Christopher A Reynolds

List of Publications by Year
in descending order

131 papers	4,223 citations	94433 37 h-index	133252 59 g-index
141 all docs	141 docs citations	141 times ranked	3750 citing authors

#	Article	IF	Citations
1	Cryo-EM structure of the active, Gs-protein complexed, human CGRP receptor. Nature, 2018, 561, 492-497.	27.8	210
2	Studies on the Mechanism of Hypoxic Selectivity in Copper Bis(Thiosemicarbazone) Radiopharmaceuticals. Journal of Medicinal Chemistry, 2002, 45, 1420-1431.	6.4	183
3	Atomic charges for variable molecular conformations. Journal of the American Chemical Society, 1992, 114, 9075-9079.	13.7	163
4	Semiempirical AM1 electrostatic potentials and AM1 electrostatic potential derived charges: A comparison with ab initio values. Journal of Computational Chemistry, 1990, 11, 159-169.	3.3	157
5	Dimerization of G-Protein-Coupled Receptors. Journal of Medicinal Chemistry, 2001, 44, 4595-4614.	6.4	139
6	The Extracellular Surface of the GLP-1 Receptor Is a Molecular Trigger for Biased Agonism. Cell, 2016, 165, 1632-1643.	28.9	126
7	Dimerization and Domain Swapping in G-Protein-Coupled Receptors A Computational Study. Neuropsychopharmacology, 2000, 23, S60-S77.	5.4	121
8	Activation of the GLP-1 receptor by a non-peptidic agonist. Nature, 2020, 577, 432-436.	27.8	119
9	Domain swapping in G-protein coupled receptor dimers. Protein Engineering, Design and Selection, 1998, 11, 1181-1193.	2.1	114
10	Towards new transition metal-based hypoxic selective agents for therapy and imaging. Journal of Inorganic Biochemistry, 2001, 85, 15-22.	3.5	95
11	Free energy calculations in molecular biophysics. Molecular Physics, 1992, 76, 251-275.	1.7	88
12	Computed redox potentials and the design of bioreductive agents. Nature, 1988, 334, 80-82.	27.8	83
13	A New Approach to Docking in the β2-Adrenergic Receptor That Exploits the Domain Structure of G-Protein-Coupled Receptors. Journal of Medicinal Chemistry, 1997, 40, 3871-3886.	6.4	75
14	Toward the active conformations of rhodopsin and the β2-adrenergic receptor. Proteins: Structure, Function and Bioinformatics, 2004, 56, 67-84.	2.6	74
15	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
16	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
17	Structure and Dynamics of Adrenomedullin Receptors AM$_1$ and AM$_2$ 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
18	Theoretical determination of partition coefficients. Journal of the American Chemical Society, 1992, 114, 3634-3639.	13.7	65

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19	Bioinformatics and molecular modelling approaches to GPCR oligomerization. Current Opinion in Pharmacology, 2010, 10, 30-37.	3.5	61
20	Modulation of Glucagon Receptor Pharmacology by Receptor Activity-modifying Protein-2 (RAMP2). Journal of Biological Chemistry, 2015, 290, 23009-23022.	3.4	61
21	Do Plants Contain G Protein-Coupled Receptors?. Plant Physiology, 2014, 164, 287-307.	4.8	56
22	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
23	Lipid-facing correlated mutations and dimerization in G-protein coupled receptors. Protein Engineering, Design and Selection, 2001, 14, 759-767.	2.1	51
24	Classical Polarization in Hybrid QM/MM Methods. Journal of Physical Chemistry A, 2006, 110, 6487-6497.	2.5	51
25	Theoretical calculation of electrode potentials: Electron-withdrawing compounds. International Journal of Quantum Chemistry, 1992, 41, 293-310.	2.0	48
26	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
27	Molecular Signature for Receptor Engagement in the Metabolic Peptide Hormone Amylin. ACS Pharmacology and Translational Science, 2018, 1, 32-49.	4.9	48
28	Structure and dynamics of the active Gs-coupled human secretin receptor. Nature Communications, 2020, 11, 4137.	12.8	46
29	Computational studies of Family A and Family B GPCRs. Biochemical Society Transactions, 2007, 35, 749-754.	3.4	45
30	Toward Improved Force Fields. 1. Multipole-Derived Atomic Charges. Journal of Physical Chemistry A, 1997, 101, 5437-5445.	2.5	43
31	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
32	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
33	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
34	Assessing the Role of Polarization in Docking. Journal of Physical Chemistry A, 2008, 112, 12157-12163.	2.5	42
35	Toward Improved Force Fields. 2. Effective Distributed Multipoles. Journal of Physical Chemistry A, 1997, 101, 5446-5455.	2.5	41
36	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

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37	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
38	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
39	The Molecular Control of Calcitonin Receptor Signaling. ACS Pharmacology and Translational Science, 2019, 2, 31-51.	4.9	38
40	The oxidation potential of 1,4-diaminobenzene. Journal of Electroanalytical Chemistry and Interfacial Electrochemistry, 1989, 258, 79-88.	0.1	37
41	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
42	Receptor activity-modifying proteins; multifunctional G protein-coupled receptor accessory proteins. Biochemical Society Transactions, 2016, 44, 568-573.	3.4	36
43	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
44	Towards improved force fields: III. Polarization through modified atomic charges. Journal of Computational Chemistry, 1999, 20, 704-712.	3.3	35
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	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
47	Modeling Polarization through Induced Atomic Charges. Journal of Physical Chemistry A, 2001, 105, 11470-11479.	2.5	34
48	Simulations on dimeric peptides: evidence for domain swapping in G-protein-coupled receptors?. Biochemical Society Transactions, 1997, 25, 1066-1071.	3.4	33
49	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
50	Dynamics of GLP-1R peptide agonist engagement are correlated with kinetics of G protein activation. Nature Communications, 2022, 13, 92.	12.8	30
51	A Linear Molecular Similarity Index. QSAR and Combinatorial Science, 1992, 11, 34-35.	1.2	29
52	Methods for determining the reliability of semiempirical electrostatic potentials and potential derived charges. Computational and Theoretical Chemistry, 1992, 256, 249-269.	1.5	29
53	Accurate redox potentials from theoretical calculations: methyl-substituted benzoquinones. Journal of the Chemical Society Chemical Communications, 1988, , 1434.	2.0	28
54	Density functional calculation of quinone electrode potentials. International Journal of Quantum Chemistry, 1995, 56, 677-687.	2.0	28

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55	A Supervised Molecular Dynamics Approach to Unbiased Ligand–Protein Unbinding. Journal of Chemical Information and Modeling, 2020, 60, 1804-1817.	5.4	28
56	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
57	Solvation effects. Protein Engineering, Design and Selection, 1989, 2, 319-327.	2.1	25
58	Relative partition coefficients from partition functions: a theoretical approach to drug transport. Journal of the Chemical Society Chemical Communications, 1989, , 1152.	2.0	25
59	Modeling GPCR active state conformations: The β_2–adrenergic receptor. Proteins: Structure, Function and Bioinformatics, 2011, 79, 1441-1457.	2.6	24
60	Extracellular loops 2 and 3 of the calcitonin receptor selectively modify agonist binding and efficacy. Biochemical Pharmacology, 2018, 150, 214-244.	4.4	24
61	Selective activation of Gαob by an adenosine A1 receptor agonist elicits analgesia without cardiorespiratory depression. Nature Communications, 2022, 13, .	12.8	23
62	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
63	Electrostatic potential and binding of drugs to the minor groove of DNA. Journal of Molecular Graphics, 1987, 5, 165-166.	1.1	18
64	Identification of Small-Molecule Positive Modulators of Calcitonin-like Receptor-Based Receptors. ACS Pharmacology and Translational Science, 2020, 3, 305-320.	4.9	17
65	Entropy and Oligomerization in GPCRs. Journal of Molecular Neuroscience, 2005, 26, 113-122.	2.3	16
66	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
67	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
68	The activation of the CGRP receptor. Biochemical Society Transactions, 2013, 41, 180-184.	3.4	14
69	Correlated mutations amongst the external residues of G-protein coupled receptors. Biochemical Society Transactions, 1997, 25, 529S-529S.	3.4	13
70	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
71	Toward a Consistent Treatment of Polarization in Model QM/MM Calculations. Journal of Physical Chemistry A, 2008, 112, 12151-12156.	2.5	13
72	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

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73	Closed loop folding units from structural alignments: Experimental foldons revisited. Journal of Computational Chemistry, 2010, 31, 2689-2701.	3.3	13
74	G-protein-coupled receptor dynamics: dimerization and activation models compared with experiment. Biochemical Society Transactions, 2012, 40, 394-399.	3.4	13
75	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
76	Rational drug design: binding free energy differences of carbonic anhydrase inhibitors. Journal of the Chemical Society Chemical Communications, 1989, , 853.	2.0	12
77	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
78	Prediction of selective bioreductive anti-tumour, anti-folate activity using a modified ab initio method for calculating enzyme–inhibitor interaction energies. Journal of the Chemical Society Perkin Transactions II, 1988, , 551-556.	0.9	11
79	Electrochromic behaviour and X-ray structure analysis of a Pechmann dye, (E)-5,5′-diphenyl-3,3′-bifuranylidene-2,2′-dione. Journal of Materials Chemistry, 1994, 4, 1201-1204.	6.7	11
80	Connectivity and binding‐site recognition: Applications relevant to drug design. Journal of Computational Chemistry, 2010, 31, 2677-2688.	3.3	11
81	Modeling Active GPCR Conformations. Methods in Enzymology, 2013, 522, 21-35.	1.0	11
82	Peeking at G-protein-coupled receptors through the molecular dynamics keyhole. Future Medicinal Chemistry, 2019, 11, 599-615.	2.3	11
83	The theoretical calculation of basicities: an homologous amine series. Computational and Theoretical Chemistry, 1990, 208, 205-221.	1.5	9
84	Conservation of closed loops. Journal of Molecular Graphics and Modelling, 2007, 26, 652-655.	2.4	9
85	Deciphering the Agonist Binding Mechanism to the Adenosine A1 Receptor. ACS Pharmacology and Translational Science, 2021, 4, 314-326.	4.9	9
86	Molecular dynamics studies reveal structural and functional features of the SARS‐CoV‐2 spike protein. BioEssays, 2022, 44, .	2.5	9
87	Ab initio calculations relevant to the mechanism of chemical carcinogenesis by N-nitrosamines. Computational and Theoretical Chemistry, 1987, 149, 345-351.	1.5	8
88	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
89	Free Energy Calculations of Pharmaceutically Important Properties. Molecular Simulation, 1990, 5, 265-275.	2.0	8
90	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

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91	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
92	Multisite Model of Allosterism for the Adenosine A1 Receptor. Journal of Chemical Information and Modeling, 2021, 61, 2001-2015.	5.4	8
93	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
94	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
95	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
96	Brownian dynamics simulations of the β2 -adrenergic receptor extracellular loops: evidence for helix movement in ligand binding?. Computational and Theoretical Chemistry, 1999, 469, 229-232.	1.5	7
97	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
98	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
99	Rational development of a high-affinity secretin receptor antagonist. Biochemical Pharmacology, 2020, 177, 113929.	4.4	7
100	Partial agonism improves the anti-hyperglycaemic efficacy of an oxyntomodulin-derived GLP-1R/GCGR co-agonist. Molecular Metabolism, 2021, 51, 101242.	6.5	7
101	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
102	Ab-initio calculations relevant to the mechanism of chemical carcinogenesis by N-nitrosamines. Computational and Theoretical Chemistry, 1986, 138, 131-139.	1.5	6
103	Energetics of Reactions Involving Transition Metal Complexes:Â Calculation of Relative Electrode Potentials for Cobalt Complexes at Various Ionic Strengths Using Density Functional and Poissonâˆ'Boltzmann Methods. Journal of the American Chemical Society, 1996, 118, 10545-10550.	13.7	6
104	Assessing the effect of dynamics on the closed-loop protein-folding hypothesis. Journal of the Royal Society Interface, 2014, 11, 20130935.	3.4	6
105	Standard transition-structure geometries. Journal of the Chemical Society, Faraday Transactions 2, 1987, 83, 961.	1.1	5
106	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
107	The statistical significance of selected senseâ€"antisense peptide interactions. Journal of Computational Chemistry, 2012, 33, 1440-1447.	3.3	5
108	Calcitonin Gene-Related Peptide Antagonists and Therapeutic Antibodies. Handbook of Experimental Pharmacology, 2018, 255, 169-192.	1.8	5

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109	Peptidomimeticâ€based approach toward inhibitors of microbial trimethylamine lyases. Chemical Biology and Drug Design, 2021, 97, 231-236.	3.2	5
110	Exploring Ligand Binding to Calcitonin Gene-Related Peptide Receptors. Frontiers in Molecular Biosciences, 2021, 8, 720561.	3.5	5
111	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
112	Potential energy surfaces from Kohn-Sham potentials. Chemical Physics Letters, 1996, 262, 533-538.	2.6	4
113	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
114	Correlated mutations in the HLA class II molecule. International Journal of Quantum Chemistry, 1999, 73, 85-96.	2.0	4
115	Identifying subset errors in multiple sequence alignments. Journal of Biomolecular Structure and Dynamics, 2014, 32, 364-371.	3.5	4
116	Correlated mutations and subtype specificity in the adrenergic receptor. Biochemical Society Transactions, 1997, 25, 434S-434S.	3.4	3
117	The Role of ICL1 and H8 in Class B1 GPCRs; Implications for Receptor Activation. Frontiers in Endocrinology, 2021, 12, 792912.	3.5	3
118	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
119	Hydrated carbonium ions as possible nitrosamine metabolites: Anab initio study. International Journal of Quantum Chemistry, 1987, 32, 123-131.	2.0	2
120	Simulations on the activation of the bradykinin B2 receptor. Biochemical Society Transactions, 1996, 24, 259-263.	3.4	2
121	Modelling G-protein coupled receptors. Theoretical and Computational Chemistry, 2001, , 341-376.	0.4	2
122	A multilayered approach to approximating solute polarization. Journal of Computational Chemistry, 2004, 25, 627-631.	3.3	2
123	Accurate redox potentials from theoretical calculations. Journal of Molecular Graphics, 1989, 7, 174-175.	1.1	1
124	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
125	Cyclophosphamides as hypoxia-activated diffusible cytotoxins: a theoretical study. , 2000, 14, 307-316.		1
126	Macromolecular Modelling on the Cray T3D. , 1999, , 229-236.		1

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127	Modelling biological systems. Chemical Modelling, 2007, , 199-238.	0.4	1
128	DOMAIN SWAPPING IN THE ACTIVATION OF G-PROTEIN COUPLED RECEPTORS. Biochemical Society Transactions, 1997, 25, 429S-429S.	3.4	0
129	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
130	Quantitative measurement of protease ligand conformation. Journal of Computer-Aided Molecular Design, 2008, 22, 105-109.	2.9	0
131	THz differential spectroscopy of Rhodopsin. , 2008, , .		0