Jana Selent

List of Publications by Year in descending order

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		236612	264894
65	2,095	25	42
papers	citations	h-index	g-index

69	69	69	3198
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	SCoV2-MD: a database for the dynamics of the SARS-CoV-2 proteome and variant impact predictions. Nucleic Acids Research, 2022, 50, D858-D866.	6.5	17
2	Simulating Time-Resolved Dynamics of Biomolecular Systems. , 2022, , 115-134.		2
3	Community guidelines for GPCR ligand bias: IUPHAR review 32. British Journal of Pharmacology, 2022, 179, 3651-3674.	2.7	84
4	In Silico Study of Allosteric Communication Networks in GPCR Signaling Bias. International Journal of Molecular Sciences, 2022, 23, 7809.	1.8	1
5	Mechanistic insights into dopaminergic and serotonergic neurotransmission â€“ concerted interactions with helices 5 and 6 drive the functional outcome. Chemical Science, 2021, 12, 10990-11003.	3.7	7
6	Electron Paramagnetic Resonance Gives Evidence for the Presence of Type 1 Gonadotropin-Releasing Hormone Receptor (GnRH-R) in Subdomains of Lipid Rafts. Molecules, 2021, 26, 973.	1.7	1
7	Dopamine D2 Receptor Agonist Binding Kineticsâ€”Role of a Conserved Serine Residue. International Journal of Molecular Sciences, 2021, 22, 4078.	1.8	5
8	Can molecular dynamics simulations improve the structural accuracy and virtual screening performance of GPCR models?. PLoS Computational Biology, 2021, 17, e1008936.	1.5	16
9	A molecular sensor for cholesterol in the human serotonin _{1A} receptor. Science Advances, 2021, 7, .	4.7	31
10	Structural dynamics bridge the gap between the genetic and functional levels of GPCRs. Current Opinion in Structural Biology, 2021, 69, 150-159.	2.6	6
11	Entrectinibâ€”A SARS-CoV-2 Inhibitor in Human Lung Tissue (HLT) Cells. International Journal of Molecular Sciences, 2021, 22, 13592.	1.8	7
12	A highly conserved Î´â€opioid receptor region determines RGS4 interaction. FEBS Journal, 2020, 287, 736-748.	2.2	5
13	GPCRmd uncovers the dynamics of the 3D-GPCRome. Nature Methods, 2020, 17, 777-787.	9.0	90
14	Ligand with Two Modes of Interaction with the Dopamine D₂ Receptorâ€“An Induced-Fit Mechanism of Insurmountable Antagonism. ACS Chemical Neuroscience, 2020, 11, 3130-3143.	1.7	8
15	Distinct phosphorylation sites in a prototypical GPCR differently orchestrate Î²-arrestin interaction, trafficking, and signaling. Science Advances, 2020, 6, .	4.7	55
16	How Do Molecular Dynamics Data Complement Static Structural Data of GPCRs. International Journal of Molecular Sciences, 2020, 21, 5933.	1.8	35
17	The European Research Network on Signal Transduction (ERNEST): Toward a Multidimensional Holistic Understanding of G Protein-Coupled Receptor Signaling. ACS Pharmacology and Translational Science, 2020, 3, 361-370.	2.5	15
18	Performance of virtual screening against GPCR homology models: Impact of template selection and treatment of binding site plasticity. PLoS Computational Biology, 2020, 16, e1007680.	1.5	35

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19	Key phosphorylation sites in <scp>GPCR</scp> s orchestrate the contribution of Î²â€Arrestin 1 in <scp>ERK</scp> 1/2 activation. EMBO Reports, 2020, 21, e49886.	2.0	48
20	Sharing Data from Molecular Simulations. Journal of Chemical Information and Modeling, 2019, 59, 4093-4099.	2.5	26
21	Conformational Sensors and Domain Swapping Reveal Structural and Functional Differences between Î²-Arrestin Isoforms. Cell Reports, 2019, 28, 3287-3299.e6.	2.9	54
22	Proteinâ€“Protein Docking in Drug Design and Discovery. Methods in Molecular Biology, 2018, 1762, 285-305.	0.4	17
23	Role of palmitoylation of cysteine 415 in functional coupling CB₁ receptor to Gî±_{i2} protein. Biotechnology and Applied Biochemistry, 2018, 65, 16-20.	1.4	12
24	Membrane cholesterol effect on the 5â€HT_{2A} receptor: Insights into the lipidâ€induced modulation of an antipsychotic drug target. Biotechnology and Applied Biochemistry, 2018, 65, 29-37.	1.4	12
25	Challenges and Opportunities in Drug Discovery of Biased Ligands. Methods in Molecular Biology, 2018, 1705, 321-334.	0.4	6
26	Synthesis, molecular modelling studies and biological evaluation of new oxoeicosanoid receptor 1 agonists. Bioorganic and Medicinal Chemistry, 2018, 26, 3580-3587.	1.4	9
27	Membrane cholesterol access into a G-protein-coupled receptor. Nature Communications, 2017, 8, 14505.	5.8	129
28	C-edge loops of arrestin function as a membrane anchor. Nature Communications, 2017, 8, 14258.	5.8	77
29	Palmitoylation of cysteine 415 of CB 1 receptor affects ligand-stimulated internalization and selective interaction with membrane cholesterol and caveolin 1. Biochimica Et Biophysica Acta - Molecular and Cell Biology of Lipids, 2017, 1862, 523-532.	1.2	24
30	Development of Fluorescent Probes that Target Serotonin 5-HT2B Receptors. Scientific Reports, 2017, 7, 10765.	1.6	15
31	Serotonin 2A receptor disulfide bridge integrity is crucial for ligand binding to different signalling states but not for its homodimerization. European Journal of Pharmacology, 2017, 815, 138-146.	1.7	11
32	Computational methods for studying G protein-coupled receptors (GPCRs). Methods in Cell Biology, 2016, 132, 359-399.	0.5	31
33	In silicoExploration of the Conformational Universe of GPCRs. Molecular Informatics, 2016, 35, 227-237.	1.4	7
34	Membrane omega-3 fatty acids modulate the oligomerisation kinetics of adenosine A2A and dopamine D2 receptors. Scientific Reports, 2016, 6, 19839.	1.6	89
35	Drugging specific conformational states of GPCRs: challenges and opportunities for computational chemistry. Drug Discovery Today, 2016, 21, 625-631.	3.2	26
36	Membrane Protein Structure, Function, and Dynamics: a Perspective from Experiments and Theory. Journal of Membrane Biology, 2015, 248, 611-640.	1.0	157

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37	Detection of New Biased Agonists for the Serotonin 5-HT_{2A} Receptor: Modeling and Experimental Validation. Molecular Pharmacology, 2015, 87, 740-746.	1.0	29
38	Multiâ€Component Protein â€“ Protein Docking Based Protocol with External Scoring for Modeling Dimers of G Proteinâ€Coupled Receptors. Molecular Informatics, 2015, 34, 246-255.	1.4	15
39	Novel insights on the structural determinants of clozapine and olanzapine multi-target binding profiles. European Journal of Medicinal Chemistry, 2014, 77, 91-95.	2.6	21
40	Electronic Sculpting of Ligand-GPCR Subtype Selectivity: The Case of Angiotensin II. ACS Chemical Biology, 2014, 9, 1420-1425.	1.6	31
41	MEMBPLUGIN: studying membrane complexity in VMD. Bioinformatics, 2014, 30, 1478-1480.	1.8	215
42	Cell Membrane Composition Affects GPCR Aggregation. Biophysical Journal, 2014, 106, 517a-518a.	0.2	0
43	A Dynamic View of Molecular Switch Behavior at Serotonin Receptors: Implications for Functional Selectivity. PLoS ONE, 2014, 9, e109312.	1.1	27
44	Application of BRET for Studying G Protein-Coupled Receptors. Mini-Reviews in Medicinal Chemistry, 2014, 14, 411-425.	1.1	19
45	Modeling Complexes of Transmembrane Proteins: Systematic Analysis of Proteinï¿¿Protein Docking Tools. Molecular Informatics, 2013, 32, 717-733.	1.4	27
46	Structure-Based Molecular Modeling Approaches to GPCR Oligomerization. Methods in Cell Biology, 2013, 117, 91-104.	0.5	10
47	Simulating G Protein-Coupled Receptors in Native-Like Membranes. Methods in Cell Biology, 2013, 117, 63-90.	0.5	13
48	Rational design of the survivin/CDK4 complex by combining proteinâ€“protein docking and molecular dynamics simulations. Journal of Molecular Modeling, 2013, 19, 1507-1514.	0.8	8
49	Novel Insights into Biased Agonism at G Protein-Coupled Receptors and their Potential for Drug Design. Current Pharmaceutical Design, 2013, 19, 5156-5166.	0.9	27
50	Crosstalk within GPCR Heteromers in Schizophrenia and Parkinsons Disease: Physical or Just Functional?. Current Medicinal Chemistry, 2012, 19, 1119-1134.	1.2	10
51	Tungstate activates BK channels in a Î² subunit- and Mg2+-dependent manner: relevance for arterial vasodilatation. Cardiovascular Research, 2012, 95, 29-38.	1.8	12
52	Fractal dimension as a measure of surface roughness of G protein-coupled receptors: implications for structure and function. Journal of Molecular Modeling, 2012, 18, 4465-4475.	0.8	17
53	Effects of palmitoylation of Cys⁴¹⁵ in helix 8 of the CB₁ cannabinoid receptor on membrane localization and signalling. British Journal of Pharmacology, 2012, 165, 2635-2651.	2.7	50
54	Membrane-Sensitive Conformational States of Helix 8 in the Metabotropic Glu2 Receptor, a Class C GPCR. PLoS ONE, 2012, 7, e42023.	1.1	31

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55	Progress in the structural prediction of G proteinâ€coupled receptors: D₃ receptor in complex with eticlopride. Proteins: Structure, Function and Bioinformatics, 2011, 79, 1695-1703.	1.5	22
56	A gain-of-function SNP in TRPC4 cation channel protects against myocardial infarction. Cardiovascular Research, 2011, 91, 465-471.	1.8	31
57	Synthesis, 3Dâ€QSAR, and Structural Modeling of Benzolactam Derivatives with Binding Affinity for the D₂ and D₃ Receptors. ChemMedChem, 2010, 5, 1300-1317.	1.6	23
58	A Novel Multilevel Statistical Method for the Study of the Relationships between Multireceptorial Binding Affinity Profiles and In Vivo Endpoints. Molecular Pharmacology, 2010, 77, 149-158.	1.0	10
59	Equine Estrogens Impair Nitric Oxide Production and Endothelial Nitric Oxide Synthase Transcription in Human Endothelial Cells Compared With the Natural 17Î²-Estradiol. Hypertension, 2010, 56, 405-411.	1.3	39
60	Induced Effects of Sodium Ions on Dopaminergic G-Protein Coupled Receptors. PLoS Computational Biology, 2010, 6, e1000884.	1.5	93
61	Synthesis, binding affinity and SAR of new benzolactam derivatives as dopamine D3 receptor ligands. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 1773-1778.	1.0	35
62	Multiâ€Receptor Binding Profile of Clozapine and Olanzapine: A Structural Study Based on the New Î²₂ Adrenergic Receptor Template. ChemMedChem, 2008, 3, 1194-1198.	1.6	51
63	Synthesis, Binding Affinity, and Molecular Docking Analysis of New Benzofuranone Derivatives as Potential Antipsychotics. Journal of Medicinal Chemistry, 2008, 51, 6085-6094.	2.9	26
64	Selective Inhibition of the Collagenase Activity of Cathepsin K. Journal of Biological Chemistry, 2007, 282, 16492-16501.	1.6	23
65	Enantiomeric N-methyl-4-piperidyl benzilates as muscarinic receptor ligands: Radioligand binding studies and docking studies to models of the three muscarinic receptors M1, M2 and M3. Bioorganic and Medicinal Chemistry, 2006, 14, 1729-1736.	1.4	6