Jana Selent

List of Publications by Year in descending order

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IANA SELENT

| # | Article | IF | CITATIONS |
|----|---|-----|-----------|
| 1 | MEMBPLUGIN: studying membrane complexity in VMD. Bioinformatics, 2014, 30, 1478-1480. | 1.8 | 215 |
| 2 | Membrane Protein Structure, Function, and Dynamics: a Perspective from Experiments and Theory. Journal of Membrane Biology, 2015, 248, 611-640. | 1.0 | 157 |
| 3 | Membrane cholesterol access into a G-protein-coupled receptor. Nature Communications, 2017, 8, 14505. | 5.8 | 129 |
| 4 | Induced Effects of Sodium Ions on Dopaminergic G-Protein Coupled Receptors. PLoS Computational Biology, 2010, 6, e1000884. | 1.5 | 93 |
| 5 | GPCRmd uncovers the dynamics of the 3D-GPCRome. Nature Methods, 2020, 17, 777-787. | 9.0 | 90 |
| 6 | Membrane omega-3 fatty acids modulate the oligomerisation kinetics of adenosine A2A and dopamine D2 receptors. Scientific Reports, 2016, 6, 19839. | 1.6 | 89 |
| 7 | Community guidelines for GPCR ligand bias: IUPHAR review 32. British Journal of Pharmacology, 2022, 179, 3651-3674. | 2.7 | 84 |
| 8 | C-edge loops of arrestin function as a membrane anchor. Nature Communications, 2017, 8, 14258. | 5.8 | 77 |
| 9 | Distinct phosphorylation sites in a prototypical GPCR differently orchestrate Î ² -arrestin interaction, trafficking, and signaling. Science Advances, 2020, 6, . | 4.7 | 55 |
| 10 | Conformational Sensors and Domain Swapping Reveal Structural and Functional Differences between β-Arrestin Isoforms. Cell Reports, 2019, 28, 3287-3299.e6. | 2.9 | 54 |
| 11 | Multiâ€Receptor Binding Profile of Clozapine and Olanzapine: A Structural Study Based on the New β ₂ Adrenergic Receptor Template. ChemMedChem, 2008, 3, 1194-1198. | 1.6 | 51 |
| 12 | Effects of palmitoylation of Cys ⁴¹⁵ in helix 8 of the CB ₁ cannabinoid receptor on membrane localization and signalling. British Journal of Pharmacology, 2012, 165, 2635-2651. | 2.7 | 50 |
| 13 | Key phosphorylation sites in <scp>GPCR</scp> s orchestrate the contribution of βâ€Arrestin 1 in <scp>ERK</scp> 1/2 activation. EMBO Reports, 2020, 21, e49886. | 2.0 | 48 |
| 14 | Equine Estrogens Impair Nitric Oxide Production and Endothelial Nitric Oxide Synthase Transcription in Human Endothelial Cells Compared With the Natural 17β-Estradiol. Hypertension, 2010, 56, 405-411. | 1.3 | 39 |
| 15 | 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 |
| 16 | How Do Molecular Dynamics Data Complement Static Structural Data of GPCRs. International Journal of Molecular Sciences, 2020, 21, 5933. | 1.8 | 35 |
| 17 | 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 |
| 18 | A gain-of-function SNP in TRPC4 cation channel protects against myocardial infarction. Cardiovascular Research, 2011, 91, 465-471. | 1.8 | 31 |

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|----|--|-----|-----------|
| 19 | Electronic Sculpting of Ligand-GPCR Subtype Selectivity: The Case of Angiotensin II. ACS Chemical Biology, 2014, 9, 1420-1425. | 1.6 | 31 |
| 20 | Computational methods for studying G protein-coupled receptors (GPCRs). Methods in Cell Biology, 2016, 132, 359-399. | 0.5 | 31 |
| 21 | A molecular sensor for cholesterol in the human serotonin _{1A} receptor. Science Advances, 2021, 7, . | 4.7 | 31 |
| 22 | Membrane-Sensitive Conformational States of Helix 8 in the Metabotropic Glu2 Receptor, a Class C GPCR. PLoS ONE, 2012, 7, e42023. | 1.1 | 31 |
| 23 | 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 |
| 24 | Modeling Complexes of Transmembrane Proteins: Systematic Analysis of ProteinProtein Docking Tools. Molecular Informatics, 2013, 32, 717-733. | 1.4 | 27 |
| 25 | A Dynamic View of Molecular Switch Behavior at Serotonin Receptors: Implications for Functional Selectivity. PLoS ONE, 2014, 9, e109312. | 1.1 | 27 |
| 26 | 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 |
| 27 | 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 |
| 28 | Drugging specific conformational states of GPCRs: challenges and opportunities for computational chemistry. Drug Discovery Today, 2016, 21, 625-631. | 3.2 | 26 |
| 29 | Sharing Data from Molecular Simulations. Journal of Chemical Information and Modeling, 2019, 59, 4093-4099. | 2.5 | 26 |
| 30 | 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 |
| 31 | Selective Inhibition of the Collagenase Activity of Cathepsin K. Journal of Biological Chemistry, 2007, 282, 16492-16501. | 1.6 | 23 |
| 32 | Synthesis, 3Dâ€QSAR, and Structural Modeling of Benzolactam Derivatives with Binding Affinity for the D ₂ and D ₃ Receptors. ChemMedChem, 2010, 5, 1300-1317. | 1.6 | 23 |
| 33 | Progress in the structural prediction of G proteinâ€coupled receptors: D ₃ receptor in complex with eticlopride. Proteins: Structure, Function and Bioinformatics, 2011, 79, 1695-1703. | 1.5 | 22 |
| 34 | 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 |
| 35 | Application of BRET for Studying G Protein-Coupled Receptors. Mini-Reviews in Medicinal Chemistry, 2014, 14, 411-425. | 1.1 | 19 |
| 36 | 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 |

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|----|--|-----|-----------|
| 37 | Protein–Protein Docking in Drug Design and Discovery. Methods in Molecular Biology, 2018, 1762, 285-305. | 0.4 | 17 |
| 38 | 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 |
| 39 | Can molecular dynamics simulations improve the structural accuracy and virtual screening performance of GPCR models?. PLoS Computational Biology, 2021, 17, e1008936. | 1.5 | 16 |
| 40 | Multi omponent Protein – Protein Docking Based Protocol with External Scoring for Modeling Dimers of G Protein oupled Receptors. Molecular Informatics, 2015, 34, 246-255. | 1.4 | 15 |
| 41 | Development of Fluorescent Probes that Target Serotonin 5-HT2B Receptors. Scientific Reports, 2017, 7, 10765. | 1.6 | 15 |
| 42 | 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 |
| 43 | Simulating G Protein-Coupled Receptors in Native-Like Membranes. Methods in Cell Biology, 2013, 117, 63-90. | 0.5 | 13 |
| 44 | Tungstate activates BK channels in a β subunit- and Mg2+-dependent manner: relevance for arterial vasodilatation. Cardiovascular Research, 2012, 95, 29-38. | 1.8 | 12 |
| 45 | Role of palmitoylation of cysteine 415 in functional coupling CB ₁ receptor to Gα _{i2} protein. Biotechnology and Applied Biochemistry, 2018, 65, 16-20. | 1.4 | 12 |
| 46 | 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 |
| 47 | 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 |
| 48 | 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 |
| 49 | Crosstalk within GPCR Heteromers in Schizophrenia and Parkinsons Disease: Physical or Just Functional?. Current Medicinal Chemistry, 2012, 19, 1119-1134. | 1.2 | 10 |
| 50 | Structure-Based Molecular Modeling Approaches to GPCR Oligomerization. Methods in Cell Biology, 2013, 117, 91-104. | 0.5 | 10 |
| 51 | Synthesis, molecular modelling studies and biological evaluation of new oxoeicosanoid receptor 1 agonists. Bioorganic and Medicinal Chemistry, 2018, 26, 3580-3587. | 1.4 | 9 |
| 52 | Rational design of the survivin/CDK4 complex by combining protein–protein docking and molecular dynamics simulations. Journal of Molecular Modeling, 2013, 19, 1507-1514. | 0.8 | 8 |
| 53 | Ligand with Two Modes of Interaction with the Dopamine D ₂ Receptor–An Induced-Fit Mechanism of Insurmountable Antagonism. ACS Chemical Neuroscience, 2020, 11, 3130-3143. | 1.7 | 8 |
| 54 | <i>In silico</i> Exploration of the Conformational Universe of GPCRs. Molecular Informatics, 2016, 35, 227-237. | 1.4 | 7 |

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| 55 | Mechanistic insights into dopaminergic and serotonergic neurotransmission – concerted interactions with helices 5 and 6 drive the functional outcome. Chemical Science, 2021, 12, 10990-11003. | 3.7 | 7 |
| 56 | Entrectinib—A SARS-CoV-2 Inhibitor in Human Lung Tissue (HLT) Cells. International Journal of Molecular Sciences, 2021, 22, 13592. | 1.8 | 7 |
| 57 | 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 |
| 58 | Challenges and Opportunities in Drug Discovery of Biased Ligands. Methods in Molecular Biology, 2018, 1705, 321-334. | 0.4 | 6 |
| 59 | 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 |
| 60 | A highly conserved δâ€opioid receptor region determines RGS4 interaction. FEBS Journal, 2020, 287, 736-748. | 2.2 | 5 |
| 61 | Dopamine D2 Receptor Agonist Binding Kinetics—Role of a Conserved Serine Residue. International Journal of Molecular Sciences, 2021, 22, 4078. | 1.8 | 5 |
| 62 | Simulating Time-Resolved Dynamics of Biomolecular Systems. , 2022, , 115-134. | | 2 |
| 63 | 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 |
| 64 | In Silico Study of Allosteric Communication Networks in GPCR Signaling Bias. International Journal of Molecular Sciences, 2022, 23, 7809. | 1.8 | 1 |
| 65 | Cell Membrane Composition Affects GPCR Aggregation, Biophysical Journal, 2014, 106, 517a-518a. | 0.2 | 0 |