David Kenneth Chalmers

List of Publications by Year
in descending order

94	2,870	196777	214428
papers	citations	29 h-index	50 g-index

97	97	97	4722
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Selective Binding of Small Molecules to Vibrio cholerae DsbA Offers a Starting Point for the Design of Novel Antibacterials. ChemMedChem, 2022, 17, .	1.6	3
2	Crystal structure of the Î±1B-adrenergic receptor reveals molecular determinants of selective ligand recognition. Nature Communications, 2022, 13, 382.	5.8	21
3	Enhanced nitric oxide production by macrophages treated with a cell-penetrating peptide conjugate. Bioorganic Chemistry, 2022, 123, 105763.	2.0	2
4	Structural Features of Iperoxoâ€“BQCA Muscarinic Acetylcholine Receptor Hybrid Ligands Determining Subtype Selectivity and Efficacy. ACS Chemical Neuroscience, 2022, 13, 97-111.	1.7	4
5	Aqueous phase behavior of the PEO-containing non-ionic surfactant C12E6: A molecular dynamics simulation study. Journal of Colloid and Interface Science, 2021, 588, 257-268.	5.0	12
6	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. Journal of Controlled Release, 2021, 331, 45-61.	4.8	6
7	Guiding the Immune Response to a Conserved Epitope in MSP2, an Intrinsically Disordered Malaria Vaccine Candidate. Vaccines, 2021, 9, 855.	2.1	2
8	Cyclosporin Structure and Permeability: From A to Z and Beyond. Journal of Medicinal Chemistry, 2021, 64, 13131-13151.	2.9	43
9	Sideâ€Chain Interactions in <scp>d</scp>/<scp>l</scp> Peptide Nanotubes: Studies by Crystallography, NMR Spectroscopy and Molecular Dynamics. Chemistry - A European Journal, 2021, 27, 14489-14500.	1.7	5
10	Molecular Dynamics Simulations and Experimental Results Provide Insight into Clinical Performance Differences between SandimmuneÂ® and NeoralÂ® Lipid-Based Formulations. Pharmaceutical Research, 2021, 38, 1531-1547.	1.7	3
11	Computational and Experimental Models of Type III Lipid-Based Formulations of Loratadine Containing Complex Nonionic Surfactants. Molecular Pharmaceutics, 2021, 18, 4354-4370.	2.3	3
12	Improving Membrane Permeation in the Beyond Rule-of-Five Space by Using Prodrugs to Mask Hydrogen Bond Donors. ACS Chemical Biology, 2020, 15, 2070-2078.	1.6	26
13	Conformational Changes in Tyrosine 11 of Neurotensin Are Required to Activate the Neurotensin Receptor 1. ACS Pharmacology and Translational Science, 2020, 3, 690-705.	2.5	16
14	INPHARMAâ€Based Determination of Ligand Binding Modes at Î±₁â€Adrenergic Receptors Explains the Molecular Basis of Subtype Selectivity. Chemistry - A European Journal, 2020, 26, 11796-11805.	1.7	12
15	Markov State Model Analysis of Haloperidol Binding to the D3 Dopamine Receptor. Journal of Chemical Theory and Computation, 2020, 16, 3879-3888.	2.3	4
16	Structural and functional characterisation of a novel peptide from the Australian sea anemone Actinia tenebrosa. Toxicon, 2019, 168, 104-112.	0.8	11
17	Production of metabolites of the anti-cancer drug noscapine using a P450BM3 mutant library. Biotechnology Reports (Amsterdam, Netherlands), 2019, 24, e00372.	2.1	12
18	(S)-(â^)-Fluorenylethylchloroformate (FLEC); preparation using asymmetric transfer hydrogenation and application to the analysis and resolution of amines. Tetrahedron, 2019, 75, 130591.	1.0	6

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19	Location of Solvated Probe Molecules Within Nonionic Surfactant Micelles Using Molecular Dynamics. Journal of Pharmaceutical Sciences, 2019, 108, 205-213.	1.6	9
20	Improvement in the Predicted Partitioning of Alcohol and Polyethylene Oxide Groups Between Water and Octanol (logP) in Molecular Dynamics Simulations. Journal of Pharmaceutical Sciences, 2019, 108, 214-222.	1.6	7
21	A Nonionic Polyethylene Oxide (PEO) Surfactant Model: Experimental and Molecular Dynamics Studies of Kolliphor EL. Journal of Pharmaceutical Sciences, 2019, 108, 193-204.	1.6	20
22	Controlled Construction of Cyclic <scp>dâ€...</scp>/<scp>â€...l</scp> Peptide Nanorods. Angewandte Chemie - International Edition, 2019, 58, 596-601.	7.2	8
23	Controlled Construction of Cyclic <scp>dâ€...</scp>/<scp>â€...l</scp> Peptide Nanorods. Angewandte Chemie, 2019, 131, 606-611.	1.6	2
24	Polymeric Precipitation Inhibitors Promote Fenofibrate Supersaturation and Enhance Drug Absorption from a Type IV Lipid-Based Formulation. Molecular Pharmaceutics, 2018, 15, 2355-2371.	2.3	40
25	The influence and manipulation of acid/base properties in drug discovery. Drug Discovery Today: Technologies, 2018, 27, 41-47.	4.0	6
26	Free Energy Methods in Drug Design: Prospects of â€œAlchemical Perturbationâ€•in Medicinal Chemistry. Journal of Medicinal Chemistry, 2018, 61, 638-649.	2.9	125
27	A Cyclic Peptide Inhibitor of the iNOSâ€“SPSB Proteinâ€“Protein Interaction as a Potential Anti-Infective Agent. ACS Chemical Biology, 2018, 13, 2930-2938.	1.6	17
28	Cyclic Hexapeptide Mimics of the LEDGF Integrase Recognition Loop in Complex with HIVâ€1 Integrase. ChemMedChem, 2018, 13, 1555-1565.	1.6	5
29	Computational Models of the Gastrointestinal Environment. 1. The Effect of Digestion on the Phase Behavior of Intestinal Fluids. Molecular Pharmaceutics, 2017, 14, 566-579.	2.3	27
30	Structure and activity of contryphan-Vc2: Importance of the d -amino acid residue. Toxicon, 2017, 129, 113-122.	0.8	13
31	Parallel and antiparallel cyclic <scp>d</scp>/<scp>l</scp> peptide nanotubes. Chemical Communications, 2017, 53, 6613-6616.	2.2	36
32	Computational Models of the Gastrointestinal Environment. 2. Phase Behavior and Drug Solubilization Capacity of a Type I Lipid-Based Drug Formulation after Digestion. Molecular Pharmaceutics, 2017, 14, 580-592.	2.3	30
33	How kanamycin A interacts with bacterial and mammalian mimetic membranes. Biochimica Et Biophysica Acta - Biomembranes, 2017, 1859, 2242-2252.	1.4	33
34	Computational Models of the Intestinal Environment. 3. The Impact of Cholesterol Content and pH on Mixed Micelle Colloids. Molecular Pharmaceutics, 2017, 14, 3684-3697.	2.3	26
35	Beta amino acidâ€modified and fluorescently labelled kisspeptin analogues with potent KISS1R activity. Journal of Peptide Science, 2016, 22, 406-414.	0.8	6
36	Redoxâ€stable cyclic peptide inhibitors of the SPSB2â€“iNOS interaction. FEBS Letters, 2016, 590, 696-704.	1.3	17

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37	Structureâ€“Activity Studies of Î²-Hairpin Peptide Inhibitors of the Plasmodium falciparum AMA1â€“RON2 Interaction. Journal of Molecular Biology, 2016, 428, 3986-3998.	2.0	22
38	Determination of ligand binding modes in weak proteinâ€“ligand complexes using sparse NMR data. Journal of Biomolecular NMR, 2016, 66, 195-208.	1.6	19
39	Design, Synthesis, and Characterization of Cyclic Peptidomimetics of the Inducible Nitric Oxide Synthase Binding Epitope That Disrupt the Proteinâ€“Protein Interaction Involving SPRY Domain-Containing Suppressor of Cytokine Signaling Box Protein (SPSB) 2 and Inducible Nitric Oxide Synthase. Journal of Medicinal Chemistry, 2016, 59, 5799-5809.	2.9	19
40	Ligand Binding Pathways of Clozapine and Haloperidol in the Dopamine D₂ and D₃ Receptors. Journal of Chemical Information and Modeling, 2016, 56, 308-321.	2.5	31
41	Homology Modeling and Docking Evaluation of Human Muscarinic Acetylcholine Receptors. Neuromethods, 2016, , 15-35.	0.2	1
42	Propargyloxyproline Regio- and Stereoisomers for Click-Conjugation of Peptides: Synthesis and Application in Linear and Cyclic Peptides. Australian Journal of Chemistry, 2015, 68, 1365.	0.5	11
43	Identification of mechanistically distinct inhibitors of HIV-1 reverse transcriptase through fragment screening. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 6979-6984.	3.3	22
44	Design, Synthesis, and Biological Evaluation of Tetraâ€Substituted Thiophenes as Inhibitors of p38Î± MAPK. ChemistryOpen, 2015, 4, 56-64.	0.9	12
45	Fragment Based Strategies for Discovery of Novel HIV-1 Reverse Transcriptase and Integrase Inhibitors. Current Topics in Medicinal Chemistry, 2015, 16, 1135-1153.	1.0	6
46	Toward activated homology models of the human M1 muscarinic acetylcholine receptor. Journal of Molecular Graphics and Modelling, 2014, 49, 91-98.	1.3	13
47	Homology Modeling of Human Muscarinic Acetylcholine Receptors. Journal of Chemical Information and Modeling, 2014, 54, 243-253.	2.5	22
48	Digestion of Phospholipids after Secretion of Bile into the Duodenum Changes the Phase Behavior of Bile Components. Molecular Pharmaceutics, 2014, 11, 2825-2834.	2.3	40
49	A Potent Cyclic Peptide Targeting SPSB2 Protein as a Potential Anti-infective Agent. Journal of Medicinal Chemistry, 2014, 57, 7006-7015.	2.9	25
50	Glyceride Lipid Formulations: Molecular Dynamics Modeling of Phase Behavior During Dispersion and Molecular Interactions Between Drugs and Excipients. Pharmaceutical Research, 2013, 30, 3238-3253.	1.7	33
51	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
52	A Chemogenomic Analysis of Ionization Constantsâ€”Implications for Drug Discovery. ChemMedChem, 2013, 8, 242-255.	1.6	40
53	(+)-Fluorenylethylchloroformate (FLEC) â€“ improved synthesis for application in chiral analysis and peptidomimetic synthesis. Organic and Biomolecular Chemistry, 2013, 11, 2571.	1.5	5
54	<scp>l</scp>-Aminoacyl-triazine Derivatives Are Isoform-Selective PI3KÎ² Inhibitors That Target Nonconserved Asp862 of PI3KÎ². ACS Medicinal Chemistry Letters, 2013, 4, 206-210.	1.3	27

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55	The significance of acid/base properties in drug discovery. Chemical Society Reviews, 2013, 42, 485-496.	18.7	236
56	The Acid/Base Profile of the Human Metabolome and Natural Products. Molecular Informatics, 2013, 32, 505-515.	1.4	11
57	Protein structure prediction based on optimal hydrophobic core formation. , 2012, , .		3
58	Synthesis and Pharmacological Evaluation of 4-Iminothiazolidinones for Inhibition of PI3 Kinase. Australian Journal of Chemistry, 2012, 65, 1396.	0.5	15
59	Virtual screening using a conformationally flexible target protein: models for ligand binding to p38Î± MAPK. Journal of Computer-Aided Molecular Design, 2012, 26, 409-423.	1.3	15
60	Molecular modeling of lipid drug formulations. Journal of Cheminformatics, 2012, 4, .	2.8	0
61	Using Molecular Dynamics to Study Liquid Phase Behavior: Simulations of the Ternary Sodium Laurate/Sodium Oleate/Water System. Langmuir, 2011, 27, 11381-11393.	1.6	35
62	Discovery of 7-Hydroxy-6-methoxy-2-methyl-3-(3,4,5-trimethoxybenzoyl)benzo[b]furan (BNC105), a Tubulin Polymerization Inhibitor with Potent Antiproliferative and Tumor Vascular Disrupting Properties. Journal of Medicinal Chemistry, 2011, 54, 6014-6027.	2.9	133
63	Status of GPCR Modeling and Docking as Reflected by Community-wide GPCR Dock 2010 Assessment. Structure, 2011, 19, 1108-1126.	1.6	269
64	Thiazolidinedioneâ€Based PI3KÎ± Inhibitors: An Analysis of Biochemical and Virtual Screening Methods. ChemMedChem, 2011, 6, 514-522.	1.6	15
65	Fragmentâ€Based Design of Ligands Targeting a Novel Site on the Integrase Enzyme of Human Immunodeficiency Virusâ€...1. ChemMedChem, 2011, 6, 258-261.	1.6	24
66	Backbone and side chain 1H, 15N and 13C assignments for the oxidised and reduced forms of the oxidoreductase protein DsbA from Staphylococcus aureus. Biomolecular NMR Assignments, 2010, 4, 25-28.	0.4	3
67	Crystal structure of the HIVâ€1 integrase core domain in complex with sucrose reveals details of an allosteric inhibitory binding site. FEBS Letters, 2010, 584, 1455-1462.	1.3	38
68	Binding Mode Prediction of PDE4 Inhibitors: A Comparison of Modelling Methods. Australian Journal of Chemistry, 2010, 63, 396.	0.5	3
69	Using the Î²₂-Adrenoceptor for Structure-Based Drug Design. Journal of Chemical Education, 2010, 87, 625-627.	1.1	7
70	Homology Modeling and Docking Evaluation of Aminergic G Protein-Coupled Receptors. Journal of Chemical Information and Modeling, 2010, 50, 626-637.	2.5	91
71	Conformational Analysis of Drug Molecules: A Practical Exercise in the Medicinal Chemistry Course. Journal of Chemical Education, 2009, 86, 477.	1.1	17
72	Probing the Fibrate Binding Specificity of Rat Liver Fatty Acid Binding Protein. Journal of Medicinal Chemistry, 2009, 52, 5344-5355.	2.9	17

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73	Molecular Dynamics of Poly(<scp>l</scp>-lysine) Dendrimers with Naphthalene Disulfonate Caps. Macromolecules, 2009, 42, 2775-2783.	2.2	37
74	Structure and Dynamics of Glyceride Lipid Formulations, with Propylene Glycol and Water. Molecular Pharmaceutics, 2009, 6, 604-614.	2.3	30
75	Molecular Dynamics of Variegated Polyamide Dendrimers. Macromolecules, 2009, 42, 2784-2794.	2.2	22
76	Solid Phase Synthesis and Circular Dichroism Analysis of (i â†'ÂiÂ+Â4) Cyclic Lactam Analogues of Kisspeptin. International Journal of Peptide Research and Therapeutics, 2008, 14, 323-331.	0.9	2
77	Quantum chemical study of the intermediate complex required for iron-mediated reactivity and antimalarial activity of dispiro-1,2,4-trioxolanes. Journal of Molecular Graphics and Modelling, 2008, 27, 394-400.	1.3	11
78	2-Aminothienopyridazines as Novel Adenosine A1 Receptor Allosteric Modulators and Antagonists. Journal of Medicinal Chemistry, 2008, 51, 6165-6172.	2.9	54
79	The Dotted Cap Notation: A concise notation for describing variegated dendrimers. New Journal of Chemistry, 2008, 32, 1543.	1.4	4
80	Molecular dynamics simulations of spontaneous bile salt aggregation. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2006, 280, 182-193.	2.3	92
81	The binding interaction of synthetic ozonide antimalarials with natural and modified Î²-cyclodextrins. Journal of Pharmaceutical Sciences, 2006, 95, 146-158.	1.6	32
82	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.	1.0	60
83	A Three-dimensional Model of the Human Immunodeficiency Virus Type 1 Integration Complex. Journal of Computer-Aided Molecular Design, 2005, 19, 301-317.	1.3	51
84	Synthesis and Antiviral Activity of Dimeric Capsid-Binding Inhibitors of Human Rhinovirus (HRV). Australian Journal of Chemistry, 2004, 57, 553.	0.5	1
85	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.	1.4	81
86	Comparisons of the Hbv and HIV Polymerase, and Antiviral Resistance Mutations. Antiviral Therapy, 2004, 9, 149-160.	0.6	112
87	An Orally Bioavailable Oxime Ether Capsid Binder with Potent Activity against Human Rhinovirus. Journal of Medicinal Chemistry, 2003, 46, 3181-3184.	2.9	47
88	Analysis of agonism by dopamine at the dopaminergic D 2 G-protein coupled receptor based on comparative modelling of rhodopsin. Molecular Simulation, 2002, 28, 865-888.	0.9	1
89	The conformational and biological analysis of a cyclic anti-obesity peptide from the C-terminal domain of human growth hormone. Chemical Biology and Drug Design, 2000, 56, 388-397.	1.2	12
90	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.	1.7	62

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91	Enantioselective Synthesis of Cyclothiazide Analogues:Â Novel Probes of the Stereospecific Actions of Benzothiadiazines at AMPA-Type Glutamate Receptors. Journal of the American Chemical Society, 1996, 118, 4550-4559.	6.6	17
92	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.	6.6	134
93	Thyroid hormone uptake by hepatocytes: structure-activity relationships of phenylanthranilic acids with inhibitory activity. Journal of Medicinal Chemistry, 1993, 36, 1272-1277.	2.9	36
94	Models for the binding of amiodarone to the thyroid hormone receptor. Journal of Computer-Aided Molecular Design, 1992, 6, 19-31.	1.3	13