel inhibitors of eukaryotic elongation factor 2 kinase: In silico, synthesis and in vitro studies. *Bioorganic Chemistry*, **2021**, 116, 105296	5.1	2
22	Identifying highly effective coumarin-based novel cholinesterase inhibitors by in silico and in vitro studies. *Journal of Molecular Graphics and Modelling*, **2022**, 108210	2.8	2
21	Discovery of selective dengue virus inhibitors using combination of molecular fingerprint-based virtual screening protocols, structure-based pharmacophore model development, molecular dynamics simulations and in vitro studies. *Journal of Molecular Graphics and Modelling*, **2017**, 77, 338	2.8	1
20	In silico design of novel hERG-neutral sildenafil-like PDE5 inhibitors. *Journal of Biomolecular Structure and Dynamics*, **2017**, 35, 2830-2852	3.6	1
19	Case Study of High-Throughput Drug Screening and Remote Data Collection for SARS-CoV-2 Main Protease by Using Serial Femtosecond X-ray Crystallography. *Crystals*, **2021**, 11, 1579	2.3	1

18	In Silico Analysis of Bacteriocins from Lactic Acid Bacteria Against SARS-CoV-2. *Probiotics and Antimicrobial Proteins*, **2021**, 1	5.5	1
17	Molecular simulations reveal the impact of RAMP1 on ligand binding and dynamics of calcitonin gene-related peptide receptor (CGRPR) heterodimer.. *Computers in Biology and Medicine*, **2021**, 141, 105130	7	1
16	The neutralization effect of Montelukast on SARS-CoV-2 is shown by multiscale in silico simulations and combined in vitro studies		1
15	Target-driven design of a coumarinyl chalcone scaffold based novel EF2 Kinase inhibitor suppresses breast cancer growthin vivo		1
14	Elucidation of interaction mechanism of hERG1 potassium channel with scorpion toxins BeKm-1 and BmTx3b. *Journal of Molecular Graphics and Modelling*, **2020**, 96, 107504	2.8	1
13	Combined ligand and structure-based virtual screening approaches for identification of novel AChE inhibitors. *Turkish Journal of Chemistry*, **2020**, 44, 574-588	1	1
12	Screening of small molecule libraries using combined text mining, ligand- and target-driven based approaches for identification of novel granzyme H inhibitors. *Journal of Molecular Graphics and Modelling*, **2021**, 105, 107876	2.8	1
11	Structural and Functional Characterization of Allatostatin Receptor Type-C of , a Potential Target for Next-Generation Pest Control Agents. *Journal of Chemical Information and Modeling*, **2021**, 61, 715-728	6.1	1
10	Identification of first-in-class plasmodium OTU inhibitors with potent anti-malarial activity. *Biochemical Journal*, **2021**, 478, 3445-3466	3.8	1
9	Design and synthesis of novel caffeic acid phenethyl ester (CAPE) derivatives and their biological activity studies in glioblastoma multiforme (GBM) cancer cell lines.. *Journal of Molecular Graphics and Modelling*, **2022**, 113, 108160	2.8	1
8	Development of imidazolone based angiotensin II receptor type I inhibitor small molecule as a chemotherapeutic agent for cell cycle inhibition **2021**, 14, 678-690		0
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4	Evolutionary association of receptor-wide amino acids with G protein coupling selectivity in aminergic GPCRs. *Life Science Alliance*, **2022**, 5, e202201439	5.8	0
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