Christopher A Reynolds

List of Publications by Year
in descending order

131	4,223	94433	133252
papers	citations	37 h-index	59 g-index

141	141	141	3750
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Dynamics of GLP-1R peptide agonist engagement are correlated with kinetics of G protein activation. Nature Communications, 2022, 13, 92.	12.8	30
2	Molecular dynamics studies reveal structural and functional features of the SARSâ€CoVâ€2 spike protein. BioEssays, 2022, 44, .	2.5	9
3	Selective activation of GÎ±ob by an adenosine A1 receptor agonist elicits analgesia without cardiorespiratory depression. Nature Communications, 2022, 13, .	12.8	23
4	Peptidomimeticâ€based approach toward inhibitors of microbial trimethylamine lyases. Chemical Biology and Drug Design, 2021, 97, 231-236.	3.2	5
5	Supervised molecular dynamics for exploring the druggability of the SARS-CoV-2 spike protein. Journal of Computer-Aided Molecular Design, 2021, 35, 195-207.	2.9	41
6	Deciphering the Agonist Binding Mechanism to the Adenosine A1 Receptor. ACS Pharmacology and Translational Science, 2021, 4, 314-326.	4.9	9
7	Multisite Model of Allosterism for the Adenosine A1 Receptor. Journal of Chemical Information and Modeling, 2021, 61, 2001-2015.	5.4	8
8	Exploring Ligand Binding to Calcitonin Gene-Related Peptide Receptors. Frontiers in Molecular Biosciences, 2021, 8, 720561.	3.5	5
9	Partial agonism improves the anti-hyperglycaemic efficacy of an oxyntomodulin-derived GLP-1R/GCGR co-agonist. Molecular Metabolism, 2021, 51, 101242.	6.5	7
10	The Role of ICL1 and H8 in Class B1 GPCRs; Implications for Receptor Activation. Frontiers in Endocrinology, 2021, 12, 792912.	3.5	3
11	Activation of the GLP-1 receptor by a non-peptidic agonist. Nature, 2020, 577, 432-436.	27.8	119
12	Addressing free fatty acid receptor 1 (FFAR1) activation using supervised molecular dynamics. Journal of Computer-Aided Molecular Design, 2020, 34, 1181-1193.	2.9	8
13	Structure and dynamics of the active Gs-coupled human secretin receptor. Nature Communications, 2020, 11, 4137.	12.8	46
14	Identification of Small-Molecule Positive Modulators of Calcitonin-like Receptor-Based Receptors. ACS Pharmacology and Translational Science, 2020, 3, 305-320.	4.9	17
15	Structure and Dynamics of Adrenomedullin Receptors AM₁ and AM₂ Reveal Key Mechanisms in the Control of Receptor Phenotype by Receptor Activity-Modifying Proteins. ACS Pharmacology and Translational Science, 2020, 3, 263-284.	4.9	71
16	A Supervised Molecular Dynamics Approach to Unbiased Ligandâ€“Protein Unbinding. Journal of Chemical Information and Modeling, 2020, 60, 1804-1817.	5.4	28
17	Rational development of a high-affinity secretin receptor antagonist. Biochemical Pharmacology, 2020, 177, 113929.	4.4	7
18	Peeking at G-protein-coupled receptors through the molecular dynamics keyhole. Future Medicinal Chemistry, 2019, 11, 599-615.	2.3	11

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19	Deconvoluting the Molecular Control of Binding and Signaling at the Amylin 3 Receptor: RAMP3 Alters Signal Propagation through Extracellular Loops of the Calcitonin Receptor. ACS Pharmacology and Translational Science, 2019, 2, 183-197.	4.9	8
20	The Molecular Control of Calcitonin Receptor Signaling. ACS Pharmacology and Translational Science, 2019, 2, 31-51.	4.9	38
21	Extracellular loops 2 and 3 of the calcitonin receptor selectively modify agonist binding and efficacy. Biochemical Pharmacology, 2018, 150, 214-244.	4.4	24
22	Calcitonin Gene-Related Peptide Antagonists and Therapeutic Antibodies. Handbook of Experimental Pharmacology, 2018, 255, 169-192.	1.8	5
23	Cryo-EM structure of the active, Gs-protein complexed, human CGRP receptor. Nature, 2018, 561, 492-497.	27.8	210
24	Photoaffinity Cross-Linking and Unnatural Amino Acid Mutagenesis Reveal Insights into Calcitonin Gene-Related Peptide Binding to the Calcitonin Receptor-like Receptor/Receptor Activity-Modifying Protein 1 (CLR/RAMP1) Complex. Biochemistry, 2018, 57, 4915-4922.	2.5	20
25	Molecular Signature for Receptor Engagement in the Metabolic Peptide Hormone Amylin. ACS Pharmacology and Translational Science, 2018, 1, 32-49.	4.9	48
26	High affinity binding of the peptide agonist TIP-39 to the parathyroid hormone 2 (PTH 2) receptor requires the hydroxyl group of Tyr-318 on transmembrane helix 5. Biochemical Pharmacology, 2017, 127, 71-81.	4.4	7
27	Genetically encoded photocross-linkers determine the biological binding site of exendin-4 peptide in the N-terminal domain of the intact human glucagon-like peptide-1 receptor (GLP-1R). Journal of Biological Chemistry, 2017, 292, 7131-7144.	3.4	41
28	Understanding the molecular functions of the second extracellular loop (ECL2) of the calcitonin gene-related peptide (CGRP) receptor using a comprehensive mutagenesis approach. Molecular and Cellular Endocrinology, 2017, 454, 39-49.	3.2	7
29	Receptor activity-modifying protein dependent and independent activation mechanisms in the coupling of calcitonin gene-related peptide and adrenomedullin receptors to Gs. Biochemical Pharmacology, 2017, 142, 96-110.	4.4	30
30	Receptor Activity-modifying Proteins 2 and 3 Generate Adrenomedullin Receptor Subtypes with Distinct Molecular Properties. Journal of Biological Chemistry, 2016, 291, 11657-11675.	3.4	36
31	Receptor activity-modifying proteins; multifunctional G protein-coupled receptor accessory proteins. Biochemical Society Transactions, 2016, 44, 568-573.	3.4	36
32	Receptor Activity-modifying Protein-directed G Protein Signaling Specificity for the Calcitonin Gene-related Peptide Family of Receptors. Journal of Biological Chemistry, 2016, 291, 21925-21944.	3.4	72
33	Key interactions by conserved polar amino acids located at the transmembrane helical boundaries in Class B GPCRs modulate activation, effector specificity and biased signalling in the glucagon-like peptide-1 receptor. Biochemical Pharmacology, 2016, 118, 68-87.	4.4	41
34	The Extracellular Surface of the GLP-1 Receptor Is a Molecular Trigger for Biased Agonism. Cell, 2016, 165, 1632-1643.	28.9	126
35	A Hydrogen-Bonded Polar Network in the Core of the Glucagon-Like Peptide-1 Receptor Is a Fulcrum for Biased Agonism: Lessons from Class B Crystal Structures. Molecular Pharmacology, 2016, 89, 335-347.	2.3	56
36	Modulation of Glucagon Receptor Pharmacology by Receptor Activity-modifying Protein-2 (RAMP2). Journal of Biological Chemistry, 2015, 290, 23009-23022.	3.4	61

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37	Do Plants Contain G Protein-Coupled Receptors?. Plant Physiology, 2014, 164, 287-307.	4.8	56
38	Assessing the effect of dynamics on the closed-loop protein-folding hypothesis. Journal of the Royal Society Interface, 2014, 11, 20130935.	3.4	6
39	One motif to bind them: A small-XXX-small motif affects transmembrane domain 1 oligomerization, function, localization, and cross-talk between two yeast GPCRs. Biochimica Et Biophysica Acta - Biomembranes, 2014, 1838, 3036-3051.	2.6	16
40	Identifying subset errors in multiple sequence alignments. Journal of Biomolecular Structure and Dynamics, 2014, 32, 364-371.	3.5	4
41	Modeling Active GPCR Conformations. Methods in Enzymology, 2013, 522, 21-35.	1.0	11
42	Similarity between class A and class B G-protein-coupled receptors exemplified through calcitonin gene-related peptide receptor modelling and mutagenesis studies. Journal of the Royal Society Interface, 2013, 10, 20120846.	3.4	43
43	The activation of the CGRP receptor. Biochemical Society Transactions, 2013, 41, 180-184.	3.4	14
44	The role of ECL2 in CGRP receptor activation: a combined modelling and experimental approach. Journal of the Royal Society Interface, 2013, 10, 20130589.	3.4	27
45	Retinitis Pigmentosa Mutants Provide Insight into the Role of the N-terminal Cap in Rhodopsin Folding, Structure, and Function. Journal of Biological Chemistry, 2013, 288, 33912-33926.	3.4	35
46	G-protein-coupled receptor dynamics: dimerization and activation models compared with experiment. Biochemical Society Transactions, 2012, 40, 394-399.	3.4	13
47	The statistical significance of selected senseâ€“antisense peptide interactions. Journal of Computational Chemistry, 2012, 33, 1440-1447.	3.3	5
48	Modeling GPCR active state conformations: The Î²₂â€adrenergic receptor. Proteins: Structure, Function and Bioinformatics, 2011, 79, 1441-1457.	2.6	24
49	Connectivity and bindingâ€site recognition: Applications relevant to drug design. Journal of Computational Chemistry, 2010, 31, 2677-2688.	3.3	11
50	Closed loop folding units from structural alignments: Experimental foldons revisited. Journal of Computational Chemistry, 2010, 31, 2689-2701.	3.3	13
51	Bioinformatics and molecular modelling approaches to GPCR oligomerization. Current Opinion in Pharmacology, 2010, 10, 30-37.	3.5	61
52	Criteria for confirming sequence periodicity identified by Fourier transform analysis: Application to GCR2, a candidate plant GPCR?. Biophysical Chemistry, 2008, 133, 28-35.	2.8	48
53	Quantitative measurement of protease ligand conformation. Journal of Computer-Aided Molecular Design, 2008, 22, 105-109.	2.9	0
54	Assessing the Role of Polarization in Docking. Journal of Physical Chemistry A, 2008, 112, 12157-12163.	2.5	42

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55	Toward a Consistent Treatment of Polarization in Model QM/MM Calculations. Journal of Physical Chemistry A, 2008, 112, 12151-12156.	2.5	13
56	The effect of MM polarization on the QM/MM transition state stabilization: application to chorismate mutase. Molecular Physics, 2008, 106, 1511-1515.	1.7	13
57	THz differential spectroscopy of Rhodopsin. , 2008, , .		0
58	Computational studies of Family A and Family B GPCRs. Biochemical Society Transactions, 2007, 35, 749-754.	3.4	45
59	Conservation of closed loops. Journal of Molecular Graphics and Modelling, 2007, 26, 652-655.	2.4	9
60	Modelling biological systems. Chemical Modelling, 2007, , 199-238.	0.4	1
61	Classical Polarization in Hybrid QM/MM Methods. Journal of Physical Chemistry A, 2006, 110, 6487-6497.	2.5	51
62	Entropy and Oligomerization in GPCRs. Journal of Molecular Neuroscience, 2005, 26, 113-122.	2.3	16
63	Toward the active conformations of rhodopsin and the Î²2-adrenergic receptor. Proteins: Structure, Function and Bioinformatics, 2004, 56, 67-84.	2.6	74
64	A multilayered approach to approximating solute polarization. Journal of Computational Chemistry, 2004, 25, 627-631.	3.3	2
65	Hypoxia-Targeting Copper Bis(selenosemicarbazone) Complexes:Â Comparison with Their Sulfur Analogues. Journal of the American Chemical Society, 2003, 125, 10040-10049.	13.7	42
66	Studies on the Mechanism of Hypoxic Selectivity in Copper Bis(Thiosemicarbazone) Radiopharmaceuticals. Journal of Medicinal Chemistry, 2002, 45, 1420-1431.	6.4	183
67	Dimerization of G-Protein-Coupled Receptors. Journal of Medicinal Chemistry, 2001, 44, 4595-4614.	6.4	139
68	Modeling Polarization through Induced Atomic Charges. Journal of Physical Chemistry A, 2001, 105, 11470-11479.	2.5	34
69	Modelling G-protein coupled receptors. Theoretical and Computational Chemistry, 2001, , 341-376.	0.4	2
70	Towards new transition metal-based hypoxic selective agents for therapy and imaging. Journal of Inorganic Biochemistry, 2001, 85, 15-22.	3.5	95
71	Lipid-facing correlated mutations and dimerization in G-protein coupled receptors. Protein Engineering, Design and Selection, 2001, 14, 759-767.	2.1	51
72	Fully polarizable QM/MM calculations: An application to the nonbonded iodine-oxygen interaction in dimethyl-2-iodobenzoylphosphonate. Journal of Computational Chemistry, 2000, 21, 478-482.	3.3	13

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73	Dimerization and Domain Swapping in G-Protein-Coupled Receptors A Computational Study. Neuropsychopharmacology, 2000, 23, S60-S77.	5.4	121
74	Cyclophosphamides as hypoxia-activated diffusible cytotoxins: a theoretical study. , 2000, 14, 307-316.		1
75	Brownian dynamics simulations of the Î² 2 -adrenergic receptor extracellular loops: evidence for helix movement in ligand binding?. Computational and Theoretical Chemistry, 1999, 469, 229-232.	1.5	7
76	Solute polarization and the design of cobalt complexes as redox-active therapeutic agents. International Journal of Quantum Chemistry, 1999, 73, 229-236.	2.0	4
77	Correlated mutations in the HLA class II molecule. International Journal of Quantum Chemistry, 1999, 73, 85-96.	2.0	4
78	Evidence for dimerization in the ?2-adrenergic receptor from the evolutionary trace method. International Journal of Quantum Chemistry, 1999, 74, 371-379.	2.0	12
79	Towards improved force fields: III. Polarization through modified atomic charges. Journal of Computational Chemistry, 1999, 20, 704-712.	3.3	35
80	Macromolecular Modelling on the Cray T3D. , 1999, , 229-236.		1
81	Exploiting the parallelisation inherent in the windowing approach to Monte Carlo energy perturbation calculations. Computational and Theoretical Chemistry, 1998, 427, 131-135.	1.5	0
82	Domain swapping in G-protein coupled receptor dimers. Protein Engineering, Design and Selection, 1998, 11, 1181-1193.	2.1	114
83	Simulations on dimeric peptides: evidence for domain swapping in G-protein-coupled receptors?. Biochemical Society Transactions, 1997, 25, 1066-1071.	3.4	33
84	DOMAIN SWAPPING IN THE ACTIVATION OF G-PROTEIN COUPLED RECEPTORS. Biochemical Society Transactions, 1997, 25, 429S-429S.	3.4	0
85	Correlated mutations and subtype specificity in the adrenergic receptor. Biochemical Society Transactions, 1997, 25, 434S-434S.	3.4	3
86	Correlated mutations amongst the external residues of G-protein coupled receptors. Biochemical Society Transactions, 1997, 25, 529S-529S.	3.4	13
87	Theoretical studies of the intramolecular mechanism for the alkoxyphosphazene to alkoxyphosphazane transformation. Journal of the Chemical Society Dalton Transactions, 1997, , 367-370.	1.1	1
88	A New Approach to Docking in the Î²2-Adrenergic Receptor That Exploits the Domain Structure of G-Protein-Coupled Receptors. Journal of Medicinal Chemistry, 1997, 40, 3871-3886.	6.4	75
89	Accurate numerical determination of Kohn-Sham potentials from electronic densities: I. Two-electron systems. Journal of Chemical Physics, 1997, 106, 9659-9667.	3.0	42
90	Toward Improved Force Fields. 1. Multipole-Derived Atomic Charges. Journal of Physical Chemistry A, 1997, 101, 5437-5445.	2.5	43

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91	Toward Improved Force Fields. 2. Effective Distributed Multipoles. Journal of Physical Chemistry A, 1997, 101, 5446-5455.	2.5	41
92	Inclusion of conserved buried water molecules in the model structure of rat submaxillary kallikrein. Journal of Computer-Aided Molecular Design, 1997, 11, 547-556.	2.9	7
93	Energetics of Reactions Involving Transition Metal Complexes:Â Calculation of Relative Electrode Potentials for Cobalt Complexes at Various Ionic Strengths Using Density Functional and Poissonâ^'Boltzmann Methods. Journal of the American Chemical Society, 1996, 118, 10545-10550.	13.7	6
94	Simulations on the activation of the bradykinin B2 receptor. Biochemical Society Transactions, 1996, 24, 259-263.	3.4	2
95	Energetics of reactions involving radical species in solution: Calculation of relative electrode potentials for nitroimidazoles using density functional and continuum methods. International Journal of Quantum Chemistry, 1996, 59, 135-145.	2.0	4
96	Potential energy surfaces from Kohn-Sham potentials. Chemical Physics Letters, 1996, 262, 533-538.	2.6	4
97	Density functional calculation of quinone electrode potentials. International Journal of Quantum Chemistry, 1995, 56, 677-687.	2.0	28
98	A Molecular Dynamics Approach to Receptor Mapping: Application to the 5HT3 and .beta.2-Adrenergic Receptors. Journal of Medicinal Chemistry, 1995, 38, 4080-4086.	6.4	15
99	Electrochromic behaviour and X-ray structure analysis of a Pechmann dye, (E)-5,5â€²-diphenyl-3,3â€²-bifuranylidene-2,2â€²-dione. Journal of Materials Chemistry, 1994, 4, 1201-1204.	6.7	11
100	Theoretical calculation of electrode potentials: Electron-withdrawing compounds. International Journal of Quantum Chemistry, 1992, 41, 293-310.	2.0	48
101	A Linear Molecular Similarity Index. QSAR and Combinatorial Science, 1992, 11, 34-35.	1.2	29
102	Atomic charges for variable molecular conformations. Journal of the American Chemical Society, 1992, 114, 9075-9079.	13.7	163
103	Theoretical determination of partition coefficients. Journal of the American Chemical Society, 1992, 114, 3634-3639.	13.7	65
104	Free energy calculations in molecular biophysics. Molecular Physics, 1992, 76, 251-275.	1.7	88
105	Methods for determining the reliability of semiempirical electrostatic potentials and potential derived charges. Computational and Theoretical Chemistry, 1992, 256, 249-269.	1.5	29
106	Errors in free-energy perturbation calculations due to neglecting the conformational variation of atomic charges. Chemical Physics Letters, 1992, 199, 257-260.	2.6	35
107	The theoretical calculation of basicities: an homologous amine series. Computational and Theoretical Chemistry, 1990, 208, 205-221.	1.5	9
108	Semiempirical AM1 electrostatic potentials and AM1 electrostatic potential derived charges: A comparison withab initio values. Journal of Computational Chemistry, 1990, 11, 159-169.	3.3	157

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109	Free Energy Calculations of Pharmaceutically Important Properties. Molecular Simulation, 1990, 5, 265-275.	2.0	8
110	Theoretical electrode potentials and conformational energies of benzoquinones and naphthoquinones in aqueous solution. Journal of the American Chemical Society, 1990, 112, 7545-7551.	13.7	71
111	Solvation effects. Protein Engineering, Design and Selection, 1989, 2, 319-327.	2.1	25
112	Accurate redox potentials from theoretical calculations. Journal of Molecular Graphics, 1989, 7, 174-175.	1.1	1
113	The oxidation potential of 1,4-diaminobenzene. Journal of Electroanalytical Chemistry and Interfacial Electrochemistry, 1989, 258, 79-88.	0.1	37
114	Identifying targets for bioreductive agents: Using GRID to predict selective binding regions of proteins. Journal of Molecular Graphics, 1989, 7, 103-108.	1.1	34
115	Relative partition coefficients from partition functions: a theoretical approach to drug transport. Journal of the Chemical Society Chemical Communications, 1989, , 1152.	2.0	25
116	Rational drug design: binding free energy differences of carbonic anhydrase inhibitors. Journal of the Chemical Society Chemical Communications, 1989, , 853.	2.0	12
117	Ab initio calculations relevant to the mechanism of chemical carcinogenesis byN-nitrosamines. VIII. Effects of hydration on various reactions involved in the formation and metabolism ofN-nitrosamines. Journal of Computational Chemistry, 1988, 9, 779-783.	3.3	8
118	Computed redox potentials and the design of bioreductive agents. Nature, 1988, 334, 80-82.	27.8	83
119	Accurate redox potentials from theoretical calculations: methyl-substituted benzoquinones. Journal of the Chemical Society Chemical Communications, 1988, , 1434.	2.0	28
120	Prediction of selective bioreductive anti-tumour, anti-folate activity using a modified ab initio method for calculating enzymeâ€“inhibitor interaction energies. Journal of the Chemical Society Perkin Transactions II, 1988, , 551-556.	0.9	11
121	Ab initio calculations relevant to the mechanism of chemical carcinogenesis by N-nitrosamines. Computational and Theoretical Chemistry, 1987, 149, 345-351.	1.5	8
122	Standard transition-structure geometries. Journal of the Chemical Society, Faraday Transactions 2, 1987, 83, 961.	1.1	5
123	Ab initio calculations relevant to the mechanism of chemical carcinogenesis by N-nitrosamines. Part 7. The nitrosation of amines by nitrosyl chloride. Journal of the Chemical Society Perkin Transactions II, 1987, , 1337.	0.9	7
124	Ab initio calculations relevant to the mechanism of chemical carcinogenesis by N-nitrosamines. Part 3.â€”Transition structures in nitrosamine formation and metabolism. Journal of the Chemical Society, Faraday Transactions 2, 1987, 83, 485-502.	1.1	5
125	Hydrated carbonium ions as possible nitrosamine metabolites: Anab initio study. International Journal of Quantum Chemistry, 1987, 32, 123-131.	2.0	2
126	Electrostatic potential and binding of drugs to the minor groove of DNA. Journal of Molecular Graphics, 1987, 5, 165-166.	1.1	18

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127	Ab initio calculations relevant to the mechanism of chemical carcinogenesis by nitrosamines. Part 5. The role of diazomethane. Journal of the Chemical Society Perkin Transactions II, 1986, , 1927.	0.9	6
128	Ab-initio calculations relevant to the mechanism of chemical carcinogenesis by N-nitrosamines. Computational and Theoretical Chemistry, 1986, 138, 131-139.	1.5	6
129	Ab-initio molecular orbital studies on a new mechanism for the interconversion of monomethylnitrosamine and methyldiazohydroxide. Theoretica Chimica Acta, 1986, 70, 421-427.	0.8	2
130	A theoretical study of N-nitrosamine metabolites: Possible alkylating species in carcinogenesis by N,N'-dimethyl nitrosamine. International Journal of Quantum Chemistry, 1986, 30, 751-762.	2.0	7
131	Ab initio calculations relevant to the mechanism of chemical carcinogenesis byN-nitrosamines. I. The nitrosation of amines. International Journal of Quantum Chemistry, 1984, 26, 167-181.	2.0	12