

# Hitoshi Goto

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/1311641/publications.pdf>

Version: 2024-02-01

68  
papers

2,533  
citations

304368

22  
h-index

189595

50  
g-index

71  
all docs

71  
docs citations

71  
times ranked

2458  
citing authors

#	ARTICLE	IF	CITATIONS
1	Corner flapping: a simple and fast algorithm for exhaustive generation of ring conformations. <i>Journal of the American Chemical Society</i> , 1989, 111, 8950-8951.	6.6	445
2	Report on the sixth blind test of organic crystal structure prediction methods. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2016, 72, 439-459.	0.5	445
3	An efficient algorithm for searching low-energy conformers of cyclic and acyclic molecules. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1993, , 187-198.	0.9	351
4	Synthesis, Absolute Configuration, and Enantiomeric Enrichment of a Cruciferous Oxindole Phytoalexin, (S)-( $\alpha^*$ )-Spirobrassinin, and Its Oxazoline Analog. <i>Journal of Organic Chemistry</i> , 2001, 66, 3940-3947.	1.7	170
5	Investigation of intramolecular interactions in n-alkanes. Cooperative energy increments associated with GG and GTG' [G = gauche, T = trans] sequences. <i>Journal of the American Chemical Society</i> , 1991, 113, 4665-4671.	6.6	105
6	Synthesis, Resolution, and Absolute Stereochemistry of ( $\alpha^*$ )-Blestriarene C. <i>Journal of Organic Chemistry</i> , 2003, 68, 2099-2108.	1.7	62
7	How many conformers are there for small n-alkanes? Consequences of asymmetric deformation in GG $\alpha^2$ segment. <i>Tetrahedron</i> , 1993, 49, 387-396.	1.0	57
8	Continuously Growing Spiral Carbon Nanoparticles as the Intermediates in the Formation of Fullerenes and Nanoions. <i>Journal of Physical Chemistry B</i> , 2002, 106, 7135-7138.	1.2	51
9	Geometrical structure of benzene and naphthalene: Ultrahigh-resolution laser spectroscopy and <i>ab initio</i> calculation. <i>Journal of Chemical Physics</i> , 2011, 135, 054305.	1.2	51
10	Cooperative Enhancement of Water Binding to Crownophane by Multiple Hydrogen Bonds: Analysis by High Level <i>ab Initio</i> Calculations. <i>Journal of the American Chemical Society</i> , 2001, 123, 4255-4258.	6.6	48
11	Structure and excited-state dynamics of anthracene: Ultrahigh-resolution spectroscopy and theoretical calculation. <i>Journal of Chemical Physics</i> , 2009, 130, 134315.	1.2	47
12	Thermosaliency in Macrocyclic-Based Soft Crystals via Anisotropic Deformation of Disilanyl Architecture. <i>Journal of the American Chemical Society</i> , 2020, 142, 12651-12657.	6.6	44
13	Viewpoint 11 "approaches to the global minimum problem. <i>Computational and Theoretical Chemistry</i> , 1993, 285, 157-168.	1.5	42
14	Absolute configuration of chiral fullerenes and covalent derivatives from their calculated circular dichroism spectra. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1998, , 1719-1724.	0.9	40
15	C100 IPR fullerenes: temperature-dependent relative IPR stabilities based on the Gibbs function. <i>Chemical Physics</i> , 2004, 306, 93-104.	0.9	40
16	Theoretical Studies on the Relative Stabilities of C96IPR Fullerenes. <i>Journal of Physical Chemistry A</i> , 2004, 108, 4479-4484.	1.1	40
17	Chemistry of Unique Chiral Olefins. 4. Theoretical Studies of the Racemization Mechanism of <i>trans</i> - and <i>cis</i> -1,1 $\alpha^*$ ,2,2 $\alpha^*$ ,3,3 $\alpha^*$ ,4,4 $\alpha^*$ -Octahydro-4,4 $\alpha^*$ -biphenanthrylidene. <i>Journal of Organic Chemistry</i> , 1999, 64, 1667-1674.	1.7	36
18	Is the CD Exciton Chirality Method Applicable to Chiral 1,1 $\alpha^*$ -Biphenanthryl Compounds?. <i>Journal of the American Chemical Society</i> , 1998, 120, 9086-9087.	6.6	31

#	ARTICLE	IF	CITATIONS
19	Proposed mechanism for diterpene synthases in the formation of phomactatriene and taxadiene. <i>Organic and Biomolecular Chemistry</i> , 2005, 3, 2713.	1.5	30
20	Computing the relative gas-phase populations of C60 and C70: beyond the traditional $\hat{H}_f$ scale. <i>Journal of Molecular Graphics and Modelling</i> , 2001, 19, 216-221.	1.3	29
21	Theoretical investigations on relative stabilities of fullerene C94. <i>Journal of Chemical Physics</i> , 2003, 118, 10534-10540.	1.2	26
22	Photoinduced molecular transformations. Part 155. General synthesis of macrocyclic ketones based on a ring expansion involving a selective $\beta$ -scission of alkoxy radicals, its application to a new synthesis of ( $\Delta^{\pm}$ )-isocaryophyllene and ( $\Delta^{\pm}$ )-caryophyllene, and a conformational analysis of the two sesquiterpenes and the radical intermediate in the synthesis by MM3 calculations. <i>Journal of the Chemical Society Perkin Transactions 1</i> , 1995, , 69-81.	0.9	24
23	Highly stereoselective spirocyclopropanation of various diazooxindoles with olefins catalyzed using Ru( $\eta^5$ -Cp) $\cdot$ Cl $_2$ -complex. <i>RSC Advances</i> , 2018, 8, 39865-39869.	1.7	19
24	Parallelization of Crystal Calculation for Large-Scale Molecular Crystal Structure Analysis. <i>Journal of Computer Aided Chemistry</i> , 2008, 9, 8-16.	0.3	15
25	A revised nomenclature for the ring conformation and a note on the conformational distance in cyclododecane. <i>Tetrahedron</i> , 1992, 48, 7131-7144.	1.0	14
26	Ultrahigh-resolution laser spectroscopy of the S1 $\rightarrow$ S0 transition of perylene. <i>Journal of Molecular Spectroscopy</i> , 2010, 260, 72-76.	0.4	14
27	Mode-selective internal conversion of perylene. <i>Molecular Physics</i> , 2011, 109, 1831-1840.	0.8	14
28	Computational chemical analysis of Ru(II)-Pheox-catalyzed highly enantioselective intramolecular cyclopropanation reactions. <i>Chirality</i> , 2019, 31, 52-61.	1.3	14
29	Origin of regioselectivity in the O-methylation of erythromycin as elucidated with the aid of computational conformational space search. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1993, , 1647-1654.	0.9	13
30	Electronic structures and redox properties of silylmethylated C60. <i>Tetrahedron</i> , 1996, 52, 5053-5064.	1.0	13
31	A frontier mode-following method for mapping saddle points of conformational interconversion in flexible molecules starting from the energy minimum. <i>Chemical Physics Letters</i> , 1998, 292, 254-258.	1.2	13
32	Prediction of favorable isomeric structures for the C <sub>100</sub> to C <sub>120</sub> 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-( <i>N,N</i> -dimethylamino)phenyl)-2-(2-cyanophenyl)disilane Crystals under External Stimuli. <i>Journal of Physical Chemistry C</i> , 2020, 124, 17450-17458.	1.5	13
34	Charge mobility calculation of organic semiconductors without use of experimental single-crystal data. <i>Scientific Reports</i> , 2020, 10, 2524.	1.6	13
35	Conformational Polymorphism Analysis of Aspirin Crystal with a Crystal Calculation Method. <i>Journal of Computer Chemistry Japan</i> , 2008, 7, 151-164.	0.0	13
36	Application of molecular mechanics to natural product chemistry. <i>Pure and Applied Chemistry</i> , 1989, 61, 597-600.	0.9	12

#	ARTICLE	IF	CITATIONS
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. <i>Journal of Organic Chemistry</i> , 1990, 55, 1129-1132.	1.7	12
38	High-speed prediction of crystal structures for organic molecules. <i>AIP Conference Proceedings</i> , 2015, , ,	0.3	11
39	Ligand Exchange Reaction on a Ru(II)â€Pheox Complex as a Mechanistic Study of Catalytic Reactions. <i>ACS Omega</i> , 2018, 3, 11286-11289.	1.6	10
40	Validation Study of QSAR/DNN Models Using the Competition Datasets. <i>Molecular Informatics</i> , 2020, 39, 1900154.	1.4	10
41	Cluster conformational analysis of a seco acid used in Woodward's total synthesis of erythromycin A. <i>Computational and Theoretical Chemistry</i> , 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. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1992, , 811-818.	0.9	7
44	Vacancy profile in reverse osmosis membranes studied by positron annihilation lifetime measurements and molecular dynamics simulations. <i>Journal of Physics: Conference Series</i> , 2013, 443, 012050.	0.3	7
45	Preparation of photonic molecular trains via soft-crystal polymerization of lanthanide complexes. <i>Nature Communications</i> , 2022, 13, .	5.8	7
46	Conformational analyses of periplanone analogs by molecular mechanics calculations. <i>Journal of Chemical Ecology</i> , 1991, 17, 779-788.	0.9	5
47	Conformational analysis of serricornin: Application of molecular mechanics calculations to stereochemical assignment of serricornin, sex pheromone of cigarette beetle ( <i>Lasioderma serricorne</i> ) Tj ETQq1 1 0.084314 rgt /Over to		
48	Chiral Synthesis of Polyketide-Derived Natural Products. 33. Stereoselective Total Synthesis of 16-Membered Macrolide Aglycons, Leuconolides and Maridonolides. Macrocylic Stereocontrol Based on Conformational Analysis of the 16-Membered Macrolide Ring.. <i>Chemical and Pharmaceutical Bulletin</i> , 1991, 39, 2819-2829.	0.6	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. <i>Journal of the Chemical Society Perkin Transactions II</i> , 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. <i>Journal of Molecular Structure</i> , 2005, 748, 9-16.	1.8	3
53	Numerical calculation on a two-step subdiffusion behavior of lateral protein movement in plasma membranes. <i>Physical Review E</i> , 2017, 96, 042410.	0.8	3
54	Journal of Computer Chemistry, Japan:Conversion of Japanese Word Manuscript into the XML Format and Web Publication Management System. <i>Journal of Computer Chemistry Japan</i> , 2011, 10, 141-146.	0.0	3

#	ARTICLE	IF	CITATIONS
55	Theoretical Electronic Circular Dichroism Study of 1,3- $\epsilon$ -Diene Derivatives for the Elucidation of ECD Spectra of 1,3-Cyclohexadiene and Its Derivatives. <i>Chirality</i> , 2015, 27, 476-478.	1.3	2
56	Soft Crystal Force Field for Reproducing the Crystal Structures of Aryl Gold Isocyanide Complexes. <i>Journal of Computer Chemistry Japan</i> , 2018, 17, 155-157.	0.0	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. <i>Journal of Computer Chemistry Japan</i> , 2016, 15, 229-231.	0.0	1
60	Crystal Structure Optimization Method for Evaluation of Mechanical Properties of Soft Crystals. <i>Nihon Kessho Gakkaishi</i> , 2021, 63, 63-68.	0.0	1
61	Conformational Analysis of Long Chain Seco-Acids Used in Woodward's Total Synthesis of Erythromycin A - Conformational Space Search as the Basis of Molecular Modeling. , 1996, , 189-197.		1
62	Crystal Structure Prediction; From the Present to the Future. <i>Nihon Kessho Gakkaishi</i> , 2020, 62, 260-268.	0.0	1
63	Spiral carbon nanoparticles. <i>AIP Conference Proceedings</i> , 2001, , .	0.3	0
64	Chiral Olefin and Molecular Motor. <i>Journal of Computer Chemistry Japan</i> , 2017, 16, A21-A22.	0.0	0
65	Development of Visualization Technique of Biological Information for Mobile Terminal Devices. <i>Journal of Computer Chemistry Japan</i> , 2014, 13, 175-176.	0.0	0
66	Development of Education Curriculum for First Level Simulation Engineering in Chemistry - Questionnaire Research and Core-Curriculum Proposal -. <i>Journal of Computer Chemistry Japan</i> , 2014, 13, 179-180.	0.0	0
67	Nomenclature of Aldohexopyranose Conformations Including Rotational Isomers of Hydroxyl Groups. <i>Journal of Computer Chemistry Japan</i> , 2014, 13, 263-267.	0.0	0
68	Improving the Accuracy of Crystal Structure Prediction Using FMO Crystal Energy: An Example of Target XXIII. <i>Journal of Computer Chemistry Japan</i> , 2021, 20, 92-93.	0.0	0