Carlos Jaime

List of Publications by Year in descending order

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120 papers	2,842 citations	201385 27 h-index	197535 49 g-index
126 all docs	126 docs citations	126 times ranked	2629 citing authors

#	Article	IF	Citations
1	Synthesis and In Vitro Studies of Photoactivatable Semisquaraine-type Pt(II) Complexes. Inorganic Chemistry, 2022, 61, 7729-7745.	1.9	1
2	Carbon nanotube transmembrane channel formation and single-stranded DNA spontaneous internalization: a dissipative particle dynamics study. Soft Matter, 2021, 17, 1028-1036.	1.2	4
3	Antibody cooperative adsorption onto AuNPs and its exploitation to force natural killer cells to kill HIV-infected T cells. Nano Today, 2021, 36, 101056.	6.2	7
4	Evidence of Enantiomers of Spiroglycol. Distinction by Using Î±,Î±â€²-Bis(trifluoromethyl)-9,10-anthracenedimethanol as a Chiral Solvating Agent and by Derivatization with Chiral Acids. Journal of Organic Chemistry, 2020, 85, 7247-7257.	1.7	7
5	Platinum nanoparticles stabilized by N-heterocyclic thiones. Synthesis and catalytic activity in mono- and di-hydroboration of alkynes. Nanoscale, 2020, 12, 6821-6831.	2.8	18
6	Inclusion complex of Callistemon viminalis essential oil prepared by kneading. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2020, 97, 109-119.	0.9	7
7	Interaction with Modified Cyclodextrin as a Way to Increase the Antimalarial Activity of Primaquine. Current Drug Discovery Technologies, 2020, 17, 670-681.	0.6	3
8	Removal of the synthetic hormone methyltestosterone from aqueous solution using a Î²-cyclodextrin/silica composite. Journal of Environmental Chemical Engineering, 2019, 7, 103492.	3.3	16
9	Chitosan as a capping agent: Insights on the stabilization of gold nanoparticles. Carbohydrate Polymers, 2019, 207, 806-814.	5.1	37
10	A study on the molecular existing interactions in nanoherbicides: A chitooligosaccharide/tripolyphosphate loaded with paraquat case. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2019, 562, 220-228.	2.3	12
11	Complexes between methyltestosterone and Î²-cyclodextrin for application in aquaculture production. Carbohydrate Polymers, 2018, 179, 386-393.	5.1	27
12	Domain Formation and Conformational Changes in Gold Nanoparticle Conjugates Studied Using DPD Simulations. Langmuir, 2017, 33, 14502-14512.	1.6	10
13	Selective deuteration of [(pyridylmethyl)sulfinyl]benzimidazole antisecretory drugs. A NMR study where DMSO- d 6 acts as deuteration agent. Journal of Pharmaceutical and Biomedical Analysis, 2016, 131, 454-463.	1.4	2
14	Pyrrole-Pyridine and Pyrrole-Naphthyridine Hosts for Anion Recognition. Molecules, 2015, 20, 9862-9878.	1.7	3
15	Computational study on the intramolecular self-organization of the macrorings of some â€˜giantâ€™ cyclodextrins (CDn, n = 40, 70, 85, 100). Organic and Biomolecular Chemistry, 2015, 13, 1680-1689.	1.5	5
16	Computational study on the conformations of CD38 and inclusion complexes of some lower-size large-ring cyclodextrins. Journal of Molecular Structure, 2014, 1056-1057, 238-245.	1.8	10
17	Configuration and conformation of alfentanil hydrochloride. Conformational study by NMR and theoretical calculations. Magnetic Resonance in Chemistry, 2014, 52, 440-447.	1.1	4
18	Molecular tweezers for enantiodiscrimination in NMR: Diâ€(R,R)â€1â€[10â€(1â€hydroxyâ€2,2,2â€trifluoroethyl)â€9â€anthryl]â€2,2,2â€trifluoroethyl benzenedicarboxylate. Chirality, 2010, 22, 548-556.	1.3	12

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19	Computational Study of Macroscopic Properties of Macromolecules with Industrial Interest. JAOCS, Journal of the American Oil Chemists' Society, 2010, 87, 271-279.	0.8	1
20	Optimal Configurations of â€œCappedâ€•Î²â€Cyclodextrin Dimers in Water Maximise Hydrophobic Association. ChemPhysChem, 2010, 11, 452-459.	1.0	5
21	Folding and self-assembling with Î²-oligomers based on (1R,2S)-2-aminocyclobutane-1-carboxylic acid. Organic and Biomolecular Chemistry, 2010, 8, 564-575.	1.5	59
22	Synthesis and structural characterization of a new chiral macrocycle derived from Î±,Î±â€²-(bistrifluoromethyl)-9,10-anthracendimethanol and terephthalic acid. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2009, 65, 419-426.	1.6	2
23	Size-Tunable Trehalose-Based Nanocavities: Synthesis, Structure, and Inclusion Properties of Large-Ring Cyclotrehalans. Journal of Organic Chemistry, 2009, 74, 2997-3008.	1.7	20
24	Molecular dynamics study on the conformational flexibility and energetics in aqueous solution of methylated Î²â€cyclodextrins. Chirality, 2008, 20, 1127-1133.	1.3	6
25	Synthesis, Structure, and Inclusion Capabilities of Trehalose-Based Cyclodextrin Analogues (Cyclotrehalans). Journal of Organic Chemistry, 2008, 73, 2967-2979.	1.7	32
26	Fine-Tuning Ligandâ^'Receptor Design for Selective Molecular Recognition of Dicarboxylic Acids. Inorganic Chemistry, 2007, 46, 10632-10638.	1.9	18
27	Molecular dynamics study of the conformational dynamics and energetics of some large-ring cyclodextrins (CDn,n= 24, 25, 26, 27, 28, 29). Chirality, 2007, 19, 203-213.	1.3	16
28	Chelate Effect in Cyclodextrin Dimers:Â A Computational (MD, MM/PBSA, and MM/GBSA) Study. Journal of Organic Chemistry, 2006, 71, 2056-2063.	1.7	34
29	Di-(R,R)-1-[10-(1-hydroxy-2,2,2-trifluoroethyl)-9-anthryl]-2,2,2-trifluoroethyl Muconate:Â A Highly Chiral Cavity for Enantiodiscrimination by NMR. Journal of Organic Chemistry, 2006, 71, 8114-8120.	1.7	27
30	Computational Studies on Two Supramolecular Structures: Cyclodextrins and Rotaxanes. Current Organic Chemistry, 2006, 10, 731-743.	0.9	6
31	Theoretical and experimental study of a praziquantel and -cyclodextrin inclusion complex using molecular mechanic calculations and -nuclear magnetic resonance. Journal of Pharmaceutical and Biomedical Analysis, 2006, 41, 1428-1432.	1.4	37
32	Chiral discrimination of ibuprofen isomers in Î²-cyclodextrin inclusion complexes: experimental (NMR) and theoretical (MD, MM/GBSA) studies. Tetrahedron, 2006, 62, 4162-4172.	1.0	46
33	Di-2,2,2-trifluoro-1-(9-anthryl)ethyl fumarate, an easy starting point for the enantioselective preparation of trans-cyclohexene-4,5-dicarboxylate derivatives by Dielsâ€“Alder reaction. Tetrahedron: Asymmetry, 2006, 17, 3237-3243.	1.8	3
34	Structural Dynamics of Some Large-Ring Cyclodextrins. A Molecular Dynamics Study: An Analysis of Force Field Performance. Theoretical Chemistry Accounts, 2006, 117, 85-97.	0.5	26
35	Enantioselective preparation and structural and conformational analysis of the chiral solvating agent Î±,Î±â€²-bis(trifluoromethyl)-1,8-anthracenedimethanol. Tetrahedron: Asymmetry, 2005, 16, 3084-3093.	1.8	27
36	Experimental (NMR) and Theoretical (MD Simulations) Studies on the Conformational Preference of Three Cycloalkanols when Included in Î²-Cyclodextrin. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2005, 51, 241-247.	1.6	5

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37	Cyclodextrinic carcerands. I. Would they form inclusion complexes? Computational study on structure and energetics. Arkivoc, 2005, 2005, 287-304.	0.3	4
38	Towards the design of hostâ€“guest complexes: biotin and urea derivatives versus artificial receptors. Biosensors and Bioelectronics, 2004, 20, 1242-1249.	5.3	20
39	Insights into the Structure of Large-Ring Cyclodextrins through Molecular Dynamics Simulations in Solution. Journal of Physical Chemistry B, 2004, 108, 6261-6274.	1.2	34
40	Computational Studies on Pseudorotaxanes by Molecular Dynamics and Free Energy Perturbation Simulations. Journal of Organic Chemistry, 2003, 68, 1539-1547.	1.7	27
41	Molecular Modelling Study of the 2:1 Î³-Cyclodextrin:C60 Complex. Dummy Atoms Simulating Bond Electron Distribution. Supramolecular Chemistry, 2003, 15, 251-260.	1.5	8
42	Shuttling Process in [2]Rotaxanes. Modeling by Molecular Dynamics and Free Energy Perturbation Simulations. Journal of Physical Chemistry B, 2003, 107, 7582-7588.	1.2	27
43	Reduction of Aromatic Imino Derivatives: Chemical, Electrochemical, and Theoretical Studies. Polycyclic Aromatic Compounds, 2003, 23, 457-470.	1.4	3
44	Diastereomeric Î²-cyclodextrin Complexes With Cizolirtine and Its Carbinol. A Molecular Dynamics Study. Supramolecular Chemistry, 2002, 14, 33-39.	1.5	5
45	Structure and Thermodynamics of Î±-, Î²-, and Î³-Cyclodextrin Dimers. Molecular Dynamics Studies of the Solvent Effect and Free Binding Energiesâ€. Journal of Organic Chemistry, 2002, 67, 8602-8609.	1.7	59
46	Molecular recognition by Î²-cyclodextrin derivatives: molecular dynamics, free-energy perturbation and molecular mechanics/ Poisson-Boltzmann surface area goals and problems. Theoretical Chemistry Accounts, 2002, 108, 286-292.	0.5	20
47	Î±- and Î²-cyclodextrin complexes with n-alkyl carboxylic acids and n-alkyl p-hydroxy benzoates. A molecular mechanics study of 1:1 and 1:2 associations. Computational and Theoretical Chemistry, 2002, 594, 207-213.	1.5	15
48	Î±-, Î²-, and Î³-Cyclodextrin Dimers. Molecular Modeling Studies by Molecular Mechanics and Molecular Dynamics Simulations. Journal of Organic Chemistry, 2001, 66, 689-692.	1.7	69
49	Effect of Î²-Cyclodextrin on the Hydrolysis of Trifluoroacetate Esters. Journal of Organic Chemistry, 2001, 66, 4399-4404.	1.7	18
50	Molecular mechanics (MM3) study of the conformations of ethyl esters of diastereoisomeric 3-substituted 4,4,4-trichloro-2-cyano-butanoic acids. Journal of Molecular Modeling, 2001, 7, 240-244.	0.8	21
51	Di[(S)-1-(9-anthryl)-2,2,2-trifluoroethyl]sulphite, a case of diastereotopic anthracene groups. Tetrahedron: Asymmetry, 2001, 12, 1737-1740.	1.8	2
52	Molecular dynamics simulation studies of liquid acetonitrile: New six-site model. Journal of Computational Chemistry, 2000, 21, 901-908.	1.5	136
53	NMR study of 9-(1-adamantylaminomethyl)-9,10-dihydroanthracene and its Î²-cyclodextrin complexes. Magnetic Resonance in Chemistry, 2000, 38, 925-931.	1.1	14
54	The CSIC Reaction on Substrates Derived From Aldehydes. Tetrahedron, 2000, 56, 2523-2531.	1.0	39

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55	Enantiodifferentiation by Complexation with Î²-Cyclodextrin: Experimental (NMR) and Theoretical (MD,) Tj ETQq1 1 0.784314 rgBT /Ov	1.0	26
56	Complexation betweentert-Butyl Ketones and Î²-Cyclodextrin. Structural Study by NMR and MD Simulations. Journal of Organic Chemistry, 2000, 65, 8139-8145.	1.7	32
57	Preparation of (R)- and (S)-1-adamantyl-9-anthrylmethanol. Conformational study and their behaviour as chiral solvating agents. Tetrahedron: Asymmetry, 1999, 10, 3719-3725.	1.8	8
58	Configurational and conformational NMR study of enantiopure 2,2-dimethyl-1-(1-naphthyl)propanol via its carbamate derivatives. Magnetic Resonance in Chemistry, 1999, 37, 885-890.	1.1	3
59	Î²-cyclodextrin bimodal complexes with n-alkylbenzenes and n-alkylcyclohexanes A molecular mechanics study. Computational and Theoretical Chemistry, 1998, 428, 195-201.	1.5	25
60	The Diels-Alder cycloaddition reaction of some substituted furans and E-1,2-bis(phenylsulfonyl)ethylene. Tetrahedron, 1998, 54, 9095-9110.	1.0	17
61	Conformational equilibria and cyclodextrin inclusion complexes. Computational study by force field calculations (MM3(92)). Journal of Molecular Structure, 1998, 442, 93-101.	1.8	15
62	Cyclodextrin Inclusion Complexes. Molecular Mechanics Calculations on the Modification of Ï€-Face Selectivityâ€. Journal of Organic Chemistry, 1997, 62, 5923-5927.	1.7	20
63	Title is missing!. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 1997, 27, 215-231.	1.6	21
64	Determination of the Inclusion Geometry for the Î²-Cyclodextrin/Benzoic Acid Complex by NMR and Molecular Modeling. Journal of Organic Chemistry, 1996, 61, 9578-9581.	1.7	115
65	Modelling of the inclusion process of Î±-, Î²-, and Î³- cyclodextrins with 1-bromoadamantane. A comparative molecular mechanics study accounting for the solvent. Journal of Molecular Structure, 1996, 377, 137-147.	1.8	15
66	Modelling of the inclusion process of Î±-, Î²-, and Î³-cyclodextrins with 1-bromoadamantane. A comparative molecular mechanics study accounting for the solvent. Computational and Theoretical Chemistry, 1996, 377, 137-147.	1.5	7
67	Preparation of enantiomers of 9-(1-amino-2,2-dimethylpropyl)-9,10-dihydroanthracene. Conformational study and their behaviour as chiral solvating agents. Tetrahedron: Asymmetry, 1996, 7, 1295-1302.	1.8	18
68	Conformational Analysis of 2,4-Disubstituted 9-Oxobicyclo[3.3.1]nonane Derivatives. Collection of Czechoslovak Chemical Communications, 1995, 60, 216-223.	1.0	0
69	Preparation of homochiral 9-anthryl-tert-butylcarbinol. The configurational and conformational NMR study of its carbamate derivatives. Tetrahedron: Asymmetry, 1995, 6, 1307-1310.	1.8	9
70	Restricted Rotation and NOE Transfer: A Conformational Study of Some Substituted (9-Anthryl)carbinol Derivatives. Journal of Organic Chemistry, 1995, 60, 27-31.	1.7	40
71	Cyclo-bis-Intercalands with Acridine Subunits Linked by Rigid Spacers. Tetrahedron Letters, 1995, 36, 5261-5264.	0.7	13
72	Conformation of tricyclo [4.3.1.12,5]undec-3-en-10-one. Magnetic Resonance in Chemistry, 1994, 32, 210-212.	1.1	2

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73	Conformational analysis of 4-aryl-2,2,6,6-tetramethyl-heptane-3,5-diones. Dipole moment determinations and molecular mechanics calculations. Tetrahedron, 1994, 50, 11213-11218.	1.0	2
74	Cyclodextrin Inclusion Complexes. MM2 Calculations Reproducing Bimodal Inclusions. Journal of Organic Chemistry, 1994, 59, 1288-1293.	1.7	50
75	MM2 calculations with atomic point charges modelling AM1 energy surfaces. Journal of Molecular Structure, 1993, 291, 105-121.	1.8	8
76	Dipole moments can be used to determine the conformation of calix[4]arenes. Recueil Des Travaux Chimiques Des Pays-Bas, 1993, 112, 367-369.	0.0	16
77	Molecular mechanics calculations on the differentiation of diastereomeric complexes ofcis-decalin with?-cyclodextrin. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 1993, 16, 55-62.	1.6	21
78	Synthesis and structure of new hosts related to 9,9â€²-bianthryl. Journal of the Chemical Society Perkin Transactions II, 1993, , 757-766.	0.9	22
79	Substituted .gamma.-lactones with vicinal hydrogen atoms. Conformational study by MM2 calculations and coupling constant analysis. Journal of Organic Chemistry, 1993, 58, 154-158.	1.7	30
80	Attempted Transformation of 2,3,5,6-Tetrachloro-4,4-dimethoxypentacyclo[5.4.0.02,6.03,10.05,9]undecane-8,11-dione toward Pentaprismane Retaining Chloro Group. Bulletin of the Chemical Society of Japan, 1992, 65, 2312-2314.	2.0	4
81	Determination of the conformation in solution of three 1,2-3,4-Di-O-methylenepyranoses: NMR and molecular mechanics studies. Magnetic Resonance in Chemistry, 1992, 30, 133-136.	1.1	2
82	Heterocyclic betaines. Aza analogs of sesquifulvalene. 1. Structural studies of 1-alkyl-4-azolylidene-1,4-dihydropyridines and azolium azolate inner salts. Journal of Organic Chemistry, 1991, 56, 4223-4233.	1.7	41
83	Conformational study of (R)-(-)-2,2,2-trifluoro-1-(9-anthryl)ethanol (Pirkle's alcohol) by dynamic NMR. Journal of Organic Chemistry, 1991, 56, 6521-6523.	1.7	11
84	Carbon-13 NMR chemical shifts. A single rule to determine the conformation of calix[4]arenes. Journal of Organic Chemistry, 1991, 56, 3372-3376.	1.7	563
85	On the possibility of determining stereochemistry in acyclic polyhydroxylated compounds by the combined vicinal coupling constant/molecular mechanics method. A test with alditol peracetates. Tetrahedron, 1991, 47, 4579-4590.	1.0	18
86	MM2' calculations on methylenecyclohexane, methylenecyclopentane, and cyclopentane. Pitfalls in the two-bond drive technique: How large should the ring be?. Journal of Computational Chemistry, 1990, 11, 411-415.	1.5	4
87	Empirical computation of13C NMR chemical shifts. Magnetic Resonance in Chemistry, 1990, 28, 42-46.	1.1	7
88	Solution geometry of .beta.-cyclodextrin-1-bromoadamantane host-guest complex as determined by 1H[1H] intermolecular NOE and MM2 calculations. Journal of Organic Chemistry, 1990, 55, 4772-4776.	1.7	59
89	Photoinduced molecular transformations. Part 109. Conformational dependence of the stereochemistry of photochemical 1,3-acyl shifts of Î²,Î³-unsaturated cyclic ketones: conformation-specific photorearrangements of steroidal Î²,Î³-unsaturated cyclic ketones, 7a-homocholest-5-en-7a-one and 4a-homo-5Î±-cholest-1-en-4-one. Journal of the Chemical Society Perkin Transactions 1, 1990, , 1247-1253.	0.9	3
90	Conformational study of peracetylated aldononitriles. Journal of Organic Chemistry, 1990, 55, 3530-3536.	1.7	11

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91	Conformational analysis of bridged biphenyls and 2,2'-bipyridines. Empirical force field calculations (MM2-V4). Journal of Organic Chemistry, 1990, 55, 2637-2644.	1.7	33
92	Determination of rotational barriers of carbon(sp2)-carbon(sp3) bonds in 2-arylpiperidines. 3. Proton dynamic nuclear magnetic resonance studies and molecular mechanics calculations of the 1,2,2-trimethyl-6-(3,4,5-trimethoxyphenyl)- and 1,5,5-trimethyl-2-(3,4,5-trimethoxyphenyl)-4-piperidones. Journal of Organic Chemistry, 1990, 55, 2307-2311.	1.7	10
93	Conformational analysis of bicyclo[3.3.1]nonaneâ€exoâ€2,exoâ€4â€dicarboxylic acid derivatives and related compounds. Chemische Berichte, 1989, 122, 1313-1322.	0.2	6
94	Empirical force field calculations (MM2-V4) on biphenyl and 2,2â€²-bipyridine. Journal of Molecular Structure, 1989, 195, 103-110.	1.8	23
95	A conformational study of bis-, tris- and tetrakis-pyrazolylmethane. Crystallography, L.S.R., dipole moments and theoretical calculations. Tetrahedron, 1989, 45, 7805-7816.	1.0	20
96	Parameterization of cyano group MM2 constants in peracetylated aldononitriles. Journal of Organic Chemistry, 1988, 53, 5363-5366.	1.7	5
97	Role of the A 1,3 allylic interaction on the stereochemistry of formation of Schiff's bases derived from bicyclo[2.2.1]hept-5-en-2-one and 7-oxabicyclo[2.2.1]hept-5-en-2-one. Journal of the Chemical Society Perkin Transactions II, 1988, , 865.	0.9	2
98	On the Reactivity of 5(4H)-Oxazolones with Amines. Heterocycles, 1988, 27, 2567.	0.4	8
99	Molecular mechanics and dipole moments as a useful combination in conformational analysis of open-chain compounds. Application to Î±-adamantyl-Î²-diketones. Journal of the Chemical Society Chemical Communications, 1987, , 1706-1708.	2.0	5
100	Computation of vicinal coupling constants in tetra- and hexa-alditol peracetates using molecular mechanics. A rational approach to conformational analysis in solution. Journal of the Chemical Society Chemical Communications, 1986, , 261-263.	2.0	27
101	Molecular mechanics calculations on the Csp3-Csp2 rotation in the N,3,3-trimethyl-2-phenyl-4-piperidone system. Journal of Organic Chemistry, 1986, 51, 3951-3955.	1.7	7
102	Di- and trisubstituted .gamma.-lactones. Conformational study by molecular mechanics calculations and coupling constant analysis. Journal of Organic Chemistry, 1986, 51, 3946-3951.	1.7	48
103	Determination of rotational barriers of c(sp2)-c(sp3) bonds in 2-arylpiperidines. II.1 1h-dnmr and 13c-dnmr studies of the trans-1,3-dimethyl-2-(3,4,5-trimethoxyphenyl)-4-piperidone. Tetrahedron, 1986, 42, 3957-3966.	1.0	15
104	Studies on structurally simple butenolides. V. reactions of protoanemonin with piperidine and -nucleophiles. Tetrahedron, 1985, 41, 5577-5587.	1.0	24
105	Kinetically and thermodynamically controlled synthesis of 2,6-disubstituted cyclohexanone semicarbazones. A molecular mechanics study of a1,3-strai. Tetrahedron, 1985, 41, 3791-3802.	1.0	7
106	Molecular mechanics analysis of restricted rotation about pivot bond in substituted bicyclohexyls and phenylcyclohexanes. Importance of successive gauche and progauche sequences in conformational dynamics. Journal of Molecular Structure, 1985, 126, 363-380.	1.8	12
107	On the Synthesis of Unsaturated 4(5H)-Imidazolines. 2. Semi-empirical SCF-MO(MNDO) Study on Geometric Factors influencing the Reaction Course. Heterocycles, 1985, 23, 2685.	0.4	1
108	Dynamic nuclear magnetic resonance and empirical force field studies of cannabidiol. Tetrahedron, 1984, 40, 2919-2927.	1.0	13

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109	Does the boat-like conformer exist for 1,8,8-trimethylbicyclo[3.2.1]Octan-3-one?. Tetrahedron Letters, 1984, 25, 3883-3886.	0.7	3
110	Photo-induced transformations. Part 69. The formation of bridged oxabicyclic compounds by intramolecular radical addition of oxyl radicals generated fromB-homocholest-5-en-7a-ol hypoiodites. Journal of the Chemical Society Perkin Transactions 1, 1984, , 575-581.	0.9	5
111	(Z)-9-(bicyclo[4.2.1]nonan-9-ylidene)bicyclo[4.2.1]nonane and some related compounds. Assignment of the configuration to the product of monoepoxidation of (E)-9-(bicyclo[4.2.1]non-3-en-9-ylidene)bicyclo-[4.2.1]non-3-ene by1H nuclear magnetic resonance spectroscopy using the shift reagent Eu(fod)3. Journal of the Chemical Society Perkin Transactions II, 1984, , 515.	0.9	3
112	Homo-Diels-Alder reaction of tricyclo[5.3.1.04,9]undeca-2,5-diene, a molecule with unusually strong through-space interaction in a 1,4-cyclooctadiene system. Journal of the American Chemical Society, 1984, 106, 1512-1514.	6.6	12
113	Crystal and molecular structure of bis(9-triptycyl) ether. Journal of the American Chemical Society, 1984, 106, 4712-4717.	6.6	30
114	Application of empirical potential energy calculations to organic chemistry. Part 22. Restricted internal rotation in substituted 1,1â€²-bipiperidines, 1-cyclohexylpiperidines, and related molecules due to 1,5-interactions across the pivot bond. Journal of the Chemical Society Perkin Transactions II, 1984, , 995-999.	0.9	6
115	A reparameterization of empirical hydrocarbon force field MM2 for improved performance in torsional energy surface calculations. Tetrahedron, 1983, 39, 2769-2778.	1.0	100
116	Recognition of paired gauchePâ€“gaucheMsequences as the source of the rotational barrier in 2,2â€²-dimethyl-1,1â€²-bipiperidines. Journal of the Chemical Society Chemical Communications, 1983, , 708-709.	2.0	5
117	Application of potential energy calculations to organic chemistry. Part 16. Further examples of enhanced lengthening of strained carbon-carbon bonds by orbital interactions. Journal of Organic Chemistry, 1983, 48, 3990-3993.	1.7	29
118	Application of empirical potential energy calculations to organic chemistry. Part 19. Conformational preference in 2,4-dimethoxybicyclo[3.3.1]nonan-9-one and related molecules. Analysis of vicinal NMR coupling constants in multiple rotor system by combined molecular mechanics and generalized Karplus equation. Journal of Organic Chemistry, 1983, 48, 4514-4519.	1.7	45
119	Stereospecific and practical syntheses of both meso-cyclopentane-1,2,3-tricarboxylic acids. Canadian Journal of Chemistry, 1982, 60, 2358-2364.	0.6	1
120	The 1,3-dimethoxytrimethylene bridge as two latent carboxyl groups: synthesis of cis-isoaposantenic and cis-apocamphoric acids. Canadian Journal of Chemistry, 1981, 59, 2848-2852.	0.6	3