# Young Kee Kang

List of Publications by Year
in descending order

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|---|---|---|---|
| 110 papers | 2,544 citations | 185998 28 h-index | 223531 46 g-index |
| 112 all docs | 112 docs citations | 112 times ranked | 2378 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | 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, 7547-7552. | 3.3 | 140 |
| 2 | 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. | 2.9 | 131 |
| 3 | Additivity of atomic static polarizabilities and dispersion coefficients. Theoretica Chimica Acta, 1982, 61, 41-48. | 0.9 | 117 |
| 4 | Ab initio MO and density functional studies on trans and cis conformers of N-methylacetamide. Computational and Theoretical Chemistry, 2001, 546, 183-193. | 1.5 | 99 |
| 5 | Free energies of hydration of solute molecules. 4. Revised treatment of the hydration shell model. The Journal of Physical Chemistry, 1988, 92, 4739-4742. | 2.9 | 98 |
| 6 | Positional preference of proline in Î±â€helices. Protein Science, 1999, 8, 1492-1499. | 3.1 | 94 |
| 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. | 2.9 | 77 |
| 8 | Conformational Preferences of Non-Prolyl and Prolyl Residues. Journal of Physical Chemistry B, 2006, 110, 21338-21348. | 1.2 | 74 |
| 9 | Internal rotation about the Câ€“N bond of amides. Computational and Theoretical Chemistry, 2004, 676, 171-176. | 1.5 | 72 |
| 10 | Cisâ€“trans isomerization and puckering of proline residue. Biophysical Chemistry, 2004, 111, 135-142. | 1.5 | 68 |
| 11 | 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. | 2.9 | 65 |
| 12 | Imide Cisâ^'Trans Isomerization ofN-Acetyl-Nâ€˜-methylprolineamide and Solvent Effects. Journal of Physical Chemistry A, 1999, 103, 5436-5439. | 1.1 | 57 |
| 13 | Pseudorotation in heterocyclic five-membered rings: tetrahydrofuran and pyrrolidine. Computational and Theoretical Chemistry, 1996, 369, 157-165. | 1.5 | 52 |
| 14 | Conformational Preferences of Proline Oligopeptides. Journal of Physical Chemistry B, 2006, 110, 17645-17655. | 1.2 | 48 |
| 15 | Assessment of density functionals with longâ€range and/or empirical dispersion corrections for conformational energy calculations of peptides. Journal of Computational Chemistry, 2010, 31, 2915-2923. | 1.5 | 46 |
| 16 | Cisâ^'Trans Isomerization and Puckering of Pseudoproline Dipeptides. Journal of Physical Chemistry B, 2002, 106, 2074-2082. | 1.2 | 44 |
| 17 | Which Functional Form Is Appropriate for Hydrogen Bond of Amides?. Journal of Physical Chemistry B, 2000, 104, 8321-8326. | 1.2 | 43 |
| 18 | Ab Initio Molecular Orbital Calculations on Low-Energy Conformers ofN-Acetyl-Nâ€˜-methylprolineamide. The Journal of Physical Chemistry, 1996, 100, 11589-11595. | 2.9 | 40 |

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|---|---|---|---|
| 19 | Ab initio and DFT conformational study of proline dipeptide. Computational and Theoretical Chemistry, 2004, 675, 37-45. | 1.5 | 40 |
| 20 | 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. | 1.2 | 38 |
| 21 | A pseudrotation model and ring-puckering of cyclopentane. Computational and Theoretical Chemistry, 1996, 362, 243-255. | 1.5 | 36 |
| 22 | Ring Flip of Proline Residue via the Transition State with an Envelope Conformation. Journal of Physical Chemistry B, 2004, 108, 5463-5465. | 1.2 | 36 |
| 23 | Thiazoleâ€Based Î³â€Building Blocks as Reverseâ€Turn Mimetic to Design a Gramicidinâ€…S Analogue: Conformational and Biological Evaluation. Chemistry - A European Journal, 2014, 20, 6713-6720. | 1.7 | 36 |
| 24 | Puckering Transition of Proline Residue in Water. Journal of Physical Chemistry B, 2007, 111, 10550-10556. | 1.2 | 34 |
| 25 | Conformational preferences and pK<sub>a</sub> value of selenocysteine residue. Biopolymers, 2011, 95, 345-353. | 1.2 | 34 |
| 26 | 12/10-Helical Î²-Peptide 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. | 6.6 | 30 |
| 27 | Intrinsic Torsional Potential Parameters for Conformational Analysis of Peptides and Proteins. The Journal of Physical Chemistry, 1996, 100, 15588-15598. | 2.9 | 29 |
| 28 | Conformational Preferences of Proline Analogues with Different Ring Size. Journal of Physical Chemistry B, 2007, 111, 3496-3507. | 1.2 | 29 |
| 29 | A Fast Method for Calculating Geometry-Dependent Net Atomic Charges for Polypeptides. Journal of Physical Chemistry B, 2001, 105, 3624-3634. | 1.2 | 27 |
| 30 | Determination of Nonbonded Potential Parameters for Peptides. The Journal of Physical Chemistry, 1995, 99, 13019-13027. | 2.9 | 25 |
| 31 | Conformational Preference and Cisâ^'Trans Isomerization of 4(R)-Substituted Proline Residues. Journal of Physical Chemistry B, 2006, 110, 1915-1927. | 1.2 | 25 |
| 32 | Conformational Preferences and cisâ^'trans Isomerization of Azaproline Residue. Journal of Physical Chemistry B, 2007, 111, 5377-5385. | 1.2 | 25 |
| 33 | Conformational preference and cisâ€“trans isomerization of 4â€methylproline residues. Biopolymers, 2011, 95, 51-61. | 1.2 | 25 |
| 34 | Puckering Transition of 4-Substituted Proline Residues. Journal of Physical Chemistry B, 2005, 109, 16982-16987. | 1.2 | 24 |
| 35 | Local Control of the Cisâ€“Trans Isomerization and Backbone Dihedral Angles in Peptides Using Trifluoromethylated Pseudoprolines. Journal of Physical Chemistry B, 2012, 116, 4069-4079. | 1.2 | 24 |
| 36 | Conformational Preferences of Pseudoproline Residues. Journal of Physical Chemistry B, 2007, 111, 12551-12562. | 1.2 | 23 |

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|---|---|---|---|
| 37 | Remote Stereoinductive Intramolecular Nitrile Oxide Cycloaddition: Asymmetric Total Synthesis and Structure Revision of (â^')-11Î²-Hydroxycurvularin. Journal of Organic Chemistry, 2016, 81, 2612-2617. | 1.7 | 20 |
| 38 | cis â€“ trans Isomerization of N -acetyl- N â€²-methylamides of 5-methylproline and 5,5-dimethylproline. Computational and Theoretical Chemistry, 2002, 585, 209-221. | 1.5 | 19 |
| 39 | Ab initio conformational study of N-acetyl-l-proline-Nâ€²,Nâ€²-dimethylamide: a model for polyproline. Biophysical Chemistry, 2005, 113, 93-101. | 1.5 | 19 |
| 40 | Comparative conformational study of N-acetyl-Nâ€²-methylprolineamide with different basis sets. Computational and Theoretical Chemistry, 2002, 593, 55-64. | 1.5 | 18 |
| 41 | Conformational preferences of Î³-aminobutyric acid in the gas phase and in water. Journal of Molecular Structure, 2012, 1024, 163-169. | 1.8 | 18 |
| 42 | The triple helical structure and stability of collagen model peptide with 4(s)â€hydroxyprolylâ€proâ€gly units. Biopolymers, 2012, 98, 111-121. | 1.2 | 18 |
| 43 | An Efficient Method for Calculating Atomic Charges of Peptides and Proteins from Electronic Populations. Journal of Physical Chemistry B, 2008, 112, 5470-5478. | 1.2 | 17 |
| 44 | Computationally designed Î²â€turn foldamers of Î³â€peptides based on 2â€(aminomethyl)cyclohexanecarboxylic acid. Biopolymers, 2012, 97, 1018-1025. | 1.2 | 17 |
| 45 | Preferred conformations of RGDX tetrapeptides to inhibit the binding of fibrinogen to platelets. Biopolymers, 2002, 63, 298-313. | 1.2 | 16 |
| 46 | Altering the Cyclization Modes: Temperature-Dependent Intramolecular 7-Endo-Dig vs 6-Endo-Dig Electrophilic Ring Closures. Organic Letters, 2017, 19, 1474-1477. | 2.4 | 16 |
| 47 | Transition of prolyl puckering in a model of polyproline. Computational and Theoretical Chemistry, 2005, 718, 17-21. | 1.5 | 15 |
| 48 | Puckering transitions of pseudoproline residues. Biopolymers, 2009, 91, 444-455. | 1.2 | 15 |
| 49 | Tailoring the Physicochemical Properties of Antimicrobial Peptides onto a Thiazole-Based Î³-Peptide Foldamer. Journal of Medicinal Chemistry, 2020, 63, 9168-9180. | 2.9 | 15 |
| 50 | Determination of Potential Parameters for Amino Acid Zwitterions. The Journal of Physical Chemistry, 1996, 100, 17670-17677. | 2.9 | 14 |
| 51 | Prospect of Thiazoleâ€based Î³â€Peptide Foldamers in Enamine Catalysis: Exploration of the Nitroâ€Michael Addition. Chemistry - A European Journal, 2019, 25, 7396-7401. | 1.7 | 14 |
| 52 | Conformational study of the dinucleotide dGpdCp-tetrapeptide Ala4 complex. Macromolecules, 1984, 17, 138-147. | 2.2 | 13 |
| 53 | Conformational Preferences and Cisâ^'Trans Isomerization of l-Lactic Acid Residue. Journal of Physical Chemistry B, 2008, 112, 9126-9134. | 1.2 | 13 |
| 54 | Conformational preferences and cisâ€“trans isomerization of <scp>L</scp>â€3,4â€dehydroproline residue. Biopolymers, 2009, 92, 387-398. | 1.2 | 13 |

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|---|---|---|---|
| 55 | Conformation and hydration of acetylcholine. Journal of Molecular Structure, 1992, 269, 231-241. | 1.8 | 12 |
| 56 | Conformational preferences and prolyl cisâ€“trans isomerization of phosphorylated Ser/Thrâ€Pro motifs. Biopolymers, 2010, 93, 330-339. | 1.2 | 12 |
| 57 | Exploring conformational preferences of alanine tetrapeptide by CCSD(T), MP2, and dispersion-corrected DFT methods. Chemical Physics Letters, 2018, 702, 69-75. | 1.2 | 12 |
| 58 | A mechanistic study supports a two-step mechanism for peptide bond formation on the ribosome. Physical Chemistry Chemical Physics, 2013, 15, 14931. | 1.3 | 11 |
| 59 | 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. | 1.2 | 11 |
| 60 | Which DFT levels of theory are appropriate in predicting the prolyl cisâ€“trans isomerization in solution?. New Journal of Chemistry, 2019, 43, 17159-17173. | 1.4 | 11 |
| 61 | Conformational study of asialo-GM1 (GA1) ganglioside. , 1997, 42, 19-35. | | 10 |
| 62 | Conformational Preferences and pKa Value of Cysteine Residue. Journal of Physical Chemistry B, 2008, 112, 11189-11193. | 1.2 | 10 |
| 63 | Conformation and hydration of aspartame. International Journal of Peptide and Protein Research, 1991, 38, 79-83. | 0.1 | 10 |
| 64 | Conformational Preferences of X-Pro Sequences: Ala-Pro and Aib-Pro Motifs. Journal of Physical Chemistry B, 2010, 114, 14077-14086. | 1.2 | 10 |
| 65 | Binding free energies of inhibitors to iron porphyrin complex as a model for Cytochrome P450. Biopolymers, 2012, 97, 219-228. | 1.2 | 10 |
| 66 | Conformational preferences of the 2-methylproline residue and its role in stabilizing Î²-turn and polyproline II structures of peptides. New Journal of Chemistry, 2014, 38, 2831. | 1.4 | 10 |
| 67 | Propensities of peptides containing the <scp>A</scp>snâ€<scp>G</scp>ly segment to form Î²â€turn and Î²â€hairpin structures. Biopolymers, 2016, 105, 653-664. | 1.2 | 10 |
| 68 | Conformational Preferences of Glycerol in the Gas Phase and in Water. Bulletin of the Korean Chemical Society, 2012, 33, 917-924. | 1.0 | 10 |
| 69 | Reagent-free intramolecular hydrofunctionalization: a regioselective 6-endo-dig cyclization of o-alkynoylphenols. Green Chemistry, 2022, 24, 2376-2384. | 4.6 | 10 |
| 70 | Strength of CHÂ·Â·Â·Ï€ interactions in the Câ€terminal subdomain of villin headpiece. Biopolymers, 2012, 97, 778-788. | 1.2 | 9 |
| 71 | Conformational preferences of helix foldamers of Î³â€peptides based on 2â€(aminomethyl)cyclohexanecarboxylic acid. Biopolymers, 2014, 101, 87-95. | 1.2 | 9 |
| 72 | C<sub>9/12</sub> Ribbonâ€Like Structures in Hybrid Peptides Alternating Î±â€and Thiazoleâ€Based Î³â€Amino Acids. Chemistry - A European Journal, 2017, 23, 17584-17591. | 1.7 | 9 |

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| 73 | Puckering transitions in cyclohexane: Revisited. Chemical Physics Letters, 2018, 702, 82-89. | 1.2 | 9 |
| 74 | Conformational study of trinucleoside tetraphosphate d(pCpGpCp): Transition of right-handed form to left-handed form. Biopolymers, 1984, 23, 511-536. | 1.2 | 8 |
| 75 | A histidine substitution confers metal binding affinity to a Schistosoma japonicum Glutathione S-transferase. Protein Expression and Purification, 2010, 73, 74-77. | 0.6 | 8 |
| 76 | Helix foldamers of Î³-peptides based on 2-aminocyclohexylacetic acid: a computational study. New Journal of Chemistry, 2014, 38, 966. | 1.4 | 8 |
| 77 | Helix foldamers of Î³-peptides based on 2-aminocyclopentylacetic acid. New Journal of Chemistry, 2015, 39, 3241-3249. | 1.4 | 8 |
| 78 | Conformational study on proline-containing tripeptides of ribonuclease T1. The Journal of Physical Chemistry, 1993, 97, 9248-9258. | 2.9 | 7 |
| 79 | Conformational preferences of 4â€²chloroproline residues. Biopolymers, 2012, 97, 629-641. | 1.2 | 7 |
| 80 | Conformational preferences of taurine in the gas phase and in water. Computational and Theoretical Chemistry, 2013, 1025, 8-15. | 1.1 | 7 |
| 81 | Allylic Azide Rearrangements Investigated by Density Functional Theory Calculations. Bulletin of the Korean Chemical Society, 2017, 38, 1419-1426. | 1.0 | 7 |
| 82 | PMFF: Development of a Physics-Based Molecular Force Field for Protein Simulation and Ligand Docking. Journal of Physical Chemistry B, 2020, 124, 974-989. | 1.2 | 7 |
| 83 | Low-energy conformations of two lysine-containing tetrapeptides of collagen: Implications for posttranslational lysine hydroxylation. Biopolymers, 1987, 26, 1781-1788. | 1.2 | 6 |
| 84 | Conformation and sweet tastes ofL-aspartyl dipeptide methyl esters. Biopolymers, 1994, 34, 1037-1048. | 1.2 | 6 |
| 85 | Ab initio MO study on model compounds of malonyl-CoA: malonic acid and malonyl methyl sulfide. Computational and Theoretical Chemistry, 1996, 369, 145-156. | 1.5 | 6 |
| 86 | Preferred conformations of a linear RGD tripeptide. Chemical Biology and Drug Design, 2000, 56, 360-372. | 1.2 | 6 |
| 87 | Conformational analysis of poly(2-hydroxyethyl methacrylate). Journal of Polymer Science Part A, 1991, 29, 393-398. | 2.5 | 5 |
| 88 | Preferred conformations of cyclic Acâ€“Cysâ€“Proâ€“Xaaâ€“Cysâ€“NHMe peptides: a model for chain reversal and active site of disulfide oxidoreductase. Biophysical Chemistry, 2003, 105, 89-104. | 1.5 | 5 |
| 89 | Influence of substituents on conformational preferences of helix foldamers of Î³â€dipeptides. Biopolymers, 2014, 101, 1077-1087. | 1.2 | 5 |
| 90 | Propensities to form the Î²-turn and Î²-hairpin structures of<scp>d</scp>-Pro-Gly and Aib-<scp>d</scp>-Ala containing peptides: a computational study. New Journal of Chemistry, 2016, 40, 8565-8578. | 1.4 | 5 |

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| 91 | Conformational analysis of some antibacterial agent 4-aminodiphenyl sulfones. Archives of Pharmacal Research, 1990, 13, 43-50. | 2.7 | 4 |
| 92 | Ab Initio Molecular Orbital Calculations onN-Î²-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. | 1.2 | 4 |
| 93 | Conformational preferences of Nâ€methoxycarbonyl proline dipeptide. Journal of Computational Chemistry, 2009, 30, 1116-1127. | 1.5 | 4 |
| 94 | Conformational preferences and antimicrobial activities of alkanediols. Computational and Theoretical Chemistry, 2015, 1064, 15-24. | 1.1 | 4 |
| 95 | Conformational preferences of Î²-sheet structures in cyclopropane-containing Î³-peptides. New Journal of Chemistry, 2015, 39, 4640-4646. | 1.4 | 4 |
| 96 | Organocatalytic Asymmetric Addition of Aldehyde to Nitroolefin by H-<scp>d</scp>-Pro-Pro-Glu-NH<sub>2</sub>: A Mechanistic Study. ACS Omega, 2019, 4, 8862-8873. | 1.6 | 4 |
| 97 | Conformational preferences of cationic Î²-peptide in water studied by CCSD(T), MP2, and DFT methods. Heliyon, 2020, 6, e04721. | 1.4 | 4 |
| 98 | Mechanistic study of hemicucurbit[6]uril formation by step-growth oligomerization and end-to-end cyclization. Chemical Physics Letters, 2017, 669, 92-98. | 1.2 | 3 |
| 99 | Conformation and activity of <sup>+</sup>H<sub>2</sub>â€Proâ€Leuâ€Glyâ€NH<sub>2</sub> and its analogues modified at the leucyl residue. International Journal of Peptide and Protein Research, 1995, 46, 381-390. | 0.1 | 2 |
| 100 | Hairpin formation promoted by the heterochiral dinipecotic acid segment: A DFT study. Biopolymers, 2015, 103, 609-617. | 1.2 | 2 |
| 101 | Conformational Preferences of Cyclopentaneâ€Based Oligoâ€Î²â€peptides in the Gas Phase and in Solution. ChemPlusChem, 2021, 86, 533-539. | 1.3 | 2 |
| 102 | Semiempirical MO study on malonyl-CoA. Part 2. Malonyl-AMP. Computational and Theoretical Chemistry, 1996, 365, 201-209. | 1.5 | 1 |
| 103 | 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, 3287-3289. | 1.2 | 1 |
| 104 | Reply to â€œcomment on â€˜binding free energies of inhibitors to iron porphyrin complex as a model for cytochrome P450â€™â€. Biopolymers, 2012, 97, 649-650. | 1.2 | 1 |
| 105 | Effects of isosteric substitutions on the conformational preference and cisâ€“trans isomerization of proline-containing peptides. New Journal of Chemistry, 2017, 41, 6593-6606. | 1.4 | 1 |
| 106 | Puckering transition of the proline residue along the pseudorotational path: revisited. New Journal of Chemistry, 2021, 45, 9780-9793. | 1.4 | 1 |
| 107 | Exploring Helical Folding in Oligomers of Cyclopentaneâ€Based Ïµâ€Amino Acids: A Computational Study. ChemistryOpen, 2022, , e202100253. | 0.9 | 1 |
| 108 | Preferred conformations of a linear RGD tripeptide. Chemical Biology and Drug Design, 2001, 58, 90-90. | 1.2 | 0 |

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|---|---|---|---|
| 109 | Proline puckering and cis-trans isomerization of proline-containing peptides. , 2002, , 420-421. | | 0 |
| 110 | Exploring Helical Folding in Oligomers of Cyclopentaneâ€Based Ïµâ€Amino Acids: A Computational Study. ChemistryOpen, 2022, 11, e202200035. | 0.9 | 0 |