Gary Tresadern

List of Publications by Year
in descending order

79 papers	2,993 citations	126708 33 h-index	182168 51 g-index
79 all docs	79 docs citations	79 times ranked	3502 citing authors

#	Article	IF	Citations
1	Recognizing Pitfalls in Virtual Screening: A Critical Review. Journal of Chemical Information and Modeling, 2012, 52, 867-881.	2.5	358
2	Large scale relative protein ligand binding affinities using non-equilibrium alchemy. Chemical Science, 2020, 11, 1140-1152.	3.7	147
3	Best Practices for Alchemical Free Energy Calculations [Article v1.0]. Living Journal of Computational Molecular Science, 2020, 2, .	2.2	125
4	Molecular blueprint of allosteric binding sites in a homologue of the agonist-binding domain of the Î±7 nicotinic acetylcholine receptor. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E2543-52.	3.3	102
5	Application of Free Energy Perturbation for the Design of BACE1 Inhibitors. Journal of Chemical Information and Modeling, 2016, 56, 1856-1871.	2.5	92
6	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.	2.3	80
7	Scaffold hopping from pyridones to imidazo[1,2-a]pyridines. New positive allosteric modulators of metabotropic glutamate 2 receptor. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 175-179.	1.0	73
8	Discovery of 3-Cyclopropylmethyl-7-(4-phenylpiperidin-1-yl)-8-trifluoromethyl[1,2,4]triazolo[4,3-a]pyridine (JNJ-42153605): A Positive Allosteric Modulator of the Metabotropic Glutamate 2 Receptor. Journal of Medicinal Chemistry, 2012, 55, 8770-8789.	2.9	71
9	1,4-Oxazine Î²-Secretase 1 (BACE1) Inhibitors: From Hit Generation to Orally Bioavailable Brain Penetrant Leads. Journal of Medicinal Chemistry, 2015, 58, 8216-8235.	2.9	67
10	Acylguanidine Beta Secretase 1 Inhibitors: A Combined Experimental and Free Energy Perturbation Study. Journal of Chemical Theory and Computation, 2017, 13, 1439-1453.	2.3	67
11	QM/MM Studies Show Substantial Tunneling for the Hydrogen-Transfer Reaction in Methylamine Dehydrogenase. Journal of the American Chemical Society, 2001, 123, 8604-8605.	6.6	62
12	Benzazaborinines as Novel Bioisosteric Replacements of Naphthalene: Propranolol as an Example. Journal of Medicinal Chemistry, 2015, 58, 9287-9295.	2.9	62
13	A comparison of ligand based virtual screening methods and application to corticotropin releasing factor 1 receptor. Journal of Molecular Graphics and Modelling, 2009, 27, 860-870.	1.3	59
14	Design and Synthesis of a Novel Series of Bicyclic Heterocycles As Potent Î³-Secretase Modulators. Journal of Medicinal Chemistry, 2012, 55, 9089-9106.	2.9	59
15	Calculations of hydrogen tunnelling and enzyme catalysis: a comparison of liver alcohol dehydrogenase, methylamine dehydrogenase and soybean lipoxygenase. Chemical Physics Letters, 2002, 358, 489-494.	1.2	56
16	Imidazo[1,2-a]pyridines: Orally Active Positive Allosteric Modulators of the Metabotropic Glutamate 2 Receptor. Journal of Medicinal Chemistry, 2012, 55, 2688-2701.	2.9	55
17	Discovery of 1-Butyl-3-chloro-4-(4-phenyl-1-piperidinyl)-(1H)-pyridone (JNJ-40411813): A Novel Positive Allosteric Modulator of the Metabotropic Glutamate 2 Receptor. Journal of Medicinal Chemistry, 2014, 57, 6495-6512.	2.9	54
18	Product ion mobility as a promising tool for assignment of positional isomers of drug metabolites. Rapid Communications in Mass Spectrometry, 2011, 25, 3497-3503.	0.7	50

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19	Pyrido[4,3-e][1,2,4]triazolo[4,3-a]pyrazines as Selective, Brain Penetrant Phosphodiesterase 2 (PDE2) Inhibitors. ACS Medicinal Chemistry Letters, 2015, 6, 282-286.	1.3	49
20	DeltaDelta neural networks for lead optimization of small molecule potency. Chemical Science, 2019, 10, 10911-10918.	3.7	48
21	Alchemical absolute proteinâ€“ligand binding free energies for drug design. Chemical Science, 2021, 12, 13958-13971.	3.7	48
22	Molecular properties affecting fast dissociation from the D2 receptor. Bioorganic and Medicinal Chemistry, 2011, 19, 2231-2241.	1.4	46
23	Extending kinome coverage by analysis of kinase inhibitor broad profiling data. Drug Discovery Today, 2015, 20, 652-658.	3.2	46
24	Accurate Prediction of GPCR Ligand Binding Affinity with Free Energy Perturbation. Journal of Chemical Information and Modeling, 2020, 60, 5563-5579.	2.5	45
25	Rational design and synthesis of aminopiperazinones as Î²-secretase (BACE) inhibitors. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 7255-7260.	1.0	44
26	Progress in the Developement of Positive Allosteric Modulators of the Metabotropic Glutamate Receptor 2. Current Medicinal Chemistry, 2011, 18, 47-68.	1.2	44
27	Predicting Binding Free Energies of PDE2 Inhibitors. The Difficulties of Protein Conformation. Scientific Reports, 2018, 8, 4883.	1.6	43
28	Structure-Based Design of a Potent, Selective, and Brain Penetrating PDE2 Inhibitor with Demonstrated Target Engagement. ACS Medicinal Chemistry Letters, 2014, 5, 1049-1053.	1.3	41
29	Molecular Switches of Allosteric Modulation of the Metabotropic Glutamate 2 Receptor. Structure, 2017, 25, 1153-1162.e4.	1.6	41
30	Molecular mechanism of positive allosteric modulation of the metabotropic glutamate receptor 2 by JNJâ€46281222. British Journal of Pharmacology, 2016, 173, 588-600.	2.7	39
31	Extreme tunnelling in methylamine dehydrogenase revealed by hybrid QM/MM calculations: potential energy surface profile for methylamine and ethanolamine substrates and kinetic isotope effect values. Molecular Physics, 2003, 101, 2775-2784.	0.8	37
32	Molecular determinants of positive allosteric modulation of the human metabotropic glutamate receptor 2. British Journal of Pharmacology, 2015, 172, 2383-2396.	2.7	37
33	Predicting Activity Cliffs with Free-Energy Perturbation. Journal of Chemical Theory and Computation, 2019, 15, 1884-1895.	2.3	37
34	Discovery of 8-Trifluoromethyl-3-cyclopropylmethyl-7-[(4-(2,4-difluorophenyl)-1-piperazinyl)methyl]-1,2,4-triazolo[4,3-a]pyridine (JNJ-46356479), a Selective and Orally Bioavailable mGlu2 Receptor Positive Allosteric Modulator (PAM). Journal of Medicinal Chemistry, 2016, 59, 8495-8507.	2.9	35
35	Discovery and Kinetic Profiling of 7-Aryl-1,2,4-triazolo[4,3-a]pyridines: Positive Allosteric Modulators of the Metabotropic Glutamate Receptor 2. Journal of Medicinal Chemistry, 2017, 60, 6704-6720.	2.9	35
36	Discovery of 1,4-Disubstituted 3-Cyano-2-pyridones: A New Class of Positive Allosteric Modulators of the Metabotropic Glutamate 2 Receptor. Journal of Medicinal Chemistry, 2012, 55, 2388-2405.	2.9	33

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37	Accuracy and Precision of Alchemical Relative Free Energy Predictions with and without Replicaâ€Exchange. Advanced Theory and Simulations, 2020, 3, 1900195.	1.3	30
38	Benchmark assessment of molecular geometries and energies from small molecule force fields. F1000Research, 2020, 9, 1390.	0.8	30
39	Direct dynamics calculations of reaction rate and kinetic isotope effects in enzyme catalysed reactions. Faraday Discussions, 2003, 122, 223-242.	1.6	29
40	The Prokaryote Ligand-Gated Ion Channel ELIC Captured in a Pore Blocker-Bound Conformation by the Alzheimerâ€™s Disease Drug Memantine. Structure, 2014, 22, 1399-1407.	1.6	27
41	Non-equilibrium approach for binding free energies in cyclodextrins in SAMPL7: force fields and software. Journal of Computer-Aided Molecular Design, 2021, 35, 49-61.	1.3	23
42	Mechanism of covalent binding of ibrutinib to Bruton's tyrosine kinase revealed by QM/MM calculations. Chemical Science, 2021, 12, 5511-5516.	3.7	22
43	Pre-Exascale Computing of Proteinâ€“Ligand Binding Free Energies with Open Source Software for Drug Design. Journal of Chemical Information and Modeling, 2022, 62, 1172-1177.	2.5	22
44	Discovery of 1,5-Disubstituted Pyridones: A New Class of Positive Allosteric Modulators of the Metabotropic Glutamate 2 Receptor. ACS Chemical Neuroscience, 2010, 1, 788-795.	1.7	21
45	Mechanisms Underlying Allosteric Molecular Switches of Metabotropic Glutamate Receptor 5. Journal of Chemical Information and Modeling, 2019, 59, 2456-2466.	2.5	21
46	Dihydrothiazolopyridone Derivatives as a Novel Family of Positive Allosteric Modulators of the Metabotropic Glutamate 5 (mGlu₅) Receptor. Journal of Medicinal Chemistry, 2013, 56, 7243-7259.	2.9	20
47	QSAR design of triazolopyridine mGlu2 receptor positive allosteric modulators. Journal of Molecular Graphics and Modelling, 2014, 53, 82-91.	1.3	20
48	Evaluation of a Series of Î²-Secretase 1 Inhibitors Containing Novel Heteroaryl-Fused-Piperazine Amidine Warheads. ACS Medicinal Chemistry Letters, 2019, 10, 1159-1165.	1.3	20
49	Design and synthesis of bicyclic heterocycles as potent Î³-secretase modulators. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 4794-4800.	1.0	18
50	Identification of Allosteric Modulators of Metabotropic Glutamate 7 Receptor Using Proteochemometric Modeling. Journal of Chemical Information and Modeling, 2017, 57, 2976-2985.	2.5	18
51	Application of ESMACS binding free energy protocols to diverse datasets: Bromodomain-containing protein 4. Scientific Reports, 2019, 9, 6017.	1.6	18
52	Anilinotriazoles as potent gamma secretase modulators. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 5805-5813.	1.0	17
53	Covalent Allosteric Probe for the Metabotropic Glutamate ReceptorÂ2: Design, Synthesis, and Pharmacological Characterization. Journal of Medicinal Chemistry, 2019, 62, 223-233.	2.9	17
54	Recent advances in quantum mechanical/molecular mechanical calculations of enzyme catalysis: hydrogen tunnelling in liver alcohol dehydrogenase and inhibition of elastase by Î±-ketoheterocycles. Theoretical Chemistry Accounts, 2003, 109, 108-117.	0.5	16

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55	A Versatile Approach to CF₃â€Containing 2â€Pyrrolidones by Tandem Michael Additionâ€“Cyclization: Exemplification in the Synthesis of Amidine Class BACE1 Inhibitors. Chemistry - A European Journal, 2015, 21, 11719-11726.	1.7	16
56	Constitutive activity of the metabotropic glutamate receptor 2 explored with a whole-cell label-free biosensor. Biochemical Pharmacology, 2018, 152, 201-210.	2.0	16
57	mGlu2 Receptor Agonism, but Not Positive Allosteric Modulation, Elicits Rapid Tolerance towards Their Primary Efficacy on Sleep Measures in Rats. PLoS ONE, 2015, 10, e0144017.	1.1	16
58	Limitations of Ligand-Only Approaches for Predicting the Reactivity of Covalent Inhibitors. Journal of Chemical Information and Modeling, 2019, 59, 4220-4227.	2.5	15
59	Modeling approaches for ligand-based 3D similarity. Future Medicinal Chemistry, 2010, 2, 1547-1561.	1.1	14
60	Design, Synthesis, and Biological Evaluation of Novel Fluorinated Ethanolamines. Chemistry - A European Journal, 2011, 17, 14772-14784.	1.7	14
61	Fragment Binding to Î²-Secretase 1 without Catalytic Aspartate Interactions Identified via Orthogonal Screening Approaches. ACS Omega, 2017, 2, 685-697.	1.6	14
62	[1,2,4]Triazolo[1,5-a]pyrimidine Phosphodiesterase 2A Inhibitors: Structure and Free-Energy Perturbation-Guided Exploration. Journal of Medicinal Chemistry, 2020, 63, 12887-12910.	2.9	14
63	Conformational Sampling with Stochastic Proximity Embedding and Self-Organizing Superimposition: Establishing Reasonable Parameters for Their Practical Use. Journal of Chemical Information and Modeling, 2009, 49, 2786-2800.	2.5	12
64	Diazaspirononane Nonsaccharide Inhibitors of O-GlcNAcase (OGA) for the Treatment of Neurodegenerative Disorders. Journal of Medicinal Chemistry, 2020, 63, 14017-14044.	2.9	10
65	Application of the ESMACS Binding Free Energy Protocol to a Multiâ€Binding Site Lactate Dehydogenase A Ligand Dataset. Advanced Theory and Simulations, 2020, 3, 1900194.	1.3	9
66	Selective inhibition of intestinal guanosine 3â€²,5â€²-cyclic monophosphate signaling by small-molecule protein kinase inhibitors. Journal of Biological Chemistry, 2018, 293, 8173-8181.	1.6	8
67	Computational Drug Design Applied to the Study of Metabotropic Glutamate Receptors. Molecules, 2019, 24, 1098.	1.7	8
68	Inhibition of the Alanine-Serine-Cysteine-1 Transporter by BMS-466442. ACS Chemical Neuroscience, 2019, 10, 2510-2517.	1.7	8
69	Monte Carlo simulations using PELE to identify a proteinâ€“protein inhibitor binding site and pose. RSC Advances, 2020, 10, 7058-7064.	1.7	7
70	Impact of allosteric modulation: Exploring the binding kinetics of glutamate and other orthosteric ligands of the metabotropic glutamate receptor 2. Biochemical Pharmacology, 2018, 155, 356-365.	2.0	6
71	Industrial medicinal chemistry insights: neuroscience hit generation at Janssen. Drug Discovery Today, 2017, 22, 1478-1488.	3.2	5
72	Computationally Guided Identification of Allosteric Agonists of the Metabotropic Glutamate 7 Receptor. ACS Chemical Neuroscience, 2019, 10, 1043-1054.	1.7	5

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73	Spiro-oxindole Piperidines and 3-(Azetidin-3-yl)-1H-benzimidazol-2-ones as mGlu₂ Receptor PAMs. ACS Medicinal Chemistry Letters, 2020, 11, 303-308.	1.3	5
74	The Impact of Experimental and Calculated Error on the Performance of Affinity Predictions. Journal of Chemical Information and Modeling, 2022, 62, 703-717.	2.5	4
75	Hydride shift in substituted phenyl glyoxals: Interpretation of experimental rate data using electronic structure and variational transition state theory calculations. Physical Chemistry Chemical Physics, 2001, 3, 3967-3972.	1.3	3
76	A Brain-Penetrant and Bioavailable Pyrazolopiperazine BACE1 Inhibitor Elicits Sustained Reduction of Amyloid Î² In Vivo. ACS Medicinal Chemistry Letters, 2022, 13, 76-83.	1.3	3
77	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.	2.5	3
78	The computational modeling of allosteric modulation of metabotropic glutamate receptors. Advances in Pharmacology, 2020, 88, 1-33.	1.2	1
79	Scaffold Hopping to Imidazo[1,2-a]pyrazin-8-one Positive Allosteric Modulators of Metabotropic Glutamate 2 Receptor. ACS Omega, 2021, 6, 22997-23006.	1.6	1