Antonio Llinas

List of Publications by Year in Descending Order

31 papers	1,438 citations	17 h-index	34 g-index
34 ext. papers	1,628 ext. citations	5.3 avg, IF	4.56 L-index

#	Paper	IF	Citations
31	Membrane Permeability in Cyclic Peptides is Modulated by Core Conformations. *Journal of Chemical Information and Modeling*, **2021**, 61, 263-269	6.1	6
30	AZD0284, a Potent, Selective, and Orally Bioavailable Inverse Agonist of Retinoic Acid Receptor-Related Orphan Receptor C2. *Journal of Medicinal Chemistry*, **2021**, 64, 13807-13829	8.3	1
29	Multisolvent Models for Solvation Free Energy Predictions Using 3D-RISM Hydration Thermodynamic Descriptors. *Journal of Chemical Information and Modeling*, **2020**, 60, 2977-2988	6.1	6
28	Identification and Optimization of Pyrrolidine Derivatives as Highly Potent Ghrelin Receptor Full Agonists. *Journal of Medicinal Chemistry*, **2020**, 63, 9705-9730	8.3	4
27	Findings of the Second Challenge to Predict Aqueous Solubility. *Journal of Chemical Information and Modeling*, **2020**, 60, 4791-4803	6.1	9
26	Discovery of Potent and Orally Bioavailable Inverse Agonists of the Retinoic Acid Receptor-Related Orphan Receptor C2. *ACS Medicinal Chemistry Letters*, **2019**, 10, 972-977	4.3	10
25	Solubility Challenge Revisited after Ten Years, with Multilab Shake-Flask Data, Using Tight (SD ~ 0.17 log) and Loose (SD ~ 0.62 log) Test Sets. *Journal of Chemical Information and Modeling*, **2019**, 59, 3036-3040	6.1	23
24	Derisking Development by a Cocrystallization Screen of a Novel Selective Inhaled JAK-STAT inhibitor. *Crystal Growth and Design*, **2019**, 19, 403-414	3.5	2
23	Property prediction and pharmacokinetic evaluation of mixed stoichiometry cocrystals of zafirlukast, a drug delivery case study. *CrystEngComm*, **2018**, 20, 1346-1351	3.3	4
22	Discovery of a Novel Oral Glucocorticoid Receptor Modulator (AZD9567) with Improved Side Effect Profile. *Journal of Medicinal Chemistry*, **2018**, 61, 1785-1799	8.3	34
21	Potent and Orally Bioavailable Inverse Agonists of RORγ Resulting from Structure-Based Design. *Journal of Medicinal Chemistry*, **2018**, 61, 7796-7813	8.3	24
20	Identification and Pharmacological Profile of an Indane Based Series of Ghrelin Receptor Full Agonists. *Journal of Medicinal Chemistry*, **2018**, 61, 5974-5987	8.3	12
19	Equilibrium solubility measurement of ionizable drugs – consensus recommendations for improving data quality. *ADMET and DMPK*, **2016**, 4, 117	1.3	47
18	Two New Polymorphic Cocrystals of Zafirlukast: Preparation, Crystal Structure, and Stability Relations. *Crystal Growth and Design*, **2015**, 15, 4162-4169	3.5	7
17	Fast and General Method To Predict the Physicochemical Properties of Druglike Molecules Using the Integral Equation Theory of Molecular Liquids. *Molecular Pharmaceutics*, **2015**, 12, 3420-32	5.6	21
16	Discovery of AZD6642, an inhibitor of 5-lipoxygenase activating protein (FLAP) for the treatment of inflammatory diseases. *Journal of Medicinal Chemistry*, **2015**, 58, 897-911	8.3	33
15	Discovery of N-[[1-[2-(tert-butylcarbamoylamino)ethyl]-4-(hydroxymethyl)-4-piperidyl]methyl]-3,5-dichloro-benzamide as a selective T-type calcium channel (Cav3.2) inhibitor. *Bioorganic and Medicinal Chemistry Letters*, **2013**, 23, 119-24	2.9	4

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14	Beyond size, ionization state, and lipophilicity: influence of molecular topology on absorption, distribution, metabolism, excretion, and toxicity for druglike compounds. *Journal of Medicinal Chemistry*, **2012**, 55, 3667-77	8.3	96
13	Oxadiazoles in medicinal chemistry. *Journal of Medicinal Chemistry*, **2012**, 55, 1817-30	8.3	357
12	Discovery of N-(1-adamantyl)-2-(4-alkylpiperazin-1-yl)acetamide derivatives as T-type calcium channel (Cav3.2) inhibitors. *Bioorganic and Medicinal Chemistry Letters*, **2011**, 21, 5557-61	2.9	6
11	Impact of input parameters on the prediction of hepatic plasma clearance using the well-stirred model. *Current Drug Metabolism*, **2010**, 11, 583-94	3.5	18
10	Polymorph control: past, present and future. *Drug Discovery Today*, **2008**, 13, 198-210	8.8	247
9	Predicting intrinsic aqueous solubility by a thermodynamic cycle. *Molecular Pharmaceutics*, **2008**, 5, 266-79	5.6	91
8	Solubility challenge: can you predict solubilities of 32 molecules using a database of 100 reliable measurements?. *Journal of Chemical Information and Modeling*, **2008**, 48, 1289-303	6.1	142
7	Concomitant Hydrate Polymorphism in the Precipitation of Sparfloxacin from Aqueous Solution. *Crystal Growth and Design*, **2008**, 8, 114-118	3.5	23
6	Diclofenac solubility: independent determination of the intrinsic solubility of three crystal forms. *Journal of Medicinal Chemistry*, **2007**, 50, 979-83	8.3	96
5	A new method for the reproducible generation of polymorphs: two forms of sulindac with very different solubilities. *Journal of Applied Crystallography*, **2007**, 40, 379-381	3.8	35
4	Amodiaquinium dichloride dihydrate from laboratory powder diffraction data. *Acta Crystallographica Section E: Structure Reports Online*, **2006**, 62, o4196-o4199		13
3	Intramolecular general acid catalysis in the aminolysis of beta-lactam antibiotics. *Organic and Biomolecular Chemistry*, **2004**, 2, 651-4	3.9	40
2	The role of a proton transfer donor in the degradation of benzylpenicillin. *Journal of Molecular Catalysis A*, **2001**, 175, 3-16		7
1	Chemical Reactivity of Penicillins and Cephalosporins. Intramolecular Involvement of the Acyl-Amido Side Chain. *Journal of Organic Chemistry*, **1998**, 63, 9052-9060	4.2	20