Young Kee Kang

List of Publications by Year in Descending Order

109 papers	2,292 citations	27 h-index	43 g-index
112 ext. papers	2,406 ext. citations	3.4 avg, IF	5.21 L-index

#	Paper	IF	Citations
109	Exploring Helical Folding in Oligomers of Cyclopentane-Based ?-Amino Acids: A Computational Study.. *ChemistryOpen*, **2022**, e202100253	2.3	1
108	Reagent-free intramolecular hydrofunctionalization: a regioselective 6-endo-dig cyclization of o-alkynoylphenols. *Green Chemistry*, **2022**, 24, 2376-2384	10	1
107	Exploring Helical Folding in Oligomers of Cyclopentane-Based ?-Amino Acids: A Computational Study.. *ChemistryOpen*, **2022**, 11, e202200035	2.3	
106	Conformational Preferences of Cyclopentane-Based Oligo-peptides in the Gas Phase and in Solution. *ChemPlusChem*, **2021**, 86, 533-539	2.8	1
105	Puckering transition of the proline residue along the pseudorotational path: revisited. *New Journal of Chemistry*, **2021**, 45, 9780-9793	3.6	1
104	PMFF: Development of a Physics-Based Molecular Force Field for Protein Simulation and Ligand Docking. *Journal of Physical Chemistry B*, **2020**, 124, 974-989	3.4	0
103	Conformational preferences of cationic peptide in water studied by CCSD(T), MP2, and DFT methods. *Heliyon*, **2020**, 6, e04721	3.6	3
102	Tailoring the Physicochemical Properties of Antimicrobial Peptides onto a Thiazole-Based Peptide Foldamer. *Journal of Medicinal Chemistry*, **2020**, 63, 9168-9180	8.3	7
101	Organocatalytic Asymmetric Addition of Aldehyde to Nitroolefin by H-d-Pro-Pro-Glu-NH: A Mechanistic Study. *ACS Omega*, **2019**, 4, 8862-8873	3.9	2
100	Prospect of Thiazole-based Peptide Foldamers in Enamine Catalysis: Exploration of the Nitro-Michael Addition. *Chemistry - A European Journal*, **2019**, 25, 7396-7401	4.8	12
99	Which DFT levels of theory are appropriate in predicting the prolyl cistrans isomerization in solution?. *New Journal of Chemistry*, **2019**, 43, 17159-17173	3.6	7
98	Exploring conformational preferences of alanine tetrapeptide by CCSD(T), MP2, and dispersion-corrected DFT methods. *Chemical Physics Letters*, **2018**, 702, 69-75	2.5	6
97	Puckering transitions in cyclohexane: Revisited. *Chemical Physics Letters*, **2018**, 702, 82-89	2.5	5
96	Mechanistic study of hemicucurbit[6]uril formation by step-growth oligomerization and end-to-end cyclization. *Chemical Physics Letters*, **2017**, 669, 92-98	2.5	2
95	Altering the Cyclization Modes: Temperature-Dependent Intramolecular 7-Endo-Dig vs 6-Endo-Dig Electrophilic Ring Closures. *Organic Letters*, **2017**, 19, 1474-1477	6.2	15
94	Effects of isosteric substitutions on the conformational preference and cistrans isomerization of proline-containing peptides. *New Journal of Chemistry*, **2017**, 41, 6593-6606	3.6	1
93	C Ribbon-Like Structures in Hybrid Peptides Alternating and Thiazole-Based Amino Acids. *Chemistry - A European Journal*, **2017**, 23, 17584-17591	4.8	8

92	Allylic Azide Rearrangements Investigated by Density Functional Theory Calculations. *Bulletin of the Korean Chemical Society*, **2017**, 38, 1419-1426	1.2	5
91	Assessment of CCSD(T), MP2, and DFT methods for the calculations of structures and interaction energies of the peptide backbone with water molecules. *Chemical Physics Letters*, **2017**, 687, 23-30	2.5	6
90	Propensities to form the Eturn and Ehairpin structures of D-Pro-Gly and Aib-D-Ala containing peptides: a computational study. *New Journal of Chemistry*, **2016**, 40, 8565-8578	3.6	0
89	12/10-Helical EPeptide with Dynamic Folding Propensity: Coexistence of Right- and Left-Handed Helices in an Enantiomeric Foldamer. *Journal of the American Chemical Society*, **2016**, 138, 13390-13395	16.4	24
88	Remote Stereoinductive Intramolecular Nitrile Oxide Cycloaddition: Asymmetric Total Synthesis and Structure Revision of (-)-11EHydroxycurvularin. *Journal of Organic Chemistry*, **2016**, 81, 2612-7	4.2	14
87	Propensities of peptides containing the Asn-Gly segment to form Eturn and Ehairpin structures. *Biopolymers*, **2016**, 105, 653-64	2.2	8
86	Conformational preferences and antimicrobial activities of alkanediols. *Computational and Theoretical Chemistry*, **2015**, 1064, 15-24	2	4
85	Conformational preferences of Esheet structures in cyclopropane-containing Epeptides. *New Journal of Chemistry*, **2015**, 39, 4640-4646	3.6	4
84	Hairpin formation promoted by the heterochiral dinipecotic acid segment: A DFT study. *Biopolymers*, **2015**, 103, 609-17	2.2	2
83	Helix foldamers of Epeptides based on 2-aminocyclopentylacetic acid. *New Journal of Chemistry*, **2015**, 39, 3241-3249	3.6	7
82	Assessment of CCSD(T), MP2, DFT-D, CBS-QB3, and G4(MP2) methods for conformational study of alanine and proline dipeptides. *Chemical Physics Letters*, **2014**, 600, 112-117	2.5	30
81	Helix foldamers of Epeptides based on 2-aminocyclohexylacetic acid: a computational study. *New Journal of Chemistry*, **2014**, 38, 966	3.6	7
80	Conformational preferences of the 2-methylproline residue and its role in stabilizing Eturn and polyproline II structures of peptides. *New Journal of Chemistry*, **2014**, 38, 2831	3.6	7
79	Thiazole-based Ebuilding blocks as reverse-turn mimetic to design a gramicidin S analogue: conformational and biological evaluation. *Chemistry - A European Journal*, **2014**, 20, 6713-20	4.8	35
78	Conformational preferences of helix foldamers of Epeptides based on 2-(aminomethyl)cyclohexanecarboxylic acid. *Biopolymers*, **2014**, 101, 87-95	2.2	8
77	Influence of substituents on conformational preferences of helix foldamers of Edipeptides. *Biopolymers*, **2014**, 101, 1077-87	2.2	5
76	A mechanistic study supports a two-step mechanism for peptide bond formation on the ribosome. *Physical Chemistry Chemical Physics*, **2013**, 15, 14931-5	3.6	11
75	Conformational preferences of taurine in the gas phase and in water. *Computational and Theoretical Chemistry*, **2013**, 1025, 8-15	2	5

74	Binding free energies of inhibitors to iron porphyrin complex as a model for Cytochrome P450. *Biopolymers*, **2012**, 97, 219-28	2.2	6
73	Conformational preferences of □aminobutyric acid in the gas phase and in water. *Journal of Molecular Structure*, **2012**, 1024, 163-169	3.4	16
72	Computationally designed □turn foldamers of □peptides based on 2-(aminomethyl)cyclohexanecarboxylic acid. *Biopolymers*, **2012**, 97, 1018-25	2.2	17
71	Local control of the cis-trans isomerization and backbone dihedral angles in peptides using trifluoromethylated pseudoprolines. *Journal of Physical Chemistry B*, **2012**, 116, 4069-79	3.4	22
70	The triple helical structure and stability of collagen model peptide with 4(S)-hydroxyprolyl-Pro-Gly units. *Biopolymers*, **2012**, 98, 111-21	2.2	15
69	Reply to "comment on □binding free energies of inhibitors to iron porphyrin complex as a model for cytochrome P450□". *Biopolymers*, **2012**, 97, 649-50	2.2	1
68	Conformational preferences of 4-chloroproline residues. *Biopolymers*, **2012**, 97, 629-41	2.2	7
67	Strength of CH□□□interactions in the C-terminal subdomain of villin headpiece. *Biopolymers*, **2012**, 97, 778-88	2.2	9
66	Conformational Preferences of Glycerol in the Gas Phase and in Water. *Bulletin of the Korean Chemical Society*, **2012**, 33, 917-924	1.2	9
65	Conformational preference and cis-trans isomerization of 4-methylproline residues. *Biopolymers*, **2011**, 95, 51-61	2.2	24
64	Conformational preferences and pK(a) value of selenocysteine residue. *Biopolymers*, **2011**, 95, 345-53	2.2	30
63	Conformational preferences of X-Pro sequences: Ala-Pro and Aib-Pro motifs. *Journal of Physical Chemistry B*, **2010**, 114, 14077-86	3.4	10
62	A histidine substitution confers metal binding affinity to a Schistosoma japonicum Glutathione S-transferase. *Protein Expression and Purification*, **2010**, 73, 74-7	2	6
61	Conformational preferences and prolyl cis-trans isomerization of phosphorylated Ser/Thr-Pro motifs. *Biopolymers*, **2010**, 93, 330-9	2.2	12
60	Assessment of density functionals with long-range and/or empirical dispersion corrections for conformational energy calculations of peptides. *Journal of Computational Chemistry*, **2010**, 31, 2915-23	3.5	44
59	Conformational preferences of N-methoxycarbonyl proline dipeptide. *Journal of Computational Chemistry*, **2009**, 30, 1116-27	3.5	4
58	Puckering transitions of pseudoproline residues. *Biopolymers*, **2009**, 91, 444-55	2.2	13
57	Conformational preferences and cis-trans isomerization of L-3,4-dehydroproline residue. *Biopolymers*, **2009**, 92, 387-98	2.2	10

56	Conformational preferences and cis-trans isomerization of L-lactic acid residue. *Journal of Physical Chemistry B*, **2008**, 112, 9126-34	3.4	13
55	The rate enhancement for prolyl cis-to-trans isomerization of cyclic CPFC peptide is caused by an increase in the vibrational entropy of the transition state. *Journal of Physical Chemistry B*, **2008**, 112, 3287-9	3.4	1
54	An efficient method for calculating atomic charges of peptides and proteins from electronic populations. *Journal of Physical Chemistry B*, **2008**, 112, 5470-8	3.4	12
53	Conformational preferences and pKa value of cysteine residue. *Journal of Physical Chemistry B*, **2008**, 112, 11189-93	3.4	10
52	Puckering transition of proline residue in water. *Journal of Physical Chemistry B*, **2007**, 111, 10550-6	3.4	34
51	Conformational preferences and cis-trans isomerization of azaproline residue. *Journal of Physical Chemistry B*, **2007**, 111, 5377-85	3.4	21
50	Conformational preferences of proline analogues with different ring size. *Journal of Physical Chemistry B*, **2007**, 111, 3496-507	3.4	28
49	Conformational preferences of pseudoproline residues. *Journal of Physical Chemistry B*, **2007**, 111, 12551-62	3.4	19
48	Conformational preferences of proline oligopeptides. *Journal of Physical Chemistry B*, **2006**, 110, 17645-55	3.4	43
47	Conformational preferences of non-prolyl and prolyl residues. *Journal of Physical Chemistry B*, **2006**, 110, 21338-48	3.4	73
46	Conformational preference and cis-trans isomerization of 4(R)-substituted proline residues. *Journal of Physical Chemistry B*, **2006**, 110, 1915-27	3.4	25
45	Puckering transition of 4-substituted proline residues. *Journal of Physical Chemistry B*, **2005**, 109, 16982-7	3.4	24
44	Transition of prolyl puckering in a model of polyproline. *Computational and Theoretical Chemistry*, **2005**, 718, 17-21		15
43	Ab initio conformational study of N-acetyl-L-proline-NR,NRdimethylamide: a model for polyproline. *Biophysical Chemistry*, **2005**, 113, 93-101	3.5	19
42	Physics-based protein-structure prediction using a hierarchical protocol based on the UNRES force field: assessment in two blind tests. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 7547-52	11.5	120
41	Ab initio and DFT conformational study of proline dipeptide. *Computational and Theoretical Chemistry*, **2004**, 675, 37-45		37
40	Internal rotation about the CN bond of amides. *Computational and Theoretical Chemistry*, **2004**, 676, 171-176		65
39	Cis-trans isomerization and puckering of proline residue. *Biophysical Chemistry*, **2004**, 111, 135-42	3.5	63

38	Ring Flip of Proline Residue via the Transition State with an Envelope Conformation. *Journal of Physical Chemistry B*, **2004**, 108, 5463-5465	3.4	36
37	Preferred conformations of cyclic Ac-Cys-Pro-Xaa-Cys-NHMe peptides: a model for chain reversal and active site of disulfide oxidoreductase. *Biophysical Chemistry*, **2003**, 105, 89-104	3.5	5
36	Preferred conformations of RGDX tetrapeptides to inhibit the binding of fibrinogen to platelets. *Biopolymers*, **2002**, 63, 298-313	2.2	14
35	cis trans Isomerization of N -acetyl- N ?-methylamides of 5-methylproline and 5,5-dimethylproline. *Computational and Theoretical Chemistry*, **2002**, 585, 209-221		19
34	Comparative conformational study of N-acetyl-N?-methylprolineamide with different basis sets. *Computational and Theoretical Chemistry*, **2002**, 593, 55-64		18
33	Cis trans Isomerization and Puckering of Pseudoproline Dipeptides. *Journal of Physical Chemistry B* , **2002**, 106, 2074-2082	3.4	41
32	Proline puckering and cis-trans isomerization of proline-containing peptides **2002**, 420-421		
31	Ab initio MO and density functional studies on trans and cis conformers of N-methylacetamide. *Computational and Theoretical Chemistry*, **2001**, 546, 183-193		92
30	A Fast Method for Calculating Geometry-Dependent Net Atomic Charges for Polypeptides. *Journal of Physical Chemistry B*, **2001**, 105, 3624-3634	3.4	26
29	Preferred conformations of a linear RGD tripeptide. *Chemical Biology and Drug Design*, **2000**, 56, 360-72		6
28	Which Functional Form Is Appropriate for Hydrogen Bond of Amides?. *Journal of Physical Chemistry B*, **2000**, 104, 8321-8326	3.4	41
27	Positional preference of proline in alpha-helices. *Protein Science*, **1999**, 8, 1492-9	6.3	81
26	Imide Cis trans Isomerization of N-Acetyl-N methylprolineamide and Solvent Effects. *Journal of Physical Chemistry A*, **1999**, 103, 5436-5439	2.8	57
25	Ab Initio Molecular Orbital Calculations on N-Mercaptoethylacetamide and Its Derivatives as Model Compounds of Coenzyme A (CoA), Acetyl-CoA, and Malonyl-CoA. *Journal of Physical Chemistry B*, **1997**, 101, 7001-7006	3.4	4
24	Conformational study of asialo-GM1 (GA1) ganglioside. *Biopolymers*, **1997**, 42, 19-35	2.2	9
23	Determination of Potential Parameters for Amino Acid Zwitterions. *The Journal of Physical Chemistry*, **1996**, 100, 17670-17677		12
22	Intrinsic Torsional Potential Parameters for Conformational Analysis of Peptides and Proteins. *The Journal of Physical Chemistry*, **1996**, 100, 15588-15598		29
21	Ab Initio Molecular Orbital Calculations on Low-Energy Conformers of N-Acetyl-N methylprolineamide. *The Journal of Physical Chemistry*, **1996**, 100, 11589-11595		40

20	A pseudrotation model and ring-puckering of cyclopentane. *Computational and Theoretical Chemistry*, **1996**, 362, 243-255		35
19	Semiempirical MO study on malonyl-CoA. Part 2. Malonyl-AMP. *Computational and Theoretical Chemistry*, **1996**, 365, 201-209		1
18	Pseudorotation in heterocyclic five-membered rings: tetrahydrofuran and pyrrolidine. *Computational and Theoretical Chemistry*, **1996**, 369, 157-165		46
17	Ab initio MO study on model compounds of malonyl-CoA: malonic acid and malonyl methyl sulfide. *Computational and Theoretical Chemistry*, **1996**, 369, 145-156		6
16	Conformation and activity of +H2-Pro-Leu-Gly-NH2 and its analogues modified at the leucyl residue. *International Journal of Peptide and Protein Research*, **1995**, 46, 381-90		2
15	Determination of Nonbonded Potential Parameters for Peptides. *The Journal of Physical Chemistry*, **1995**, 99, 13019-13027		25
14	Conformation and sweet tastes of L-aspartyl dipeptide methyl esters. *Biopolymers*, **1994**, 34, 1037-48	2.2	5
13	Conformational study on proline-containing tripeptides of ribonuclease T1. *The Journal of Physical Chemistry*, **1993**, 97, 9248-9258		7
12	Conformation and hydration of acetylcholine. *Journal of Molecular Structure*, **1992**, 269, 231-241	3.4	11
11	Conformation and hydration of aspartame. *International Journal of Peptide and Protein Research*, **1991**, 38, 79-83		10
10	Conformational analysis of poly(2-hydroxyethyl methacrylate). *Journal of Polymer Science Part A*, **1991**, 29, 393-398	2.5	3
9	Conformational analysis of some antibacterial agent 4-aminodiphenyl sulfones. *Archives of Pharmacal Research*, **1990**, 13, 43-50	6.1	3
8	Free energies of hydration of solute molecules. 4. Revised treatment of the hydration shell model. *The Journal of Physical Chemistry*, **1988**, 92, 4739-4742		87
7	Free energies of hydration of solute molecules. 3. Application of the hydration shell model to charged organic molecules. *The Journal of Physical Chemistry*, **1987**, 91, 4118-4120		73
6	Free energies of hydration of solute molecules. 1. Improvement of the hydration shell model by exact computations of overlapping volumes. *The Journal of Physical Chemistry*, **1987**, 91, 4105-4109		118
5	Free energies of hydration of solute molecules. 2. Application of the hydration shell model to nonionic organic molecules. *The Journal of Physical Chemistry*, **1987**, 91, 4109-4117		61
4	Low-energy conformations of two lysine-containing tetrapeptides of collagen: implications for posttranslational lysine hydroxylation. *Biopolymers*, **1987**, 26, 1781-8	2.2	6
3	Conformational study of trinucleoside tetraphosphate d(pCpGpCp): Transition of right-handed form to left-handed form. *Biopolymers*, **1984**, 23, 511-536	2.2	8

2	Conformational study of the dinucleotide dGpdCp-tetrapeptide Ala4 complex. *Macromolecules*, **1984**, 17, 138-147	5.5	13
1	Additivity of atomic static polarizabilities and dispersion coefficients. *Theoretica Chimica Acta*, **1982**, 61, 41-48		111