

Alessio Lodola

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	In silico drug discovery of melatonin receptor ligands with therapeutic potential.. <i>Expert Opinion on Drug Discovery</i> , 2022 , 1-12	6.2	1
114	Impact of Warhead Modulations on the Covalent Inhibition of SARS-CoV-2 M Explored by QM/MM Simulations.. <i>ACS Catalysis</i> , 2022 , 12, 698-708	13.1	2
113	Analysis of ADAM12-Mediated Ephrin-A1 Cleavage and Its Biological Functions. <i>International Journal of Molecular Sciences</i> , 2021 , 22,	6.3	2
112	Different roles for the acyl chain and the amine leaving group in the substrate selectivity of -Acylethanolamine acid amidase. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2021 , 36, 1411-1423	5.6	0
111	A sulfonyl fluoride derivative inhibits EGFR by covalent modification of the catalytic lysine. <i>European Journal of Medicinal Chemistry</i> , 2021 , 225, 113786	6.8	4
110	Discovery of SARS-CoV-2 M peptide inhibitors from modelling substrate and ligand binding. <i>Chemical Science</i> , 2021 , 12, 13686-13703	9.4	14
109	Free-Energy Simulations Support a Lipophilic Binding Route for Melatonin Receptors.. <i>Journal of Chemical Information and Modeling</i> , 2021 ,	6.1	3
108	Phenotype Screening of an Azole-bisindole Chemical Library Identifies URB1483 as a New Antileishmanial Agent Devoid of Toxicity on Human Cells.. <i>ACS Omega</i> , 2021 , 6, 35699-35710	3.9	0
107	-Acylethanolamine Acid Amidase (NAAA): Structure, Function, and Inhibition. <i>Journal of Medicinal Chemistry</i> , 2020 , 63, 7475-7490	8.3	31
106	Ephrin or not? Six tough questions on Eph targeting. <i>Expert Opinion on Therapeutic Targets</i> , 2020 , 24, 403-415	6.4	3
105	Optimization of EphA2 antagonists based on a lithocholic acid core led to the identification of UniPR505, a new 3 β -carbamoyloxy derivative with antiangiogenetic properties. <i>European Journal of Medicinal Chemistry</i> , 2020 , 189, 112083	6.8	2
104	Benzisothiazolinone Derivatives as Potent Allosteric Monoacylglycerol Lipase Inhibitors That Functionally Mimic Sulfenylation of Regulatory Cysteines. <i>Journal of Medicinal Chemistry</i> , 2020 , 63, 1261-1280	8.3	3
103	Drug-gut microbiota metabolic interactions: the case of UniPR1331, selective antagonist of the Eph-ephrin system, in mice. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2020 , 180, 113067	3.5	2
102	N-Acylethanolamine Acid Amidase (NAAA): Mechanism of Palmitoylethanolamide Hydrolysis Revealed by Mechanistic Simulations. <i>ACS Catalysis</i> , 2020 , 10, 11797-11813	13.1	8
101	New classes of potent heparanase inhibitors from ligand-based virtual screening. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2020 , 35, 1685-1696	5.6	4
100	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. <i>Chemical Science</i> , 2020 , 12, 1433-1444	9.4	50
99	Design and SAR Analysis of Covalent Inhibitors Driven by Hybrid QM/MM Simulations. <i>Methods in Molecular Biology</i> , 2020 , 2114, 307-337	1.4	7

98	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. <i>Frontiers in Oncology</i> , 2019 , 9, 179	5.3	23
97	Targeting the Eph/Ephrin System as Anti-Inflammatory Strategy in IBD. <i>Frontiers in Pharmacology</i> , 2019 , 10, 691	5.6	6
96	Fibroblast growth factor receptor inhibitors: patent review (2015-2019). <i>Expert Opinion on Therapeutic Patents</i> , 2019 , 29, 965-977	6.8	7
95	Balancing reactivity and antitumor activity: heteroarylthioacetamide derivatives as potent and time-dependent inhibitors of EGFR. <i>European Journal of Medicinal Chemistry</i> , 2019 , 162, 507-524	6.8	8
94	Inhibition of Eph/ephrin interaction with the small molecule UniPR500 improves glucose tolerance in healthy and insulin-resistant mice. <i>Pharmacological Research</i> , 2019 , 141, 319-330	10.2	7
93	L718Q mutant EGFR escapes covalent inhibition by stabilizing a non-reactive conformation of the lung cancer drug osimertinib. <i>Chemical Science</i> , 2018 , 9, 2740-2749	9.4	51
92	Tetrahydroquinoline Ring as a Versatile Bioisostere of Tetralin for Melatonin Receptor Ligands. <i>Journal of Medicinal Chemistry</i> , 2018 , 61, 3726-3737	8.3	11
91	N-tert-butyloxycarbonyl-Phe-Leu-Phe-Leu-Phe (BOC2) inhibits the angiogenic activity of heparin-binding growth factors. <i>Angiogenesis</i> , 2018 , 21, 47-59	10.6	24
90	Identification of Bivalent Ligands with Melatonin Receptor Agonist and Fatty Acid Amide Hydrolase (FAAH) Inhibitory Activity That Exhibit Ocular Hypotensive Effect in the Rabbit. <i>Journal of Medicinal Chemistry</i> , 2018 , 61, 7902-7916	8.3	10
89	Combined Quantum Mechanics and Molecular Mechanics Studies of Enzymatic Reaction Mechanisms. <i>Advances in Protein Chemistry and Structural Biology</i> , 2018 , 113, 1-32	5.3	5
88	UniPR1331, a small molecule targeting Eph/ephrin interaction, prolongs survival in glioblastoma and potentiates the effect of antiangiogenic therapy in mice. <i>Oncotarget</i> , 2018 , 9, 24347-24363	3.3	16
87	Pharmacological evaluation of new bioavailable small molecules targeting Eph/ephrin interaction. <i>Biochemical Pharmacology</i> , 2018 , 147, 21-29	6	14
86	Theoretical Model of EphA2-Ephrin A1 Inhibition. <i>Molecules</i> , 2018 , 23,	4.8	3
85	Metadynamics Simulations Distinguish Short- and Long-Residence-Time Inhibitors of Cyclin-Dependent Kinase 8. <i>Journal of Chemical Information and Modeling</i> , 2017 , 57, 159-169	6.1	37
84	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. <i>Journal of Medicinal Chemistry</i> , 2017 , 60, 4304-4315	8.3	10
83	Metadynamics for Perspective Drug Design: Computationally Driven Synthesis of New Protein-Protein Interaction Inhibitors Targeting the EphA2 Receptor. <i>Journal of Medicinal Chemistry</i> , 2017 , 60, 787-796	8.3	21
82	Targeting Eph/ephrin system in cancer therapy. <i>European Journal of Medicinal Chemistry</i> , 2017 , 142, 152-162	6.2	47
81	Mechanistic Insights into the Reaction of Chlorination of Tryptophan Catalyzed by Tryptophan 7-Halogenase. <i>Scientific Reports</i> , 2017 , 7, 17395	4.9	19

80	Biochemical characterization of EphA2 antagonists with improved physico-chemical properties by cell-based assays and surface plasmon resonance analysis. <i>Biochemical Pharmacology</i> , 2016 , 99, 18-30	6	4
79	Free-energy studies reveal a possible mechanism for oxidation-dependent inhibition of MGL. <i>Scientific Reports</i> , 2016 , 6, 31046	4.9	6
78	Exploiting Free-Energy Minima to Design Novel EphA2 Protein-Protein Antagonists: From Simulation to Experiment and Return. <i>Chemistry - A European Journal</i> , 2016 , 22, 8048-52	4.8	12
77	Targeting glioblastoma with UniPR1331, a new and stable bioavailable small molecule inhibiting Eph β ephrin interaction: In vitro and in vivo evidence. <i>European Journal of Cancer</i> , 2016 , 69, S30-S31	7.5	2
76	Combined inhibition of the EGFR/AKT pathways by a novel conjugate of quinazoline with isothiocyanate. <i>European Journal of Medicinal Chemistry</i> , 2016 , 117, 283-91	6.8	11
75	Fatty acid amide hydrolase inhibitors: a patent review (2009-2014). <i>Expert Opinion on Therapeutic Patents</i> , 2015 , 25, 1247-66	6.8	42
74	(5)-Cholenoyl-amino acids as selective and orally available antagonists of the Eph-ephrin system. <i>European Journal of Medicinal Chemistry</i> , 2015 , 103, 312-24	6.8	26
73	Highly Potent and Selective MT2 Melatonin Receptor Full Agonists from Conformational Analysis of 1-Benzyl-2-acylaminomethyl-tetrahydroquinolines. <i>Journal of Medicinal Chemistry</i> , 2015 , 58, 7512-25	8.3	31
72	The ellagitannin colonic metabolite urolithin D selectively inhibits EphA2 phosphorylation in prostate cancer cells. <i>Molecular Nutrition and Food Research</i> , 2015 , 59, 2155-67	5.9	26
71	Comparative Analysis of Virtual Screening Approaches in the Search for Novel EphA2 Receptor Antagonists. <i>Molecules</i> , 2015 , 20, 17132-51	4.8	4
70	Amino Acid Derivatives as Palmitoylethanolamide Prodrugs: Synthesis, In Vitro Metabolism and In Vivo Plasma Profile in Rats. <i>PLoS ONE</i> , 2015 , 10, e0128699	3.7	20
69	Pushing the boundaries of vinylogous reactivity: catalytic enantioselective mukaiyama aldol reactions of highly unsaturated 2-silyloxyindoles. <i>Chemistry - A European Journal</i> , 2015 , 21, 6433-42	4.8	17
68	Quantum mechanics/molecular mechanics modeling of covalent addition between EGFR-cysteine 797 and N-(4-anilinoquinazolin-6-yl) acrylamide. <i>Journal of Chemical Information and Modeling</i> , 2015 , 55, 589-99	6.1	33
67	Targeting the Eph-ephrin System with Protein-Protein Interaction (PPI) Inhibitors. <i>Current Drug Targets</i> , 2015 , 16, 1048-56	3	9
66	Combining ligand- and structure-based approaches for the discovery of new inhibitors of the EPHA2-ephrin-A1 interaction. <i>Journal of Chemical Information and Modeling</i> , 2014 , 54, 2621-6	6.1	11
65	Predicting the reactivity of nitrile-carrying compounds with cysteine: a combined computational and experimental study. <i>ACS Medicinal Chemistry Letters</i> , 2014 , 5, 501-5	4.3	50
64	Synthesis and characterization of new bivalent agents as melatonin- and histamine H3-ligands. <i>International Journal of Molecular Sciences</i> , 2014 , 15, 16114-33	6.3	6
63	Physical Nature of Fatty Acid Amide Hydrolase Interactions with Its Inhibitors: Testing a Simple Nonempirical Scoring Model. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 14727-36	3.4	8

62	On the use of 2,5-dimethyl-pyrrol-1-yl-benzoic acid derivatives as Eph-ephrin antagonists. <i>Journal of Virology</i> , 2014 , 88, 12173	6.6	4
61	Are we using the right pharmacological tools to target EphA4?. <i>ACS Chemical Neuroscience</i> , 2014 , 5, 1146-7	5.7	14
60	Target hopping as a useful tool for the identification of novel EphA2 protein-protein antagonists. <i>ChemMedChem</i> , 2014 , 9, 67-72	3.7	17
59	Insights in the mechanism of action and inhibition of N-acylethanolamine acid amidase by means of computational methods. <i>Advances in Protein Chemistry and Structural Biology</i> , 2014 , 96, 219-34	5.3	3
58	UniPR129 is a competitive small molecule Eph-ephrin antagonist blocking in vitro angiogenesis at low micromolar concentrations. <i>British Journal of Pharmacology</i> , 2014 , 171, 5195-208	8.6	31
57	Therapeutic perspectives of Eph-ephrin system modulation. <i>Drug Discovery Today</i> , 2014 , 19, 661-9	8.8	33
56	VGF-Derived Peptide TLQP-21 2014 , 49		
55	Structure-based virtual screening of MT2 melatonin receptor: influence of template choice and structural refinement. <i>Journal of Chemical Information and Modeling</i> , 2013 , 53, 821-35	6.1	28
54	Long-lasting inhibition of EGFR autophosphorylation in A549 tumor cells by intracellular accumulation of non-covalent inhibitors. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2013 , 23, 5290-4	2.9	2
53	Amino acid conjugates of lithocholic acid as antagonists of the EphA2 receptor. <i>Journal of Medicinal Chemistry</i> , 2013 , 56, 2936-47	8.3	40
52	Computational enzymology. <i>Methods in Molecular Biology</i> , 2013 , 924, 67-89	1.4	11
51	Conformational effects on the pro-S hydrogen abstraction reaction in cyclooxygenase-1: an integrated QM/MM and MD study. <i>Biophysical Journal</i> , 2013 , 104, L5-7	2.9	21
50	Quantum mechanics/molecular mechanics modeling of fatty acid amide hydrolase reactivation distinguishes substrate from irreversible covalent inhibitors. <i>Journal of Medicinal Chemistry</i> , 2013 , 56, 2500-12	8.3	28
49	Nonempirical energetic analysis of reactivity and covalent inhibition of fatty acid amide hydrolase. <i>Journal of Physical Chemistry B</i> , 2013 , 117, 6656-66	3.4	10
48	Homology models of melatonin receptors: challenges and recent advances. <i>International Journal of Molecular Sciences</i> , 2013 , 14, 8093-121	6.3	27
47	Synthesis and structure-activity relationships of amino acid conjugates of cholanic acid as antagonists of the EphA2 receptor. <i>Molecules</i> , 2013 , 18, 13043-60	4.8	12
46	Dibasic biphenyl H3 receptor antagonists: Steric tolerance for a lipophilic side chain. <i>European Journal of Medicinal Chemistry</i> , 2012 , 48, 214-30	6.8	10
45	MT1-selective melatonin receptor ligands: synthesis, pharmacological evaluation, and molecular dynamics investigation of N-[(3-O-substituted)anilino]alkyl]amides. <i>ChemMedChem</i> , 2012 , 7, 1954-64	3.7	21

44	The increasing role of QM/MM in drug discovery. <i>Advances in Protein Chemistry and Structural Biology</i> , 2012 , 87, 337-62	5.3	39
43	Irreversible inhibition of epidermal growth factor receptor activity by 3-aminopropanamides. <i>Journal of Medicinal Chemistry</i> , 2012 , 55, 2251-64	8.3	48
42	Structure-activity relationships and mechanism of action of Eph-ephrin antagonists: interaction of cholanic acid with the EphA2 receptor. <i>ChemMedChem</i> , 2012 , 7, 1071-83	3.7	28
41	N-(2-oxo-3-oxetanyl)carbamic acid esters as N-acylethanolamine acid amidase inhibitors: synthesis and structure-activity and structure-property relationships. <i>Journal of Medicinal Chemistry</i> , 2012 , 55, 4824-36	8.3	44
40	A catalytic mechanism for cysteine N-terminal nucleophile hydrolases, as revealed by free energy simulations. <i>PLoS ONE</i> , 2012 , 7, e32397	3.7	55
39	A catalytically silent FAAH-1 variant drives anandamide transport in neurons. <i>Nature Neuroscience</i> , 2011 , 15, 64-9	25.5	134
38	Covalent inhibitors of fatty acid amide hydrolase: a rationale for the activity of piperidine and piperazine aryl ureas. <i>Journal of Medicinal Chemistry</i> , 2011 , 54, 6612-23	8.3	33
37	Lithocholic acid is an Eph-ephrin ligand interfering with Eph-kinase activation. <i>PLoS ONE</i> , 2011 , 6, e18128	3.7	55
36	Biphenyl-3-yl alkylcarbamates as fatty acid amide hydrolase (FAAH) inhibitors: steric effects of N-alkyl chain on rat plasma and liver stability. <i>European Journal of Medicinal Chemistry</i> , 2011 , 46, 4466-73	6.8	16
35	Application of a SCC-DFTB QM/MM approach to the investigation of the catalytic mechanism of fatty acid amide hydrolase. <i>Journal of Molecular Modeling</i> , 2011 , 17, 2375-83	2	17
34	Understanding the role of carbamate reactivity in fatty acid amide hydrolase inhibition by QM/MM mechanistic modelling. <i>Chemical Communications</i> , 2011 , 47, 2517-9	5.8	21
33	Catalytic, asymmetric hypervinylogous Mukaiyama aldol reactions of extended furan-based silyl enolates. <i>Organic Letters</i> , 2011 , 13, 4738-41	6.2	26
32	Epidermal growth factor receptor irreversible inhibitors: chemical exploration of the cysteine-trap portion. <i>Mini-Reviews in Medicinal Chemistry</i> , 2011 , 11, 1019-30	3.2	36
31	Application of computational methods to the design of fatty acid amide hydrolase (FAAH) inhibitors based on a carbamic template structure. <i>Advances in Protein Chemistry and Structural Biology</i> , 2011 , 85, 1-26	5.3	10
30	Novel irreversible epidermal growth factor receptor inhibitors by chemical modulation of the cysteine-trap portion. <i>Journal of Medicinal Chemistry</i> , 2010 , 53, 2038-50	8.3	44
29	Structural Fluctuations in Enzyme-Catalyzed Reactions: Determinants of Reactivity in Fatty Acid Amide Hydrolase from Multivariate Statistical Analysis of Quantum Mechanics/Molecular Mechanics Paths. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 2948-60	6.4	53
28	Synthesis and structure-activity relationships of N-(2-oxo-3-oxetanyl)amides as N-acylethanolamine-hydrolyzing acid amidase inhibitors. <i>Journal of Medicinal Chemistry</i> , 2010 , 53, 5770-81	8.3	49
27	Structure-property relationships of a class of carbamate-based fatty acid amide hydrolase (FAAH) inhibitors: chemical and biological stability. <i>ChemMedChem</i> , 2009 , 4, 1495-504	3.7	32

26	A critical cysteine residue in monoacylglycerol lipase is targeted by a new class of isothiazolinone-based enzyme inhibitors. <i>British Journal of Pharmacology</i> , 2009 , 157, 974-83	8.6	65
25	Discovery of potent and reversible monoacylglycerol lipase inhibitors. <i>Chemistry and Biology</i> , 2009 , 16, 1045-52		80
24	5-Benzylidene-hydantoin: synthesis and antiproliferative activity on A549 lung cancer cell line. <i>European Journal of Medicinal Chemistry</i> , 2009 , 44, 3471-9	6.8	34
23	Selective N-acylethanolamine-hydrolyzing acid amidase inhibition reveals a key role for endogenous palmitoylethanolamide in inflammation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009 , 106, 20966-71	11.5	179
22	Insights into the mechanism and inhibition of fatty acid amide hydrolase from quantum mechanics/molecular mechanics (QM/MM) modelling. <i>Biochemical Society Transactions</i> , 2009 , 37, 363-7	5.1	34
21	Pharmacological tools in endocannabinoid neurobiology. <i>Current Topics in Behavioral Neurosciences</i> , 2009 , 1, 87-110	3.4	5
20	Applications and Advances of QM/MM Methods in Computational Enzymology. <i>Annual Reports in Computational Chemistry</i> , 2008 , 155-169	1.8	7
19	Synthesis and quantitative structure-activity relationship of fatty acid amide hydrolase inhibitors: modulation at the N-portion of biphenyl-3-yl alkylcarbamates. <i>Journal of Medicinal Chemistry</i> , 2008 , 51, 3487-98	8.3	59
18	Dual mechanisms of action of the 5-benzylidene-hydantoin UPR1024 on lung cancer cell lines. <i>Molecular Cancer Therapeutics</i> , 2008 , 7, 361-70	6.1	55
17	Relationship between chiroptical properties, structural changes and interactions in enzymes: a computational study on beta-lactamases from class A. <i>Computational Biology and Chemistry</i> , 2008 , 32, 167-75	3.6	7
16	Aromatic interactions and rotational strengths within protein environment: An electronic structural study on β -lactamases from class A. <i>Chemical Physics Letters</i> , 2008 , 456, 89-95	2.5	6
15	Identification of productive inhibitor binding orientation in fatty acid amide hydrolase (FAAH) by QM/MM mechanistic modelling. <i>Chemical Communications</i> , 2008 , 214-6	5.8	58
14	Conformational effects in enzyme catalysis: reaction via a high energy conformation in fatty acid amide hydrolase. <i>Biophysical Journal</i> , 2007 , 92, L20-2	2.9	69
13	Synthesis, enantiomeric resolution, and structure-activity relationship study of a series of 10,11-dihydro-5H-dibenzo[a,d]cycloheptene MT2 receptor antagonists. <i>ChemMedChem</i> , 2007 , 2, 1741-9	3.7	11
12	Correlation between energetics of collisionally activated decompositions, interaction energy and biological potency of carbamate FAAH inhibitors. <i>Journal of Mass Spectrometry</i> , 2007 , 42, 1624-7	2.2	8
11	N-(substituted-anilinoethyl)amides: design, synthesis, and pharmacological characterization of a new class of melatonin receptor ligands. <i>Journal of Medicinal Chemistry</i> , 2007 , 50, 6618-26	8.3	70
10	Synthesis and structure-activity relationships of FAAH inhibitors: cyclohexylcarbamic acid biphenyl esters with chemical modulation at the proximal phenyl ring. <i>ChemMedChem</i> , 2006 , 1, 130-9	3.7	53
9	Design and synthesis of N-(3,3-diphenylpropenyl)alkanamides as a novel class of high-affinity MT2-selective melatonin receptor ligands. <i>Journal of Medicinal Chemistry</i> , 2006 , 49, 7393-403	8.3	24

8	5-benzylidene-hydantoin s as new EGFR inhibitors with antiproliferative activity. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2006 , 16, 4021-5	2.9	64
7	MT2 selective melatonin receptor antagonists: design and structure-activity relationships. <i>Arkivoc</i> , 2006 , 2006, 8-16	0.9	12
6	QM/MM modelling of oleamide hydrolysis in fatty acid amide hydrolase (FAAH) reveals a new mechanism of nucleophile activation. <i>Chemical Communications</i> , 2005 , 4399-401	5.8	59
5	Application of 3D-QSAR in the rational design of receptor ligands and enzyme inhibitors. <i>Chemistry and Biodiversity</i> , 2005 , 2, 1438-51	2.5	8
4	Cyclohexylcarbamic acid 3S or 4Ssubstituted biphenyl-3-yl esters as fatty acid amide hydrolase inhibitors: synthesis, quantitative structure-activity relationships, and molecular modeling studies. <i>Journal of Medicinal Chemistry</i> , 2004 , 47, 4998-5008	8.3	239
3	Synthesis, pharmacological evaluation, and structure-activity relationships of benzopyran derivatives with potent SERM activity. <i>Bioorganic and Medicinal Chemistry</i> , 2004 , 12, 3763-82	3.4	18
2	Getting it right: modeling of pH, solvent and "nearly" everything else in virtual screening of biological targets. <i>Journal of Molecular Graphics and Modelling</i> , 2004 , 22, 479-86	2.8	25
1	Discovery of SARS-CoV-2 Mpro Peptide Inhibitors from Modelling Substrate and Ligand Binding		1