Ann M Vos

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Molecular mechanisms of retroviral integrase inhibition and the evolution of viral resistance. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 20057-20062.	7.1	275
2	A Theoretical Study of the Alkylation Reaction of Toluene with Methanol Catalyzed by Acidic Mordenite. Journal of the American Chemical Society, 2001, 123, 2799-2809.	13.7	177
3	Resistance Mutations in Human Immunodeficiency Virus Type 1 Integrase Selected with Elvitegravir Confer Reduced Susceptibility to a Wide Range of Integrase Inhibitors. Journal of Virology, 2008, 82, 10366-10374.	3.4	153
4	Molecular blueprint of allosteric binding sites in a homologue of the agonist-binding domain of the α7 nicotinic acetylcholine receptor. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E2543-52.	7.1	102
5	Reactivity Descriptors and Rate Constants for Electrophilic Aromatic Substitution:Â Acid Zeolite Catalyzed Methylation of Benzene and Toluene. Journal of Physical Chemistry B, 2002, 106, 2026-2034.	2.6	90
6	1,4-Oxazine Î ² -Secretase 1 (BACE1) Inhibitors: From Hit Generation to Orally Bioavailable Brain Penetrant Leads. Journal of Medicinal Chemistry, 2015, 58, 8216-8235.	6.4	67
7	Primary mutations selected in vitro with raltegravir confer large fold changes in susceptibility to first-generation integrase inhibitors, but minor fold changes to inhibitors with second-generation resistance profiles. Virology, 2010, 402, 338-346.	2.4	58
8	Minisci-Photoredox-Mediated α-Heteroarylation of N-Protected Secondary Amines: Remarkable Selectivity of Azetidines. Organic Letters, 2018, 20, 6003-6006.	4.6	56
9	Structure-Based Site of Metabolism Prediction for Cytochrome P450 2D6. Journal of Medicinal Chemistry, 2011, 54, 6098-6105.	6.4	44
10	Synthesis and Evaluation of <i>N</i> -Phenyl-3-sulfamoyl-benzamide Derivatives as Capsid Assembly Modulators Inhibiting Hepatitis B Virus (HBV). Journal of Medicinal Chemistry, 2018, 61, 6247-6260.	6.4	40
11	1a/1b Subtype Profiling of Nonnucleoside Polymerase Inhibitors of Hepatitis C Virus. Journal of Virology, 2010, 84, 2923-2934.	3.4	39
12	Resistance to raltegravir highlights integrase mutations at codon 148 in conferring cross-resistance to a second-generation HIV-1 integrase inhibitor. Antiviral Research, 2011, 91, 167-176.	4.1	30
13	Reactivity Descriptors and Rate Constants for Acid Zeolite Catalyzed Ethylation and Isopropylation of Benzene. Journal of Physical Chemistry B, 2003, 107, 2001-2008.	2.6	29
14	Antiviral profiling of the capsid assembly modulator BAY41-4109 on full-length HBV genotype A-H clinical isolates and core site-directed mutants inÂvitro. Antiviral Research, 2017, 144, 205-215.	4.1	28
15	NO2 disproportionation for the IR characterisation of basic zeolites. Chemical Communications, 2005, , 1049.	4.1	20
16	Evaluation of a Series of β-Secretase 1 Inhibitors Containing Novel Heteroaryl-Fused-Piperazine Amidine Warheads. ACS Medicinal Chemistry Letters, 2019, 10, 1159-1165.	2.8	20
17	A computational and conceptual DFT approach to the kinetics of acid zeolite catalyzed electrophilic aromatic substitution reactions. Computational and Theoretical Chemistry, 2006, 762, 69-78.	1.5	18
	Discovery of		

18 3-({5-Chĺoro-1-[3-(methylsulfonyl)propyl]-1<i>H</i>indol-2-yl}methyl)-1-(2,2,2-trifluoroethyl)-1,3-dihydro-2<i>H</i>-imidazo[4,5-<i>c</i (JNJ-53718678), a Potent and Orally Bioavailable Fusion Inhibitor of Respiratory Syncytial Virus. Journal of Medicinal Chemistry, 2020, 63, 8046-8058.

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19	NO+: Infrared probe for basic zeolites. Studies in Surface Science and Catalysis, 2005, 158, 663-670.	1.5	14
20	Probing the basicity of zeolite frameworks with N2O4: A DFT approach. Microporous and Mesoporous Materials, 2006, 90, 370-376.	4.4	14
21	Fragment Binding to β-Secretase 1 without Catalytic Aspartate Interactions Identified via Orthogonal Screening Approaches. ACS Omega, 2017, 2, 685-697.	3.5	14
22	DFT study on the electrophilic aromatic substitution catalyzed byÂLewisÂacids. Journal of Catalysis, 2003, 220, 333-346.	6.2	13
23	Calculation of reaction rate constants for hydrogen–deuterium exchange reactions of methane catalysed by acid zeolites. Chemical Communications, 2001, , 1108-1109.	4.1	10
24	Preparation of 4′‧pirocyclobutyl Nucleoside Analogues as Novel and Versatile Adenosine Scaffolds. Chemistry - A European Journal, 2019, 25, 15419-15423.	3.3	10
25	JNJ-67569762, A 2-Aminotetrahydropyridine-Based Selective BACE1 Inhibitor Targeting the S3 Pocket: From Discovery to Clinical Candidate. Journal of Medicinal Chemistry, 2021, 64, 14175-14191.	6.4	10
26	Development and implementation of an enterprise-wide predictive model for early absorption, distribution, metabolismÂand excretion properties. Future Medicinal Chemistry, 2021, 13, 1639-1654.	2.3	7
27	3,3-Difluoro-3,4,5,6-tetrahydropyridin-2-amines: Potent and permeable BACE-1 inhibitors. Bioorganic and Medicinal Chemistry Letters, 2020, 30, 126999.	2.2	3
28	A Brain-Penetrant and Bioavailable Pyrazolopiperazine BACE1 Inhibitor Elicits Sustained Reduction of Amyloid β In Vivo. ACS Medicinal Chemistry Letters, 2022, 13, 76-83.	2.8	3
29	Divide and Conquer. Pocket-Opening Mixed-Solvent Simulations in the Perspective of Docking Virtual Screening Applications for Drug Discovery. Journal of Chemical Information and Modeling, 2022, 62, 533-543.	5.4	3
30	Modulating physicochemical properties of tetrahydropyridine-2-amine BACE1 inhibitors with electron-withdrawing groups: A systematic study. European Journal of Medicinal Chemistry, 2022, 228, 114028.	5.5	0