Anna Vulpetti

List of Publications by Year
in descending order

55 papers	3,369 citations	172386 29 h-index	161767 54 g-index
56 all docs	56 docs citations	56 times ranked	4492 citing authors

#	Article	IF	Citations
1	Identification of compounds with binding affinity to proteins via magnetization transfer from bulk water. Journal of Biomolecular NMR, 2000, 18, 65-68.	1.6	412
2	Comparability of Mixed IC50 Data â€“ A Statistical Analysis. PLoS ONE, 2013, 8, e61007.	1.1	211
3	The Experimental Uncertainty of Heterogeneous Public K_i Data. Journal of Medicinal Chemistry, 2012, 55, 5165-5173.	2.9	183
4	Fluorine as a Hydrogenâ€Bond Acceptor: Experimental Evidence and Computational Calculations. Chemistry - A European Journal, 2014, 20, 11058-11068.	1.7	153
5	3-Aminopyrazole Inhibitors of CDK2/Cyclin A as Antitumor Agents. 1. Lead Finding. Journal of Medicinal Chemistry, 2004, 47, 3367-3380.	2.9	150
6	Potent and Selective Aurora Inhibitors Identified by the Expansion of a Novel Scaffold for Protein Kinase Inhibition. Journal of Medicinal Chemistry, 2005, 48, 3080-3084.	2.9	147
7	Assessment of Docking Poses:â€‰ Interactions-Based Accuracy Classification (IBAC) versus Crystal Structure Deviations. Journal of Chemical Information and Computer Sciences, 2004, 44, 871-881.	2.8	116
8	Ligand-Based Fluorine NMR Screening: Principles and Applications in Drug Discovery Projects. Journal of Medicinal Chemistry, 2019, 62, 2218-2244.	2.9	115
9	Fluorine local environment: from screening to drug design. Drug Discovery Today, 2012, 17, 890-897.	3.2	113
10	Design and NMR-Based Screening of LEF, a Library of Chemical Fragments with Different Local Environment of Fluorine. Journal of the American Chemical Society, 2009, 131, 12949-12959.	6.6	112
11	Identification of N,1,4,4-Tetramethyl-8-{[4-(4-methylpiperazin-1-yl)phenyl]amino}-4,5-dihydro-1H-pyrazolo[4,3-h]quinazoline-3-ca (PHA-848125), a Potent, Orally Available Cyclin Dependent Kinase Inhibitor. Journal of Medicinal Chemistry, 2009, 52, 5152-5163.	2.9	111
12	3-Aminopyrazole Inhibitors of CDK2/Cyclin A as Antitumor Agents. 2. Lead Optimization. Journal of Medicinal Chemistry, 2005, 48, 2944-2956.	2.9	98
13	Predicting Polypharmacology by Binding Site Similarity: From Kinases to the Protein Universe. Journal of Chemical Information and Modeling, 2010, 50, 1418-1431.	2.5	93
14	Discovery of LOU064 (Remibrutinib), a Potent and Highly Selective Covalent Inhibitor of Brutonâ€™s Tyrosine Kinase. Journal of Medicinal Chemistry, 2020, 63, 5102-5118.	2.9	92
15	Fluorineâ€“Protein Interactions and ¹⁹Fâ€…NMR Isotropic Chemical Shifts: An Empirical Correlation with Implications for Drug Design. ChemMedChem, 2011, 6, 104-114.	1.6	90
16	Sequence and structural analysis of kinase ATP pocket residues. Il Farmaco, 2004, 59, 759-765.	0.9	87
17	Weak Intermolecular Hydrogen Bonds with Fluorine: Detection and Implications for Enzymatic/Chemical Reactions, Chemical Properties, and Ligand/Protein Fluorine NMR Screening. Chemistry - A European Journal, 2016, 22, 7592-7601.	1.7	71
18	Intermolecular and Intramolecular Hydrogen Bonds Involving Fluorine Atoms: Implications for Recognition, Selectivity, and Chemical Properties. ChemMedChem, 2012, 7, 262-272.	1.6	70

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19	Small-molecule factor D inhibitors targeting the alternative complement pathway. Nature Chemical Biology, 2016, 12, 1105-1110.	3.9	68
20	Tautomer Preference in PDB Complexes and its Impact on Structure-Based Drug Discovery. Journal of Chemical Information and Modeling, 2010, 50, 1062-1074.	2.5	62
21	Optimization of 6,6-dimethyl pyrrolo[3,4-c]pyrazoles: Identification of PHA-793887, a potent CDK inhibitor suitable for intravenous dosing. Bioorganic and Medicinal Chemistry, 2010, 18, 1844-1853.	1.4	58
22	3-Amino-1,4,5,6-tetrahydropyrrolo[3,4-c]pyrazoles: A new class of CDK2 inhibitors. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 1084-1090.	1.0	56
23	NMR-Based Quality Control Approach for the Identification of False Positives and False Negatives in High Throughput Screening. Current Drug Discovery Technologies, 2006, 3, 115-124.	0.6	56
24	Polyfluorinated Amino Acids for Sensitive19F NMR-Based Screening and Kinetic Measurements. Journal of the American Chemical Society, 2007, 129, 5665-5672.	6.6	48
25	Design and Generation of Highly Diverse Fluorinated Fragment Libraries and their Efficient Screening with Improved ¹⁹Fâ€…NMR Methodology. ChemMedChem, 2013, 8, 2057-2069.	1.6	48
26	Structure-Based Approaches to Improve Selectivity:â€‰ CDK2â^'GSK3Î² Binding Site Analysis. Journal of Chemical Information and Modeling, 2005, 45, 1282-1290.	2.5	45
27	Technical and practical aspects of ¹⁹F NMRâ€based screening: toward sensitive highâ€throughput screening with rapid deconvolution. Magnetic Resonance in Chemistry, 2012, 50, 592-597.	1.1	38
28	Identification of Potent Pyrazolo[4,3-h]quinazoline-3-carboxamides as Multi-Cyclin-Dependent Kinase Inhibitors. Journal of Medicinal Chemistry, 2010, 53, 2171-2187.	2.9	36
29	Combined use of computational chemistry, NMR screening, and Xâ€ray crystallography for identification and characterization of fluorophilic protein environments. Proteins: Structure, Function and Bioinformatics, 2010, 78, 3281-3291.	1.5	30
30	Discovery of Highly Potent and Selective Small-Molecule Reversible Factor D Inhibitors Demonstrating Alternative Complement Pathway Inhibition in Vivo. Journal of Medicinal Chemistry, 2017, 60, 5717-5735.	2.9	27
31	Chemogenomics in drug discovery: computational methods based on the comparison of binding sites. Future Medicinal Chemistry, 2012, 4, 1971-1979.	1.1	26
32	Synthesis and Biological Evaluation of New Triazoloâ€•and Imidazolopyridine RORÎ³t Inverse Agonists. ChemMedChem, 2016, 11, 2640-2648.	1.6	26
33	Comprehensive and Highâ€Throughput Exploration of Chemical Space Using Broadband ¹⁹Fâ€…NMRâ€Based Screening. Angewandte Chemie - International Edition, 2020, 59, 14809-14817.	7.2	24
34	Subpocket Analysis Method for Fragment-Based Drug Discovery. Journal of Chemical Information and Modeling, 2013, 53, 131-141.	2.5	23
35	19F NMR chemical shift prediction with fluorine fingerprint descriptor. Journal of Fluorine Chemistry, 2010, 131, 570-577.	0.9	22
36	Structure-Based Library Design and Fragment Screening for the Identification of Reversible Complement Factor D Protease Inhibitors. Journal of Medicinal Chemistry, 2017, 60, 1946-1958.	2.9	22

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37	Optimizing a Weakly Binding Fragment into a Potent RORÎ³t Inverse Agonist with Efficacy in an in Vivo Inflammation Model. Journal of Medicinal Chemistry, 2018, 61, 6724-6735.	2.9	22
38	6-Substituted Pyrrolo[3,4-c]pyrazoles: An Improved Class of CDK2 Inhibitors. ChemMedChem, 2007, 2, 841-852.	1.6	21
39	Quality Issues with Public Domain Chemogenomics Data. Molecular Informatics, 2013, 32, 898-905.	1.4	21
40	Structure-based drug design to the discovery of new 2-aminothiazole CDK2 inhibitors. Journal of Molecular Graphics and Modelling, 2006, 24, 341-348.	1.3	20
41	Fluorine NMR functional screening: from purified enzymes to human intact living cells. Journal of Biomolecular NMR, 2020, 74, 613-631.	1.6	20
42	Virtual screening to enrich a compound collection with CDK2 inhibitors using docking, scoring, and composite scoring models. Proteins: Structure, Function and Bioinformatics, 2005, 60, 629-643.	1.5	19
43	Hydrogen Bond Acceptor Propensity of Different Fluorine Atom Types: An Analysis of Experimentally and Computationally Derived Parameters. Chemistry - A European Journal, 2021, 27, 8764-8773.	1.7	18
44	Making sure there's a "give" associated with the "take": producing and using open-source software in big pharma. Journal of Cheminformatics, 2011, 3, .	2.8	16
45	Design, Synthesis, and Preclinical Characterization of Selective Factor D Inhibitors Targeting the Alternative Complement Pathway. Journal of Medicinal Chemistry, 2019, 62, 4656-4668.	2.9	16
46	Application of the rule of shielding in the design of novel fluorinated structural motifs and peptidomimetics. Journal of Fluorine Chemistry, 2013, 152, 129-135.	0.9	15
47	Design of Potent and Selective Covalent Inhibitors of Brutonâ€™s Tyrosine Kinase Targeting an Inactive Conformation. ACS Medicinal Chemistry Letters, 2019, 10, 1467-1472.	1.3	15
48	Discovery and Design of First Benzylamine-Based Ligands Binding to an Unlocked Conformation of the Complement Factor D. ACS Medicinal Chemistry Letters, 2018, 9, 490-495.	1.3	9
49	Largeâ€Scale Evaluation of CavBase for Analyzing the Polypharmacology of Kinase Inhibitors. Molecular Informatics, 2011, 30, 923-925.	1.4	5
50	Fluorine NMR spectroscopy and computational calculations for assessing intramolecular hydrogen bond involving fluorine and for characterizing the dynamic of a fluorinated molecule. Journal of Fluorine Chemistry, 2017, 202, 34-40.	0.9	4
51	Efficient Screening of Targetâ€Specific Selected Compounds in Mixtures by ¹⁹ F NMR Binding Assay with Predicted ¹⁹ F NMR Chemical Shifts. ChemMedChem, 2022, , .	1.6	4
52	Comprehensive and Highâ€Throughput Exploration of Chemical Space Using Broadband 19 Fâ€…NMRâ€Based Screening. Angewandte Chemie, 2020, 132, 14919-14927.	1.6	3
53	Pyrazoles as Efficient Adenine-Mimetic Heterocycles for the Discovery of CDK Inhibitors. Enzyme Inhibitors Series, 2006, , 323-347.	0.1	1
54	Assessment of Docking Poses: Interactions-Based Accuracy Classification (IBAC) versus Crystal Structure Deviations.. ChemInform, 2004, 35, no.	0.1	0

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55	Innentitelbild: Comprehensive and Highâ€Throughput Exploration of Chemical Space Using Broadband ¹⁹Fâ€…NMRâ€Based Screening (Angew. Chem. 35/2020). Angewandte Chemie, 2020, 132, 14806-14806.	1.6	0