Xavier Lucas

List of Publications by Year
in descending order

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36 papers	2,170 citations	394390 19 h-index	330122 37 g-index
39 all docs	39 docs citations	39 times ranked	3046 citing authors

#	Article	IF	Citations
1	Targeting Xanthine Oxidase by Natural Products as a Therapeutic Approach for Mental Disorders. Current Pharmaceutical Design, 2021, 27, 367-382.	1.9	16
2	Development and Benchmarking of Open Force Field v1.0.0â€"the Parsley Small-Molecule Force Field. Journal of Chemical Theory and Computation, 2021, 17, 6262-6280.	5.3	80
3	Structureâ€Based Design of a Macrocyclic PROTAC. Angewandte Chemie - International Edition, 2020, 59, 1727-1734.	13.8	150
4	Structureâ€Based Design of a Macrocyclic PROTAC. Angewandte Chemie, 2020, 132, 1744-1751.	2.0	13
5	4-Acyl Pyrroles as Dual BET-BRD7/9 Bromodomain Inhibitors Address BETi Insensitive Human Cancer Cell Lines. Journal of Medicinal Chemistry, 2020, 63, 15603-15620.	6.4	11
6	The ChemicalToolbox: reproducible, user-friendly cheminformatics analysis on the Galaxy platform. Journal of Cheminformatics, 2020, 12, 40.	6.1	21
7	Hidden Specificities in Enzyme Catalysis: Structural Basis of Substrate Structureâ€Selectivity Relationship of a Ketoreductase. ChemBioChem, 2019, 20, 1150-1154.	2.6	6
8	Thioamide substitution to probe the hydroxyproline recognition of VHL ligands. Bioorganic and Medicinal Chemistry, 2018, 26, 2992-2995.	3.0	13
9	Targeting Ligandable Pockets on Plant Homeodomain (PHD) Zinc Finger Domains by a Fragment-Based Approach. ACS Chemical Biology, 2018, 13, 915-921.	3.4	25
10	3-Fluoro-4-hydroxyprolines: Synthesis, Conformational Analysis, and Stereoselective Recognition by the VHL E3 Ubiquitin Ligase for Targeted Protein Degradation. Journal of the American Chemical Society, 2018, 140, 9299-9313.	13.7	102
11	Surface Probing by Fragment-Based Screening and Computational Methods Identifies Ligandable Pockets on the von Hippelâ€"Lindau (VHL) E3 Ubiquitin Ligase. Journal of Medicinal Chemistry, 2018, 61, 7387-7393.	6.4	21
12	Recognition of substrate degrons by E3 ubiquitin ligases and modulation by small-molecule mimicry strategies. Current Opinion in Structural Biology, 2017, 44, 101-110.	5.7	74
13	Structural basis of molecular recognition of helical histone H3 tail by PHD finger domains. Biochemical Journal, 2017, 474, 1633-1651.	3.7	31
14	Structural basis of PROTAC cooperative recognition for selective protein degradation. Nature Chemical Biology, 2017, 13, 514-521.	8.0	758
15	Beyond the BET Family: Targeting CBP/p300 with 4â€Acyl Pyrroles. Angewandte Chemie - International Edition, 2017, 56, 12476-12480.	13.8	26
16	Beyond the BET Family: Targeting CBP/p300 with 4â€Acyl Pyrroles. Angewandte Chemie, 2017, 129, 12650-12654.	2.0	5
17	Preparation data of the bromodomains BRD3(1), BRD3(2), BRD4(1), and BRPF1B and crystallization of BRD4(1)-inhibitor complexes. Data in Brief, 2016, 7, 1370-1374.	1.0	1
18	StreptomeDB 2.0â€"an extended resource of natural products produced by streptomycetes. Nucleic Acids Research, 2016, 44, D509-D514.	14.5	70

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19	4-Acyl Pyrrole Derivatives Yield Novel Vectors for Designing Inhibitors of the Acetyl-Lysine Recognition Site of BRD4(1). Journal of Medicinal Chemistry, 2016, 59, 1518-1530.	6.4	51
20	A thorough anionâ€“Ï€ interaction study in biomolecules: on the importance of cooperativity effects. Chemical Science, 2016, 7, 1038-1050.	7.4	188
21	Target Fishing by Crossâ€Docking to Explain Polypharmacological Effects. ChemMedChem, 2015, 10, 1209-1217.	3.2	21
22	The Purchasable Chemical Space: A Detailed Picture. Journal of Chemical Information and Modeling, 2015, 55, 915-924.	5.4	38
23	Targeting the BET family for the treatment of leukemia. Epigenomics, 2014, 6, 153-155.	2.1	8
24	Using chiral molecules as an approach to address lowâ€druggability recognition sites. Journal of Computational Chemistry, 2014, 35, 2114-2121.	3.3	4
25	Metabolic pathway monitoring of phenalinolactone biosynthesis from Streptomyces sp. TÃ¼46071 by liquid chromatography/mass spectrometry coupling. Rapid Communications in Mass Spectrometry, 2014, 28, 1459-1467.	1.5	5
26	Dynamic information system for small molecules. Journal of Cheminformatics, 2014, 6, .	6.1	0
27	ChemicalToolBoX and its application on the study of the drug like and purchasable space. Journal of Cheminformatics, 2014, 6, .	6.1	3
28	StreptomeDB: a resource for natural compounds isolated from Streptomyces species. Nucleic Acids Research, 2013, 41, D1130-D1136.	14.5	107
29	4â€Acyl Pyrroles: Mimicking Acetylated Lysines in Histone Code Reading. Angewandte Chemie - International Edition, 2013, 52, 14055-14059.	13.8	102
30	Discovery of the Inhibitory Effect of a Phosphatidylinositol Derivative on P-Glycoprotein by Virtual Screening Followed by In Vitro Cellular Studies. PLoS ONE, 2013, 8, e60679.	2.5	7
31	Virtual screening strategies in drug design â€“ methods and applications. Biotechnologia, 2011, 3, 249-264.	0.9	36
32	The Role of the Ethynyl Substituent on the Ï€â€“Ï€ Stacking Affinity of Benzene: A Theoretical Study. ChemPhysChem, 2011, 12, 283-288.	2.1	3
33	Erroneous behaviour of the widely used MP2(full)/aug-cc-pVXZ (X=D,T) level of theory for evaluating the BSSE in ionâ€“Ï€ complexes. Chemical Physics Letters, 2010, 489, 254-258.	2.6	20
34	Substituent Effects in Ionâˆ’Ï€ Interactions: Fine-Tuning via the Ethynyl Group. Journal of Physical Chemistry A, 2010, 114, 1926-1930.	2.5	22
35	Very Longâ€Range Effects: Cooperativity between Anionâ€“Ï€ and Hydrogenâ€Bonding Interactions. ChemPhysChem, 2009, 10, 2256-2264.	2.1	80
36	Counterintuitive Substituent Effect of the Ethynyl Group in Ionâˆ’Ï€ Interactions. Journal of Physical Chemistry A, 2009, 113, 10367-10375.	2.5	43