Vittorio Limongelli

List of Publications by Year
in descending order

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	Discovery of Bile Acid Derivatives as Potent ACE2 Activators by Virtual Screening and Essential Dynamics. Journal of Chemical Information and Modeling, 2022, 62, 196-209.	2.5	15
2	Discovery of a Potent and Orally Active Dual GPBAR1/CysLT1R Modulator for the Treatment of Metabolic Fatty Liver Disease. Frontiers in Pharmacology, 2022, 13, 858137.	1.6	4
3	Perspectives on High-Throughput Ligand/Protein Docking With Martini MD Simulations. Frontiers in Molecular Biosciences, 2021, 8, 657222.	1.6	25
4	Drug Repurposing on G Protein-Coupled Receptors Using a Computational Profiling Approach. Frontiers in Molecular Biosciences, 2021, 8, 673053.	1.6	4
5	Structural Basis for Developing Multitarget Compounds Acting on Cysteinyl Leukotriene Receptor 1 and G-Protein-Coupled Bile Acid Receptor 1. Journal of Medicinal Chemistry, 2021, 64, 16512-16529.	2.9	3
6	Improving Small-Molecule Force Field Parameters in Ligand Binding Studies. Frontiers in Molecular Biosciences, 2021, 8, 760283.	1.6	8
7	Ligand binding free energy and kinetics calculation in 2020. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1455.	6.2	86
8	Proteinâ€“ligand binding with the coarse-grained Martini model. Nature Communications, 2020, 11, 3714.	5.8	139
9	Ligand binding free-energy calculations with funnel metadynamics. Nature Protocols, 2020, 15, 2837-2866.	5.5	96
10	Identification of cysteinyl-leukotriene-receptor 1 antagonists as ligands for the bile acid receptor GPBAR1. Biochemical Pharmacology, 2020, 177, 113987.	2.0	5
11	GPBAR1 Activation by C6-Substituted Hyodeoxycholane Analogues Protect against Colitis. ACS Medicinal Chemistry Letters, 2020, 11, 818-824.	1.3	8
12	Binding of the Anti-FIV Peptide C8 to Differently Charged Membrane Models: From First Docking to Membrane Tubulation. Frontiers in Chemistry, 2020, 8, 493.	1.8	2
13	Bioinformatics and Biosimulations as Toolbox for Peptides and Peptidomimetics Design: Where Are We?. Frontiers in Molecular Biosciences, 2020, 7, 66.	1.6	34
14	Promoting transparency and reproducibility in enhanced molecular simulations. Nature Methods, 2019, 16, 670-673.	9.0	655
15	DDT - Drug Discovery Tool: a fast and intuitive graphics user interface for docking and molecular dynamics analysis. Bioinformatics, 2019, 35, 5328-5330.	1.8	7
16	Ligand Binding, Unbinding, and Allosteric Effects: Deciphering Small-Molecule Modulation of HSP90. Journal of Chemical Theory and Computation, 2019, 15, 6368-6381.	2.3	42
17	Structural Insight into the Binding Mode of FXR and GPBAR1 Modulators. Handbook of Experimental Pharmacology, 2019, 256, 111-136.	0.9	8
18	Introduction of Nonacidic Side Chains on 6-Ethylcholane Scaffolds in the Identification of Potent Bile Acid Receptor Agonists with Improved Pharmacokinetic Properties. Molecules, 2019, 24, 1043.	1.7	3

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19	Homo and Heterodimeric Structures of CCR5 and CXCR4: Molecular Dynamics Simulation as an Alternative to X-Ray Diffraction. Biophysical Journal, 2019, 116, 344a.	0.2	1
20	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. Scientific Reports, 2019, 9, 2504.	1.6	13
21	Molecular Modeling for Nanomaterialâ€"Biology Interactions: Opportunities, Challenges, and Perspectives. Frontiers in Bioengineering and Biotechnology, 2019, 7, 268.	2.0	55
22	Investigation around the Oxadiazole Core in the Discovery of a New Chemotype of Potent and Selective FXR Antagonists. ACS Medicinal Chemistry Letters, 2019, 10, 504-510.	1.3	27
23	Accelerating the Calculation of Proteinâ€"Ligand Binding Free Energy and Residence Times Using Dynamically Optimized Collective Variables. Journal of Chemical Theory and Computation, 2019, 15, 743-750.	2.3	44
24	Novel Isoxazole Derivatives with Potent FXR Agonistic Activity Prevent Acetaminophen-Induced Liver Injury. ACS Medicinal Chemistry Letters, 2019, 10, 407-412.	1.3	27
25	The Molecular Mechanism Underlying Ligand Binding to the Membrane-Embedded Site of a G-Protein-Coupled Receptor. Journal of Chemical Theory and Computation, 2018, 14, 2761-2770.	2.3	46
26	Disruption of TFGÎ²-SMAD3 pathway by the nuclear receptor SHP mediates the antifibrotic activities of BAR704, a novel highly selective FXR ligand. Pharmacological Research, 2018, 131, 17-31.	3.1	25
27	Ligand binding to telomeric G-quadruplex DNA investigated by funnel-metadynamics simulations. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E2136-E2145.	3.3	91
28	Hyodeoxycholic acid derivatives as liver X receptor Î± and G-protein-coupled bile acid receptor agonists. Scientific Reports, 2017, 7, 43290.	1.6	30
29	Unbinding Kinetics of a p38 MAP Kinase Type II Inhibitor from Metadynamics Simulations. Journal of the American Chemical Society, 2017, 139, 4780-4788.	6.6	187
30	Epoxide functionalization on cholane side chains in the identification of G-protein coupled bile acid receptor (GPBAR1) selective agonists. RSC Advances, 2017, 7, 32877-32885.	1.7	4
31	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. Frontiers in Pharmacology, 2017, 8, 162.	1.6	23
32	Conformational Changes in the Epidermal Growth Factor Receptor: Role of the Transmembrane Domain Investigated by Coarse-Grained MetaDynamics Free Energy Calculations. Journal of the American Chemical Society, 2016, 138, 10611-10622.	6.6	103
33	The Free Energy Landscape of GABA Binding to a Pentameric Ligand-Gated Ion Channel and Its Disruption by Mutations. Journal of Chemical Theory and Computation, 2016, 12, 3398-3406.	2.3	41
34	Structure-based drug design targeting the cell membrane receptor GPBAR1: exploiting the bile acid scaffold towards selective agonism. Scientific Reports, 2015, 5, 16605.	1.6	23
35	Energetics and Structural Characterization of the large-scale Functional Motion of Adenylate Kinase. Scientific Reports, 2015, 5, 8425.	1.6	50
36	Kinetics of proteinâ€"ligand unbinding: Predicting pathways, rates, and rate-limiting steps. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E386-91.	3.3	311

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37	Funnel-Metadynamics and Solution NMR to Estimate Proteinâ€“Ligand Affinities. Journal of the American Chemical Society, 2015, 137, 1273-1281.	6.6	44
38	The Glycan Role in the Glycopeptide Immunogenicity Revealed by Atomistic Simulations and Spectroscopic Experiments on the Multiple Sclerosis Biomarker CSF114(Glc). Scientific Reports, 2015, 5, 9200.	1.6	13
39	Steroidal scaffolds as FXR and GPBAR1 ligands: from chemistry to therapeutical application. Future Medicinal Chemistry, 2015, 7, 1109-1135.	1.1	32
40	G-triplex structure and formation propensity. Nucleic Acids Research, 2014, 42, 13393-13404.	6.5	71
41	Mechanistic insight into ligand binding to G-quadruplex DNA. Nucleic Acids Research, 2014, 42, 5447-5455.	6.5	79
42	Indolylarylsulfones Carrying a Heterocyclic Tail as Very Potent and Broad Spectrum HIV-1 Non-nucleoside Reverse Transcriptase Inhibitors. Journal of Medicinal Chemistry, 2014, 57, 9945-9957.	2.9	42
43	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). Journal of Medicinal Chemistry, 2014, 57, 7687-7701.	2.9	62
44	Design, Synthesis, and Biological Evaluation of Potent Dual Agonists of Nuclear and Membrane Bile Acid Receptors. Journal of Medicinal Chemistry, 2014, 57, 937-954.	2.9	79
45	Highly Enhanced Conformational Sampling of the Transmembrane Domain of Egf Receptor Sheds Light on the Activation Mechanism. Biophysical Journal, 2014, 106, 307a.	0.2	0
46	Insights on pregnane-X-receptor modulation. Natural and semisynthetic steroids from Theonella marine sponges. European Journal of Medicinal Chemistry, 2014, 73, 126-134.	2.6	14
47	Incisterols, highly degraded marine sterols, are a new chemotype of PXR agonists. Steroids, 2014, 83, 80-85.	0.8	14
48	Marine and Semi-Synthetic Hydroxysteroids as New Scaffolds for Pregnane X Receptor Modulation. Marine Drugs, 2014, 12, 3091-3115.	2.2	13
49	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. Journal of Medicinal Chemistry, 2013, 56, 4701-4717.	2.9	49
50	Funnel metadynamics as accurate binding free-energy method. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 6358-6363.	3.3	337
51	The Gâ€Triplex DNA. Angewandte Chemie - International Edition, 2013, 52, 2269-2273.	7.2	133
52	Sampling protein motion and solvent effect during ligand binding. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 1467-1472.	3.3	100
53	Investigating the Mechanism of Substrate Uptake and Release in the Glutamate Transporter Homologue Glt_{Ph} through Metadynamics Simulations. Journal of the American Chemical Society, 2012, 134, 453-463.	6.6	66
54	Tailoring of Integrin Ligands: Probing the Charge Capability of the Metal Ion-Dependent Adhesion Site. Journal of Medicinal Chemistry, 2012, 55, 871-882.	2.9	12

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55	New Insight into the Central Benzodiazepine Receptorâ€“Ligand Interactions: Design, Synthesis, Biological Evaluation, and Molecular Modeling of 3-Substituted 6-Phenyl-4H-imidazo[1,5-a][1,4]benzodiazepines and Related Compounds. Journal of Medicinal Chemistry, 2011, 54, 5694-5711.	2.9	45
56	Î³-Glutamyl 16-diaminopropane derivative of vasoactive intestinal peptide: a potent anti-oxidative agent for human epidermoid cancer cells. Amino Acids, 2010, 39, 661-670.	1.2	4
57	Design, Synthesis and Biological Evaluation of Carboxy Analogues of Arginine Methyltransferase Inhibitorâ€…1 (AMIâ€‑1). ChemMedChem, 2010, 5, 398-414.	1.6	60
58	Molecular basis of cyclooxygenase enzymes (COXs) selective inhibition. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 5411-5416.	3.3	187
59	Stop Fitan: Antispasmodic Effect of Natural Extract of Chestnut Wood in Guinea Pig Ileum and Proximal Colon Smooth Muscle. Journal of Medicinal Food, 2010, 13, 1104-1110.	0.8	33
60	Potent Arylsulfonamide Inhibitors of Tumor Necrosis Factor-Î± Converting Enzyme Able to Reduce Activated Leukocyte Cell Adhesion Molecule Shedding in Cancer Cell Models. Journal of Medicinal Chemistry, 2010, 53, 2622-2635.	2.9	37
61	NovelN²-Substituted Pyrazolo[3,4-d]pyrimidine Adenosine A₃Receptor Antagonists: Inhibition of A₃-Mediated Human Glioblastoma Cell Proliferation^{â€}. Journal of Medicinal Chemistry, 2010, 53, 3954-3963.	2.9	50
62	Structural and Conformational Requisites in DNA Quadruplex Groove Binding: Another Piece to the Puzzle. Journal of the American Chemical Society, 2010, 132, 6425-6433.	6.6	111
63	Membrane charge dependent states of the Î²-amyloid fragment AÎ² (16â€“35) with differently charged micelle aggregates. Biochimica Et Biophysica Acta - Biomembranes, 2010, 1798, 660-671.	1.4	24
64	Breaking the Dogma of the Metalâ€Coordinating Carboxylate Group in Integrin Ligands: Introducing Hydroxamic Acids to the MIDAS To Tune Potency and Selectivity. Angewandte Chemie - International Edition, 2009, 48, 4436-4440.	7.2	35
65	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 (Angew. Chem. Int. Ed.) Tj ETQq1 1 0.784314 rgBT /Over	7.2	0
66	Acetic Acid Aldose Reductase Inhibitors Bearing a Five-Membered Heterocyclic Core with Potent Topical Activity in a Visual Impairment Rat Model. Journal of Medicinal Chemistry, 2008, 51, 3182-3193.	2.9	47
67	Design, Synthesis, and Biological Evaluation of Novel Aminobisphosphonates Possessing an in Vivo Antitumor Activity Through a Î³Î´-T Lymphocytes-Mediated Activation Mechanism. Journal of Medicinal Chemistry, 2008, 51, 6800-6807.	2.9	70
68	Ethyl 8-Fluoro-6-(3-nitrophenyl)-4H-imidazo[1,5-a][1,4]benzodiazepine-3-carboxylate as Novel, Highly Potent, and Safe Antianxiety Agent. Journal of Medicinal Chemistry, 2008, 51, 4730-4743.	2.9	38
69	Ensemble-Docking Approach on BACE-1: Pharmacophore Perception and Guidelines for Drug Design. ChemMedChem, 2007, 2, 667-678.	1.6	43
70	Homology Modeling of NR2B Modulatory Domain of NMDA Receptor and Analysis of Ifenprodil Binding. ChemMedChem, 2007, 2, 1498-1510.	1.6	38
71	Modeling of Cdc25B Dual Specifity Protein Phosphatase Inhibitors: Docking of Ligands and Enzymatic Inhibition Mechanism. ChemMedChem, 2006, 1, 540-550.	1.6	64