Alessio Lodola

List of Publications by Citations

115 papers	3,078 citations	33 h-index	50 g-index
134 ext. papers	3,536 ext. citations	5.6 avg, IF	4.85 L-index

#	Paper	IF	Citations
115	Cyclohexylcarbamic acid 3S or 4Ssubstituted biphenyl-3-yl esters as fatty acid amide hydrolase inhibitors: synthesis, quantitative structure-activity relationships, and molecular modeling studies. *Journal of Medicinal Chemistry*, **2004**, 47, 4998-5008	8.3	239
114	Selective N-acylethanolamine-hydrolyzing acid amidase inhibition reveals a key role for endogenous palmitoylethanolamide in inflammation. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 20966-71	11.5	179
113	A catalytically silent FAAH-1 variant drives anandamide transport in neurons. *Nature Neuroscience*, **2011**, 15, 64-9	25.5	134
112	Discovery of potent and reversible monoacylglycerol lipase inhibitors. *Chemistry and Biology*, **2009**, 16, 1045-52		80
111	N-(substituted-anilinoethyl)amides: design, synthesis, and pharmacological characterization of a new class of melatonin receptor ligands. *Journal of Medicinal Chemistry*, **2007**, 50, 6618-26	8.3	70
110	Conformational effects in enzyme catalysis: reaction via a high energy conformation in fatty acid amide hydrolase. *Biophysical Journal*, **2007**, 92, L20-2	2.9	69
109	A critical cysteine residue in monoacylglycerol lipase is targeted by a new class of isothiazolinone-based enzyme inhibitors. *British Journal of Pharmacology*, **2009**, 157, 974-83	8.6	65
108	5-benzylidene-hydantoins as new EGFR inhibitors with antiproliferative activity. *Bioorganic and Medicinal Chemistry Letters*, **2006**, 16, 4021-5	2.9	64
107	Synthesis and quantitative structure-activity relationship of fatty acid amide hydrolase inhibitors: modulation at the N-portion of biphenyl-3-yl alkylcarbamates. *Journal of Medicinal Chemistry*, **2008**, 51, 3487-98	8.3	59
106	QM/MM modelling of oleamide hydrolysis in fatty acid amide hydrolase (FAAH) reveals a new mechanism of nucleophile activation. *Chemical Communications*, **2005**, 4399-401	5.8	59
105	Identification of productive inhibitor binding orientation in fatty acid amide hydrolase (FAAH) by QM/MM mechanistic modelling. *Chemical Communications*, **2008**, 214-6	5.8	58
104	Lithocholic acid is an Eph-ephrin ligand interfering with Eph-kinase activation. *PLoS ONE*, **2011**, 6, e18128	3.7	55
103	Dual mechanisms of action of the 5-benzylidene-hydantoin UPR1024 on lung cancer cell lines. *Molecular Cancer Therapeutics*, **2008**, 7, 361-70	6.1	55
102	A catalytic mechanism for cysteine N-terminal nucleophile hydrolases, as revealed by free energy simulations. *PLoS ONE*, **2012**, 7, e32397	3.7	55
101	Structural Fluctuations in Enzyme-Catalyzed Reactions: Determinants of Reactivity in Fatty Acid Amide Hydrolase from Multivariate Statistical Analysis of Quantum Mechanics/Molecular Mechanics Paths. *Journal of Chemical Theory and Computation*, **2010**, 6, 2948-60	6.4	53
100	Synthesis and structure-activity relationships of FAAH inhibitors: cyclohexylcarbamic acid biphenyl esters with chemical modulation at the proximal phenyl ring. *ChemMedChem*, **2006**, 1, 130-9	3.7	53
99	L718Q mutant EGFR escapes covalent inhibition by stabilizing a non-reactive conformation of the lung cancer drug osimertinib. *Chemical Science*, **2018**, 9, 2740-2749	9.4	51

98	Predicting the reactivity of nitrile-carrying compounds with cysteine: a combined computational and experimental study. *ACS Medicinal Chemistry Letters*, **2014**, 5, 501-5	4.3	50
97	Mechanism of inhibition of SARS-CoV-2 M by peptidyl Michael acceptor explained by QM/MM simulations and design of new derivatives with tunable chemical reactivity. *Chemical Science*, **2020**, 12, 1433-1444	9.4	50
96	Synthesis and structure-activity relationships of N-(2-oxo-3-oxetanyl)amides as N-acylethanolamine-hydrolyzing acid amidase inhibitors. *Journal of Medicinal Chemistry*, **2010**, 53, 5770-81	8.3	49
95	Irreversible inhibition of epidermal growth factor receptor activity by 3-aminopropanamides. *Journal of Medicinal Chemistry*, **2012**, 55, 2251-64	8.3	48
94	Targeting Eph/ephrin system in cancer therapy. *European Journal of Medicinal Chemistry*, **2017**, 142, 152-162	6.8	47
93	N-(2-oxo-3-oxetanyl)carbamic acid esters as N-acylethanolamine acid amidase inhibitors: synthesis and structure-activity and structure-property relationships. *Journal of Medicinal Chemistry*, **2012**, 55, 4824-36	8.3	44
92	Novel irreversible epidermal growth factor receptor inhibitors by chemical modulation of the cysteine-trap portion. *Journal of Medicinal Chemistry*, **2010**, 53, 2038-50	8.3	44
91	Fatty acid amide hydrolase inhibitors: a patent review (2009-2014). *Expert Opinion on Therapeutic Patents*, **2015**, 25, 1247-66	6.8	42
90	Amino acid conjugates of lithocholic acid as antagonists of the EphA2 receptor. *Journal of Medicinal Chemistry*, **2013**, 56, 2936-47	8.3	40
89	The increasing role of QM/MM in drug discovery. *Advances in Protein Chemistry and Structural Biology*, **2012**, 87, 337-62	5.3	39
88	Metadynamics Simulations Distinguish Short- and Long-Residence-Time Inhibitors of Cyclin-Dependent Kinase 8. *Journal of Chemical Information and Modeling*, **2017**, 57, 159-169	6.1	37
87	Epidermal growth factor receptor irreversible inhibitors: chemical exploration of the cysteine-trap portion. *Mini-Reviews in Medicinal Chemistry*, **2011**, 11, 1019-30	3.2	36
86	5-Benzylidene-hydantoins: synthesis and antiproliferative activity on A549 lung cancer cell line. *European Journal of Medicinal Chemistry*, **2009**, 44, 3471-9	6.8	34
85	Insights into the mechanism and inhibition of fatty acid amide hydrolase from quantum mechanics/molecular mechanics (QM/MM) modelling. *Biochemical Society Transactions*, **2009**, 37, 363-7	5.1	34
84	Quantum mechanics/molecular mechanics modeling of covalent addition between EGFR-cysteine 797 and N-(4-anilinoquinazolin-6-yl) acrylamide. *Journal of Chemical Information and Modeling*, **2015** , 55, 589-99	6.1	33
83	Therapeutic perspectives of Eph-ephrin system modulation. *Drug Discovery Today*, **2014**, 19, 661-9	8.8	33
82	Covalent inhibitors of fatty acid amide hydrolase: a rationale for the activity of piperidine and piperazine aryl ureas. *Journal of Medicinal Chemistry*, **2011**, 54, 6612-23	8.3	33
81	Structure-property relationships of a class of carbamate-based fatty acid amide hydrolase (FAAH) inhibitors: chemical and biological stability. *ChemMedChem*, **2009**, 4, 1495-504	3.7	32

80	Highly Potent and Selective MT2 Melatonin Receptor Full Agonists from Conformational Analysis of 1-Benzyl-2-acylaminomethyl-tetrahydroquinolines. *Journal of Medicinal Chemistry*, **2015**, 58, 7512-25	8.3	31
79	-Acylethanolamine Acid Amidase (NAAA): Structure, Function, and Inhibition. *Journal of Medicinal Chemistry*, **2020**, 63, 7475-7490	8.3	31
78	UniPR129 is a competitive small molecule Eph-ephrin antagonist blocking in vitro angiogenesis at low micromolar concentrations. *British Journal of Pharmacology*, **2014**, 171, 5195-208	8.6	31
77	Structure-based virtual screening of MT2 melatonin receptor: influence of template choice and structural refinement. *Journal of Chemical Information and Modeling*, **2013**, 53, 821-35	6.1	28
76	Quantum mechanics/molecular mechanics modeling of fatty acid amide hydrolase reactivation distinguishes substrate from irreversible covalent inhibitors. *Journal of Medicinal Chemistry*, **2013**, 56, 2500-12	8.3	28
75	Structure-activity relationships and mechanism of action of Eph-ephrin antagonists: interaction of cholanic acid with the EphA2 receptor. *ChemMedChem*, **2012**, 7, 1071-83	3.7	28
74	Homology models of melatonin receptors: challenges and recent advances. *International Journal of Molecular Sciences*, **2013**, 14, 8093-121	6.3	27
73	[5)-Cholenoyl-amino acids as selective and orally available antagonists of the Eph-ephrin system. *European Journal of Medicinal Chemistry*, **2015**, 103, 312-24	6.8	26
72	The ellagitannin colonic metabolite urolithin D selectively inhibits EphA2 phosphorylation in prostate cancer cells. *Molecular Nutrition and Food Research*, **2015**, 59, 2155-67	5.9	26
71	Catalytic, asymmetric hypervinylogous Mukaiyama aldol reactions of extended furan-based silyl enolates. *Organic Letters*, **2011**, 13, 4738-41	6.2	26
70	Getting it right: modeling of pH, solvent and "nearly" everything else in virtual screening of biological targets. *Journal of Molecular Graphics and Modelling*, **2004**, 22, 479-86	2.8	25
69	N-tert-butyloxycarbonyl-Phe-Leu-Phe-Leu-Phe (BOC2) inhibits the angiogenic activity of heparin-binding growth factors. *Angiogenesis*, **2018**, 21, 47-59	10.6	24
68	Design and synthesis of N-(3,3-diphenylpropenyl)alkanamides as a novel class of high-affinity MT2-selective melatonin receptor ligands. *Journal of Medicinal Chemistry*, **2006**, 49, 7393-403	8.3	24
67	Expanding the Arsenal of FGFR Inhibitors: A Novel Chloroacetamide Derivative as a New Irreversible Agent With Anti-proliferative Activity Against FGFR1-Amplified Lung Cancer Cell Lines. *Frontiers in Oncology*, **2019**, 9, 179	5.3	23
66	Metadynamics for Perspective Drug Design: Computationally Driven Synthesis of New Protein-Protein Interaction Inhibitors Targeting the EphA2 Receptor. *Journal of Medicinal Chemistry* , **2017**, 60, 787-796	8.3	21
65	Conformational effects on the pro-S hydrogen abstraction reaction in cyclooxygenase-1: an integrated QM/MM and MD study. *Biophysical Journal*, **2013**, 104, L5-7	2.9	21
64	MT1-selective melatonin receptor ligands: synthesis, pharmacological evaluation, and molecular dynamics investigation of N-{[(3-O-substituted)anilino]alkyl}amides. *ChemMedChem*, **2012**, 7, 1954-64	3.7	21
63	Understanding the role of carbamate reactivity in fatty acid amide hydrolase inhibition by QM/MM mechanistic modelling. *Chemical Communications*, **2011**, 47, 2517-9	5.8	21

62	Amino Acid Derivatives as Palmitoylethanolamide Prodrugs: Synthesis, In Vitro Metabolism and In Vivo Plasma Profile in Rats. *PLoS ONE*, **2015**, 10, e0128699	3.7	20
61	Mechanistic Insights into the Reaction of Chlorination of Tryptophan Catalyzed by Tryptophan 7-Halogenase. *Scientific Reports*, **2017**, 7, 17395	4.9	19
60	Synthesis, pharmacological evaluation, and structure-activity relationships of benzopyran derivatives with potent SERM activity. *Bioorganic and Medicinal Chemistry*, **2004**, 12, 3763-82	3.4	18
59	Pushing the boundaries of vinylogous reactivity: catalytic enantioselective mukaiyama aldol reactions of highly unsaturated 2-silyloxyindoles. *Chemistry - A European Journal*, **2015**, 21, 6433-42	4.8	17
58	Target hopping as a useful tool for the identification of novel EphA2 protein-protein antagonists. *ChemMedChem*, **2014**, 9, 67-72	3.7	17
57	Application of a SCC-DFTB QM/MM approach to the investigation of the catalytic mechanism of fatty acid amide hydrolase. *Journal of Molecular Modeling*, **2011**, 17, 2375-83	2	17
56	Biphenyl-3-yl alkylcarbamates as fatty acid amide hydrolase (FAAH) inhibitors: steric effects of N-alkyl chain on rat plasma and liver stability. *European Journal of Medicinal Chemistry*, **2011**, 46, 4466-73	6.8	16
55	UniPR1331, a small molecule targeting Eph/ephrin interaction, prolongs survival in glioblastoma and potentiates the effect of antiangiogenic therapy in mice. *Oncotarget*, **2018**, 9, 24347-24363	3.3	16
54	Are we using the right pharmacological tools to target EphA4?. *ACS Chemical Neuroscience*, **2014**, 5, 1146-7	5.7	14
53	Pharmacological evaluation of new bioavailable small molecules targeting Eph/ephrin interaction. *Biochemical Pharmacology*, **2018**, 147, 21-29	6	14
52	Discovery of SARS-CoV-2 M peptide inhibitors from modelling substrate and ligand binding. *Chemical Science*, **2021**, 12, 13686-13703	9.4	14
51	Synthesis and structure-activity relationships of amino acid conjugates of cholanic acid as antagonists of the EphA2 receptor. *Molecules*, **2013**, 18, 13043-60	4.8	12
50	MT2 selective melatonin receptor antagonists: design and structure-activity relationships. *Arkivoc*, **2006**, 2006, 8-16	0.9	12
49	Exploiting Free-Energy Minima to Design Novel EphA2 Protein-Protein Antagonists: From Simulation to Experiment and Return. *Chemistry - A European Journal*, **2016**, 22, 8048-52	4.8	12
48	Tetrahydroquinoline Ring as a Versatile Bioisostere of Tetralin for Melatonin Receptor Ligands. *Journal of Medicinal Chemistry*, **2018**, 61, 3726-3737	8.3	11
47	Combining ligand- and structure-based approaches for the discovery of new inhibitors of the EPHA2-ephrin-A1 interaction. *Journal of Chemical Information and Modeling*, **2014**, 54, 2621-6	6.1	11
46	Computational enzymology. *Methods in Molecular Biology*, **2013**, 924, 67-89	1.4	11
45	Synthesis, enantiomeric resolution, and structure-activity relationship study of a series of 10,11-dihydro-5H-dibenzo[a,d]cycloheptene MT2 receptor antagonists. *ChemMedChem*, **2007**, 2, 1741-9	3.7	11

44	Combined inhibition of the EGFR/AKT pathways by a novel conjugate of quinazoline with isothiocyanate. *European Journal of Medicinal Chemistry*, **2016**, 117, 283-91	6.8	11
43	Atropisomerism and Conformational Equilibria: Impact on PI3K□Inhibition of 2-((6-Amino-9H-purin-9-yl)methyl)-5-methyl-3-(o-tolyl)quinazolin-4(3H)-one (IC87114) and Its Conformationally Restricted Analogs. *Journal of Medicinal Chemistry*, **2017**, 60, 4304-4315	8.3	10
42	Identification of Bivalent Ligands with Melatonin Receptor Agonist and Fatty Acid Amide Hydrolase (FAAH) Inhibitory Activity That Exhibit Ocular Hypotensive Effect in the Rabbit. *Journal of Medicinal Chemistry*, **2018**, 61, 7902-7916	8.3	10
41	Dibasic biphenyl H3 receptor antagonists: Steric tolerance for a lipophilic side chain. *European Journal of Medicinal Chemistry*, **2012**, 48, 214-30	6.8	10
40	Nonempirical energetic analysis of reactivity and covalent inhibition of fatty acid amide hydrolase. *Journal of Physical Chemistry B*, **2013**, 117, 6656-66	3.4	10
39	Application of computational methods to the design of fatty acid amide hydrolase (FAAH) inhibitors based on a carbamic template structure. *Advances in Protein Chemistry and Structural Biology*, **2011**, 85, 1-26	5.3	10
38	Targeting the Eph-ephrin System with Protein-Protein Interaction (PPI) Inhibitors. *Current Drug Targets*, **2015**, 16, 1048-56	3	9
37	Physical Nature of Fatty Acid Amide Hydrolase Interactions with Its Inhibitors: Testing a Simple Nonempirical Scoring Model. *Journal of Physical Chemistry B*, **2014**, 118, 14727-36	3.4	8
36	Correlation between energetics of collisionally activated decompositions, interaction energy and biological potency of carbamate FAAH inhibitors. *Journal of Mass Spectrometry*, **2007**, 42, 1624-7	2.2	8
35	Application of 3D-QSAR in the rational design of receptor ligands and enzyme inhibitors. *Chemistry and Biodiversity*, **2005**, 2, 1438-51	2.5	8
34	N-Acylethanolamine Acid Amidase (NAAA): Mechanism of Palmitoylethanolamide Hydrolysis Revealed by Mechanistic Simulations. *ACS Catalysis*, **2020**, 10, 11797-11813	13.1	8
33	Balancing reactivity and antitumor activity: heteroarylthioacetamide derivatives as potent and time-dependent inhibitors of EGFR. *European Journal of Medicinal Chemistry*, **2019**, 162, 507-524	6.8	8
32	Fibroblast growth factor receptor inhibitors: patent review (2015-2019). *Expert Opinion on Therapeutic Patents*, **2019**, 29, 965-977	6.8	7
31	Applications and Advances of QM/MM Methods in Computational Enzymology. *Annual Reports in Computational Chemistry*, **2008**, 155-169	1.8	7
30	Relationship between chiroptical properties, structural changes and interactions in enzymes: a computational study on beta-lactamases from class A. *Computational Biology and Chemistry*, **2008**, 32, 167-75	3.6	7
29	Inhibition of Eph/ephrin interaction with the small molecule UniPR500 improves glucose tolerance in healthy and insulin-resistant mice. *Pharmacological Research*, **2019**, 141, 319-330	10.2	7
28	Design and SAR Analysis of Covalent Inhibitors Driven by Hybrid QM/MM Simulations. *Methods in Molecular Biology*, **2020**, 2114, 307-337	1.4	7
27	Free-energy studies reveal a possible mechanism for oxidation-dependent inhibition of MGL. *Scientific Reports*, **2016**, 6, 31046	4.9	6

26	Targeting the Eph/Ephrin System as Anti-Inflammatory Strategy in IBD. *Frontiers in Pharmacology*, **2019**, 10, 691	5.6	6
25	Synthesis and characterization of new bivalent agents as melatonin- and histamine H3-ligands. *International Journal of Molecular Sciences*, **2014**, 15, 16114-33	6.3	6
24	Aromatic interactions and rotational strengths within protein environment: An electronic structural study on β-lactamases from class A. *Chemical Physics Letters*, **2008**, 456, 89-95	2.5	6
23	Combined Quantum Mechanics and Molecular Mechanics Studies of Enzymatic Reaction Mechanisms. *Advances in Protein Chemistry and Structural Biology*, **2018**, 113, 1-32	5.3	5
22	Pharmacological tools in endocannabinoid neurobiology. *Current Topics in Behavioral Neurosciences*, **2009**, 1, 87-110	3.4	5
21	Biochemical characterization of EphA2 antagonists with improved physico-chemical properties by cell-based assays and surface plasmon resonance analysis. *Biochemical Pharmacology*, **2016**, 99, 18-30	6	4
20	Comparative Analysis of Virtual Screening Approaches in the Search for Novel EphA2 Receptor Antagonists. *Molecules*, **2015**, 20, 17132-51	4.8	4
19	On the use of 2,5-dimethyl-pyrrol-1-yl-benzoic acid derivatives as EPH-ephrin antagonists. *Journal of Virology*, **2014**, 88, 12173	6.6	4
18	New classes of potent heparanase inhibitors from ligand-based virtual screening. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2020**, 35, 1685-1696	5.6	4
17	A sulfonyl fluoride derivative inhibits EGFR by covalent modification of the catalytic lysine. *European Journal of Medicinal Chemistry*, **2021**, 225, 113786	6.8	4
16	Ephrin or not? Six tough questions on Eph targeting. *Expert Opinion on Therapeutic Targets*, **2020**, 24, 403-415	6.4	3
15	Insights in the mechanism of action and inhibition of N-acylethanolamine acid amidase by means of computational methods. *Advances in Protein Chemistry and Structural Biology*, **2014**, 96, 219-34	5.3	3
14	Benzisothiazolinone Derivatives as Potent Allosteric Monoacylglycerol Lipase Inhibitors That Functionally Mimic Sulfenylation of Regulatory Cysteines. *Journal of Medicinal Chemistry*, **2020**, 63, 1261-1280	8.3	3
13	Theoretical Model of EphA2-Ephrin A1 Inhibition. *Molecules*, **2018**, 23,	4.8	3
12	Free-Energy Simulations Support a Lipophilic Binding Route for Melatonin Receptors.. *Journal of Chemical Information and Modeling*, **2021**,	6.1	3
11	Optimization of EphA2 antagonists based on a lithocholic acid core led to the identification of UniPR505, a new 3-carbamoyloxy derivative with antiangiogenetic properties. *European Journal of Medicinal Chemistry*, **2020**, 189, 112083	6.8	2
10	Long-lasting inhibition of EGFR autophosphorylation in A549 tumor cells by intracellular accumulation of non-covalent inhibitors. *Bioorganic and Medicinal Chemistry Letters*, **2013**, 23, 5290-4	2.9	2
9	Drug-gut microbiota metabolic interactions: the case of UniPR1331, selective antagonist of the Eph-ephrin system, in mice. *Journal of Pharmaceutical and Biomedical Analysis*, **2020**, 180, 113067	3.5	2

8	Analysis of ADAM12-Mediated Ephrin-A1 Cleavage and Its Biological Functions. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	2
7	Targeting glioblastoma with UniPR1331, a new and stable bioavailable small molecule inhibiting Eph□ephrin interaction: In vitro and in vivo evidence. *European Journal of Cancer*, **2016**, 69, S30-S31	7.5	2
6	Impact of Warhead Modulations on the Covalent Inhibition of SARS-CoV-2 M Explored by QM/MM Simulations.. *ACS Catalysis*, **2022**, 12, 698-708	13.1	2
5	Discovery of SARS-CoV-2 Mpro Peptide Inhibitors from Modelling Substrate and Ligand Binding		1
4	In silico drug discovery of melatonin receptor ligands with therapeutic potential.. *Expert Opinion on Drug Discovery*, **2022**, 1-12	6.2	1
3	Different roles for the acyl chain and the amine leaving group in the substrate selectivity of -Acylethanolamine acid amidase. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2021**, 36, 1411-1423	5.6	0
2	Phenotype Screening of an Azole-bisindole Chemical Library Identifies URB1483 as a New Antileishmanial Agent Devoid of Toxicity on Human Cells.. *ACS Omega*, **2021**, 6, 35699-35710	3.9	0
1	VGF-Derived Peptide TLQP-21 **2014**, 49		