# Gary Tresadern

## List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/4694213/publications.pdf

Version: 2024-02-01

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|---|---|---|---|
| 79 papers | 2,993 citations | 126907 33 h-index | 182427 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. | 5.4 | 358 |
| 2 | Large scale relative protein ligand binding affinities using non-equilibrium alchemy. Chemical Science, 2020, 11, 1140-1152. | 7.4 | 147 |
| 3 | Best Practices for Alchemical Free Energy Calculations [Article v1.0]. Living Journal of Computational Molecular Science, 2020, 2, . | 6.4 | 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. | 7.1 | 102 |
| 5 | Application of Free Energy Perturbation for the Design of BACE1 Inhibitors. Journal of Chemical Information and Modeling, 2016, 56, 1856-1871. | 5.4 | 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. | 5.3 | 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. | 2.2 | 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. | 6.4 | 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. | 6.4 | 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. | 5.3 | 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. | 13.7 | 62 |
| 12 | Benzazaborinines as Novel Bioisosteric Replacements of Naphthalene: Propranolol as an Example. Journal of Medicinal Chemistry, 2015, 58, 9287-9295. | 6.4 | 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. | 2.4 | 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. | 6.4 | 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. | 2.6 | 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. | 6.4 | 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. | 6.4 | 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. | 1.5 | 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. | 2.8 | 49 |
| 20 | DeltaDelta neural networks for lead optimization of small molecule potency. Chemical Science, 2019, 10, 10911-10918. | 7.4 | 48 |
| 21 | Alchemical absolute proteinâ€“ligand binding free energies for drug design. Chemical Science, 2021, 12, 13958-13971. | 7.4 | 48 |
| 22 | Molecular properties affecting fast dissociation from the D2 receptor. Bioorganic and Medicinal Chemistry, 2011, 19, 2231-2241. | 3.0 | 46 |
| 23 | Extending kinome coverage by analysis of kinase inhibitor broad profiling data. Drug Discovery Today, 2015, 20, 652-658. | 6.4 | 46 |
| 24 | Accurate Prediction of GPCR Ligand Binding Affinity with Free Energy Perturbation. Journal of Chemical Information and Modeling, 2020, 60, 5563-5579. | 5.4 | 45 |
| 25 | Rational design and synthesis of aminopiperazinones as Î²-secretase (BACE) inhibitors. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 7255-7260. | 2.2 | 44 |
| 26 | Progress in the Developement of Positive Allosteric Modulators of the Metabotropic Glutamate Receptor 2. Current Medicinal Chemistry, 2011, 18, 47-68. | 2.4 | 44 |
| 27 | Predicting Binding Free Energies of PDE2 Inhibitors. The Difficulties of Protein Conformation. Scientific Reports, 2018, 8, 4883. | 3.3 | 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. | 2.8 | 41 |
| 29 | Molecular Switches of Allosteric Modulation of the Metabotropic Glutamate 2 Receptor. Structure, 2017, 25, 1153-1162.e4. | 3.3 | 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. | 5.4 | 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. | 1.7 | 37 |
| 32 | Molecular determinants of positive allosteric modulation of the human metabotropic glutamate receptor 2. British Journal of Pharmacology, 2015, 172, 2383-2396. | 5.4 | 37 |
| 33 | Predicting Activity Cliffs with Free-Energy Perturbation. Journal of Chemical Theory and Computation, 2019, 15, 1884-1895. | 5.3 | 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. | 6.4 | 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. | 6.4 | 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. | 6.4 | 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. | 2.8 | 30 |
| 38 | Benchmark assessment of molecular geometries and energies from small molecule force fields. F1000Research, 2020, 9, 1390. | 1.6 | 30 |
| 39 | Direct dynamics calculations of reaction rate and kinetic isotope effects in enzyme catalysed reactions. Faraday Discussions, 2003, 122, 223-242. | 3.2 | 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. | 3.3 | 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. | 2.9 | 23 |
| 42 | Mechanism of covalent binding of ibrutinib to Bruton's tyrosine kinase revealed by QM/MM calculations. Chemical Science, 2021, 12, 5511-5516. | 7.4 | 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. | 5.4 | 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. | 3.5 | 21 |
| 45 | Mechanisms Underlying Allosteric Molecular Switches of Metabotropic Glutamate Receptor 5. Journal of Chemical Information and Modeling, 2019, 59, 2456-2466. | 5.4 | 21 |
| 46 | Dihydrothiazolopyridone Derivatives as a Novel Family of Positive Allosteric Modulators of the Metabotropic Glutamate 5 (mGlu<sub>5</sub>) Receptor. Journal of Medicinal Chemistry, 2013, 56, 7243-7259. | 6.4 | 20 |
| 47 | QSAR design of triazolopyridine mGlu2 receptor positive allosteric modulators. Journal of Molecular Graphics and Modelling, 2014, 53, 82-91. | 2.4 | 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. | 2.8 | 20 |
| 49 | Design and synthesis of bicyclic heterocycles as potent Î³-secretase modulators. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 4794-4800. | 2.2 | 18 |
| 50 | Identification of Allosteric Modulators of Metabotropic Glutamate 7 Receptor Using Proteochemometric Modeling. Journal of Chemical Information and Modeling, 2017, 57, 2976-2985. | 5.4 | 18 |
| 51 | Application of ESMACS binding free energy protocols to diverse datasets: Bromodomain-containing protein 4. Scientific Reports, 2019, 9, 6017. | 3.3 | 18 |
| 52 | Anilinotriazoles as potent gamma secretase modulators. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 5805-5813. | 2.2 | 17 |
| 53 | Covalent Allosteric Probe for the Metabotropic Glutamate ReceptorÂ2: Design, Synthesis, and Pharmacological Characterization. Journal of Medicinal Chemistry, 2019, 62, 223-233. | 6.4 | 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. | 1.4 | 16 |

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|---|---|---|---|
| 55 | A Versatile Approach to CF<sub>3</sub>â€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. | 3.3 | 16 |
| 56 | Constitutive activity of the metabotropic glutamate receptor 2 explored with a whole-cell label-free biosensor. Biochemical Pharmacology, 2018, 152, 201-210. | 4.4 | 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. | 2.5 | 16 |
| 58 | Limitations of Ligand-Only Approaches for Predicting the Reactivity of Covalent Inhibitors. Journal of Chemical Information and Modeling, 2019, 59, 4220-4227. | 5.4 | 15 |
| 59 | Modeling approaches for ligand-based 3D similarity. Future Medicinal Chemistry, 2010, 2, 1547-1561. | 2.3 | 14 |
| 60 | Design, Synthesis, and Biological Evaluation of Novel Fluorinated Ethanolamines. Chemistry - A European Journal, 2011, 17, 14772-14784. | 3.3 | 14 |
| 61 | Fragment Binding to Î²-Secretase 1 without Catalytic Aspartate Interactions Identified via Orthogonal Screening Approaches. ACS Omega, 2017, 2, 685-697. | 3.5 | 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. | 6.4 | 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. | 5.4 | 12 |
| 64 | Diazaspirononane Nonsaccharide Inhibitors of O-GlcNAcase (OGA) for the Treatment of Neurodegenerative Disorders. Journal of Medicinal Chemistry, 2020, 63, 14017-14044. | 6.4 | 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. | 2.8 | 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. | 3.4 | 8 |
| 67 | Computational Drug Design Applied to the Study of Metabotropic Glutamate Receptors. Molecules, 2019, 24, 1098. | 3.8 | 8 |
| 68 | Inhibition of the Alanine-Serine-Cysteine-1 Transporter by BMS-466442. ACS Chemical Neuroscience, 2019, 10, 2510-2517. | 3.5 | 8 |
| 69 | Monte Carlo simulations using PELE to identify a proteinâ€“protein inhibitor binding site and pose. RSC Advances, 2020, 10, 7058-7064. | 3.6 | 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. | 4.4 | 6 |
| 71 | Industrial medicinal chemistry insights: neuroscience hit generation at Janssen. Drug Discovery Today, 2017, 22, 1478-1488. | 6.4 | 5 |
| 72 | Computationally Guided Identification of Allosteric Agonists of the Metabotropic Glutamate 7 Receptor. ACS Chemical Neuroscience, 2019, 10, 1043-1054. | 3.5 | 5 |

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|---|---|---|---|
| 73 | Spiro-oxindole Piperidines and 3-(Azetidin-3-yl)-1H-benzimidazol-2-ones as mGlu<sub>2</sub> Receptor PAMs. ACS Medicinal Chemistry Letters, 2020, 11, 303-308. | 2.8 | 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. | 5.4 | 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. | 2.8 | 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. | 2.8 | 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. | 5.4 | 3 |
| 78 | The computational modeling of allosteric modulation of metabotropic glutamate receptors. Advances in Pharmacology, 2020, 88, 1-33. | 2.0 | 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. | 3.5 | 1 |