

# Giuseppe Deganutti

## List of Publications by Year in descending order

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Version: 2024-02-01

35  
papers

1,121  
citations

471061

17  
h-index

433756

31  
g-index

46  
all docs

46  
docs citations

46  
times ranked

1218  
citing authors

#	ARTICLE	IF	CITATIONS
1	Cryo-EM structure of the active, Gs-protein complexed, human CGRP receptor. <i>Nature</i> , 2018, 561, 492-497.	13.7	210
2	Activation of the GLP-1 receptor by a non-peptidic agonist. <i>Nature</i> , 2020, 577, 432-436.	13.7	119
3	Deciphering the Complexity of Ligand-Protein Recognition Pathways Using Supervised Molecular Dynamics (SuMD) Simulations. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 687-705.	2.5	88
4	Structure and Dynamics of Adrenomedullin Receptors AM <sub>1</sub> and AM <sub>2</sub> Reveal Key Mechanisms in the Control of Receptor Phenotype by Receptor Activity-Modifying Proteins. <i>ACS Pharmacology and Translational Science</i> , 2020, 3, 263-284.	2.5	71
5	Understanding allosteric interactions in G protein-coupled receptors using Supervised Molecular Dynamics: A prototype study analysing the human A <sub>3</sub> adenosine receptor positive allosteric modulator LUF6000. <i>Bioorganic and Medicinal Chemistry</i> , 2015, 23, 4065-4071.	1.4	53
6	Molecular Signature for Receptor Engagement in the Metabolic Peptide Hormone Amylin. <i>ACS Pharmacology and Translational Science</i> , 2018, 1, 32-49.	2.5	48
7	Structure and dynamics of the active Gs-coupled human secretin receptor. <i>Nature Communications</i> , 2020, 11, 4137.	5.8	46
8	Supervised molecular dynamics for exploring the druggability of the SARS-CoV-2 spike protein. <i>Journal of Computer-Aided Molecular Design</i> , 2021, 35, 195-207.	1.3	41
9	Exploring the recognition pathway at the human A <sub>2A</sub> adenosine receptor of the endogenous agonist adenosine using supervised molecular dynamics simulations. <i>MedChemComm</i> , 2015, 6, 1081-1085.	3.5	36
10	Estimation of kinetic and thermodynamic ligand-binding parameters using computational strategies. <i>Future Medicinal Chemistry</i> , 2017, 9, 507-523.	1.1	30
11	Dynamics of GLP-1R peptide agonist engagement are correlated with kinetics of G protein activation. <i>Nature Communications</i> , 2022, 13, 92.	5.8	30
12	AquaMMapS: An Alternative Tool to Monitor the Role of Water Molecules During Protein-Ligand Association. <i>ChemMedChem</i> , 2018, 13, 522-531.	1.6	29
13	A Supervised Molecular Dynamics Approach to Unbiased Ligand-Protein Unbinding. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 1804-1817.	2.5	28
14	Comparison of the Human A <sub>2A</sub> Adenosine Receptor Recognition by Adenosine and Inosine: New Insight from Supervised Molecular Dynamics Simulations. <i>ChemMedChem</i> , 2017, 12, 1319-1326.	1.6	26
15	Extracellular loops 2 and 3 of the calcitonin receptor selectively modify agonist binding and efficacy. <i>Biochemical Pharmacology</i> , 2018, 150, 214-244.	2.0	24
16	A <sub>2A</sub> and A <sub>2B</sub> adenosine receptors: The extracellular loop 2 determines high (A <sub>2A</sub> ) or low affinity (A <sub>2B</sub> ) for adenosine. <i>Biochemical Pharmacology</i> , 2020, 172, 1137-118.	2.0	24
17	Structural and functional diversity among agonist-bound states of the GLP-1 receptor. <i>Nature Chemical Biology</i> , 2022, 18, 256-263.	3.9	24
18	Selective activation of G <sub>i/o</sub> by an adenosine A <sub>1</sub> receptor agonist elicits analgesia without cardiorespiratory depression. <i>Nature Communications</i> , 2022, 13, .	5.8	23

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19	Impact of proteinâ€“ligand solvation and desolvation on transition state thermodynamic properties of adenosine A2A ligand binding kinetics. <i>In Silico Pharmacology</i> , 2017, 5, 16.	1.8	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. <i>Molecules</i> , 2017, 22, 818.	1.7	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. <i>Molecules</i> , 2019, 24, 2752.	1.7	14
22	Peeking at G-protein-coupled receptors through the molecular dynamics keyhole. <i>Future Medicinal Chemistry</i> , 2019, 11, 599-615.	1.1	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. <i>Journal of Computer-Aided Molecular Design</i> , 2018, 32, 1337-1346.	1.3	9
24	Deciphering the Agonist Binding Mechanism to the Adenosine A1 Receptor. <i>ACS Pharmacology and Translational Science</i> , 2021, 4, 314-326.	2.5	9
25	Molecular dynamics studies reveal structural and functional features of the SARSâ€“CoVâ€“2 spike protein. <i>BioEssays</i> , 2022, 44, .	1.2	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. <i>ACS Pharmacology and Translational Science</i> , 2019, 2, 183-197.	2.5	8
27	Addressing free fatty acid receptor 1 (FFAR1) activation using supervised molecular dynamics. <i>Journal of Computer-Aided Molecular Design</i> , 2020, 34, 1181-1193.	1.3	8
28	Multisite Model of Allosterism for the Adenosine A1 Receptor. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 2001-2015.	2.5	8
29	Could Adenosine Recognize its Receptors with a Stoichiometry Other than 1â€“:â€“1?. <i>Molecular Informatics</i> , 2018, 37, e1800009.	1.4	7
30	Partial agonism improves the anti-hyperglycaemic efficacy of an oxyntomodulin-derived GLP-1R/GCGR co-agonist. <i>Molecular Metabolism</i> , 2021, 51, 101242.	3.0	7
31	New Insights into Key Determinants for Adenosine 1 Receptor Antagonists Selectivity Using Supervised Molecular Dynamics Simulations. <i>Biomolecules</i> , 2020, 10, 732.	1.8	5
32	Peptidomimeticâ€“based approach toward inhibitors of microbial trimethylamine lyases. <i>Chemical Biology and Drug Design</i> , 2021, 97, 231-236.	1.5	5
33	Exploring Ligand Binding to Calcitonin Gene-Related Peptide Receptors. <i>Frontiers in Molecular Biosciences</i> , 2021, 8, 720561.	1.6	5
34	Insights into agonist-elicited activation of the human glucose-dependent insulinotropic polypeptide receptor. <i>Biochemical Pharmacology</i> , 2021, 192, 114715.	2.0	5
35	New Trends in Inspecting GPCRâ€“ligand Recognition Process: the Contribution of the Molecular Modeling Section (MMS) at the University of Padova. <i>Molecular Informatics</i> , 2016, 35, 440-448.	1.4	3