Andreas Verras

List of Publications by Year
in descending order

75 papers	3,260 citations	279798 23 h-index	149698 56 g-index
77 all docs	77 docs citations	77 times ranked	3084 citing authors

#	Article	IF	Citations
1	NMR Dataâ€Driven Docking of HDM2â€Inhibitor Complexes. ChemBioChem, 2022, , .	2.6	0
2	Oxetane Promise Delivered: Discovery of Long-Acting IDO1 Inhibitors Suitable for Q3W Oral or Parenteral Dosing. Journal of Medicinal Chemistry, 2022, 65, 6001-6016.	6.4	8
3	Diminishing GSH-Adduct Formation of Tricyclic Diazepine-based Mutant IDH1 Inhibitors. ACS Medicinal Chemistry Letters, 2022, 13, 734-741.	2.8	1
4	Development of High-Throughput Assays for Evaluation of Hematopoietic Progenitor Kinase 1 Inhibitors. SLAS Discovery, 2021, 26, 88-99.	2.7	15
5	Carbamate and N-Pyrimidine Mitigate Amide Hydrolysis: Structure-Based Drug Design of Tetrahydroquinoline IDO1 Inhibitors. ACS Medicinal Chemistry Letters, 2021, 12, 389-396.	2.8	14
6	Identification of Potent Reverse Indazole Inhibitors for HPK1. ACS Medicinal Chemistry Letters, 2021, 12, 459-466.	2.8	16
7	Discovery of Diaminopyrimidine Carboxamide HPK1 Inhibitors as Preclinical Immunotherapy Tool Compounds. ACS Medicinal Chemistry Letters, 2021, 12, 653-661.	2.8	18
8	Projected Dose Optimization of Amino- and Hydroxypyrrolidine Purine PI3KÎ´ Immunomodulators. Journal of Medicinal Chemistry, 2021, 64, 5137-5156.	6.4	7
9	Structural insights on ligand recognition at the human leukotriene B4 receptor 1. Nature Communications, 2021, 12, 2971.	12.8	13
10	Discovery of a new series of PI3K-Î´ inhibitors from Virtual Screening. Bioorganic and Medicinal Chemistry Letters, 2021, 42, 128046.	2.2	1
11	Discovery of the First Non-cGMP Mimetic Small Molecule Activators of cGMP-Dependent Protein Kinase 1 Î± (PKG1Î±). ACS Medicinal Chemistry Letters, 2021, 12, 1275-1282.	2.8	3
12	Utilization of Metabolite Identification and Structural Data to Guide Design of Low-Dose IDO1 Inhibitors. ACS Medicinal Chemistry Letters, 2021, 12, 1435-1440.	2.8	7
13	SAR towards indoline and 3-azaindoline classes of IDO1 inhibitors. Bioorganic and Medicinal Chemistry Letters, 2021, 47, 128214.	2.2	4
14	Discovery of IDO1 inhibitors containing a decahydroquinoline, decahydro-1,6-naphthyridine, or octahydro-1H-pyrrolo[3,2-c]pyridine scaffold. Bioorganic and Medicinal Chemistry Letters, 2021, 49, 128314.	2.2	7
15	Discovery of MK-4688: an Efficient Inhibitor of the HDM2â€“p53 Proteinâ€“Protein Interaction. Journal of Medicinal Chemistry, 2021, 64, 16213-16241.	6.4	14
16	Discovery and optimization of heteroaryl piperazines as potent and selective PI3KÎ´ inhibitors. Bioorganic and Medicinal Chemistry Letters, 2020, 30, 126715.	2.2	9
17	Discovery of Potent and Orally Available Bicyclo[1.1.1]pentane-Derived Indoleamine-2,3-dioxygenase 1 (IDO1) Inhibitors. ACS Medicinal Chemistry Letters, 2020, 11, 1548-1554.	2.8	44
18	Optimization of Versatile Oxindoles as Selective PI3KÎ´ Inhibitors. ACS Medicinal Chemistry Letters, 2020, 11, 2461-2469.	2.8	11

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19	Strategic Incorporation of Polarity in Heme-Displacing Inhibitors of Indoleamine-2,3-dioxygenase-1 (IDO1). ACS Medicinal Chemistry Letters, 2020, 11, 550-557.	2.8	28
20	Design of selective PI3KÎ´ inhibitors using an iterative scaffold-hopping workflow. Bioorganic and Medicinal Chemistry Letters, 2019, 29, 2575-2580.	2.2	13
21	Discovery of Amino-cyclobutarene-derived Indoleamine-2,3-dioxygenase 1 (IDO1) Inhibitors for Cancer Immunotherapy. ACS Medicinal Chemistry Letters, 2019, 10, 1530-1536.	2.8	38
22	Structure Overhaul Affords a Potent Purine PI3KÎ´ Inhibitor with Improved Tolerability. Journal of Medicinal Chemistry, 2019, 62, 4370-4382.	6.4	13
23	Workflows and performances in the ranking prediction of 2016 D3R Grand Challenge 2: lessons learned from a collaborative effort. Journal of Computer-Aided Molecular Design, 2018, 32, 129-142.	2.9	8
24	Performance of multiple docking and refinement methods in the pose prediction D3R prospective Grand Challenge 2016. Journal of Computer-Aided Molecular Design, 2018, 32, 113-127.	2.9	7
25	Repurposing a Histamine Detection Platform for High-Throughput Screening of Histidine Decarboxylase. SLAS Discovery, 2018, 23, 974-981.	2.7	2
26	Microscale High-Throughput Experimentation as an Enabling Technology in Drug Discovery: Application in the Discovery of (Piperidinyl)pyridinyl-1H-benzimidazole Diacylglycerol Acyltransferase 1 Inhibitors. Journal of Medicinal Chemistry, 2017, 60, 3594-3605.	6.4	65
27	Informing the Selection of Screening Hit Series with in Silico Absorption, Distribution, Metabolism, Excretion, and Toxicity Profiles. Journal of Medicinal Chemistry, 2017, 60, 6771-6780.	6.4	17
28	Discovery of Spirocyclic Aldosterone Synthase Inhibitors as Potential Treatments for Resistant Hypertension. ACS Medicinal Chemistry Letters, 2017, 8, 128-132.	2.8	12
29	The Discovery of 3-((4-Chloro-3-methoxyphenyl)amino)-1-((3R,4S)-4-cyanotetrahydro-2H-pyran-3-yl)-1H-pyrazole-4-carboxa a Highly Ligand Efficient and Efficacious Janus Kinase 1 Selective Inhibitor with Favorable Pharmacokinetic Properties. Journal of Medicinal Chemistry, 2017, 60, 9676-9690.	6.4	15
30	Is Multitask Deep Learning Practical for Pharma?. Journal of Chemical Information and Modeling, 2017, 57, 2068-2076.	5.4	191
31	Discovery and Pharmacology of a Novel Class of Diacylglycerol Acyltransferase 2 Inhibitors. Journal of Medicinal Chemistry, 2015, 58, 9345-9353.	6.4	22
32	High-resolution crystal structures of factor XIa coagulation factor in complex with nonbasic high-affinity synthetic inhibitors. Acta Crystallographica Section F: Structural Biology Communications, 2012, 68, 404-408.	0.7	12
33	1H-Imidazo[4,5-c]pyridine-4-carbonitrile as cathepsin S inhibitors: Separation of desired cellular activity from undesired tissue accumulation through optimization of basic nitrogen pka. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 932-935.	2.2	8
34	Design and optimization of a series of novel 2-cyano-pyrimidines as cathepsin K inhibitors. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 1524-1527.	2.2	23
35	Dioxo-triazines as a novel series of cathepsin K inhibitors. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 1488-1490.	2.2	21
36	4-(3-Trifluoromethylphenyl)-pyrimidine-2-carbonitrile as cathepsin S inhibitors: N3, not N1 is critically important. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 4507-4510.	2.2	20

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37	2-Phenyl-9H-purine-6-carbonitrile derivatives as selective cathepsin S inhibitors. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 4447-4450.	2.2	12
38	6-Phenyl-1H-imidazo[4,5-c]pyridine-4-carbonitrile as cathepsin S inhibitors. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 4350-4354.	2.2	17
39	Optimisation of 2-cyano-pyrimidine inhibitors of cathepsin K: Improving selectivity over hERG. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 6237-6241.	2.2	8
40	Trifluoromethylphenyl as P2 for ketoamide-based cathepsin S inhibitors. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 6890-6894.	2.2	18
41	X-Ray Structures of the LXRÎ± LBD in Its Homodimeric Form and Implications for Heterodimer Signaling. Journal of Molecular Biology, 2010, 399, 120-132.	4.2	44
42	Quantitative assessment of the effect of basis set superposition error on the electron density of molecular complexes by means of quantum molecular similarity measures. International Journal of Quantum Chemistry, 2009, 109, 2572-2580.	2.0	0
43	Incorporating protein flexibility into docking and structure-based drug design. Expert Opinion on Drug Discovery, 2006, 1, 335-349.	5.0	30
44	Unsupervised guided docking of covalently bound ligands. Journal of Computer-Aided Molecular Design, 2004, 18, 635-650.	2.9	18
45	Tautomeric conjugate acids of 2-aminopyrroles: effect of substituents, solvation and cosolute. Theoretical Chemistry Accounts, 2004, 111, 223-230.	1.4	3
46	Second-order atomic Fukui indices from the electron-pair density in the framework of the atoms in molecules theory. Journal of Computational Chemistry, 2004, 25, 439-446.	3.3	13
47	Guided Docking Approaches to Structure-Based Design and Screening. Current Topics in Medicinal Chemistry, 2004, 4, 687-700.	2.1	62
48	The Delocalization Index as an Electronic Aromaticity Criterion: Application to a Series of Planar Polycyclic Aromatic Hydrocarbons. Chemistry - A European Journal, 2003, 9, 400-406.	3.3	396
49	An Insight into the Local Aromaticities of Polycyclic Aromatic Hydrocarbons and Fullerenes. Chemistry - A European Journal, 2003, 9, 1113-1122.	3.3	125
50	Electron pairing analysis of the Fischer-type chromiumâ€“carbene complexes (CO)5Crî˜...C(X)R (X=H, OH,) Tj ETQq0 0 0 rgBT /Overlock	1.9	18
51	Molecular Dynamics Study of [2]Rotaxanes:Â Influence of Solvation and Cation on Co-conformation. Journal of Organic Chemistry, 2003, 68, 4663-4673.	3.2	24
52	TOPOLOGICAL ANALYSIS OF HYDROGEN-BONDED COMPLEXES. , 2002, , 1615-1641.		0
53	Ligand-induced changes in the binding sites of proteins. Bioinformatics, 2002, 18, 939-948.	4.1	46
54	ELECTRON CORRELATION STUDIES BY MEANS OF ELECTRON-PAIR DENSITY FUNCTIONS. , 2002, , 577-611.		2

#	Article	IF	Citations
55	BIELECTRONIC DENSITIES: ANALYSIS AND APPLICATIONS IN MOLECULAR STRUCTURE AND CHEMICAL REACTIVITY. , 2002, , 831-870.		2
56	A chemical Hamiltonian approach study of the basis set superposition error changes on electron densities and one- and two-center energy components. Journal of Chemical Physics, 2002, 116, 6443-6457.	3.0	8
57	Electron localization and delocalization in open-shell molecules. Journal of Computational Chemistry, 2002, 23, 1347-1356.	3.3	34
58	The calculation of electron localization and delocalization indices at the Hartree-Fock, density functional and post-Hartree-Fock levels of theory. Theoretical Chemistry Accounts, 2002, 107, 362-371.	1.4	187
59	Electron-pairing analysis from localization and delocalization indices in the framework of the atoms-in-molecules theory. Theoretical Chemistry Accounts, 2002, 108, 214-224.	1.4	175
60	Aminoimidazo[1,2-a]pyridines: regioselective synthesis of substituted imidazonaphthyridines, azacarbolines and cyclazines. Tetrahedron, 2002, 58, 295-307.	1.9	22
61	New Insights in Chemical Reactivity by Means of Electron Pairing Analysis. Journal of Physical Chemistry A, 2001, 105, 2052-2063.	2.5	34
62	Effects of Solvation on the Pairing of Electrons in a Series of Simple Molecules and in the Menshutkin Reaction. Journal of Physical Chemistry A, 2001, 105, 6249-6257.	2.5	32
63	Electronâ€“electron counterbalance density for molecules: Exchange and correlation effects. Journal of Chemical Physics, 2001, 115, 1987-1994.	3.0	11
64	Determination of the integrated x-ray scattering intensities through the electron-pair relative-motion density at the origin. Physical Review A, 2001, 64, .	2.5	7
65	Atomic transferability within the exchange-correlation density. Journal of Computational Chemistry, 2000, 21, 1361-1374.	3.3	11
66	Similarity-driven flexible ligand docking. Proteins: Structure, Function and Bioinformatics, 2000, 40, 623-636.	2.6	87
67	Charge-density concentration and electron-electron coalescence density in atoms and molecules. Physical Review A, 2000, 62, .	2.5	7
68	The mapping of the local contributions of Fermi and Coulomb correlation into intracule and extracule density distributions. Journal of Chemical Physics, 2000, 113, 2530-2543.	3.0	9
69	Effect of basis set superposition error on the electron density of molecular complexes. Journal of Chemical Physics, 2000, 112, 10106-10115.	3.0	24
70	Interpretation of Molecular Intracule and Extracule Density Distributions in Terms of Valence Bond Structures:â€‰ Two-Electron Systems and Processes. Journal of Physical Chemistry A, 2000, 104, 8445-8454.	2.5	11
71	Comparative electronic analysis between hydrogen transfers in the CH₄/CH₃⁺, CH₄/CH₃^{â€¢}, and CH₄/CH₃⁻ systems: on the electronic nature of the hydrogen (H⁻, H^{â€¢}, H⁺) being transferred. II. Analysis of electron-pair interactions from intracule and â€“tracule densities. Canadian Journal of Chemistry, 2000, 78, 328-337.	1.1	7
72	The Lewis Model and Beyond. Journal of Physical Chemistry A, 1999, 103, 304-314.	2.5	944

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73	Second-order quantum similarity measures from intracule and extracule densities. Theoretical Chemistry Accounts, 1998, 99, 44-52.	1.4	11
74	The relevance of the Laplacian of intracule and extracule density distributions for analyzing electronâ€“electron interactions in molecules. Journal of Chemical Physics, 1997, 107, 3576-3583.	3.0	28
75	Application of Molecular Quantum Similarity to QSAR. QSAR and Combinatorial Science, 1997, 16, 25-32.	1.2	58