

Vittorio Limongelli

List of Publications by Year in descending order

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Version: 2024-02-01

71
papers

4,329
citations

101384

36
h-index

114278

63
g-index

75
all docs

75
docs citations

75
times ranked

5132
citing authors

#	ARTICLE	IF	CITATIONS
1	Promoting transparency and reproducibility in enhanced molecular simulations. <i>Nature Methods</i> , 2019, 16, 670-673.	9.0	655
2	Funnel metadynamics as accurate binding free-energy method. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, 6358-6363.	3.3	337
3	Kinetics of protein-ligand unbinding: Predicting pathways, rates, and rate-limiting steps. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, E386-91.	3.3	311
4	Molecular basis of cyclooxygenase enzymes (COXs) selective inhibition. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010, 107, 5411-5416.	3.3	187
5	Unbinding Kinetics of a p38 MAP Kinase Type II Inhibitor from Metadynamics Simulations. <i>Journal of the American Chemical Society</i> , 2017, 139, 4780-4788.	6.6	187
6	Protein-ligand binding with the coarse-grained Martini model. <i>Nature Communications</i> , 2020, 11, 3714.	5.8	139
7	The G-quadruplex DNA. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 2269-2273.	7.2	133
8	Structural and Conformational Requisites in DNA Quadruplex Groove Binding: Another Piece to the Puzzle. <i>Journal of the American Chemical Society</i> , 2010, 132, 6425-6433.	6.6	111
9	Conformational Changes in the Epidermal Growth Factor Receptor: Role of the Transmembrane Domain Investigated by Coarse-Grained MetaDynamics Free Energy Calculations. <i>Journal of the American Chemical Society</i> , 2016, 138, 10611-10622.	6.6	103
10	Sampling protein motion and solvent effect during ligand binding. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 1467-1472.	3.3	100
11	Ligand binding free-energy calculations with funnel metadynamics. <i>Nature Protocols</i> , 2020, 15, 2837-2866.	5.5	96
12	Ligand binding to telomeric G-quadruplex DNA investigated by funnel-metadynamics simulations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, E2136-E2145.	3.3	91
13	Ligand binding free energy and kinetics calculation in 2020. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2020, 10, e1455.	6.2	86
14	Mechanistic insight into ligand binding to G-quadruplex DNA. <i>Nucleic Acids Research</i> , 2014, 42, 5447-5455.	6.5	79
15	Design, Synthesis, and Biological Evaluation of Potent Dual Agonists of Nuclear and Membrane Bile Acid Receptors. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 937-954.	2.9	79
16	G-triplex structure and formation propensity. <i>Nucleic Acids Research</i> , 2014, 42, 13393-13404.	6.5	71
17	Design, Synthesis, and Biological Evaluation of Novel Aminobisphosphonates Possessing an in Vivo Antitumor Activity Through a ^{131}T Lymphocytes-Mediated Activation Mechanism. <i>Journal of Medicinal Chemistry</i> , 2008, 51, 6800-6807.	2.9	70
18	Investigating the Mechanism of Substrate Uptake and Release in the Glutamate Transporter Homologue Glt _{Ph} through Metadynamics Simulations. <i>Journal of the American Chemical Society</i> , 2012, 134, 453-463.	6.6	66

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19	Modeling of Cdc25B Dual Specificity Protein Phosphatase Inhibitors: Docking of Ligands and Enzymatic Inhibition Mechanism. <i>ChemMedChem</i> , 2006, 1, 540-550.	1.6	64
20	Modification on Ursodeoxycholic Acid (UDCA) Scaffold. Discovery of Bile Acid Derivatives As Selective Agonists of Cell-Surface G-Protein Coupled Bile Acid Receptor 1 (GP-BAR1). <i>Journal of Medicinal Chemistry</i> , 2014, 57, 7687-7701.	2.9	62
21	Design, Synthesis and Biological Evaluation of Carboxy Analogues of Arginine Methyltransferase Inhibitor...1 (AMI...1). <i>ChemMedChem</i> , 2010, 5, 398-414.	1.6	60
22	Molecular Modeling for Nanomaterial-Biology Interactions: Opportunities, Challenges, and Perspectives. <i>Frontiers in Bioengineering and Biotechnology</i> , 2019, 7, 268.	2.0	55
23	Novel <i>N</i> ² -Substituted Pyrazolo[3,4- <i>d</i>]pyrimidine Adenosine A ₃ Receptor Antagonists: Inhibition of A ₃ -Mediated Human Glioblastoma Cell Proliferation. <i>Journal of Medicinal Chemistry</i> , 2010, 53, 3954-3963.	2.9	50
24	Energetics and Structural Characterization of the large-scale Functional Motion of Adenylate Kinase. <i>Scientific Reports</i> , 2015, 5, 8425.	1.6	50
25	Binding Mechanism of the Farnesoid X Receptor Marine Antagonist Suvanine Reveals a Strategy To Forestall Drug Modulation on Nuclear Receptors. Design, Synthesis, and Biological Evaluation of Novel Ligands. <i>Journal of Medicinal Chemistry</i> , 2013, 56, 4701-4717.	2.9	49
26	Acetic Acid Aldose Reductase Inhibitors Bearing a Five-Membered Heterocyclic Core with Potent Topical Activity in a Visual Impairment Rat Model. <i>Journal of Medicinal Chemistry</i> , 2008, 51, 3182-3193.	2.9	47
27	The Molecular Mechanism Underlying Ligand Binding to the Membrane-Embedded Site of a G-Protein-Coupled Receptor. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2761-2770.	2.3	46
28	New Insight into the Central Benzodiazepine Receptor-Ligand Interactions: Design, Synthesis, Biological Evaluation, and Molecular Modeling of 3-Substituted 6-Phenyl-4- <i>H</i> -imidazo[1,5- <i>a</i>][1,4]benzodiazepines and Related Compounds. <i>Journal of Medicinal Chemistry</i> , 2011, 54, 5694-5711.	2.9	45
29	Funnel-Metadynamics and Solution NMR to Estimate Protein-Ligand Affinities. <i>Journal of the American Chemical Society</i> , 2015, 137, 1273-1281.	6.6	44
30	Accelerating the Calculation of Protein-Ligand Binding Free Energy and Residence Times Using Dynamically Optimized Collective Variables. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 743-750.	2.3	44
31	Ensemble-Docking Approach on BACE-1: Pharmacophore Perception and Guidelines for Drug Design. <i>ChemMedChem</i> , 2007, 2, 667-678.	1.6	43
32	Indolylarylsulfones Carrying a Heterocyclic Tail as Very Potent and Broad Spectrum HIV-1 Non-nucleoside Reverse Transcriptase Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 9945-9957.	2.9	42
33	Ligand Binding, Unbinding, and Allosteric Effects: Deciphering Small-Molecule Modulation of HSP90. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 6368-6381.	2.3	42
34	The Free Energy Landscape of GABA Binding to a Pentameric Ligand-Gated Ion Channel and Its Disruption by Mutations. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3398-3406.	2.3	41
35	Homology Modeling of NR2B Modulatory Domain of NMDA Receptor and Analysis of Ifenprodil Binding. <i>ChemMedChem</i> , 2007, 2, 1498-1510.	1.6	38
36	Ethyl 8-Fluoro-6-(3-nitrophenyl)-4- <i>H</i> -imidazo[1,5- <i>a</i>][1,4]benzodiazepine-3-carboxylate as Novel, Highly Potent, and Safe Antianxiety Agent. <i>Journal of Medicinal Chemistry</i> , 2008, 51, 4730-4743.	2.9	38

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37	Potent Arylsulfonamide Inhibitors of Tumor Necrosis Factor- α Converting Enzyme Able to Reduce Activated Leukocyte Cell Adhesion Molecule Shedding in Cancer Cell Models. <i>Journal of Medicinal Chemistry</i> , 2010, 53, 2622-2635.	2.9	37
38	Breaking the Dogma of the Metal-Coordinating Carboxylate Group in Integrin Ligands: Introducing Hydroxamic Acids to the MIDAS To Tune Potency and Selectivity. <i>Angewandte Chemie - International Edition</i> , 2009, 48, 4436-4440.	7.2	35
39	Bioinformatics and Biosimulations as Toolbox for Peptides and Peptidomimetics Design: Where Are We?. <i>Frontiers in Molecular Biosciences</i> , 2020, 7, 66.	1.6	34
40	Stop Fitan: Antispasmodic Effect of Natural Extract of Chestnut Wood in Guinea Pig Ileum and Proximal Colon Smooth Muscle. <i>Journal of Medicinal Food</i> , 2010, 13, 1104-1110.	0.8	33
41	Steroidal scaffolds as FXR and GPBAR1 ligands: from chemistry to therapeutical application. <i>Future Medicinal Chemistry</i> , 2015, 7, 1109-1135.	1.1	32
42	Hyodeoxycholic acid derivatives as liver X receptor α and G-protein-coupled bile acid receptor agonists. <i>Scientific Reports</i> , 2017, 7, 43290.	1.6	30
43	Investigation around the Oxadiazole Core in the Discovery of a New Chemotype of Potent and Selective FXR Antagonists. <i>ACS Medicinal Chemistry Letters</i> , 2019, 10, 504-510.	1.3	27
44	Novel Isoxazole Derivatives with Potent FXR Agonistic Activity Prevent Acetaminophen-Induced Liver Injury. <i>ACS Medicinal Chemistry Letters</i> , 2019, 10, 407-412.	1.3	27
45	Disruption of TGF β -SMAD3 pathway by the nuclear receptor SHP mediates the antifibrotic activities of BAR704, a novel highly selective FXR ligand. <i>Pharmacological Research</i> , 2018, 131, 17-31.	3.1	25
46	Perspectives on High-Throughput Ligand/Protein Docking With Martini MD Simulations. <i>Frontiers in Molecular Biosciences</i> , 2021, 8, 657222.	1.6	25
47	Membrane charge dependent states of the β -amyloid fragment A β (16-35) with differently charged micelle aggregates. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2010, 1798, 660-671.	1.4	24
48	Structure-based drug design targeting the cell membrane receptor GPBAR1: exploiting the bile acid scaffold towards selective agonism. <i>Scientific Reports</i> , 2015, 5, 16605.	1.6	23
49	Targeting Bile Acid Receptors: Discovery of a Potent and Selective Farnesoid X Receptor Agonist as a New Lead in the Pharmacological Approach to Liver Diseases. <i>Frontiers in Pharmacology</i> , 2017, 8, 162.	1.6	23
50	Discovery of Bile Acid Derivatives as Potent ACE2 Activators by Virtual Screening and Essential Dynamics. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 196-209.	2.5	15
51	Insights on pregnane-X-receptor modulation. Natural and semisynthetic steroids from <i>Theonella</i> marine sponges. <i>European Journal of Medicinal Chemistry</i> , 2014, 73, 126-134.	2.6	14
52	Incisterols, highly degraded marine sterols, are a new chemotype of PXR agonists. <i>Steroids</i> , 2014, 83, 80-85.	0.8	14
53	Marine and Semi-Synthetic Hydroxysteroids as New Scaffolds for Pregnane X Receptor Modulation. <i>Marine Drugs</i> , 2014, 12, 3091-3115.	2.2	13
54	The Glycan Role in the Glycopeptide Immunogenicity Revealed by Atomistic Simulations and Spectroscopic Experiments on the Multiple Sclerosis Biomarker CSF114(Glc). <i>Scientific Reports</i> , 2015, 5, 9200.	1.6	13

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55	Discovery of ((1,2,4-oxadiazol-5-yl)pyrrolidin-3-yl)ureidyl derivatives as selective non-steroidal agonists of the G-protein coupled bile acid receptor-1. <i>Scientific Reports</i> , 2019, 9, 2504.	1.6	13
56	Tailoring of Integrin Ligands: Probing the Charge Capability of the Metal Ion-Dependent Adhesion Site. <i>Journal of Medicinal Chemistry</i> , 2012, 55, 871-882.	2.9	12
57	Structural Insight into the Binding Mode of FXR and GPBAR1 Modulators. <i>Handbook of Experimental Pharmacology</i> , 2019, 256, 111-136.	0.9	8
58	GPBAR1 Activation by C6-Substituted Hyodeoxycholane Analogues Protect against Colitis. <i>ACS Medicinal Chemistry Letters</i> , 2020, 11, 818-824.	1.3	8
59	Improving Small-Molecule Force Field Parameters in Ligand Binding Studies. <i>Frontiers in Molecular Biosciences</i> , 2021, 8, 760283.	1.6	8
60	DDT - Drug Discovery Tool: a fast and intuitive graphics user interface for docking and molecular dynamics analysis. <i>Bioinformatics</i> , 2019, 35, 5328-5330.	1.8	7
61	Identification of cysteinyl-leukotriene-receptor 1 antagonists as ligands for the bile acid receptor GPBAR1. <i>Biochemical Pharmacology</i> , 2020, 177, 113987.	2.0	5
62	$\hat{\beta}$ -Glutamyl 16-diaminopropane derivative of vasoactive intestinal peptide: a potent anti-oxidative agent for human epidermoid cancer cells. <i>Amino Acids</i> , 2010, 39, 661-670.	1.2	4
63	Epoxide functionalization on cholane side chains in the identification of G-protein coupled bile acid receptor (GPBAR1) selective agonists. <i>RSC Advances</i> , 2017, 7, 32877-32885.	1.7	4
64	Drug Repurposing on G Protein-Coupled Receptors Using a Computational Profiling Approach. <i>Frontiers in Molecular Biosciences</i> , 2021, 8, 673053.	1.6	4
65	Discovery of a Potent and Orally Active Dual GPBAR1/CysLT1R Modulator for the Treatment of Metabolic Fatty Liver Disease. <i>Frontiers in Pharmacology</i> , 2022, 13, 858137.	1.6	4
66	Introduction of Nonacidic Side Chains on 6-Ethylcholane Scaffolds in the Identification of Potent Bile Acid Receptor Agonists with Improved Pharmacokinetic Properties. <i>Molecules</i> , 2019, 24, 1043.	1.7	3
67	Structural Basis for Developing Multitarget Compounds Acting on Cysteinyl Leukotriene Receptor 1 and G-Protein-Coupled Bile Acid Receptor 1. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 16512-16529.	2.9	3
68	Binding of the Anti-FIV Peptide C8 to Differently Charged Membrane Models: From First Docking to Membrane Tubulation. <i>Frontiers in Chemistry</i> , 2020, 8, 493.	1.8	2
69	Homo and Heterodimeric Structures of CCR5 and CXCR4: Molecular Dynamics Simulation as an Alternative to X-Ray Diffraction. <i>Biophysical Journal</i> , 2019, 116, 344a.	0.2	1
70	Cover Picture: Breaking the Dogma of the Metal-Coordinating Carboxylate Group in Integrin Ligands: Introducing Hydroxamic Acids to the MIDAS To Tune Potency and Selectivity (<i>Angew. Chem. Int. Ed.</i>) Tj ETQq0 0 0 ngB /Overlock 10 Tf		
71	Highly Enhanced Conformational Sampling of the Transmembrane Domain of Egf Receptor Sheds Light on the Activation Mechanism. <i>Biophysical Journal</i> , 2014, 106, 307a.	0.2	0