Hitoshi Goto

List of Publications by Year
in descending order

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68	2,533	304743 22	189892 50
papers	citations	h-index	g-index

71	71	71	2458
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Corner flapping: a simple and fast algorithm for exhaustive generation of ring conformations. Journal of the American Chemical Society, 1989, 111, 8950-8951.	13.7	445
2	Report on the sixth blind test of organic crystal structure prediction methods. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 439-459.	1.1	445
3	An efficient algorithm for searching low-energy conformers of cyclic and acyclic molecules. Journal of the Chemical Society Perkin Transactions II, 1993, , 187-198.	0.9	351
4	Synthesis, Absolute Configuration, and Enantiomeric Enrichment of a Cruciferous Oxindole Phytoalexin, (S)-(â˜')-Spirobrassinin, and Its Oxazoline Analog. Journal of Organic Chemistry, 2001, 66, 3940-3947.	3.2	170
5	Investigation of intramolecular interactions in n-alkanes. Cooperative energy increments associated with GG and GTG' [G = gauche, T = trans] sequences. Journal of the American Chemical Society, 1991, 113, 4665-4671.	13.7	105
6	Synthesis, Resolution, and Absolute Stereochemistry of (â˜')-Blestriarene C. Journal of Organic Chemistry, 2003, 68, 2099-2108.	3.2	62
7	How many conformers are there for small n-alkanes? Consequences of asymmetric deformation in GGâ€² segment. Tetrahedron, 1993, 49, 387-396.	1.9	57
8	Continuously Growing Spiral Carbon Nanoparticles as the Intermediates in the Formation of Fullerenes and Nanoonions. Journal of Physical Chemistry B, 2002, 106, 7135-7138.	2.6	51
9	Geometrical structure of benzene and naphthalene: Ultrahigh-resolution laser spectroscopy and abâ€‰initio calculation. Journal of Chemical Physics, 2011, 135, 054305.	3.0	51
10	Cooperative Enhancement of Water Binding to Crownophane by Multiple Hydrogen Bonds:â€‰ Analysis by High Level ab Initio Calculations. Journal of the American Chemical Society, 2001, 123, 4255-4258.	13.7	48
11	Structure and excited-state dynamics of anthracene: Ultrahigh-resolution spectroscopy and theoretical calculation. Journal of Chemical Physics, 2009, 130, 134315.	3.0	47
12	Thermosalience in Macrocycle-Based Soft Crystals via Anisotropic Deformation of Disilanyl Architecture. Journal of the American Chemical Society, 2020, 142, 12651-12657.	13.7	44
13	Viewpoint 11 â€" approaches to the global minimum problem. Computational and Theoretical Chemistry, 1993, 285, 157-168.	1.5	42
14	Absolute configuration of chiral fullerenes and covalent derivatives from their calculated circular dichroism spectra. Journal of the Chemical Society Perkin Transactions II, 1998, , 1719-1724.	0.9	40
15	C100 IPR fullerenes: temperature-dependent relative stabilities based on the Gibbs function. Chemical Physics, 2004, 306, 93-104.	1.9	40
16	Theoretical Studies on the Relative Stabilities of C96IPR Fullerenes. Journal of Physical Chemistry A, 2004, 108, 4479-4484.	2.5	40
17	Chemistry of Unique Chiral Olefins. 4. Theoretical Studies of the Racemization Mechanism oftrans-andcis-1,1â€˜,2,2â€˜,3,3â€˜,4,4â€˜-Octahydro-4,4â€˜-biphenanthrylidenes. Journal of Organic Chemistry, 1999, 64, 1667-1674.	3.2	36
18	Is the CD Exciton Chirality Method Applicable to Chiral 1,1â€˜-Biphenanthryl Compounds?. Journal of the American Chemical Society, 1998, 120, 9086-9087.	13.7	31

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19	Proposed mechanism for diterpene synthases in the formation of phomactatriene and taxadiene. Organic and Biomolecular Chemistry, 2005, 3, 2713.	2.8	30
20	Computing the relative gas-phase populations of C60 and C70: beyond the traditional Î”Hf,298o scale. Journal of Molecular Graphics and Modelling, 2001, 19, 216-221.	2.4	29
21	Theoretical investigations on relative stabilities of fullerene C94. Journal of Chemical Physics, 2003, 118, 10534-10540.	3.0	26
22	Photoinduced molecular transformations. Part 155. General synthesis of macrocyclic ketones based on a ring expansion involving a selective Î²-scission of alkoxyl radicals, its application to a new synthesis of (Â±)-isocaryophyllene and (Â±)-caryophyllene, and a conformational analysis of the two sesquiterpenes and the radical intermediate in the synthesis by MM3 calculations. Journal of the Chemical Society Perkin Transactions 1, 1995, , 69-81.	0.9	24
23	Highly stereoselective spirocyclopropanation of various diazooxindoles with olefins catalyzed using Ru(<scp>ii</scp>)-complex. RSC Advances, 2018, 8, 39865-39869.	3.6	19
24	Parallelization of Crystal Calculation for Large-Scale Molecular Crystal Structure Analysis. Journal of Computer Aided Chemistry, 2008, 9, 8-16.	0.3	15
25	A revised nomenclature for the ring conformation and a note on the conformational distance in cyclododecane. Tetrahedron, 1992, 48, 7131-7144.	1.9	14
26	Ultrahigh-resolution laser spectroscopy of the S1 1B2â†•S0 1A transition of perylene. Journal of Molecular Spectroscopy, 2010, 260, 72-76.	1.2	14
27	Mode-selective internal conversion of perylene. Molecular Physics, 2011, 109, 1831-1840.	1.7	14
28	Computational chemical analysis of Ru(II)â€Pheoxâ€“catalyzed highly enantioselective intramolecular cyclopropanation reactions. Chirality, 2019, 31, 52-61.	2.6	14
29	Origin of regioselectivity in the O-methylation of erythromycin as elucidated with the aid of computational conformational space search. Journal of the Chemical Society Perkin Transactions II, 1993, , 1647-1654.	0.9	13
30	Electronic structures and redox properties of silylmethylated C60. Tetrahedron, 1996, 52, 5053-5064.	1.9	13
31	A frontier mode-following method for mapping saddle points of conformational interconversion in flexible molecules starting from the energy minimum. Chemical Physics Letters, 1998, 292, 254-258.	2.6	13
32	Prediction of favorable isomeric structures for the C₁₀₀ to C₁₂₀ giant fullerenes. An application of the phason line criteria. , 1996, 1, 163-171.		13
33	Selective Formation and SHG Intensity of Noncentrosymmetric and Centrosymmetric 1,1,2,2-Tetramethyl-1-(4-(N,N-dimethylamino)phenyl)-2-(2â€²-cyanophenyl)disilane Crystals under External Stimuli. Journal of Physical Chemistry C, 2020, 124, 17450-17458.	3.1	13
34	Charge mobility calculation of organic semiconductors without use of experimental single-crystal data. Scientific Reports, 2020, 10, 2524.	3.3	13
35	Conformational Polymorphism Analysis of Aspirin Crystal with a Crystal Calculation Method. Journal of Computer Chemistry Japan, 2008, 7, 151-164.	0.1	13
36	Application of molecular mechanics to natural product chemistry. Pure and Applied Chemistry, 1989, 61, 597-600.	1.9	12

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37	Chiral synthesis of polyketide-derived natural products. 28. Synthesis of 16-membered macrolide aglycons, carbonolide A, leuconolides, and maridonolides, via carbonolide B type compounds by virtue of completely stereoselective epoxidation and reduction based on the conformational control of macrolide rings with protecting groups. Journal of Organic Chemistry, 1990, 55, 1129-1132.	3.2	12
38	High-speed prediction of crystal structures for organic molecules. AIP Conference Proceedings, 2015, , .	0.4	11
39	Ligand Exchange Reaction on a Ru(II)â€“Pheox Complex as a Mechanistic Study of Catalytic Reactions. ACS Omega, 2018, 3, 11286-11289.	3.5	10
40	Validation Study of QSAR/DNN Models Using the Competition Datasets. Molecular Informatics, 2020, 39, 1900154.	2.5	10
41	Cluster conformational analysis of a seco acid used in Woodward's total synthesis of erythromycin A. Computational and Theoretical Chemistry, 1997, 398-399, 229-236.	1.5	9
42	Molecular activity prediction using deep learning software library. , 2016, , .		8
43	Combined molecular mechanics (MM2) and molecular orbital (AM1) study of periplanone-B and analogues. Evaluation of biological activity from electronic properties and geometries. Journal of the Chemical Society Perkin Transactions II, 1992, , 811-818.	0.9	7
44	Vacancy profile in reverse osmosis membranes studied by positron annihilation lifetime measurements and molecular dynamics simulations. Journal of Physics: Conference Series, 2013, 443, 012050.	0.4	7
45	Preparation of photonic molecular trains via soft-crystal polymerization of lanthanide complexes. Nature Communications, 2022, 13, .	12.8	7
46	Conformational analyses of periplanone analogs by molecular mechanics calculations. Journal of Chemical Ecology, 1991, 17, 779-788.	1.8	5
47	Conformational analysis of serricornin: Application of molecular mechanics calculations to stereochemical assignment of serricornin, sex pheromone of cigarette beetle (Lasioderma serricorne) Tj ETQq1 1 0.784314 rgBT /Ove	1.8	4
48	Chiral Synthesis of Polyketide-Derived Natural Products. 33. Stereoselective Total Synthesis of 16-Membered Macrolide Aglycons, Leuconolides and Maridonolides. Macrocyclic Stereocontrol Based on Conformational Analysis of the 16-Membered Macrolide Ring.. Chemical and Pharmaceutical Bulletin, 1991, 39, 2819-2829.	1.3	4
49	Combined molecular mechanics (MM2) and molecular orbital (AM1) study of reriplanone-a and analogues. Evaluation of biological activity from electronic properties and geometries. Part 2. Journal of the Chemical Society Perkin Transactions II, 1993, , 1167-1173.	0.9	3
50	The phaseon line: a new criterion for the stability of fullerenes. , 1996, 1, 151-162.		3
51	Implementation and performance evaluation of CONFLEX-G. , 2004, , .		3
52	Molecular mechanics (CONFLEX/MM3) search/minimization study of the conformations of ornoside and escuside. Journal of Molecular Structure, 2005, 748, 9-16.	3.6	3
53	Numerical calculation on a two-step subdiffusion behavior of lateral protein movement in plasma membranes. Physical Review E, 2017, 96, 042410.	2.1	3
54	Journal of Computer Chemistry, Japan:Conversion of Japanese Word Manuscript into the XML Format and Web Publication Management System. Journal of Computer Chemistry Japan, 2011, 10, 141-146.	0.1	3

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55	Theoretical Electronic Circular Dichroism Study of 1,3â€Diene Derivatives for the Elucidation of ECD Spectra of 1,3â€Cyclohexadiene and Its Derivatives. Chirality, 2015, 27, 476-478.	2.6	2
56	Soft Crystal Force Field for Reproducing the Crystal Structures of Aryl Gold Isocyanide Complexes. Journal of Computer Chemistry Japan, 2018, 17, 155-157.	0.1	2
57	FAST ALGORITHM FOR COVERING CONFORMATIONAL SPACE BY MOLECULAR MECHANICS. , 1991, , 411-416.		2
58	Drug discovery using grid technology. , 2006, , 227-248.		2
59	Investigation of a Virtual Nested Two-dimensional Lattice Model for Representing the Diffusive Motion of a Transmembrane Protein in Cell Membrane. Journal of Computer Chemistry Japan, 2016, 15, 229-231.	0.1	1
60	Crystal Structure Optimization Method for Evaluation of Mechanical Properties of Soft Crystals. Nihon Kessho Gakkaishi, 2021, 63, 63-68.	0.0	1
61	Conformational Analysis of Long Chain Seco-Acids Used in Woodwardâ€™s Total Synthesis of Erythromycin A â€" Conformational Space Search as the Basis of Molecular Modeling. , 1996, , 189-197.		1
62	Crystal Structure Prediction; From the Present to the Future. Nihon Kessho Gakkaishi, 2020, 62, 260-268.	0.0	1
63	Spiral carbon nanoparticles. AIP Conference Proceedings, 2001, , .	0.4	0
64	Chiral Olefin and Molecular Motor. Journal of Computer Chemistry Japan, 2017, 16, A21-A22.	0.1	0
65	Development of Visualization Technique of Biological Information for Mobile Terminal Devices. Journal of Computer Chemistry Japan, 2014, 13, 175-176.	0.1	0
66	Development of Education Curriculum for First Level Simulation Engineering in Chemistry - Questionnaire Research and Core-Curriculum Proposal -. Journal of Computer Chemistry Japan, 2014, 13, 179-180.	0.1	0
67	Nomenclature of Aldohexopyranose Conformations IncludingRotational Isomers of Hydroxyl Groups. Journal of Computer Chemistry Japan, 2014, 13, 263-267.	0.1	0
68	Improving the Accuracy of Crystal Structure Prediction Using FMO Crystal Energy: An Example of Target XXIII. Journal of Computer Chemistry Japan, 2021, 20, 92-93.	0.1	0