

# Serdar Durdagi

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Mechanistic insight into the impact of a bivalent ligand on the structure and dynamics of a GPCR oligomer.. <i>Computational and Structural Biotechnology Journal</i> , <b>2022</b> , 20, 925-936	6.8	2
160	Design and synthesis of novel caffeic acid phenethyl ester (CAPE) derivatives and their biological activity studies in glioblastoma multiforme (GBM) cancer cell lines.. <i>Journal of Molecular Graphics and Modelling</i> , <b>2022</b> , 113, 108160	2.8	1
159	Identifying highly effective coumarin-based novel cholinesterase inhibitors by in silico and in vitro studies. <i>Journal of Molecular Graphics and Modelling</i> , <b>2022</b> , 108210	2.8	2
158	Evolutionary association of receptor-wide amino acids with G protein-coupling selectivity in aminergic GPCRs. <i>Life Science Alliance</i> , <b>2022</b> , 5, e202201439	5.8	0
157	Case Study of High-Throughput Drug Screening and Remote Data Collection for SARS-CoV-2 Main Protease by Using Serial Femtosecond X-ray Crystallography. <i>Crystals</i> , <b>2021</b> , 11, 1579	2.3	1
156	In Silico Analysis of Bacteriocins from Lactic Acid Bacteria Against SARS-CoV-2. <i>Probiotics and Antimicrobial Proteins</i> , <b>2021</b> , 1	5.5	1
155	Development of imidazolone based angiotensin II receptor type I inhibitor small molecule as a chemotherapeutic agent for cell cycle inhibition <b>2021</b> , 14, 678-690		0
154	Molecular simulations reveal the impact of RAMP1 on ligand binding and dynamics of calcitonin gene-related peptide receptor (CGRPR) heterodimer.. <i>Computers in Biology and Medicine</i> , <b>2021</b> , 141, 105130	7	1
153	The neutralization effect of montelukast on SARS-CoV-2 is shown by multiscale in silico simulations and combined in vitro studies. <i>Molecular Therapy</i> , <b>2021</b> ,	11.7	8
152	Hybrid and TR-FRET-Guided Discovery of Novel BCL-2 Inhibitors. <i>ACS Pharmacology and Translational Science</i> , <b>2021</b> , 4, 1111-1123	5.9	2
151	Structures of MERS-CoV macro domain in aqueous solution with dynamics: Impacts of parallel tempering simulation techniques and CHARMM36m and AMBER99SB force field parameters. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2021</b> , 89, 1289-1299	4.2	0
150	Screening of small molecule libraries using combined text mining, ligand- and target-driven based approaches for identification of novel granzyme H inhibitors. <i>Journal of Molecular Graphics and Modelling</i> , <b>2021</b> , 105, 107876	2.8	1
149	Identifying new piperazine-based PARP1 inhibitors using text mining and integrated molecular modeling approaches. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2021</b> , 39, 681-690	3.6	6
148	An Integrated in silico Approach and in vitro Study for the Discovery of Small-Molecule USP7 Inhibitors as Potential Cancer Therapies. <i>ChemMedChem</i> , <b>2021</b> , 16, 555-567	3.7	3
147	Drug Re-positioning Studies for Novel HIV-1 Inhibitors Using Binary QSAR Models and Multi-target-driven In Silico Studies. <i>Molecular Informatics</i> , <b>2021</b> , 40, e2000012	3.8	4
146	Structural and Functional Characterization of Allatostatin Receptor Type-C of , a Potential Target for Next-Generation Pest Control Agents. <i>Journal of Chemical Information and Modeling</i> , <b>2021</b> , 61, 715-728	6.1	1
145	Target-Driven Design of a Coumarinyl Chalcone Scaffold Based Novel EF2 Kinase Inhibitor Suppresses Breast Cancer Growth. <i>ACS Pharmacology and Translational Science</i> , <b>2021</b> , 4, 926-940	5.9	0

144	Near-physiological-temperature serial crystallography reveals conformations of SARS-CoV-2 main protease active site for improved drug repurposing. <i>Structure</i> , <b>2021</b> , 29, 1382-1396.e6	5.2	6
143	Binary-QSAR guided virtual screening of FDA approved drugs and compounds in clinical investigation against SARS-CoV-2 main protease. <i>Turkish Journal of Biology</i> , <b>2021</b> , 45, 459-468	3.1	0
142	Screening of Clinically Approved and Investigation Drugs as Potential Inhibitors of SARS-CoV-2: A Combined in silico and in vitro Study. <i>Molecular Informatics</i> , <b>2021</b> , e2100062	3.8	3
141	Instant determination of the artemisinin from various <i>Artemisia annua</i> L. extracts by LC-ESI-MS/MS and their in-silico modelling and in vitro antiviral activity studies against SARS-CoV-2. <i>Phytochemical Analysis</i> , <b>2021</b> ,	3.4	3
140	Identification of first-in-class plasmodium OTU inhibitors with potent anti-malarial activity. <i>Biochemical Journal</i> , <b>2021</b> , 478, 3445-3466	3.8	1
139	New nimesulide derivatives with amide/sulfonamide moieties: Selective COX-2 inhibition and antitumor effects. <i>European Journal of Medicinal Chemistry</i> , <b>2021</b> , 221, 113566	6.8	4
138	Synthesis, molecular docking and molecular dynamics studies of novel tacrine-carbamate derivatives as potent cholinesterase inhibitors. <i>Bioorganic Chemistry</i> , <b>2021</b> , 115, 105225	5.1	5
137	Transcription factor NF- $\kappa$ B as target for SARS-CoV-2 drug discovery efforts using inflammation-based QSAR screening model. <i>Journal of Molecular Graphics and Modelling</i> , <b>2021</b> , 108, 107968	2.8	5
136	Novel inhibitors of eukaryotic elongation factor 2 kinase: In silico, synthesis and in vitro studies. <i>Bioorganic Chemistry</i> , <b>2021</b> , 116, 105296	5.1	2
135	In silico characterization of adipokinetic hormone receptor and screening for pesticide candidates against stick insect, <i>Carausius morosus</i> . <i>Journal of Molecular Graphics and Modelling</i> , <b>2020</b> , 101, 107720	2.8	2
134	Development of Small Molecule MEIS Inhibitors that modulate HSC activity. <i>Scientific Reports</i> , <b>2020</b> , 10, 7994	4.9	12
133	Virtual drug repurposing study against SARS-CoV-2 TMPRSS2 target. <i>Turkish Journal of Biology</i> , <b>2020</b> , 44, 185-191	3.1	19
132	Design, Synthesis, and Molecular Modeling Studies of Novel Coumarin Carboxamide Derivatives as eEF-2K Inhibitors. <i>Journal of Chemical Information and Modeling</i> , <b>2020</b> , 60, 1766-1778	6.1	11
131	Bis benzothiophene Schiff bases: synthesis and in silico-guided biological activity studies. <i>Turkish Journal of Chemistry</i> , <b>2020</b> , 44, 1164-1176	1	2
130	Physics-driven identification of clinically approved and investigation drugs against human neutrophil serine protease 4 (NSP4): A virtual drug repurposing study. <i>Journal of Molecular Graphics and Modelling</i> , <b>2020</b> , 101, 107744	2.8	2
129	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. <i>Medicinal Chemistry Research</i> , <b>2020</b> , 29, 189-198	2.2	3
128	Elucidation of interaction mechanism of hERG1 potassium channel with scorpion toxins BeKm-1 and BmTx3b. <i>Journal of Molecular Graphics and Modelling</i> , <b>2020</b> , 96, 107504	2.8	1
127	Proposing novel MDM2 inhibitors: Combined physics-driven high-throughput virtual screening and in vitro studies. <i>Chemical Biology and Drug Design</i> , <b>2020</b> , 96, 684-700	2.9	3

126	Integrated Binary QSAR-Driven Virtual Screening and In Vitro Studies for Finding Novel hMAO-B-Selective Inhibitors. <i>Journal of Chemical Information and Modeling</i> , <b>2020</b> , 60, 4047-4055	6.1	3
125	Combined ligand and structure-based virtual screening approaches for identification of novel AChE inhibitors. <i>Turkish Journal of Chemistry</i> , <b>2020</b> , 44, 574-588	1	1
124	Potent novel inhibitors against hepatitis C virus NS3 (HCV NS3 GT-3a) protease domain. <i>Journal of Molecular Graphics and Modelling</i> , <b>2020</b> , 101, 107727	2.8	2
123	Synthesis, anticholinesterase activity and molecular modeling studies of novel carvacrol-substituted amide derivatives. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2020</b> , 38, 841-859	3.6	5
122	Formation of the inclusion complex of water soluble fluorescent calix[4]arene and naringenin: solubility, cytotoxic effect and molecular modeling studies. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2020</b> , 38, 3801-3813	3.6	9
121	In vitro and in silico studies of nitrobenzamide derivatives as potential anti-neuroinflammatory agents. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2020</b> , 38, 4655-4668	3.6	2
120	Screening of FDA approved drugs for finding potential inhibitors against Granzyme B as a potent drug-repurposing target. <i>Journal of Molecular Graphics and Modelling</i> , <b>2020</b> , 95, 107462	2.8	9
119	Drug repurposing studies of PARP inhibitors as a new therapy for inherited retinal degeneration. <i>Cellular and Molecular Life Sciences</i> , <b>2020</b> , 77, 2199-2216	10.3	12
118	Novel AChE and BChE inhibitors using combined virtual screening, text mining and in vitro binding assays. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2020</b> , 38, 3342-3358	3.6	8
117	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. <i>Frontiers in Chemistry</i> , <b>2020</b> , 8, 167	5	12
116	Inhibition of acetylcholinesterase and butyrylcholinesterase with uracil derivatives: kinetic and computational studies. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , <b>2019</b> , 34, 429-437	5.6	41
115	Host-Guest Interactions between Candesartan and Its Prodrug Candesartan Cilexetil in Complex with 2-Hydroxypropyl- $\beta$ -cyclodextrin: On the Biological Potency for Angiotensin II Antagonism. <i>Molecular Pharmaceutics</i> , <b>2019</b> , 16, 1255-1271	5.6	13
114	Current status of multiscale simulations on GPCRs. <i>Current Opinion in Structural Biology</i> , <b>2019</b> , 55, 93-103	3.1	8
113	Effects of Cholesterol on GPCR Function: Insights from Computational and Experimental Studies. <i>Advances in Experimental Medicine and Biology</i> , <b>2019</b> , 1135, 89-103	3.6	17
112	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. <i>Bioorganic Chemistry</i> , <b>2019</b> , 87, 838-850	5.1	32
111	Novel tumor necrosis factor- $\alpha$ (TNF- $\alpha$ ) inhibitors from small molecule library screening for their therapeutic activity profiles against rheumatoid arthritis using target-driven approaches and binary QSAR models. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2019</b> , 37, 2464-2476	3.6	9
110	Toward Understanding the Impact of Dimerization Interfaces in Angiotensin II Type 1 Receptor. <i>Journal of Chemical Information and Modeling</i> , <b>2019</b> , 59, 4314-4327	6.1	6
109	Combined molecular modeling and cholinesterase inhibition studies on some natural and semisynthetic O-alkylcoumarin derivatives. <i>Bioorganic Chemistry</i> , <b>2019</b> , 84, 355-362	5.1	9

108	Targeting the NF- $\kappa$ B complex via fragment-based E-Pharmacophore virtual screening and binary QSAR models. <i>Journal of Molecular Graphics and Modelling</i> , <b>2019</b> , 86, 264-277	2.8	20
107	Combinatorial peptide library screening for discovery of diverse $\alpha$ -glucosidase inhibitors using molecular dynamics simulations and binary QSAR models. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2019</b> , 37, 726-740	3.6	49
106	Oligomerization and cooperativity in GPCRs from the perspective of the angiotensin AT1 and dopamine D2 receptors. <i>Neuroscience Letters</i> , <b>2019</b> , 700, 30-37	3.3	11
105	Molecular modeling and in vitro approaches towards cholinesterase inhibitory effect of some natural xanthohumol, naringenin, and acyl phloroglucinol derivatives. <i>Phytomedicine</i> , <b>2018</b> , 42, 25-33	6.5	23
104	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. <i>ACS Chemical Neuroscience</i> , <b>2018</b> , 9, 1768-1782	5.7	20
103	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. <i>European Journal of Medicinal Chemistry</i> , <b>2018</b> , 145, 279-289	6.8	13
102	Structural Investigation of the Dopamine-2 Receptor Agonist Bromocriptine Binding to Dimeric D2R and D2R States. <i>Journal of Chemical Information and Modeling</i> , <b>2018</b> , 58, 826-836	6.1	3
101	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. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2018</b> , 36, 609-620	3.6	8
100	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. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2018</b> , 36, 993-1008	3.6	3
99	Structure-based design of hERG-neutral antihypertensive oxazalone and imidazolone derivatives. <i>Journal of Molecular Graphics and Modelling</i> , <b>2018</b> , 79, 103-117	2.8	12
98	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. <i>Journal of Molecular Graphics and Modelling</i> , <b>2018</b> , 79, 88-102	2.8	13
97	Application of Multiscale Simulation Tools on GPCRs. An Example with Angiotensin II Type 1 Receptor. <i>Methods in Molecular Biology</i> , <b>2018</b> , 1824, 431-448	1.4	
96	Investigating the molecular mechanism of staphylococcal DNA gyrase inhibitors: A combined ligand-based and structure-based resources pipeline. <i>Journal of Molecular Graphics and Modelling</i> , <b>2018</b> , 85, 122-129	2.8	21
95	Proposing novel TNF $\alpha$ inhibitor Scaffolds using fragment-docking based e-pharmacophore modeling and binary QSAR-based virtual screening protocols pipeline. <i>Journal of Molecular Graphics and Modelling</i> , <b>2018</b> , 85, 111-121	2.8	4
94	In vitro and in silico approaches to appraise <i>Polygonum maritimum</i> L. as a source of innovative products with anti-ageing potential. <i>Industrial Crops and Products</i> , <b>2018</b> , 111, 391-399	5.9	16
93	A QM protein-ligand investigation of antipsychotic drugs with the dopamine D2 Receptor (D2R). <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2018</b> , 36, 2668-2677	3.6	6
92	Atomistic molecular dynamics simulations of typical and atypical antipsychotic drugs at the dopamine D2 receptor (D2R) elucidates their inhibition mechanism. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2017</b> , 35, 738-754	3.6	14
91	Virtual screening of small molecules databases for discovery of novel PARP-1 inhibitors: combination of in silico and in vitro studies. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2017</b> , 35, 1899-1915	3.6	11

90	The signaling pathway of dopamine D2 receptor (D2R) activation using normal mode analysis (NMA) and the construction of pharmacophore models for D2R ligands. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2017</b> , 35, 2040-2048	3.6	9
89	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. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , <b>2017</b> , 32, 311-330	5.6	20
88	Cholesterol up-regulates neuronal G protein-gated inwardly rectifying potassium (GIRK) channel activity in the hippocampus. <i>Journal of Biological Chemistry</i> , <b>2017</b> , 292, 6135-6147	5.4	31
87	Analysis of the Glutamate Agonist LY404,039 Binding to Nonstatic Dopamine Receptor D2 Dimer Structures and Consensus Docking. <i>ACS Chemical Neuroscience</i> , <b>2017</b> , 8, 1404-1415	5.7	15
86	First universal pharmacophore model for hERG1 K channel activators: actHER. <i>Journal of Molecular Graphics and Modelling</i> , <b>2017</b> , 74, 153-170	2.8	4
85	Identification of novel serotonin reuptake inhibitors targeting central and allosteric binding sites: A virtual screening and molecular dynamics simulations study. <i>Journal of Molecular Graphics and Modelling</i> , <b>2017</b> , 74, 193-202	2.8	5
84	Biological Insights of the Dopaminergic Stabilizer ACR16 at the Binding Pocket of Dopamine D2 Receptor. <i>ACS Chemical Neuroscience</i> , <b>2017</b> , 8, 826-836	5.7	14
83	Synthesis, anticholinesterase activity and molecular modeling study of novel carbamate-substituted thymol/carvacrol derivatives. <i>Bioorganic and Medicinal Chemistry</i> , <b>2017</b> , 25, 1352-1363	3.4	31
82	Solubility profiles, hydration and desolvation of curcumin complexed with $\beta$ -cyclodextrin and hydroxypropyl- $\beta$ -cyclodextrin. <i>Journal of Molecular Structure</i> , <b>2017</b> , 1134, 91-98	3.4	17
81	Synthesis, biological activity and multiscale molecular modeling studies for coumaryl-carboxamide derivatives as selective carbonic anhydrase IX inhibitors. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , <b>2017</b> , 32, 1042-1052	5.6	23
80	Effects of propolis, caffeic acid phenethyl ester, and pollen on renal injury in hypertensive rat: An experimental and theoretical approach. <i>Cell Biochemistry and Function</i> , <b>2017</b> , 35, 304-314	4.2	24
79	The synthesis of novel sulfamides derived from benzylphenethylamines as acetylcholinesterase, butyrylcholinesterase and carbonic anhydrase enzymes inhibitors. <i>Bioorganic Chemistry</i> , <b>2017</b> , 74, 238-250	5.1	55
78	Structural investigation of vesnarinone at the pore domains of open and open-inactivated states of hERG1 K channel. <i>Journal of Molecular Graphics and Modelling</i> , <b>2017</b> , 77, 399-412	2.8	3
77	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. <i>Journal of Molecular Graphics and Modelling</i> , <b>2017</b> , 77, 338	2.8	1
76	Structure-based design of hERG-neutral antihypertensive oxazolone and imidazolone derivatives. <i>Journal of Molecular Graphics and Modelling</i> , <b>2017</b> , 77, 240-249	2.8	
75	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. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , <b>2017</b> , 32, 84-98	5.6	7
74	In silico design of novel hERG-neutral sildenafil-like PDE5 inhibitors. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2017</b> , 35, 2830-2852	3.6	1
73	In silico investigation of PARP-1 catalytic domains in holo and apo states for the design of high-affinity PARP-1 inhibitors. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , <b>2016</b> , 31, 112-20	5.6	15

72	Discovering novel carbonic anhydrase type IX (CA IX) inhibitors from seven million compounds using virtual screening and in vitro analysis. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , <b>2016</b> , 31, 425-33	5.6	10
71	Characterization, in Vivo Evaluation, and Molecular Modeling of Different Propofol-Cyclodextrin Complexes To Assess Their Drug Delivery Potential at the Blood-Brain Barrier Level. <i>Journal of Chemical Information and Modeling</i> , <b>2016</b> , 56, 1914-1922	6.1	27
70	Role of the pH in state-dependent blockade of hERG currents. <i>Scientific Reports</i> , <b>2016</b> , 6, 32536	4.9	20
69	Synthesis of Some Novel Norbornene-Fused Pyridazines as Potent Inhibitors of Carbonic Anhydrase and Acetylcholinesterase. <i>Journal of Heterocyclic Chemistry</i> , <b>2016</b> , 53, 2049-2056	1.9	34
68	Kinetic and in silico studies of hydroxy-based inhibitors of carbonic anhydrase isoforms I and II. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , <b>2016</b> , 31, 31-7	5.6	10
67	Binding Interactions of Dopamine and Apomorphine in D2High and D2Low States of Human Dopamine D2 Receptor Using Computational and Experimental Techniques. <i>ACS Chemical Neuroscience</i> , <b>2016</b> , 7, 185-95	5.7	34
66	Mutated form (G52E) of inactive diphtheria toxin CRM197: molecular simulations clearly display effect of the mutation to NAD binding. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2016</b> , 34, 2462-8 <sup>3,6</sup>		4
65	Kinetic and docking studies of cytosolic/tumor-associated carbonic anhydrase isozymes I, II and IX with some hydroxylic compounds. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , <b>2016</b> , 31, 1214-20 <sup>5,6</sup>		2
64	Leveraging NMR and X-ray Data of the Free Ligands to Build Better Drugs Targeting Angiotensin II Type 1 G-Protein Coupled Receptor. <i>Current Medicinal Chemistry</i> , <b>2016</b> , 23, 36-59	4.3	18
63	Virtual screening of eighteen million compounds against dengue virus: Combined molecular docking and molecular dynamics simulations study. <i>Journal of Molecular Graphics and Modelling</i> , <b>2016</b> , 66, 99-107	2.8	29
62	Acetylcholinesterase and carbonic anhydrase inhibitory properties of novel urea and sulfamide derivatives incorporating dopaminergic 2-aminotetralin scaffolds. <i>Bioorganic and Medicinal Chemistry</i> , <b>2016</b> , 24, 2318-29	3.4	103
61	Investigation of inhibition of human glucose 6-phosphate dehydrogenase by some <sup>99m</sup> Tc chelators by in silico and in vitro methods. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , <b>2016</b> , 31, 141-147 <sup>5,6</sup>		6
60	NS1643 interacts around L529 of hERG to alter voltage sensor movement on the path to activation. <i>Biophysical Journal</i> , <b>2015</b> , 108, 1400-1413	2.9	23
59	Discovery of potent carbonic anhydrase and acetylcholine esterase inhibitors: novel sulfamoylcarbamates and sulfamides derived from acetophenones. <i>Bioorganic and Medicinal Chemistry</i> , <b>2015</b> , 23, 3592-602	3.4	119
58	Carbonic anhydrase inhibitors: Design, synthesis, kinetic, docking and molecular dynamics analysis of novel glycine and phenylalanine sulfonamide derivatives. <i>Bioorganic and Medicinal Chemistry</i> , <b>2015</b> , 23, 7353-8	3.4	33
57	Molecular Simulations of Solved Co-crystallized X-Ray Structures Identify Action Mechanisms of PDE Inhibitors. <i>Biophysical Journal</i> , <b>2015</b> , 109, 1163-8	2.9	13
56	Interaction of carbonic anhydrase isozymes I, II, and IX with some pyridine and phenol hydrazinecarbothioamide derivatives. <i>Bioorganic and Medicinal Chemistry Letters</i> , <b>2015</b> , 25, 5636-41	2.9	34
55	Investigation of Inhibition Mechanism of Chemokine Receptor CCR5 by Micro-second Molecular Dynamics Simulations. <i>Scientific Reports</i> , <b>2015</b> , 5, 13180	4.9	33

54	Fullerene-based inhibitors of HIV-1 protease. <i>Journal of Peptide Science</i> , <b>2015</b> , 21, 862-70	2.1	25
53	Structural modeling of the N-terminal signal-receiving domain of IB $\beta$ . <i>Frontiers in Molecular Biosciences</i> , <b>2015</b> , 2, 32	5.6	5
52	Modeling and protein engineering studies of active and inactive states of human dopamine D2 receptor (D2R) and investigation of drug/receptor interactions. <i>Molecular Diversity</i> , <b>2015</b> , 19, 321-32	3.1	25
51	Insights into the molecular basis of action of the AT1 antagonist losartan using a combined NMR spectroscopy and computational approach. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , <b>2014</b> , 1838, 1031-46	3.8	29
50	Designing of multi-targeted molecules using combination of molecular screening and in silico drug cardiotoxicity prediction approaches. <i>Journal of Molecular Graphics and Modelling</i> , <b>2014</b> , 50, 16-34	2.8	3
49	Rehabilitating drug-induced long-QT promoters: in-silico design of hERG-neutral cisapride analogues with retained pharmacological activity. <i>BMC Pharmacology &amp; Toxicology</i> , <b>2014</b> , 15, 14	2.6	14
48	Elucidation of conformational states, dynamics, and mechanism of binding in human $\beta$ opioid receptor complexes. <i>Journal of Chemical Information and Modeling</i> , <b>2014</b> , 54, 2294-308	6.1	25
47	Carbonic anhydrase inhibitory properties of novel benzylsulfamides using molecular modeling and experimental studies. <i>Bioorganic Chemistry</i> , <b>2014</b> , 56, 75-82	5.1	99
46	Structure driven design of novel human ether-a-go-go-related-gene channel (hERG1) activators. <i>PLoS ONE</i> , <b>2014</b> , 9, e105553	3.7	14
45	Inhibition of mammalian carbonic anhydrases I-XIV with grayanotoxin III: solution and in silico studies. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , <b>2014</b> , 29, 469-75	5.6	31
44	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. <i>Bioorganic and Medicinal Chemistry</i> , <b>2013</b> , 21, 1477-82	3.4	10
43	AT1 antagonists: a patent review (2008 - 2012). <i>Expert Opinion on Therapeutic Patents</i> , <b>2013</b> , 23, 1483-946.8		24
42	Kinetic and in silico analysis of thiazolidin-based inhibitors of $\beta$ carbonic anhydrase isoenzymes. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , <b>2013</b> , 28, 370-4	5.6	11
41	Molecular insights into the AT1 antagonism based on biophysical and in silico studies of telmisartan. <i>Medicinal Chemistry Research</i> , <b>2013</b> , 22, 4842-4857	2.2	8
40	Rehabilitation Studies for withdrawn Drugs from the Market: Derivation of Non-hERG1 Channel Blocker Cisapride Analogues using Multi-Faceted Approaches. <i>Biophysical Journal</i> , <b>2013</b> , 104, 266a	2.9	2
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5	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
4	The neutralization effect of Montelukast on SARS-CoV-2 is shown by multiscale in silico simulations and combined in vitro studies		1
3	Near-Physiological-Temperature Serial Femtosecond X-ray Crystallography Reveals Novel Conformations of SARS-CoV-2 Main Protease Active Site for Improved Drug Repurposing		2
2	Target-driven design of a coumarinyl chalcone scaffold based novel EF2 Kinase inhibitor suppresses breast cancer growth in vivo		1
1	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. <i>New Journal of Chemistry</i> ,	3.6	2

