Christopher A Reynolds

List of Publications by Year in Descending Order

127 papers	3,496 citations	34 h-index	55 g-index
141 ext. papers	3,893 ext. citations	6.7 avg, IF	5.07 L-index

#	Paper	IF	Citations
127	Dynamics of GLP-1R peptide agonist engagement are correlated with kinetics of G protein activation.. *Nature Communications*, **2022**, 13, 92	17.4	3
126	The Role of ICL1 and H8 in Class B1 GPCRs; Implications for Receptor Activation.. *Frontiers in Endocrinology*, **2021**, 12, 792912	5.7	0
125	Multisite Model of Allosterism for the Adenosine A1 Receptor. *Journal of Chemical Information and Modeling*, **2021**, 61, 2001-2015	6.1	2
124	Peptidomimetic-based approach toward inhibitors of microbial trimethylamine lyases. *Chemical Biology and Drug Design*, **2021**, 97, 231-236	2.9	1
123	Supervised molecular dynamics for exploring the druggability of the SARS-CoV-2 spike protein. *Journal of Computer-Aided Molecular Design*, **2021**, 35, 195-207	4.2	23
122	Deciphering the Agonist Binding Mechanism to the Adenosine A1 Receptor. *ACS Pharmacology and Translational Science*, **2021**, 4, 314-326	5.9	5
121	Exploring Ligand Binding to Calcitonin Gene-Related Peptide Receptors. *Frontiers in Molecular Biosciences*, **2021**, 8, 720561	5.6	0
120	Partial agonism improves the anti-hyperglycaemic efficacy of an oxyntomodulin-derived GLP-1R/GCGR co-agonist. *Molecular Metabolism*, **2021**, 51, 101242	8.8	2
119	Identification of Small-Molecule Positive Modulators of Calcitonin-like Receptor-Based Receptors. *ACS Pharmacology and Translational Science*, **2020**, 3, 305-320	5.9	9
118	Structure and Dynamics of Adrenomedullin Receptors AM and AM Reveal Key Mechanisms in the Control of Receptor Phenotype by Receptor Activity-Modifying Proteins. *ACS Pharmacology and Translational Science*, **2020**, 3, 263-284	5.9	42
117	A Supervised Molecular Dynamics Approach to Unbiased Ligand-Protein Unbinding. *Journal of Chemical Information and Modeling*, **2020**, 60, 1804-1817	6.1	14
116	Rational development of a high-affinity secretin receptor antagonist. *Biochemical Pharmacology*, **2020**, 177, 113929	6	2
115	Activation of the GLP-1 receptor by a non-peptidic agonist. *Nature*, **2020**, 577, 432-436	50.4	74
114	Addressing free fatty acid receptor 1 (FFAR1) activation using supervised molecular dynamics. *Journal of Computer-Aided Molecular Design*, **2020**, 34, 1181-1193	4.2	4
113	Structure and dynamics of the active Gs-coupled human secretin receptor. *Nature Communications*, **2020**, 11, 4137	17.4	26
112	Peeking at G-protein-coupled receptors through the molecular dynamics keyhole. *Future Medicinal Chemistry*, **2019**, 11, 599-615	4.1	8
111	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	5.9	7

110	The Molecular Control of Calcitonin Receptor Signaling. *ACS Pharmacology and Translational Science*, **2019**, 2, 31-51	5.9	30
109	Calcitonin Gene-Related Peptide Antagonists and Therapeutic Antibodies. *Handbook of Experimental Pharmacology*, **2019**, 255, 169-192	3.2	4
108	Extracellular loops 2 and 3 of the calcitonin receptor selectively modify agonist binding and efficacy. *Biochemical Pharmacology*, **2018**, 150, 214-244	6	18
107	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	3.2	14
106	Molecular Signature for Receptor Engagement in the Metabolic Peptide Hormone Amylin. *ACS Pharmacology and Translational Science*, **2018**, 1, 32-49	5.9	33
105	Cryo-EM structure of the active, G-protein complexed, human CGRP receptor. *Nature*, **2018**, 561, 492-497	50.4	141
104	High affinity binding of the peptide agonist TIP-39 to the parathyroid hormone 2 (PTH) receptor requires the hydroxyl group of Tyr-318 on transmembrane helix 5. *Biochemical Pharmacology*, **2017**, 127, 71-81	6	7
103	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	5.4	33
102	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	4.4	4
101	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	6	22
100	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	5.4	52
99	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	6	32
98	The Extracellular Surface of the GLP-1 Receptor Is a Molecular Trigger for Biased Agonism. *Cell*, **2016**, 165, 1632-1643	56.2	102
97	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, 335-47	4.3	43
96	Receptor Activity-modifying Proteins 2 and 3 Generate Adrenomedullin Receptor Subtypes with Distinct Molecular Properties. *Journal of Biological Chemistry*, **2016**, 291, 11657-75	5.4	34
95	Receptor activity-modifying proteins; multifunctional G protein-coupled receptor accessory proteins. *Biochemical Society Transactions*, **2016**, 44, 568-73	5.1	29
94	Modulation of Glucagon Receptor Pharmacology by Receptor Activity-modifying Protein-2 (RAMP2). *Journal of Biological Chemistry*, **2015**, 290, 23009-22	5.4	49
93	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, 3036-51	3.8	14

92	Identifying subset errors in multiple sequence alignments. *Journal of Biomolecular Structure and Dynamics*, **2014**, 32, 364-71	3.6	4
91	Do plants contain g protein-coupled receptors?. *Plant Physiology*, **2014**, 164, 287-307	6.6	45
90	Assessing the effect of dynamics on the closed-loop protein-folding hypothesis. *Journal of the Royal Society Interface*, **2014**, 11, 20130935	4.1	5
89	Modeling active GPCR conformations. *Methods in Enzymology*, **2013**, 522, 21-35	1.7	11
88	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	4.1	38
87	The activation of the CGRP receptor. *Biochemical Society Transactions*, **2013**, 41, 180-4	5.1	11
86	The role of ECL2 in CGRP receptor activation: a combined modelling and experimental approach. *Journal of the Royal Society Interface*, **2013**, 10, 20130589	4.1	22
85	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	5.4	29
84	G-protein-coupled receptor dynamics: dimerization and activation models compared with experiment. *Biochemical Society Transactions*, **2012**, 40, 394-9	5.1	13
83	The statistical significance of selected sense-antisense peptide interactions. *Journal of Computational Chemistry*, **2012**, 33, 1440-7	3.5	5
82	Modeling GPCR active state conformations: the [illegible]-adrenergic receptor. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 1441-57	4.2	23
81	Bioinformatics and molecular modelling approaches to GPCR oligomerization. *Current Opinion in Pharmacology*, **2010**, 10, 30-7	5.1	51
80	Connectivity and binding-site recognition: applications relevant to drug design. *Journal of Computational Chemistry*, **2010**, 31, 2677-88	3.5	11
79	Closed loop folding units from structural alignments: experimental foldons revisited. *Journal of Computational Chemistry*, **2010**, 31, 2689-701	3.5	11
78	Assessing the role of polarization in docking. *Journal of Physical Chemistry A*, **2008**, 112, 12157-63	2.8	36
77	Toward a consistent treatment of polarization in model QM/MM calculations. *Journal of Physical Chemistry A*, **2008**, 112, 12151-6	2.8	13
76	The effect of MM polarization on the QM/MM transition state stabilization: application to chorismate mutase. *Molecular Physics*, **2008**, 106, 1511-1515	1.7	11
75	Criteria for confirming sequence periodicity identified by Fourier transform analysis: application to GCR2, a candidate plant GPCR?. *Biophysical Chemistry*, **2008**, 133, 28-35	3.5	46

74	Quantitative measurement of protease ligand conformation. *Journal of Computer-Aided Molecular Design*, **2008**, 22, 105-9	4.2	
73	Conservation of closed loops. *Journal of Molecular Graphics and Modelling*, **2007**, 26, 652-5	2.8	8
72	Computational studies of Family A and Family B GPCRs. *Biochemical Society Transactions*, **2007**, 35, 749-54	3.1	43
71	Classical polarization in hybrid QM/MM methods. *Journal of Physical Chemistry A*, **2006**, 110, 6487-97	2.8	48
70	Entropy and oligomerization in GPCRs. *Journal of Molecular Neuroscience*, **2005**, 26, 113-22	3.3	15
69	Toward the active conformations of rhodopsin and the beta2-adrenergic receptor. *Proteins: Structure, Function and Bioinformatics*, **2004**, 56, 67-84	4.2	66
68	A multilayered approach to approximating solute polarization. *Journal of Computational Chemistry*, **2004**, 25, 627-31	3.5	2
67	Hypoxia-targeting copper bis(selenosemicarbazone) complexes: comparison with their sulfur analogues. *Journal of the American Chemical Society*, **2003**, 125, 10040-9	16.4	39
66	Studies on the mechanism of hypoxic selectivity in copper bis(thiosemicarbazone) radiopharmaceuticals. *Journal of Medicinal Chemistry*, **2002**, 45, 1420-31	8.3	162
65	Modelling G-protein coupled receptors. *Theoretical and Computational Chemistry*, **2001**, 341-376		1
64	Towards new transition metal-based hypoxic selective agents for therapy and imaging. *Journal of Inorganic Biochemistry*, **2001**, 85, 15-22	4.2	89
63	Lipid-facing correlated mutations and dimerization in G-protein coupled receptors. *Protein Engineering, Design and Selection*, **2001**, 14, 759-67	1.9	49
62	Dimerization of G-protein-coupled receptors. *Journal of Medicinal Chemistry*, **2001**, 44, 4595-614	8.3	129
61	Modeling Polarization through Induced Atomic Charges. *Journal of Physical Chemistry A*, **2001**, 105, 1147[illegible]1479	2.8	31
60	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	3.5	12
59	Dimerization and domain swapping in G-protein-coupled receptors: a computational study. *Neuropsychopharmacology*, **2000**, 23, S60-77	8.7	113
58	Cyclophosphamides as hypoxia-activated diffusible cytotoxins: a theoretical study. *Journal of Computer-Aided Molecular Design*, **2000**, 14, 307-16	4.2	0
57	Brownian dynamics simulations of the □2 -adrenergic receptor extracellular loops: evidence for helix movement in ligand binding?. *Computational and Theoretical Chemistry*, **1999**, 469, 229-232		6

56	Solute polarization and the design of cobalt complexes as redox-active therapeutic agents. *International Journal of Quantum Chemistry*, **1999**, 73, 229-236	2.1	3
55	Correlated mutations in the HLA class II molecule. *International Journal of Quantum Chemistry*, **1999**, 73, 85-96	2.1	4
54	Evidence for dimerization in the β-adrenergic receptor from the evolutionary trace method. *International Journal of Quantum Chemistry*, **1999**, 74, 371-379	2.1	11
53	Towards improved force fields: III. Polarization through modified atomic charges. *Journal of Computational Chemistry*, **1999**, 20, 704-712	3.5	34
52	Macromolecular Modelling on the Cray T3D **1999**, 229-236		1
51	Exploiting the parallelisation inherent in the windowing approach to Monte Carlo energy perturbation calculations. *Computational and Theoretical Chemistry*, **1998**, 427, 131-135		
50	Domain swapping in G-protein coupled receptor dimers. *Protein Engineering, Design and Selection*, **1998**, 11, 1181-93	1.9	102
49	Simulations on dimeric peptides: evidence for domain swapping in G-protein-coupled receptors?. *Biochemical Society Transactions*, **1997**, 25, 1066-71	5.1	32
48	DOMAIN SWAPPING IN THE ACTIVATION OF G-PROTEIN COUPLED RECEPTORS. *Biochemical Society Transactions*, **1997**, 25, 429S-429S	5.1	
47	Correlated mutations and subtype specificity in the adrenergic receptor. *Biochemical Society Transactions*, **1997**, 25, 434S	5.1	3
46	Correlated mutations amongst the external residues of G-protein coupled receptors. *Biochemical Society Transactions*, **1997**, 25, 529S	5.1	10
45	A new approach to docking in the beta 2-adrenergic receptor that exploits the domain structure of G-protein-coupled receptors. *Journal of Medicinal Chemistry*, **1997**, 40, 3871-86	8.3	68
44	Accurate numerical determination of Kohn-Sham potentials from electronic densities: I. Two-electron systems. *Journal of Chemical Physics*, **1997**, 106, 9659-9667	3.9	39
43	Toward Improved Force Fields. 1. Multipole-Derived Atomic Charges. *Journal of Physical Chemistry A*, **1997**, 101, 5437-5445	2.8	39
42	Toward Improved Force Fields. 2. Effective Distributed Multipoles. *Journal of Physical Chemistry A*, **1997**, 101, 5446-5455	2.8	38
41	Inclusion of conserved buried water molecules in the model structure of rat submaxillary kallikrein. *Journal of Computer-Aided Molecular Design*, **1997**, 11, 547-56	4.2	6
40	Energetics of Reactions Involving Transition Metal Complexes: Calculation of Relative Electrode Potentials for Cobalt Complexes at Various Ionic Strengths Using Density Functional and Poisson−Boltzmann Methods. *Journal of the American Chemical Society*, **1996**, 118, 10545-10550	16.4	4
39	Simulations on the activation of the bradykinin B2 receptor. *Biochemical Society Transactions*, **1996**, 24, 259-63	5.1	2

38	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	2.1	4
37	Potential energy surfaces from Kohn-Sham potentials. *Chemical Physics Letters*, **1996**, 262, 533-538	2.5	4
36	Density functional calculation of quinone electrode potentials. *International Journal of Quantum Chemistry*, **1995**, 56, 677-687	2.1	25
35	A molecular dynamics approach to receptor mapping: application to the 5HT3 and beta 2-adrenergic receptors. *Journal of Medicinal Chemistry*, **1995**, 38, 4080-6	8.3	14
34	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		11
33	Theoretical calculation of electrode potentials: Electron-withdrawing compounds. *International Journal of Quantum Chemistry*, **1992**, 41, 293-310	2.1	42
32	A Linear Molecular Similarity Index. *QSAR and Combinatorial Science*, **1992**, 11, 34-35		24
31	Atomic charges for variable molecular conformations. *Journal of the American Chemical Society*, **1992**, 114, 9075-9079	16.4	147
30	Theoretical determination of partition coefficients. *Journal of the American Chemical Society*, **1992**, 114, 3634-3639	16.4	59
29	Free energy calculations in molecular biophysics. *Molecular Physics*, **1992**, 76, 251-275	1.7	79
28	Methods for determining the reliability of semiempirical electrostatic potentials and potential derived charges. *Computational and Theoretical Chemistry*, **1992**, 256, 249-269		27
27	Errors in free-energy perturbation calculations due to neglecting the conformational variation of atomic charges. *Chemical Physics Letters*, **1992**, 199, 257-260	2.5	31
26	The theoretical calculation of basicities: an homologous amine series. *Computational and Theoretical Chemistry*, **1990**, 208, 205-221		8
25	Semiempirical AM1 electrostatic potentials and AM1 electrostatic potential derived charges: A comparison with ab initio values. *Journal of Computational Chemistry*, **1990**, 11, 159-169	3.5	146
24	Free Energy Calculations of Pharmaceutically Important Properties. *Molecular Simulation*, **1990**, 5, 265-275		8
23	Theoretical electrode potentials and conformational energies of benzoquinones and naphthoquinones in aqueous solution. *Journal of the American Chemical Society*, **1990**, 112, 7545-7551	16.4	61
22	Solvation effects. *Protein Engineering, Design and Selection*, **1989**, 2, 319-27	1.9	23
21	The oxidation potential of 1,4-diaminobenzene: Calculation versus experiment. *Journal of Electroanalytical Chemistry and Interfacial Electrochemistry*, **1989**, 258, 79-88		37

20	Identifying targets for bioreductive agents: using GRID to predict selective binding regions of proteins. *Journal of Molecular Graphics*, **1989**, 7, 103-8, 100		30
19	Relative partition coefficients from partition functions: a theoretical approach to drug transport. *Journal of the Chemical Society Chemical Communications*, **1989**, 1152		22
18	Rational drug design: binding free energy differences of carbonic anhydrase inhibitors. *Journal of the Chemical Society Chemical Communications*, **1989**, 853		12
17	Ab initio calculations relevant to the mechanism of chemical carcinogenesis by N-nitrosamines. VIII. Effects of hydration on various reactions involved in the formation and metabolism of N-nitrosamines. *Journal of Computational Chemistry*, **1988**, 9, 779-783	3.5	7
16	Computed redox potentials and the design of bioreductive agents. *Nature*, **1988**, 334, 80-2	50.4	74
15	Accurate redox potentials from theoretical calculations: methyl-substituted benzoquinones. *Journal of the Chemical Society Chemical Communications*, **1988**, 1434		26
14	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		10
13	Ab initio calculations relevant to the mechanism of chemical carcinogenesis by N-nitrosamines. *Computational and Theoretical Chemistry*, **1987**, 149, 345-351		6
12	Standard transition-structure geometries. *Journal of the Chemical Society, Faraday Transactions 2*, **1987**, 83, 961		4
11	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		6
10	Ab initio calculations relevant to the mechanism of chemical carcinogenesis by N-nitrosamines. Part 3.□Transition structures in nitrosamine formation and metabolism. *Journal of the Chemical Society, Faraday Transactions 2*, **1987**, 83, 485-502		3
9	Hydrated carbonium ions as possible nitrosamine metabolites: An ab initio study. *International Journal of Quantum Chemistry*, **1987**, 32, 123-131	2.1	2
8	Electrostatic potential and binding of drugs to the minor groove of DNA. *Journal of Molecular Graphics*, **1987**, 5, 165-166		16
7	Ab-initio molecular orbital studies on a new mechanism for the interconversion of monomethylnitrosamine and methyldiazohydroxide. *Theoretica Chimica Acta*, **1986**, 70, 421-427		2
6	A theoretical study of N-nitrosamine metabolites: Possible alkylating species in carcinogenesis by N,NSdimethyl nitrosamine. *International Journal of Quantum Chemistry*, **1986**, 30, 751-762	2.1	7
5	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		5
4	Ab-initio calculations relevant to the mechanism of chemical carcinogenesis by N-nitrosamines. *Computational and Theoretical Chemistry*, **1986**, 138, 131-139		5
3	Ab initio calculations relevant to the mechanism of chemical carcinogenesis by N-nitrosamines. I. The nitrosation of amines. *International Journal of Quantum Chemistry*, **1984**, 26, 167-181	2.1	10

List of Publications

2	A biased adenosine A1R agonist elicits analgesia without cardiorespiratory depression	5
1	Dynamics of GLP-1R peptide agonist engagement are correlated with kinetics of G protein activation	3