Kevin J Naidoo

List of Publications by Year in Descending Order

78 papers	1,847 citations	25 h-index	41 g-index
79 ext. papers	1,963 ext. citations	4.9 avg, IF	4.85 L-index

#	Paper	IF	Citations
78	Multidimensional Free Energy and Accelerated Quantum Library Methods Provide a Gateway to Glycoenzyme Conformational, Electronic, and Reaction Mechanisms. *Accounts of Chemical Research*, **2021**, 54, 4120-4130	24.3	0
77	Anisotropic numerical potentials for coarse-grained modeling from high-speed multidimensional lookup table and interpolation algorithms. *Journal of Computational Chemistry*, **2021**, 42, 666-675	3.5	
76	Comparative ligand structural analytics illustrated on variably glycosylated MUC1 antigen-antibody binding. *Beilstein Journal of Organic Chemistry*, **2020**, 16, 2540-2550	2.5	1
75	ProtoCaller: Robust Automation of Binding Free Energy Calculations. *Journal of Chemical Information and Modeling*, **2020**, 60, 1917-1921	6.1	9
74	BRIDGE: An Open Platform for Reproducible Protein-Ligand Simulations and Free Energy of Binding Calculations. *Bio-protocol*, **2020**, 10, e3731	0.9	
73	BRIDGE: An Open Platform for Reproducible High-Throughput Free Energy Simulations. *Journal of Chemical Information and Modeling*, **2020**, 60, 5290-5295	6.1	5
72	Biomolecular Reaction and Interaction Dynamics Global Environment (BRIDGE). *Bioinformatics*, **2019**, 35, 3508-3509	7.2	9
71	Denoising Autoencoder Self-Organizing Map (DASOM). *Neural Networks*, **2018**, 105, 112-131	9.1	28
70	Producing DFT/MM enzyme reaction trajectories from SCC-DFTB/MM driving forces to probe the underlying electronics of a glycosyltransferase reaction. *Journal of Computational Chemistry*, **2017**, 38, 1789-1798	3.5	4
69	Solution structures of chloroquine-ferriheme complexes modeled using MD simulation and investigated by EXAFS spectroscopy. *Journal of Inorganic Biochemistry*, **2016**, 154, 114-25	4.2	10
68	Multidimensional Reaction Dynamics Reveal How the Enzyme TcTS Suppresses Competing Side Reactions and Their Side Products. *ACS Catalysis*, **2016**, 6, 6384-6392	13.1	3
67	Glycosyltransferase Gene Expression Profiles Classify Cancer Types and Propose Prognostic Subtypes. *Scientific Reports*, **2016**, 6, 26451	4.9	40
66	The Glycome Analytics Platform: an integrative framework for glycobioinformatics. *Bioinformatics*, **2016**, 32, 3005-11	7.2	5
65	Conformational and electrostatic analysis of S1 donor analogue glycomimetic inhibitors of ST3Gal-I mammalian sialyltransferase. *Bioorganic and Medicinal Chemistry*, **2016**, 24, 4998-5005	3.4	2
64	Quantum supercharger library: hyper-parallel integral derivatives algorithms for ab initio QM/MM dynamics. *Journal of Computational Chemistry*, **2015**, 36, 1410-9	3.5	4
63	Quantum supercharger library: hyper-parallelism of the Hartree-Fock method. *Journal of Computational Chemistry*, **2015**, 36, 1399-409	3.5	4
62	Profiling transition-state configurations on the Trypanosoma cruzi trans-sialidase free-energy reaction surfaces. *Journal of Physical Chemistry B*, **2015**, 119, 1192-201	3.4	5

61	Computational rationale for the selective inhibition of the herpes simplex virus type 1 uracil-DNA glycosylase enzyme. *Journal of Chemical Information and Modeling*, **2014**, 54, 3362-72	6.1	4
60	Simple Link Atom Saccharide Hybrid (SLASH) Treatment for Glycosidic Bonds at the QM/MM Boundary. *Journal of Chemical Theory and Computation*, **2014**, 10, 1727-38	6.4	3
59	AM1/d-CB1: A Semiempirical Model for QM/MM Simulations of Chemical Glycobiology Systems. *Journal of Chemical Theory and Computation*, **2014**, 10, 4694-4707	6.4	30
58	Evaluating AM1/d-CB1 for Chemical Glycobiology QM/MM Simulations. *Journal of Chemical Theory and Computation*, **2014**, 10, 4708-17	6.4	13
57	Molecular structures and solvation of free monomeric and dimeric ferriheme in aqueous solution: insights from molecular dynamics simulations and extended X-ray absorption fine structure spectroscopy. *Inorganic Chemistry*, **2014**, 53, 10811-24	5.1	11
56	Conformational preferences of plumbagin with phenyl-1-thioglucoside conjugates in solution and bound to MshB determined by aromatic association. *Carbohydrate Research*, **2013**, 371, 52-60	2.9	8
55	PNP diminishes guanosine glycosidic bond strength through restrictive ring pucker as a precursor to phosphorylation. *Journal of Physical Chemistry B*, **2013**, 117, 6019-26	3.4	1
54	Interpreting medium ring canonical conformers by a triangular plane tessellation of the macrocycle. *Journal of Chemical Physics*, **2013**, 138, 184110	3.9	5
53	Experimental and time-dependent density functional theory characterization of the UV-visible spectra of monomeric and □xo dimeric ferriprotoporphyrin IX. *Inorganic Chemistry*, **2012**, 51, 10233-50	5.1	19
52	An enzyme-initiated Smiles rearrangement enables the development of an assay of MshB, the GlcNAc-Ins deacetylase of mycothiol biosynthesis. *Organic and Biomolecular Chemistry*, **2012**, 10, 5278-88	3.9	4
51	Multidimensional free energy volumes offer unique insights into reaction mechanisms, molecular conformation and association. *Physical Chemistry Chemical Physics*, **2012**, 14, 9026-36	3.6	9
50	Hydration-determined orientational preferences in aromatic association from benzene dimer free energy volumes. *Journal of Physical Chemistry B*, **2012**, 116, 324-31	3.4	10
49	Molecular details from computational reaction dynamics for the cellobiohydrolase I glycosylation reaction. *Journal of the American Chemical Society*, **2011**, 133, 19474-82	16.4	41
48	Conformational preferences in diglycosyl disulfides: NMR and molecular modeling studies. *Carbohydrate Research*, **2011**, 346, 2612-21	2.9	8
47	FEARCF a multidimensional free energy method for investigating conformational landscapes and chemical reaction mechanisms. *Science China Chemistry*, **2011**, 54, 1962-1973	7.9	11
46	Acceleration of the GAMESS-UK electronic structure package on graphical processing units. *Journal of Computational Chemistry*, **2011**, 32, 2313-8	3.5	37
45	The extent of conformational rigidity determines hydration in nonaromatic hexacyclic systems. *Journal of Physical Chemistry B*, **2011**, 115, 2608-16	3.4	9
44	Using solvent binding and dielectric friction to interpret the hydration behavior of complex anions. *Journal of Physical Chemistry B*, **2011**, 115, 1045-55	3.4	10

43	Implementation of CASTfill Low-Dross Pouring System for Ingot Casting. *Materials Science Forum*, **2011**, 693, 227-234	0.4	
42	Experimentally consistent ion association predicted for metal solutions from free energy simulations. *Journal of Physical Chemistry B*, **2010**, 114, 7286-93	3.4	16
41	Pyranose ring transition state is derived from cellobiohydrolase I induced conformational stability and glycosidic bond polarization. *Journal of the American Chemical Society*, **2010**, 132, 12800-3	16.4	37
40	Ring puckering: a metric for evaluating the accuracy of AM1, PM3, PM3CARB-1, and SCC-DFTB carbohydrate QM/MM simulations. *Journal of Physical Chemistry B*, **2010**, 114, 17142-54	3.4	73
39	Computing free energy hypersurfaces for anisotropic intermolecular associations. *Journal of Computational Chemistry*, **2010**, 31, 308-16	3.5	4
38	Optimal configurations of "capped" beta-cyclodextrin dimers in water maximise hydrophobic association. *ChemPhysChem*, **2010**, 11, 452-9	3.2	4
37	Molecular Associations Determined from Free Energy Calculations **2010**, 1-20		1
36	Calculating Ring Pucker Free Energy Surfaces From Reaction Coordinate Forces **2009**,		2
35	Free Energies from Adaptive Reaction Coordinate Forces (FEARCF): an application to ring puckering. *Molecular Physics*, **2009**, 107, 1243-1250	1.7	40
34	NMR studies of molecular conformations in alpha-cyclodextrin. *Journal of Physical Chemistry B*, **2008**, 112, 8434-6	3.4	18
33	Glucose orientation and dynamics in alpha-, beta-, and gamma-cyclodextrins. *Journal of Physical Chemistry B*, **2008**, 112, 15151-7	3.4	23
32	Conformational flexibility of sulphur linked saccharides a possible key to their glycosidase inhibitor activity. *Molecular Simulation*, **2008**, 34, 391-402	2	5
31	C-2-aryl O-substituted HI-236 derivatives as non-nucleoside HIV-1 reverse-transcriptase inhibitors. *Bioorganic and Medicinal Chemistry*, **2008**, 16, 10270-80	3.4	21
30	Stereoelectronic and solvation effects determine hydroxymethyl conformational preferences in monosaccharides. *Journal of Physical Chemistry B*, **2008**, 112, 15450-9	3.4	47
29	Haemozoin (beta-haematin) biomineralization occurs by self-assembly near the lipid/water interface. *FEBS Letters*, **2006**, 580, 5105-10	3.8	111
28	Free energy surfaces for the alpha(1 --> 4)-glycosidic linkage: implications for polysaccharide solution structure and dynamics. *Journal of Physical Chemistry B*, **2005**, 109, 7468-74	3.4	47
27	Glycosidic linkage rotations determine amylose stretching mechanism. *Journal of the American Chemical Society*, **2005**, 127, 12-3	16.4	42
26	Ramachandran free-energy surfaces for disaccharides: trehalose, a case study. *Carbohydrate Research*, **2005**, 340, 875-9	2.9	20

25	Molecular Properties Related to the Anomalous Solubility of Cyclodextrin. *Journal of Physical Chemistry B*, **2004**, 108, 4236-4238	3.4	87
24	Implementation of an adaptive umbrella sampling method for the calculation of multidimensional potential of mean force of chemical reactions in solution. *Journal of Computational Chemistry*, **2003**, 24, 1775-81	3.5	50
23	Contact ion pair between Na+ and PtCl(6)(2-) favored in methanol. *Journal of the American Chemical Society*, **2003**, 125, 13330-1	16.4	33
22	Evaluating Intramolecular Hydrogen Bond Strengths in (1) Linked Disaccharides from Electron Density Relationships. *Journal of Physical Chemistry B*, **2003**, 107, 9558-9566	3.4	31
21	The role of water in the design of glycosidic linkage flexibility. *Molecular Physics*, **2003**, 101, 2687-2694	1.7	23
20	Carbohydrate solution simulations: producing a force field with experimentally consistent primary alcohol rotational frequencies and populations. *Journal of Computational Chemistry*, **2002**, 23, 1236-43	3.5	258
19	Modeling the (1->6) Branch Point of Amylopectin in Solution. *Journal of Physical Chemistry B*, **2002**, 106, 5091-5098	3.4	17
18	Geometric hydration shells for anionic platinum group metal chloro complexes. *Inorganic Chemistry*, **2002**, 41, 1845-9	5.1	36
17	AN NMR INVESTIGATION INTO THE DYNAMICS OF PANOSE, AN (1->4) AND (1->6)-LINKED TRISACCHARIDE. *Spectroscopy Letters*, **2002**, 35, 625-632	1.1	3
16	Water structure about the dimer and hexamer repeat units of amylose from molecular dynamics computer simulations. *Journal of Computational Chemistry*, **2001**, 22, 445-456	3.5	68
15	Modeling platinum group metal complexes in aqueous solution. *Inorganic Chemistry*, **2001**, 40, 2352-7	5.1	33
14	Molecular Dynamics and NMR Study of the (1->4) and (1->6) Glycosidic Linkages: Maltose and Isomaltose. *Journal of Physical Chemistry B*, **2001**, 105, 4742-4751	3.4	58
13	Water structure about the dimer and hexamer repeat units of amylose from molecular dynamics computer simulations **2001**, 22, 445		1
12	The synthesis, characterization and properties of alkyl complexes of the type [Cp*Fe(CO)2R] (Cp*=5-C5(CH3)5; R=n-C3H7 to n-C12H25); the X-ray crystal and molecular structure of [Cp*Fe(CO)2(n-C5H11)] and molecular orbital and density functional calculations on the hydride elimination of [CpFe(CO)2(CH2CH3)]. *Journal of Organometallic Chemistry*, **1999**, 587, 28-37	2.3	23
11	Force-field parameterisation, synthesis and crystal structure of a novel tricarbonylchromium arene complex. *Journal of Organometallic Chemistry*, **1999**, 588, 176-185	2.3	5
10	Computational Investigations into the Potential Use of Poly(benzyl phenyl ether) Dendrimers as Supports for Organometallic Catalysts. *Macromolecules*, **1999**, 32, 331-341	5.5	49
9	Calculation of the Ramachandran Potential of Mean Force for a Disaccharide in Aqueous Solution. *Journal of the American Chemical Society*, **1999**, 121, 2244-2252	16.4	62
8	Organometallic dendrimers. *Advances in Dendritic Macromolecules*, **1999**, 1-60		24

7	Molecular dynamics simulations of a glycoprotein: the lectin from Erythrina corallodendron. *Computational and Theoretical Chemistry*, **1997**, 395-396, 469-475		5
6	The application of simulated annealing to the conformational analysis of disaccharides. *Chemical Physics*, **1997**, 224, 263-273	2.3	18
5	Melting of two-dimensional colloidal crystals: A simulation study of the Yukawa system. *Journal of Chemical Physics*, **1994**, 100, 3114-3121	3.9	46
4	Two-dimensional melting revisited. *Molecular Physics*, **1993**, 80, 1-24	1.7	26
3	Lel 2 ob and ob2lel cage complexes based on [Co(pn)3]3+(pn = propane-1,2-diamine): synthesis, resolution, and tentative identity of their fac and mer geometrical isomers. *Journal of the Chemical Society Chemical Communications*, **1989**, 998		3
2	71.36 The Oldest Mathematical Artefact. *Mathematical Gazette*, **1987**, 71, 294	0.1	14
1	Tessellate & Montage: Molecular analytics of cyclic conformations. *F1000Research*,6, 2113	3.6	