Serdar Durdagi

List of Publications by Year
in descending order

167 papers	3,857 citations	117453 34 h-index	182168 51 g-index
184 all docs	184 docs citations	184 times ranked	4599 citing authors

#	Article	IF	Citations
1	In Silico Analysis of Bacteriocins from Lactic Acid Bacteria Against SARS-CoV-2. Probiotics and Antimicrobial Proteins, 2023, 15, 17-29.	1.9	18
2	Challenges and limitations in the studies of glycoproteins: A computational chemist's perspective. Proteins: Structure, Function and Bioinformatics, 2022, 90, 322-339.	1.5	0
3	Screening of Clinically Approved and Investigation Drugs as Potential Inhibitors of SARSâ€CoVâ€2: A Combinedin silicoandinâ€...vitroStudy. Molecular Informatics, 2022, 41, e2100062.	1.4	9
4	Instant determination of the artemisinin from various Artemisia annua L. extracts by LCâ€ESIâ€MS/MS and their inâ€silico modelling and in vitro antiviral activity studies against SARSâ€CoVâ€2. Phytochemical Analysis, 2022, 33, 303-319.	1.2	12
5	The neutralization effect of montelukast on SARS-CoV-2 is shown by multiscale in silico simulations and combined inÂvitro studies. Molecular Therapy, 2022, 30, 963-974.	3.7	21
6	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, 2022, 141, 105130.	3.9	3
7	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.	1.9	6
8	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.	1.3	6
9	Synthesis and Aldose Reductase Inhibition Effects of Novel Nâ€Benzylâ€4â€Methoxyaniline Derivatives. Chemistry and Biodiversity, 2022, 19, .	1.0	1
10	Identifying highly effective coumarin-based novel cholinesterase inhibitors by in silico and in vitro studies. Journal of Molecular Graphics and Modelling, 2022, 115, 108210.	1.3	14
11	Evolutionary association of receptor-wide amino acids with G proteinâ€“coupling selectivity in aminergic GPCRs. Life Science Alliance, 2022, 5, e202201439.	1.3	4
12	Review on In silico Methods, High-throughput Screening Techniques, and Cell Culture Based In Vitro Assays for SARS-CoV-2... Current Medicinal Chemistry, 2022, 29, .	1.2	3
13	Identifying new piperazine-based PARP1 inhibitors using text mining and integrated molecular modeling approaches. Journal of Biomolecular Structure and Dynamics, 2021, 39, 681-690.	2.0	11
14	An Integrated in silico Approach and inâ€...vitro Study for the Discovery of Smallâ€Molecule USP7 Inhibitors as Potential Cancer Therapies. ChemMedChem, 2021, 16, 555-567.	1.6	7
15	Drug Reâ€positioning Studies for Novel HIVâ€1 Inhibitors Using Binary QSAR Models and Multiâ€targetâ€driven In Silico Studies. Molecular Informatics, 2021, 40, e2000012.	1.4	6
16	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, 2021, 45, 18443-18452.	1.4	4
17	Structural and Functional Characterization of Allatostatin Receptor Type-C of Thaumetopoea pityocampa, a Potential Target for Next-Generation Pest Control Agents. Journal of Chemical Information and Modeling, 2021, 61, 715-728.	2.5	4
18	Target-Driven Design of a Coumarinyl Chalcone Scaffold Based Novel EF2 Kinase Inhibitor Suppresses Breast Cancer Growth In Vivo. ACS Pharmacology and Translational Science, 2021, 4, 926-940.	2.5	5

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19	Hybrid In Silico and TR-FRET-Guided Discovery of Novel BCL-2 Inhibitors. ACS Pharmacology and Translational Science, 2021, 4, 1111-1123.	2.5	3
20	Structures of <scp>MERSâ€CoV</scp> macro domain in aqueous solution with dynamics: Impacts of parallel tempering simulation techniques and <scp>CHARMM36m</scp> and <scp>AMBER99SB</scp> force field parameters. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1289-1299.	1.5	2
21	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.	1.3	2
22	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.	1.6	28
23	Binary-QSAR guided virtual screening of FDA approved drugs and compounds in clinical investigation against SARS-CoV-2 main protease. Turkish Journal of Biology, 2021, 45, 459-468.	2.1	2
24	Identification of first-in-class plasmodium OTU inhibitors with potent anti-malarial activity. Biochemical Journal, 2021, 478, 3445-3466.	1.7	2
25	New nimesulide derivatives with amide/sulfonamide moieties: Selective COX-2 inhibition and antitumor effects. European Journal of Medicinal Chemistry, 2021, 221, 113566.	2.6	21
26	Synthesis, molecular docking and molecular dynamics studies of novel tacrine-carbamate derivatives as potent cholinesterase inhibitors. Bioorganic Chemistry, 2021, 115, 105225.	2.0	19
27	Transcription factor NF-ÎºB as target for SARS-CoV-2 drug discovery efforts using inflammation-based QSAR screening model. Journal of Molecular Graphics and Modelling, 2021, 108, 107968.	1.3	8
28	Novel inhibitors of eukaryotic elongation factor 2 kinase: In silico, synthesis and in vitro studies. Bioorganic Chemistry, 2021, 116, 105296.	2.0	4
29	Development of imidazolone based angiotensin II receptor type I inhibitor small molecule as a chemotherapeutic agent for cell cycle inhibition. International Journal of Transgender Health, 2021, 14, 678-690.	1.1	2
30	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.	1.0	9
31	Synthesis, anticholinesterase activity and molecular modeling studies of novel carvacrol-substituted amide derivatives. Journal of Biomolecular Structure and Dynamics, 2020, 38, 841-859.	2.0	9
32	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.	2.0	13
33	In vitro and in silico studies of nitrobenzamide derivatives as potential anti-neuroinflammatory agents. Journal of Biomolecular Structure and Dynamics, 2020, 38, 4655-4668.	2.0	4
34	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.	1.3	13
35	Drug repurposing studies of PARP inhibitors as a new therapy for inherited retinal degeneration. Cellular and Molecular Life Sciences, 2020, 77, 2199-2216.	2.4	20
36	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.	2.0	11

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37	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.	1.1	3
38	Elucidation of interaction mechanism of hERG1 potassium channel with scorpion toxins BeKm-1 and BmTx3b. Journal of Molecular Graphics and Modelling, 2020, 96, 107504.	1.3	3
39	Proposing novel MDM2 inhibitors: Combined physicsâ€driven highâ€throughput virtual screening and in vitro studies. Chemical Biology and Drug Design, 2020, 96, 684-700.	1.5	4
40	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.	2.5	7
41	Combined ligand and structure-based virtual screening approaches for identification of novel AChE inhibitors. Turkish Journal of Chemistry, 2020, 44, 574-588.	0.5	2
42	Potent novel inhibitors against hepatitis C virus NS3 (HCV NS3 GT-3a) protease domain. Journal of Molecular Graphics and Modelling, 2020, 101, 107727.	1.3	4
43	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.	1.3	8
44	Development of Small Molecule MEIS Inhibitors that modulate HSC activity. Scientific Reports, 2020, 10, 7994.	1.6	22
45	Virtual drug repurposing study against SARS-CoV-2 TMPRSS2 target. Turkish Journal of Biology, 2020, 44, 185-191.	2.1	22
46	An Integrated Computational Approach for the Discovery of Ubiquitin Specific Protease 7 (USP7) Inhibitors as Potential Cancer Therapies. Biophysical Journal, 2020, 118, 47a.	0.2	1
47	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.	2.5	17
48	Integrating Ligand and Target-Driven Based Virtual Screening Approaches With in vitro 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.	1.8	17
49	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.	1.3	4
50	Bis benzothiophene Schiff bases: synthesis and in silico-guided biological activity studies. Turkish Journal of Chemistry, 2020, 44, 1164-1176.	0.5	6
51	Novel tumor necrosis factor-Î± (TNF-Î±) 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.	2.0	21
52	Toward Understanding the Impact of Dimerization Interfaces in Angiotensin II Type 1 Receptor. Journal of Chemical Information and Modeling, 2019, 59, 4314-4327.	2.5	13
53	Inhibition of acetylcholinesterase and butyrylcholinesterase with uracil derivatives: kinetic and computational studies. Journal of Enzyme Inhibition and Medicinal Chemistry, 2019, 34, 429-437.	2.5	76
54	Hostâ€“Guest Interactions between Candesartan and Its Prodrug Candesartan Cilexetil in Complex with 2-Hydroxypropyl-Î²-cyclodextrin: On the Biological Potency for Angiotensin II Antagonism. Molecular Pharmaceutics, 2019, 16, 1255-1271.	2.3	17

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55	Current status of multiscale simulations on GPCRs. Current Opinion in Structural Biology, 2019, 55, 93-103.	2.6	17
56	Effects of Cholesterol on GPCR Function: Insights from Computational and Experimental Studies. Advances in Experimental Medicine and Biology, 2019, 1135, 89-103.	0.8	32
57	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.	2.0	49
58	Integration of Text Mining and Binary QSAR Models for Novel Anti-Hypertensive Antagonist Scaffolds. Biophysical Journal, 2019, 116, 478a.	0.2	1
59	Combined molecular modeling and cholinesterase inhibition studies on some natural and semisynthetic O-alkylcoumarin derivatives. Bioorganic Chemistry, 2019, 84, 355-362.	2.0	16
60	Targeting the NF-Î¹B/ÍÎ¹BÎ± complex via fragment-based E-Pharmacophore virtual screening and binary QSAR models. Journal of Molecular Graphics and Modelling, 2019, 86, 264-277.	1.3	28
61	Combinatorial peptide library screening for discovery of diverse Î±-glucosidase inhibitors using molecular dynamics simulations and binary QSAR models. Journal of Biomolecular Structure and Dynamics, 2019, 37, 726-740.	2.0	74
62	Oligomerization and cooperativity in GPCRs from the perspective of the angiotensin AT1 and dopamine D2 receptors. Neuroscience Letters, 2019, 700, 30-37.	1.0	17
63	Abstract 4787: New and potent small molecule as EF2K inhibitor: A novel EF2K inhibitor. , 2019, , .		0
64	Molecular modeling and in vitro approaches towards cholinesterase inhibitory effect of some natural xanthohumol, naringenin, and acyl phloroglucinol derivatives. Phytomedicine, 2018, 42, 25-33.	2.3	29
65	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.	1.7	33
66	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.	2.6	21
67	Structural Investigation of the Dopamine-2 Receptor Agonist Bromocriptine Binding to Dimeric D2HighR and D2LowR States. Journal of Chemical Information and Modeling, 2018, 58, 826-836.	2.5	3
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.	2.0	14
69	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.	2.0	12
70	Structure-based design of hERG-neutral antihypertensive oxazalone and imidazolone derivatives. Journal of Molecular Graphics and Modelling, 2018, 79, 103-117.	1.3	18
71	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.	1.3	23
72	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.	2.5	26

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73	A QM proteinâ€“ligand investigation of antipsychotic drugs with the dopamine D2 Receptor (D2R). Journal of Biomolecular Structure and Dynamics, 2018, 36, 2668-2677.	2.0	6
74	Application of Multiscale Simulation Tools on GPCRs. An Example with Angiotensin II Type 1 Receptor. Methods in Molecular Biology, 2018, 1824, 431-448.	0.4	0
75	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.	1.3	42
76	Proposing novel TNFÎ± 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.	1.3	8
77	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.	2.0	14
78	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.	2.0	16
79	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.	2.0	13
80	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 Medicinal Chemistry, 2017, 32, 311-330.	2.5	26
81	Cholesterol up-regulates neuronal G protein-gated inwardly rectifying potassium (GIRK) channel activity in the hippocampus. Journal of Biological Chemistry, 2017, 292, 6135-6147.	1.6	37
82	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.	1.7	23
83	First universal pharmacophore model for hERG1 K + channel activators: acthER. Journal of Molecular Graphics and Modelling, 2017, 74, 153-170.	1.3	9
84	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.	1.3	8
85	Biological Insights of the Dopaminergic Stabilizer ACR16 at the Binding Pocket of Dopamine D2 Receptor. ACS Chemical Neuroscience, 2017, 8, 826-836.	1.7	15
86	Synthesis, anticholinesterase activity and molecular modeling study of novel carbamate-substituted thymol/carvacrol derivatives. Bioorganic and Medicinal Chemistry, 2017, 25, 1352-1363.	1.4	45
87	Solubility profiles, hydration and desolvation of curcumin complexed with Î³-cyclodextrin and hydroxypropyl-Î³-cyclodextrin. Journal of Molecular Structure, 2017, 1134, 91-98.	1.8	26
88	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.	2.5	28
89	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.	1.4	35
90	The synthesis of novel sulfamides derived from Î²-benzylphenethylamines as acetylcholinesterase, butyrylcholinesterase and carbonic anhydrase enzymes inhibitors. Bioorganic Chemistry, 2017, 74, 238-250.	2.0	64

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91	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.	1.3	6
92	Publisher Note. Journal of Molecular Graphics and Modelling, 2017, 77, 338.	1.3	2
93	Publisher's note. Journal of Molecular Graphics and Modelling, 2017, 77, 240.	1.3	1
94	Discovery of Klotho peptide antagonists against Wnt3 and Wnt3a target proteins using combination of protein engineering, proteinâ€“protein docking, peptide docking and molecular dynamics simulations. Journal of Enzyme Inhibition and Medicinal Chemistry, 2017, 32, 84-98.	2.5	11
95	In silico design of novel hERG-neutral sildenafil-like PDE5 inhibitors. Journal of Biomolecular Structure and Dynamics, 2017, 35, 2830-2852.	2.0	3
96	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.	1.3	42
97	Acetylcholinesterase and carbonic anhydrase inhibitory properties of novel urea and sulfamide derivatives incorporating dopaminergic 2-aminotetralin scaffolds. Bioorganic and Medicinal Chemistry, 2016, 24, 2318-2329.	1.4	131
98	Investigation of inhibition of human glucose 6-phosphate dehydrogenase by some 99mTc chelators byin silicoandin vitromethods. Journal of Enzyme Inhibition and Medicinal Chemistry, 2016, 31, 141-147.	2.5	9
99	Characterization, in Vivo Evaluation, and Molecular Modeling of Different Propofolâ€“Cyclodextrin Complexes To Assess Their Drug Delivery Potential at the Bloodâ€“Brain Barrier Level. Journal of Chemical Information and Modeling, 2016, 56, 1914-1922.	2.5	39
100	Role of the pH in state-dependent blockade of hERG currents. Scientific Reports, 2016, 6, 32536.	1.6	31
101	Synthesis of Some Novel Norborneneâ€Fused Pyridazines as Potent Inhibitors of Carbonic Anhydrase and Acetylcholinesterase. Journal of Heterocyclic Chemistry, 2016, 53, 2049-2056.	1.4	39
102	Kinetic andin silicostudies of hydroxy-based inhibitors of carbonic anhydrase isoforms I and II. Journal of Enzyme Inhibition and Medicinal Chemistry, 2016, 31, 31-37.	2.5	14
103	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, 185-195.	1.7	45
104	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, 2462-2468.	2.0	4
105	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, 1214-1220.	2.5	4
106	In silicoinvestigation of PARP-1 catalytic domains inholoandapostates for the design of high-affinity PARP-1 inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2016, 31, 112-120.	2.5	21
107	Protein Engineering Studies for C-C Chemokine Receptor Type 2 (CCR2). Current Enzyme Inhibition, 2016, 12, 110-114.	0.3	0
108	Investigation of Inhibition Mechanism of Chemokine Receptor CCR5 by Micro-second Molecular Dynamics Simulations. Scientific Reports, 2015, 5, 13180.	1.6	40

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109	Fullerene-based inhibitors of HIV-1 protease. Journal of Peptide Science, 2015, 21, 862-870.	0.8	31
110	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, 2015, 23, 36-59.	1.2	20
111	Structural modeling of the N-terminal signalâ€“receiving domain of IÎºBÎ±. Frontiers in Molecular Biosciences, 2015, 2, 32.	1.6	5
112	Recent Developments of Carbonic Anhydrase Inhibitors as Potential Drugs. BioMed Research International, 2015, 2015, 1-2.	0.9	4
113	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, 321-332.	2.1	29
114	NS1643 Interacts around L529 of hERG to Alter Voltage Sensor Movement on the Path to Activation. Biophysical Journal, 2015, 108, 1400-1413.	0.2	27
115	Discovery of potent carbonic anhydrase and acetylcholine esterase inhibitors: Novel sulfamoylcarbamates and sulfamides derived from acetophenones. Bioorganic and Medicinal Chemistry, 2015, 23, 3592-3602.	1.4	137
116	Discovering novel carbonic anhydrase type IX (CA IX) inhibitors from seven million compounds using virtual screening andin vitroanalysis. Journal of Enzyme Inhibition and Medicinal Chemistry, 2015, 31, 1-9.	2.5	10
117	Carbonic anhydrase inhibitors: Design, synthesis, kinetic, docking and molecular dynamics analysis of novel glycine and phenylalanine sulfonamide derivatives. Bioorganic and Medicinal Chemistry, 2015, 23, 7353-7358.	1.4	39
118	Molecular Simulations of Solved Co-crystallized X-Ray Structures Identify Action Mechanisms of PDEÎ´ Inhibitors. Biophysical Journal, 2015, 109, 1163-1168.	0.2	15
119	Interaction of carbonic anhydrase isozymes I, II, and IX with some pyridine and phenol hydrazinecarbothioamide derivatives. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 5636-5641.	1.0	41
120	Structure Driven Design of Novel Human Ether-A-Go-Go-Related-Gene Channel (hERG1) Activators. PLoS ONE, 2014, 9, e105553.	1.1	16
121	Development and Validation Studies of Universal Pharmacophore Models for hERG Channel Openers. Biophysical Journal, 2014, 106, 15a.	0.2	1
122	Inhibition of mammalian carbonic anhydrases I-XIV with grayanotoxin III: solution and in silico studies. Journal of Enzyme Inhibition and Medicinal Chemistry, 2014, 29, 469-475.	2.5	33
123	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, 1031-1046.	1.4	35
124	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.	1.3	4
125	Rehabilitating drug-induced long-QT promoters: In-silico design of hERG-neutral cisapride analogues with retained pharmacological activity. BMC Pharmacology & Toxicology, 2014, 15, 14.	1.0	16
126	Elucidation of Conformational States, Dynamics, and Mechanism of Binding in Human Î¼-Opioid Receptor Complexes. Journal of Chemical Information and Modeling, 2014, 54, 2294-2308.	2.5	25

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127	Carbonic anhydrase inhibitory properties of novel benzylsulfamides using molecular modeling and experimental studies. Bioorganic Chemistry, 2014, 56, 75-82.	2.0	113
128	Synthesis of 1,4-bis(indolin-1-ylmethyl)benzene derivatives and their structureâ€“activity relationships for the interaction of human carbonic anhydrase isoforms I and II. Bioorganic and Medicinal Chemistry, 2013, 21, 1477-1482.	1.4	12
129	AT1 antagonists: a patent review (2008 â€“ 2012). Expert Opinion on Therapeutic Patents, 2013, 23, 1483-1494.	2.4	25
130	Kinetic and in silico analysis of thiazolidin-based inhibitors of Î±-carbonic anhydrase isoenzymes. Journal of Enzyme Inhibition and Medicinal Chemistry, 2013, 28, 370-374.	2.5	14
131	Molecular insights into the AT1 antagonism based on biophysical and in silico studies of telmisartan. Medicinal Chemistry Research, 2013, 22, 4842-4857.	1.1	8
132	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.	0.2	2
133	Identification of Novel Cholesterol-binding Regions in Kir2 Channels. Journal of Biological Chemistry, 2013, 288, 31154-31164.	1.6	95
134	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.	0.2	2
135	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, 467-475.	2.5	39
136	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, 441-452.	1.3	29
137	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, 2760-2774.	2.5	68
138	The discovery of new potent non-peptide Angiotensin II AT1 receptor blockers: A concise synthesis, molecular docking studies and biological evaluation ofÂN-substituted 5-butylimidazole derivatives. European Journal of Medicinal Chemistry, 2012, 55, 358-374.	2.6	31
139	Proteinâ€“Protein Interactions: Inhibition of Mammalian Carbonic Anhydrases Iâ€“XV by the Murine Inhibitor of Carbonic Anhydrase and Other Members of the Transferrin Family. Journal of Medicinal Chemistry, 2012, 55, 5529-5535.	2.9	27
140	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.	2.6	4
141	Structureâ€“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.	2.6	54
142	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, 463-474.	2.5	88
143	Design, synthesis and biological evaluation of novel nitroaromatic compounds as potent glutathione reductase inhibitors. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 5398-5402.	1.0	48
144	Binding of novel fullerene inhibitors to HIV-1 protease: insight through molecular dynamics and molecular mechanics Poissonâ€“Boltzmann surface area calculations. Journal of Computer-Aided Molecular Design, 2011, 25, 959-976.	1.3	45

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145	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, 865-875.	1.2	20
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