Giuseppe Deganutti

List of Publications by Year
in descending order

35	1,121	471509	434195
papers	citations	17 h-index	31 g-index

46	46	46	1218
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Cryo-EM structure of the active, Gs-protein complexed, human CGRP receptor. Nature, 2018, 561, 492-497.	27.8	210
2	Activation of the GLP-1 receptor by a non-peptidic agonist. Nature, 2020, 577, 432-436.	27.8	119
3	Deciphering the Complexity of Ligandâ€"Protein Recognition Pathways Using Supervised Molecular Dynamics (SuMD) Simulations. Journal of Chemical Information and Modeling, 2016, 56, 687-705.	5.4	88
4	Structure and Dynamics of Adrenomedullin Receptors AM₁ and AM₂ Reveal Key Mechanisms in the Control of Receptor Phenotype by Receptor Activity-Modifying Proteins. ACS Pharmacology and Translational Science, 2020, 3, 263-284.	4.9	71
5	Understanding allosteric interactions in G protein-coupled receptors using Supervised Molecular Dynamics: A prototype study analysing the human A3 adenosine receptor positive allosteric modulator LUF6000. Bioorganic and Medicinal Chemistry, 2015, 23, 4065-4071.	3.0	53
6	Molecular Signature for Receptor Engagement in the Metabolic Peptide Hormone Amylin. ACS Pharmacology and Translational Science, 2018, 1, 32-49.	4.9	48
7	Structure and dynamics of the active Gs-coupled human secretin receptor. Nature Communications, 2020, 11, 4137.	12.8	46
8	Supervised molecular dynamics for exploring the druggability of the SARS-CoV-2 spike protein. Journal of Computer-Aided Molecular Design, 2021, 35, 195-207.	2.9	41
9	Exploring the recognition pathway at the human A_{2A} adenosine receptor of the endogenous agonist adenosine using supervised molecular dynamics simulations. MedChemComm, 2015, 6, 1081-1085.	3.4	36
10	Estimation of kinetic and thermodynamic ligand-binding parameters using computational strategies. Future Medicinal Chemistry, 2017, 9, 507-523.	2.3	30
11	Dynamics of GLP-1R peptide agonist engagement are correlated with kinetics of G protein activation. Nature Communications, 2022, 13, 92.	12.8	30
12	AquaMMapS: An Alternative Tool to Monitor the Role of Water Molecules During Proteinâ€"Ligand Association. ChemMedChem, 2018, 13, 522-531.	3.2	29
13	A Supervised Molecular Dynamics Approach to Unbiased Ligandâ€"Protein Unbinding. Journal of Chemical Information and Modeling, 2020, 60, 1804-1817.	5.4	28
14	Comparison of the Human A_{2A} Adenosine Receptor Recognition by Adenosine and Inosine: New Insight from Supervised Molecular Dynamics Simulations. ChemMedChem, 2017, 12, 1319-1326.	3.2	26
15	Extracellular loops 2 and 3 of the calcitonin receptor selectively modify agonist binding and efficacy. Biochemical Pharmacology, 2018, 150, 214-244.	4.4	24
16	A2A and A2B adenosine receptors: The extracellular loop 2 determines high (A2A) or low affinity (A2B) for adenosine. Biochemical Pharmacology, 2020, 172, 113718.	4.4	24
17	Structural and functional diversity among agonist-bound states of the GLP-1 receptor. Nature Chemical Biology, 2022, 18, 256-263.	8.0	24
18	Selective activation of GÎ±ob by an adenosine A1 receptor agonist elicits analgesia without cardiorespiratory depression. Nature Communications, 2022, 13, .	12.8	23

#	Article	IF	Citations
19	Impact of proteinâ€“ligand solvation and desolvation on transition state thermodynamic properties of adenosine A2A ligand binding kinetics. In Silico Pharmacology, 2017, 5, 16.	3.3	20
20	Supporting the Identification of Novel Fragment-Based Positive Allosteric Modulators Using a Supervised Molecular Dynamics Approach: A Retrospective Analysis Considering the Human A2A Adenosine Receptor as a Key Example. Molecules, 2017, 22, 818.	3.8	19
21	Revisiting the Allosteric Regulation of Sodium Cation on the Binding of Adenosine at the Human A2A Adenosine Receptor: Insights from Supervised Molecular Dynamics (SuMD) Simulations. Molecules, 2019, 24, 2752.	3.8	14
22	Peeking at G-protein-coupled receptors through the molecular dynamics keyhole. Future Medicinal Chemistry, 2019, 11, 599-615.	2.3	11
23	Could the presence of sodium ion influence the accuracy and precision of the ligand-posing in the human A2A adenosine receptor orthosteric binding site using a molecular docking approach? Insights from Dockbench. Journal of Computer-Aided Molecular Design, 2018, 32, 1337-1346.	2.9	9
24	Deciphering the Agonist Binding Mechanism to the Adenosine A1 Receptor. ACS Pharmacology and Translational Science, 2021, 4, 314-326.	4.9	9
25	Molecular dynamics studies reveal structural and functional features of the SARSâ€CoVâ€2 spike protein. BioEssays, 2022, 44, .	2.5	9
26	Deconvoluting the Molecular Control of Binding and Signaling at the Amylin 3 Receptor: RAMP3 Alters Signal Propagation through Extracellular Loops of the Calcitonin Receptor. ACS Pharmacology and Translational Science, 2019, 2, 183-197.	4.9	8
27	Addressing free fatty acid receptor 1 (FFAR1) activation using supervised molecular dynamics. Journal of Computer-Aided Molecular Design, 2020, 34, 1181-1193.	2.9	8
28	Multisite Model of Allosterism for the Adenosine A1 Receptor. Journal of Chemical Information and Modeling, 2021, 61, 2001-2015.	5.4	8
29	Could Adenosine Recognize its Receptors with a Stoichiometry Other than 1â€‰:â€‰1?. Molecular Informatics, 2018, 37, e1800009.	2.5	7
30	Partial agonism improves the anti-hyperglycaemic efficacy of an oxyntomodulin-derived GLP-1R/GCGR co-agonist. Molecular Metabolism, 2021, 51, 101242.	6.5	7
31	New Insights into Key Determinants for Adenosine 1 Receptor Antagonists Selectivity Using Supervised Molecular Dynamics Simulations. Biomolecules, 2020, 10, 732.	4.0	5
32	Peptidomimeticâ€based approach toward inhibitors of microbial trimethylamine lyases. Chemical Biology and Drug Design, 2021, 97, 231-236.	3.2	5
33	Exploring Ligand Binding to Calcitonin Gene-Related Peptide Receptors. Frontiers in Molecular Biosciences, 2021, 8, 720561.	3.5	5
34	Insights into agonist-elicited activation of the human glucose-dependent insulinotropic polypeptide receptor. Biochemical Pharmacology, 2021, 192, 114715.	4.4	5
35	New Trends in Inspecting GPCRâ€ligand Recognition Process: the Contribution of the Molecular Modeling Section (MMS) at the University of Padova. Molecular Informatics, 2016, 35, 440-448.	2.5	3