

David Kenneth Chalmers

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/8314057/publications.pdf>

Version: 2024-02-01

94
papers

2,870
citations

172443

29
h-index

189881

50
g-index

97
all docs

97
docs citations

97
times ranked

4250
citing authors

#	ARTICLE	IF	CITATIONS
1	Status of GPCR Modeling and Docking as Reflected by Community-wide GPCR Dock 2010 Assessment. Structure, 2011, 19, 1108-1126.	3.3	269
2	The significance of acid/base properties in drug discovery. Chemical Society Reviews, 2013, 42, 485-496.	38.1	236
3	Pro-D-NMe-Amino Acid and D-Pro-NMe-Amino Acid: Simple, Efficient Reverse-Turn Constraints. Journal of the American Chemical Society, 1995, 117, 5927-5937.	13.7	134
4	Discovery of 7-Hydroxy-6-methoxy-2-methyl-3-(3,4,5-trimethoxybenzoyl)benzo[<i>b</i>]furan (BNC105), a Tubulin Polymerization Inhibitor with Potent Antiproliferative and Tumor Vascular Disrupting Properties. Journal of Medicinal Chemistry, 2011, 54, 6014-6027.	6.4	133
5	Free Energy Methods in Drug Design: Prospects of α -Chemical Perturbation in Medicinal Chemistry. Journal of Medicinal Chemistry, 2018, 61, 638-649.	6.4	125
6	Comparisons of the Hbv and HIV Polymerase, and Antiviral Resistance Mutations. Antiviral Therapy, 2004, 9, 149-160.	1.0	112
7	Molecular dynamics simulations of spontaneous bile salt aggregation. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2006, 280, 182-193.	4.7	92
8	Homology Modeling and Docking Evaluation of Aminergic G Protein-Coupled Receptors. Journal of Chemical Information and Modeling, 2010, 50, 626-637.	5.4	91
9	Potent and Long-Acting Dimeric Inhibitors of Influenza Virus Neuraminidase Are Effective at a Once-Weekly Dosing Regimen. Antimicrobial Agents and Chemotherapy, 2004, 48, 4542-4549.	3.2	81
10	Electrochemical Cyclization of Dipeptides To Form Novel Bicyclic, Reverse-Turn Peptidomimetics. 2. Synthesis and Conformational Analysis of 6,5-Bicyclic Systems. Journal of Organic Chemistry, 1996, 61, 1198-1204.	3.2	62
11	Parallel Screening of Low Molecular Weight Fragment Libraries: Do Differences in Methodology Affect Hit Identification?. Journal of Biomolecular Screening, 2013, 18, 147-159.	2.6	61
12	2-Ethoxybenzoxazole as a bioisosteric replacement of an ethyl benzoate group in a human rhinovirus (HRV) capsid binder. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 2051-2055.	2.2	60
13	2-Aminothienopyridazines as Novel Adenosine A1 Receptor Allosteric Modulators and Antagonists. Journal of Medicinal Chemistry, 2008, 51, 6165-6172.	6.4	54
14	A Three-dimensional Model of the Human Immunodeficiency Virus Type 1 Integration Complex. Journal of Computer-Aided Molecular Design, 2005, 19, 301-317.	2.9	51
15	An Orally Bioavailable Oxime Ether Capsid Binder with Potent Activity against Human Rhinovirus. Journal of Medicinal Chemistry, 2003, 46, 3181-3184.	6.4	47
16	Cyclosporin Structure and Permeability: From A to Z and Beyond. Journal of Medicinal Chemistry, 2021, 64, 13131-13151.	6.4	43
17	A Chemogenomic Analysis of Ionization Constants's Implications for Drug Discovery. ChemMedChem, 2013, 8, 242-255.	3.2	40
18	Digestion of Phospholipids after Secretion of Bile into the Duodenum Changes the Phase Behavior of Bile Components. Molecular Pharmaceutics, 2014, 11, 2825-2834.	4.6	40

#	ARTICLE	IF	CITATIONS
19	Polymeric Precipitation Inhibitors Promote Fenofibrate Supersaturation and Enhance Drug Absorption from a Type IV Lipid-Based Formulation. <i>Molecular Pharmaceutics</i> , 2018, 15, 2355-2371.	4.6	40
20	Crystal structure of the HIV-1 integrase core domain in complex with sucrose reveals details of an allosteric inhibitory binding site. <i>FEBS Letters</i> , 2010, 584, 1455-1462.	2.8	38
21	Molecular Dynamics of Poly(<i>l</i> -lysine) Dendrimers with Naphthalene Disulfonate Caps. <i>Macromolecules</i> , 2009, 42, 2775-2783.	4.8	37
22	Thyroid hormone uptake by hepatocytes: structure-activity relationships of phenylanthranilic acids with inhibitory activity. <i>Journal of Medicinal Chemistry</i> , 1993, 36, 1272-1277.	6.4	36
23	Parallel and antiparallel cyclic <i>d</i> / <i>l</i> peptide nanotubes. <i>Chemical Communications</i> , 2017, 53, 6613-6616.	4.1	36
24	Using Molecular Dynamics to Study Liquid Phase Behavior: Simulations of the Ternary Sodium Laurate/Sodium Oleate/Water System. <i>Langmuir</i> , 2011, 27, 11381-11393.	3.5	35
25	Glyceride Lipid Formulations: Molecular Dynamics Modeling of Phase Behavior During Dispersion and Molecular Interactions Between Drugs and Excipients. <i>Pharmaceutical Research</i> , 2013, 30, 3238-3253.	3.5	33
26	How kanamycin A interacts with bacterial and mammalian mimetic membranes. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2017, 1859, 2242-2252.	2.6	33
27	The binding interaction of synthetic ozonide antimalarials with natural and modified β -cyclodextrins. <i>Journal of Pharmaceutical Sciences</i> , 2006, 95, 146-158.	3.3	32
28	Ligand Binding Pathways of Clozapine and Haloperidol in the Dopamine D ₂ and D ₃ Receptors. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 308-321.	5.4	31
29	Structure and Dynamics of Glyceride Lipid Formulations, with Propylene Glycol and Water. <i>Molecular Pharmaceutics</i> , 2009, 6, 604-614.	4.6	30
30	Computational Models of the Gastrointestinal Environment. 2. Phase Behavior and Drug Solubilization Capacity of a Type I Lipid-Based Drug Formulation after Digestion. <i>Molecular Pharmaceutics</i> , 2017, 14, 580-592.	4.6	30
31	<i>l</i> -Aminoacyl-triazine Derivatives Are Isoform-Selective PI3K β Inhibitors That Target Nonconserved Asp862 of PI3K β . <i>ACS Medicinal Chemistry Letters</i> , 2013, 4, 206-210.	2.8	27
32	Computational Models of the Gastrointestinal Environment. 1. The Effect of Digestion on the Phase Behavior of Intestinal Fluids. <i>Molecular Pharmaceutics</i> , 2017, 14, 566-579.	4.6	27
33	Computational Models of the Intestinal Environment. 3. The Impact of Cholesterol Content and pH on Mixed Micelle Colloids. <i>Molecular Pharmaceutics</i> , 2017, 14, 3684-3697.	4.6	26
34	Improving Membrane Permeation in the Beyond Rule-of-Five Space by Using Prodrugs to Mask Hydrogen Bond Donors. <i>ACS Chemical Biology</i> , 2020, 15, 2070-2078.	3.4	26
35	A Potent Cyclic Peptide Targeting SPSB2 Protein as a Potential Anti-infective Agent. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 7006-7015.	6.4	25
36	Fragment-Based Design of Ligands Targeting a Novel Site on the Integrase Enzyme of Human Immunodeficiency Virus-1. <i>ChemMedChem</i> , 2011, 6, 258-261.	3.2	24

#	ARTICLE	IF	CITATIONS
37	Molecular Dynamics of Variegated Polyamide Dendrimers. <i>Macromolecules</i> , 2009, 42, 2784-2794.	4.8	22
38	Homology Modeling of Human Muscarinic Acetylcholine Receptors. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 243-253.	5.4	22
39	Identification of mechanistically distinct inhibitors of HIV-1 reverse transcriptase through fragment screening. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 6979-6984.	7.1	22
40	Structure-Activity Studies of β -Hairpin Peptide Inhibitors of the Plasmodium falciparum AMA1-RON2 Interaction. <i>Journal of Molecular Biology</i> , 2016, 428, 3986-3998.	4.2	22
41	Crystal structure of the β 1B-adrenergic receptor reveals molecular determinants of selective ligand recognition. <i>Nature Communications</i> , 2022, 13, 382.	12.8	21
42	A Nonionic Polyethylene Oxide (PEO) Surfactant Model: Experimental and Molecular Dynamics Studies of Kolliphor EL. <i>Journal of Pharmaceutical Sciences</i> , 2019, 108, 193-204.	3.3	20
43	Determination of ligand binding modes in weak protein-ligand complexes using sparse NMR data. <i>Journal of Biomolecular NMR</i> , 2016, 66, 195-208.	2.8	19
44	Design, Synthesis, and Characterization of Cyclic Peptidomimetics of the Inducible Nitric Oxide Synthase Binding Epitope That Disrupt the Protein-Protein Interaction Involving SPRY Domain-Containing Suppressor of Cytokine Signaling Box Protein (SPSB) 2 and Inducible Nitric Oxide Synthase. <i>Journal of Medicinal Chemistry</i> , 2016, 59, 5799-5809.	6.4	19
45	Enantioselective Synthesis of Cyclothiazide Analogues: A Novel Probes of the Stereospecific Actions of Benzothiadiazines at AMPA-Type Glutamate Receptors. <i>Journal of the American Chemical Society</i> , 1996, 118, 4550-4559.	13.7	17
46	Conformational Analysis of Drug Molecules: A Practical Exercise in the Medicinal Chemistry Course. <i>Journal of Chemical Education</i> , 2009, 86, 477.	2.3	17
47	Probing the Fibrate Binding Specificity of Rat Liver Fatty Acid Binding Protein. <i>Journal of Medicinal Chemistry</i> , 2009, 52, 5344-5355.	6.4	17
48	Redox-stable cyclic peptide inhibitors of the SPSB2-iNOS interaction. <i>FEBS Letters</i> , 2016, 590, 696-704.	2.8	17
49	A Cyclic Peptide Inhibitor of the iNOS-SPSB Protein-Protein Interaction as a Potential Anti-Infective Agent. <i>ACS Chemical Biology</i> , 2018, 13, 2930-2938.	3.4	17
50	Conformational Changes in Tyrosine 11 of Neurotensin Are Required to Activate the Neurotensin Receptor 1. <i>ACS Pharmacology and Translational Science</i> , 2020, 3, 690-705.	4.9	16
51	Thiazolidinedione-Based PI3K Inhibitors: An Analysis of Biochemical and Virtual Screening Methods. <i>ChemMedChem</i> , 2011, 6, 514-522.	3.2	15
52	Synthesis and Pharmacological Evaluation of 4-Iminothiazolidinones for Inhibition of PI3 Kinase. <i>Australian Journal of Chemistry</i> , 2012, 65, 1396.	0.9	15
53	Virtual screening using a conformationally flexible target protein: models for ligand binding to p38 MAPK. <i>Journal of Computer-Aided Molecular Design</i> , 2012, 26, 409-423.	2.9	15
54	Models for the binding of amiodarone to the thyroid hormone receptor. <i>Journal of Computer-Aided Molecular Design</i> , 1992, 6, 19-31.	2.9	13

#	ARTICLE	IF	CITATIONS
55	Toward activated homology models of the human M1 muscarinic acetylcholine receptor. <i>Journal of Molecular Graphics and Modelling</i> , 2014, 49, 91-98.	2.4	13
56	Structure and activity of contryphan-Vc2: Importance of the d -amino acid residue. <i>Toxicon</i> , 2017, 129, 113-122.	1.6	13
57	The conformational and biological analysis of a cyclic anti-obesity peptide from the C-terminal domain of human growth hormone. <i>Chemical Biology and Drug Design</i> , 2000, 56, 388-397.	1.1	12
58	Design, Synthesis, and Biological Evaluation of Tetra-Substituted Thiophenes as Inhibitors of p38 MAPK. <i>ChemistryOpen</i> , 2015, 4, 56-64.	1.9	12
59	Production of metabolites of the anti-cancer drug noscapine using a P450BM3 mutant library. <i>Biotechnology Reports (Amsterdam, Netherlands)</i> , 2019, 24, e00372.	4.4	12
60	INPHARMA-Based Determination of Ligand Binding Modes at β_1 -Adrenergic Receptors Explains the Molecular Basis of Subtype Selectivity. <i>Chemistry - A European Journal</i> , 2020, 26, 11796-11805.	3.3	12
61	Aqueous phase behavior of the PEO-containing non-ionic surfactant C12E6: A molecular dynamics simulation study. <i>Journal of Colloid and Interface Science</i> , 2021, 588, 257-268.	9.4	12
62	Quantum chemical study of the intermediate complex required for iron-mediated reactivity and antimalarial activity of dispiro-1,2,4-trioxolanes. <i>Journal of Molecular Graphics and Modelling</i> , 2008, 27, 394-400.	2.4	11
63	The Acid/Base Profile of the Human Metabolome and Natural Products. <i>Molecular Informatics</i> , 2013, 32, 505-515.	2.5	11
64	Propargyloxyproline Regio- and Stereoisomers for Click-Conjugation of Peptides: Synthesis and Application in Linear and Cyclic Peptides. <i>Australian Journal of Chemistry</i> , 2015, 68, 1365.	0.9	11
65	Structural and functional characterisation of a novel peptide from the Australian sea anemone <i>Actinia tenebrosa</i> . <i>Toxicon</i> , 2019, 168, 104-112.	1.6	11
66	Location of Solvated Probe Molecules Within Nonionic Surfactant Micelles Using Molecular Dynamics. <i>Journal of Pharmaceutical Sciences</i> , 2019, 108, 205-213.	3.3	9
67	Controlled Construction of Cyclic Peptide Nanorods. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 596-601.	13.8	8
68	Using the β_2 -Adrenoceptor for Structure-Based Drug Design. <i>Journal of Chemical Education</i> , 2010, 87, 625-627.	2.3	7
69	Improvement in the Predicted Partitioning of Alcohol and Polyethylene Oxide Groups Between Water and Octanol (logP) in Molecular Dynamics Simulations. <i>Journal of Pharmaceutical Sciences</i> , 2019, 108, 214-222.	3.3	7
70	Beta amino acid-modified and fluorescently labelled kisspeptin analogues with potent KISS1R activity. <i>Journal of Peptide Science</i> , 2016, 22, 406-414.	1.4	6
71	The influence and manipulation of acid/base properties in drug discovery. <i>Drug Discovery Today: Technologies</i> , 2018, 27, 41-47.	4.0	6
72	(S)-Fluorenylchloroformate (FLEC); preparation using asymmetric transfer hydrogenation and application to the analysis and resolution of amines. <i>Tetrahedron</i> , 2019, 75, 130591.	1.9	6

#	ARTICLE	IF	CITATIONS
73	Interaction with biliary and pancreatic fluids drives supersaturation and drug absorption from lipid-based formulations of low (saquinavir) and high (fenofibrate) permeability poorly soluble drugs. <i>Journal of Controlled Release</i> , 2021, 331, 45-61.	9.9	6
74	Fragment Based Strategies for Discovery of Novel HIV-1 Reverse Transcriptase and Integrase Inhibitors. <i>Current Topics in Medicinal Chemistry</i> , 2015, 16, 1135-1153.	2.1	6
75	(+)-Fluorenylethylchloroformate (FLEC) – improved synthesis for application in chiral analysis and peptidomimetic synthesis. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 2571.	2.8	5
76	Cyclic Hexapeptide Mimics of the LEDGF Integrase Recognition Loop in Complex with HIV-1 Integrase. <i>ChemMedChem</i> , 2018, 13, 1555-1565.	3.2	5
77	Side-Chain Interactions in α -Peptide Nanotubes: Studies by Crystallography, NMR Spectroscopy and Molecular Dynamics. <i>Chemistry - A European Journal</i> , 2021, 27, 14489-14500.	3.3	5
78	The Dotted Cap Notation: A concise notation for describing variegated dendrimers. <i>New Journal of Chemistry</i> , 2008, 32, 1543.	2.8	4
79	Markov State Model Analysis of Haloperidol Binding to the D3 Dopamine Receptor. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3879-3888.	5.3	4
80	Structural Features of Iperoxo-BQCA Muscarinic Acetylcholine Receptor Hybrid Ligands Determining Subtype Selectivity and Efficacy. <i>ACS Chemical Neuroscience</i> , 2022, 13, 97-111.	3.5	4
81	Backbone and side chain ¹ H, ¹⁵ N and ¹³ C assignments for the oxidised and reduced forms of the oxidoreductase protein DsbA from <i>Staphylococcus aureus</i> . <i>Biomolecular NMR Assignments</i> , 2010, 4, 25-28.	0.8	3
82	Binding Mode Prediction of PDE4 Inhibitors: A Comparison of Modelling Methods. <i>Australian Journal of Chemistry</i> , 2010, 63, 396.	0.9	3
83	Protein structure prediction based on optimal hydrophobic core formation. , 2012, , .		3
84	Molecular Dynamics Simulations and Experimental Results Provide Insight into Clinical Performance Differences between Sandimmune® and Neoral® Lipid-Based Formulations. <i>Pharmaceutical Research</i> , 2021, 38, 1531-1547.	3.5	3
85	Computational and Experimental Models of Type III Lipid-Based Formulations of Loratadine Containing Complex Nonionic Surfactants. <i>Molecular Pharmaceutics</i> , 2021, 18, 4354-4370.	4.6	3
86	Selective Binding of Small Molecules to <i>Vibrio cholerae</i> DsbA Offers a Starting Point for the Design of Novel Antibacterials. <i>ChemMedChem</i> , 2022, 17, .	3.2	3
87	Solid Phase Synthesis and Circular Dichroism Analysis of (i)-Cyclic Lactam Analogues of Kisspeptin. <i>International Journal of Peptide Research and Therapeutics</i> , 2008, 14, 323-331.	1.9	2
88	Controlled Construction of Cyclic α -Peptide Nanorods. <i>Angewandte Chemie</i> , 2019, 131, 606-611.	2.0	2
89	Guiding the Immune Response to a Conserved Epitope in MSP2, an Intrinsically Disordered Malaria Vaccine Candidate. <i>Vaccines</i> , 2021, 9, 855.	4.4	2
90	Enhanced nitric oxide production by macrophages treated with a cell-penetrating peptide conjugate. <i>Bioorganic Chemistry</i> , 2022, 123, 105763.	4.1	2

#	ARTICLE	IF	CITATIONS
91	Analysis of agonism by dopamine at the dopaminergic D ₂ G-protein coupled receptor based on comparative modelling of rhodopsin. <i>Molecular Simulation</i> , 2002, 28, 865-888.	2.0	1
92	Synthesis and Antiviral Activity of Dimeric Capsid-Binding Inhibitors of Human Rhinovirus (HRV). <i>Australian Journal of Chemistry</i> , 2004, 57, 553.	0.9	1
93	Homology Modeling and Docking Evaluation of Human Muscarinic Acetylcholine Receptors. <i>Neuroinformatics</i> , 2016, , 15-35.	0.3	1
94	Molecular modeling of lipid drug formulations. <i>Journal of Cheminformatics</i> , 2012, 4, .	6.1	0