Zhuyan Guo

List of Publications by Year in descending order

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37	1,996	304368	344852
papers	citations	22 h-index	36 g-index

37	37	37	1824
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Kinetics of protein folding: Nucleation mechanism, time scales, and pathways. Biopolymers, 1995, 36, 83-102.	1.2	340
2	Discovery of (1R,5S)-N-[3-Amino-1-(cyclobutylmethyl)-2,3-dioxopropyl]-3-[2(S)-[[[(1,1-dimethylethyl)amino]carbonyl]amino]-3,3-dimethyl-1-oxobutyl]-6,6-dimethyl-3-azabicyclo[3.1.0]hexan-2(S)-carboxamide (SCH 503034), a Selective, Potent, Orally Bioavailable Hepatitis C Virus NS3 Protease Inhibitor:Â A Potential Therapeutic Agent for the Treatment of Hepatitis C Infection. Journal of Medicinal Chemistry, 2006, 49, 6074-6086.	2.9	248
3	Characterization of resistance mutations against HCV ketoamide protease inhibitors. Antiviral Research, 2008, 77, 177-185.	1.9	131
4	Folding kinetics of proteins: A model study. Journal of Chemical Physics, 1992, 97, 525-535.	1.2	116
5	Thermodynamics of protein folding: A statistical mechanical study of a small all-Î² protein. , 1997, 42, 745-757.		106
6	Discovery of the HCV NS3/4A Protease Inhibitor (1R,5S)-N-[3-Amino-1-(cyclobutylmethyl)-2,3-dioxopropyl]-3-[2(S)-[[[(1,1-dimethylethyl)amino]carbonyl]amino]-3,3-dimethyl-1-oxobutyl]-6,6-dimethyl-3-azabicyclo[3.1.0]hexan-2(S)-carboxamide (Sch 503034) II. Key Steps in Structure-Based Optimization. Journal of Medicinal Chemistry, 2007, 50, 2310-2318.	2.9	99
7	Toward Fast and Accurate Binding Affinity Prediction with pmemdGTI: An Efficient Implementation of GPU-Accelerated Thermodynamic Integration. Journal of Chemical Theory and Computation, 2017, 13, 3077-3084.	2.3	93
8	Exploring the space of protein folding Hamiltonians: The balance of forces in a minimalist Î²-barrel model. Journal of Chemical Physics, 1998, 109, 2895-2903.	1.2	92
9	Nucleation mechanism for protein folding and theoretical predictions for hydrogen-exchange labeling experiments. Biopolymers, 1995, 35, 137-140.	1.2	86
10	The nucleation-collapse mechanism in protein folding: evidence for the non-uniqueness of the folding nucleus. Folding & Design, 1997, 2, 377-391.	4.5	68
11	Discovery and SAR of hydantoin TACE inhibitors. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 1877-1880.	1.0	48
12	Impact of Naturally Occurring Variants of HCV Protease on the Binding of Different Classes of Protease Inhibitors. Biochemistry, 2006, 45, 1353-1361.	1.2	44
13	Rapid Screening of Binding Affinities:Â Application of the Î»-Dynamics Method to a Trypsin-Inhibitor System. Journal of the American Chemical Society, 1998, 120, 1920-1921.	6.6	41
14	Efficient Sampling of Ligand Orientations and Conformations in Free Energy Calculations Using the Î»-Dynamics Method. Journal of Physical Chemistry B, 2000, 104, 6903-6910.	1.2	38
15	Identification of HCV protease inhibitor resistance mutations by selection pressure-based method. Nucleic Acids Research, 2009, 37, e74-e74.	6.5	38
16	Discovery of MK-8831, A Novel Spiro-Proline Macrocycle as a Pan-Genotypic HCV-NS3/4a Protease Inhibitor. ACS Medicinal Chemistry Letters, 2016, 7, 111-116.	1.3	31
17	Discovery of novel hydroxamates as highly potent tumor necrosis factor-Î± converting enzyme inhibitors. Part II: Optimization of the S3â€² pocket. Bioorganic and Medicinal Chemistry Letters, 2008, 18, 5809-5814.	1.0	30
18	Discovery of Novel Hydroxamates as Highly Potent Tumor Necrosis Factor-Î± Converting Enzyme Inhibitors: Part Iî—¸Discovery of Two Binding Modesâ€. Journal of Medicinal Chemistry, 2008, 51, 725-736.	2.9	28

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19	The introduction of P4 substituted 1-methylcyclohexyl groups into BoceprevirÂ®: A change in direction in the search for a second generation HCV NS3 protease inhibitor. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 2617-2621.	1.0	27
20	The discovery of novel tartrate-based TNF-Î± converting enzyme (TACE) inhibitors. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 1189-1193.	1.0	26
21	2-(2-Aminothiazol-4-yl)pyrrolidine-based tartrate diamides as potent, selective and orally bioavailable TACE inhibitors. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 3172-3176.	1.0	25
22	The importance of protonation and tautomerization in relative binding affinity prediction: a comparison of AMBER TI and SchrÃ¶dinger FEP. Journal of Computer-Aided Molecular Design, 2016, 30, 533-539.	1.3	25
23	Biaryl substituted hydantoin compounds as TACE inhibitors. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 5286-5289.	1.0	23
24	Discovery of novel spirocyclopropyl hydroxamate and carboxylate compounds as TACE inhibitors. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 54-57.	1.0	22
25	Toward the Back-Up of Boceprevir (SCH 503034): Discovery of New Extended P₄-Capped Ketoamide Inhibitors of Hepatitis C Virus NS3 Serine Protease with Improved Potency and Pharmacokinetic Profiles. Journal of Medicinal Chemistry, 2009, 52, 3679-3688.	2.9	22
26	Novel Quinoline-Based P2â€“P4 Macrocyclic Derivatives As Pan-Genotypic HCV NS3/4a Protease Inhibitors. ACS Medicinal Chemistry Letters, 2014, 5, 264-269.	1.3	22
27	Computational Study of the Effects of Mutations A156T, D168V, and D168Q on the Binding of HCV Protease Inhibitors. Journal of Chemical Theory and Computation, 2006, 2, 1657-1663.	2.3	20
28	Novel TNF-Î± converting enzyme (TACE) inhibitors as potential treatment for inflammatory diseases. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 7283-7287.	1.0	20
29	Design and Synthesis of P2â€“P4 Macrocycles Containing a Unique Spirocyclic Proline: A New Class of HCV NS3/4A Inhibitors. ACS Medicinal Chemistry Letters, 2016, 7, 1173-1178.	1.3	20
30	Application of the Î»-Dynamics Method To Evaluate the Relative Binding Free Energies of Inhibitors to HCV Protease. Journal of Medicinal Chemistry, 2003, 46, 5360-5364.	2.9	18
31	Discovery of potent sulfonamide P4-capped ketoamide second generation inhibitors of hepatitis C virus NS3 serine protease with favorable pharmacokinetic profiles in preclinical species. Bioorganic and Medicinal Chemistry, 2010, 18, 1854-1865.	1.4	14
32	Structure and activity relationships of tartrate-based TACE inhibitors. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 4812-4815.	1.0	14
33	Fused bi-heteroaryl substituted hydantoin compounds as TACE inhibitors. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 3037-3042.	1.0	8
34	Towards the second generation of Boceprevir: Dithianes as an alternative P2 substituent for 2,2-dimethyl cycloproyl proline in HCV NS3 protease inhibitors. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 1689-1692.	1.0	6
35	Generation of a Chimeric Hepatitis C Replicon Encoding a Genotype-6a NS3 Protease and Assessment of Boceprevir (SCH503034) Sensitivity and Drug-Associated Mutations. Antiviral Therapy, 2015, 20, 271-280.	0.6	4
36	Key steps in the structure-based optimization of the hepatitis C virus NS3/4A protease inhibitor SCH503034. Journal of Synchrotron Radiation, 2008, 15, 204-207.	1.0	2

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37	Discovery of hydroxy pyrimidine Factor IXa inhibitors. Bioorganic and Medicinal Chemistry Letters, 2020, 30, 127279.	1.0	1