

# Julio C Facelli

## List of Publications by Year in descending order

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193  
papers

5,761  
citations

109264

35  
h-index

98753

67  
g-index

220  
all docs

220  
docs citations

220  
times ranked

4676  
citing authors

#	ARTICLE	IF	CITATIONS
1	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.	0.5	445
2	A third blind test of crystal structure prediction. Acta Crystallographica Section B: Structural Science, 2005, 61, 511-527.	1.8	373
3	Significant progress in predicting the crystal structures of small organic molecules "a report on the fourth blind test. Acta Crystallographica Section B: Structural Science, 2009, 65, 107-125.	1.8	371
4	Towards crystal structure prediction of complex organic compounds "a report on the fifth blind test. Acta Crystallographica Section B: Structural Science, 2011, 67, 535-551.	1.8	358
5	Low-temperature carbon-13 magnetic resonance in solids. 3. Linear and pseudolinear molecules. Journal of the American Chemical Society, 1984, 106, 7672-7676.	6.6	143
6	Determination of molecular symmetry in crystalline naphthalene using solid-state NMR. Nature, 1993, 365, 325-327.	13.7	109
7	15N Chemical Shift Principal Values in Nitrogen Heterocycles. Journal of the American Chemical Society, 1997, 119, 9804-9809.	6.6	106
8	Chemical shift tensors: Theory and application to molecular structural problems. Progress in Nuclear Magnetic Resonance Spectroscopy, 2011, 58, 176-201.	3.9	106
9	Advances in Theoretical and Physical Aspects of Spin-Spin Coupling Constants. Annual Reports on NMR Spectroscopy, 2003, 51, 167-260.	0.7	102
10	Advances in theoretical and physical aspects of spin-spin coupling constants. Annual Reports on NMR Spectroscopy, 2000, 41, 55-184.	0.7	100
11	Calculations of chemical shieldings: Theory and applications. Concepts in Magnetic Resonance, 2004, 20A, 42-69.	1.3	94
12	Three-Dimensional Structure of the Siskin Green River Oil Shale Kerogen Model: A Comparison between Calculated and Observed Properties. Energy & Fuels, 2013, 27, 702-710.	2.5	94
13	A review of the applications of data mining and machine learning for the prediction of biomedical properties of nanoparticles. Computer Methods and Programs in Biomedicine, 2016, 132, 93-103.	2.6	89
14	15N Chemical Shift Tensors in Nucleic Acid Bases. Journal of the American Chemical Society, 1998, 120, 9863-9869.	6.6	80
15	Carbon-13 NMR and polarized IR spectra of vicinally labeled cyclobutadiene-13C2 in an argon matrix: interconversion of valence tautomers. Journal of the American Chemical Society, 1988, 110, 2648-2650.	6.6	77
16	Intermolecular shielding contributions studied by modeling the C13 chemical-shift tensors of organic single crystals with plane waves. Journal of Chemical Physics, 2009, 131, 144503.	1.2	75
17	13C Dipolar NMR Spectrum of Matrix-Isolated o-Benzynes-1,2-13C2. Journal of the American Chemical Society, 1996, 118, 846-852.	6.6	72
18	Modified genetic algorithm to model crystal structures. I. Benzene, naphthalene and anthracene. Journal of Chemical Physics, 2002, 116, 5984-5991.	1.2	69

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19	Modeling NMR Chemical Shift: A Survey of Density Functional Theory Approaches for Calculating Tensor Properties. <i>Journal of Physical Chemistry A</i> , 2005, 109, 1180-1187.	1.1	67
20	Effects of Hydrogen Bonding in the Calculation of $^{15}\text{N}$ Chemical Shift Tensors: Benzamide. <i>Journal of the American Chemical Society</i> , 1996, 118, 5488-5489.	6.6	63
21	Carbon-13 chemical shift tensors in polycyclic aromatic compounds. 2. Single-crystal study of naphthalene. <i>Journal of the American Chemical Society</i> , 1991, 113, 750-753.	6.6	59
22	Carbon-13 Chemical Shift Tensors in Polycyclic Aromatic Compounds. 5. Single-Crystal Study of Acenaphthene. <i>Journal of the American Chemical Society</i> , 1995, 117, 2336-2343.	6.6	56
23	Modified genetic algorithms to model cluster structures in medium-size silicon clusters. <i>Physical Review A</i> , 2004, 69, .	1.0	54
24	Density Functional Theory Calculations of the Structure and the $^{15}\text{N}$ and $^{13}\text{C}$ Chemical Shifts of Methyl Bacteriopheophorbide and Bacteriochlorophylla. <i>Journal of Physical Chemistry B</i> , 1998, 102, 2111-2116.	1.2	52
25	A comparison of the IGLO and LORG methods for the calculations of nuclear magnetic shieldings. <i>Journal of Computational Chemistry</i> , 1990, 11, 32-44.	1.5	47
26	Carbon-13 Shift Tensors in Polycyclic Aromatic Compounds. 8.1A Low-Temperature NMR Study of Coronene and Corannulene. <i>Journal of Physical Chemistry A</i> , 2000, 104, 149-155.	1.1	47
27	Carbon-13 shielding tensors: experimental and theoretical determination. <i>Accounts of Chemical Research</i> , 1987, 20, 152-158.	7.6	45
28	The use of partially restricted molecular orbitals to investigate transmission mechanisms of spin-spin coupling constants. I. The $\sigma$ and $\pi$ contributions within the FPT INDO method. <i>Theoretica Chimica Acta</i> , 1981, 59, 17-24.	0.9	43
29	Relationship of $^{13}\text{C}$ NMR chemical shift tensors to diffraction structures. <i>Acta Crystallographica Section B: Structural Science</i> , 1995, 51, 540-546.	1.8	43
30	$^{13}\text{C}$ NMR Investigation of Solid-State Polymorphism in 10-Deacetyl Baccatin III. <i>Journal of the American Chemical Society</i> , 2002, 124, 10589-10595.	6.6	43
31	Carbon-13 chemical-shift tensors in single-crystal methoxybenzenes. <i>Journal of the Chemical Society Faraday Transactions I</i> , 1988, 84, 3673.	1.0	42
32	Experimental and theoretical study of the methoxy group conformational effect on $^{13}\text{C}$ chemical shifts in ortho-substituted anisoles. <i>Magnetic Resonance in Chemistry</i> , 1989, 27, 158-161.	1.1	42
33	Carbon-13 Chemical Shift Tensors in Polycyclic Aromatic Compounds. 6.1 Single-Crystal Study of Perylene. <i>Journal of the American Chemical Society</i> , 1996, 118, 4880-4888.	6.6	42
34	Gene co-expression network analysis for identifying modules and functionally enriched pathways in SCA2. <i>Human Molecular Genetics</i> , 2017, 26, 3069-3080.	1.4	40
35	Low-temperature carbon-13 magnetic resonance in solids. 5. Chemical shielding anisotropy of the $^{13}\text{CH}_2$ group. <i>Journal of the American Chemical Society</i> , 1985, 107, 6749-6754.	6.6	38
36	$^{15}\text{N}$ Chemical Shift Tensors of Uracil Determined from $^{15}\text{N}$ Powder Pattern and $^{15}\text{N}$ - $^{13}\text{C}$ Dipolar NMR Spectroscopy. <i>The Journal of Physical Chemistry</i> , 1995, 99, 10454-10458.	2.9	38

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37	Carbon-13 chemical shift tensors of carboxylic acids: GIAO calculations in acetic acid + methylamine dimer. <i>Molecular Physics</i> , 1995, 86, 865-872.	0.8	37
38	Low temperature <sup>13</sup> C NMR magnetic resonance in solids 4. Cyclopropane, bicyclo[1.1.0]butane and [1.1.1]propellane. <i>Theoretica Chimica Acta</i> , 1985, 68, 421-430.	0.9	36
39	Effects of protonation on acetone: nuclear magnetic resonance and ab initio studies. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1992, 88, 2459-2463.	1.7	36
40	Modeling NMR chemical shifts: a comparison of charge models for solid state effects on <sup>15</sup> N chemical shift tensors. <i>Solid State Nuclear Magnetic Resonance</i> , 1998, 10, 185-189.	1.5	36
41	Modified genetic algorithms to model cluster structures in medium-sized silicon clusters: Si <sub>18</sub> ~Si <sub>60</sub> . <i>Physical Review A</i> , 2006, 73, .	1.0	35
42	Low-temperature carbon-13 magnetic resonance in solids. 7. Methyl carbons. <i>Journal of the American Chemical Society</i> , 1986, 108, 6464-6470.	6.6	34
43	Carbon-13 chemical shielding tensors in polycyclic aromatic compounds. 1. Single-crystal study of pyrene. <i>Journal of the American Chemical Society</i> , 1987, 109, 2639-2644.	6.6	34
44	Solid State <sup>15</sup> N and <sup>13</sup> C NMR Study of Several Metal 5,10,15,20-Tetraphenylporphyrin Complexes. <i>Journal of the American Chemical Society</i> , 1997, 119, 7114-7120.	6.6	34
45	Low-temperature carbon-13 magnetic resonance. 8. Chemical shielding anisotropy of olefinic carbons. <i>Journal of the American Chemical Society</i> , 1988, 110, 3386-3392.	6.6	33
46	Transmission mechanisms of inter-proton long-range couplings in substituted anisoles. <i>Magnetic Resonance in Chemistry</i> , 1981, 17, 199-203.	0.7	32
47	Carbonates, Thiocarbonates, and the Corresponding Monoalkyl Derivatives: III. The <sup>13</sup> C Chemical Shift Tensors in Potassium Carbonate, Bicarbonate and Related Monomethyl Derivatives. <i>Solid State Nuclear Magnetic Resonance</i> , 2002, 22, 29-49.	1.5	32
48	Ab initio study of the internal rotation barrier of formamide and the formamide-H <sub>2</sub> O complex. <i>International Journal of Quantum Chemistry</i> , 1993, 45, 123-132.	1.0	30
49	Carbon-13 Chemical Shift Tensors in Polycyclic Aromatic Compounds. 7.1 Symmetry Augmented Chemical Shift~Chemical Shift Correlation Spectroscopy and Single Crystal Study of Triphenylene. <i>Journal of the American Chemical Society</i> , 1998, 120, 9305-9311.	6.6	30
50	Predicting the start week of respiratory syncytial virus outbreaks using real time weather variables. <i>BMC Medical Informatics and Decision Making</i> , 2010, 10, 68.	1.5	30
51	Quantitative determination of different carbon types in fusinite and anthracite coals from carbon-13 nuclear magnetic resonance chemical shielding line-shape analysis. <i>Analytical Chemistry</i> , 1988, 60, 1574-1579.	3.2	29
52	Crystal structure prediction of flexible molecules using parallel genetic algorithms with a standard force field. <i>Journal of Computational Chemistry</i> , 2009, 30, 1973-1985.	1.5	29
53	Carbon-13 Chemical Shift Tensors and Molecular Conformation of Anisole. <i>The Journal of Physical Chemistry</i> , 1996, 100, 8268-8272.	2.9	28
54	Optimization of Crystal Structures of Archetypical Pharmaceutical Compounds: A Plane-Wave DFT-D Study Using Quantum Espresso. <i>Crystal Growth and Design</i> , 2013, 13, 2181-2189.	1.4	28

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55	Iglo calculations of the antisymmetric components of nuclear magnetic shielding tensors. <i>Chemical Physics Letters</i> , 1984, 112, 147-149.	1.2	27
56	Low-temperature carbon-13 magnetic resonance in solids. 6. Methine carbons. <i>Journal of the American Chemical Society</i> , 1986, 108, 4268-4272.	6.6	27
57	Theoretical study of the in-plane components of the <sup>13</sup> C shielding tensors in condensed aromatic hydrocarbons. <i>Theoretica Chimica Acta</i> , 1987, 71, 277-288.	0.9	27
58	A general framework to understand parallel performance in heterogeneous clusters: analysis of a new adaptive parallel genetic algorithm. <i>Journal of Parallel and Distributed Computing</i> , 2005, 65, 48-57.	2.7	26
59	Crystal structure prediction from first principles: The crystal structures of glycine. <i>Chemical Physics Letters</i> , 2015, 626, 20-24.	1.2	26
60	Carbon-13 Chemical Shielding Tensors in Sugars: Sucrose and Methyl- <sup>13</sup> C-D-Glucopyranoside. , 1993, , 367-384.		26
61	Utility of gene-specific algorithms for predicting pathogenicity of uncertain gene variants. <i>Journal of the American Medical Informatics Association: JAMIA</i> , 2012, 19, 207-211.	2.2	25
62	Theoretical study of the adsorption of H on Sin clusters, (n=3-10). <i>Journal of Chemical Physics</i> , 2005, 123, 214302.	1.2	24
63	Molecular Structure and Carbon-13 Chemical Shielding Tensors Obtained from Nuclear Magnetic Resonance. <i>Topics in Stereochemistry</i> , 2007, , 1-61.	2.0	24
64	Alarm Settings of Continuous Glucose Monitoring Systems and Associations to Glucose Outcomes in Type 1 Diabetes. <i>Journal of the Endocrine Society</i> , 2020, 4, bvz005.	0.1	24
65	Effects of electronic resonance interaction on methoxy group NMR parameters: theoretical and experimental study of substituted 2-methoxypyridines. <i>The Journal of Physical Chemistry</i> , 1993, 97, 91-93.	2.9	23
66	A Nonsynonymous Variant in the GOLM1 Gene in Cutaneous Malignant Melanoma. <i>Journal of the National Cancer Institute</i> , 2018, 110, 1380-1385.	3.0	23
67	A theoretical study of the acetate <sup>13</sup> C chemical shift tensor in cadmium acetate dihydrate. <i>Chemical Physics Letters</i> , 1999, 302, 499-504.	1.2	22
68	Modeling the <sup>13</sup> C chemical-shift tensor in organic single crystals by quantum mechanical methods: finite basis set effects. <i>Magnetic Resonance in Chemistry</i> , 2006, 44, 390-400.	1.1	22
69	Comparative pharmacokinetics of PAMAM-OH dendrimers and HPMA copolymers in ovarian tumor-bearing mice. <i>Drug Delivery and Translational Research</i> , 2013, 3, 260-271.	3.0	22
70	Molecular dynamics analysis of the aggregation propensity of polyglutamine segments. <i>PLoS ONE</i> , 2017, 12, e0178333.	1.1	22
71	Carbon-13 chemical shift tensors in aromatic compounds. 4. Substituted naphthalenes. <i>Journal of the American Chemical Society</i> , 1992, 114, 2832-2836.	6.6	21
72	NMR at Cryogenic Temperatures: A <sup>13</sup> C NMR Study of Ferrocene. <i>Journal of Physical Chemistry A</i> , 1998, 102, 7692-7697.	1.1	21

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73	Ab initio molecular orbital studies of chemical shielding in transition-metal compounds: molybdenum-95 shielding in molybdate and thiomolybdate [MoOnS(4-n)] <sup>2-</sup> anions. <i>Journal of the American Chemical Society</i> , 1989, 111, 7619-7621.	6.6	20
74	Computational Science and Engineering Online (CSE-Online): A Cyber-Infrastructure for Scientific Computing. <i>Journal of Chemical Information and Modeling</i> , 2006, 46, 971-984.	2.5	20
75	Ring Current Effects in Crystals. Evidence from <sup>13</sup> C Chemical Shift Tensors for Intermolecular Shielding in 4,7-Di- <i>t</i> -butylacenaphthene versus 4,7-Di- <i>t</i> -butylacenaphthylene. <i>Journal of Physical Chemistry A</i> , 2007, 111, 2020-2027.	1.1	20
76	Septo-hippocampal networks in chronic epilepsy. <i>Experimental Neurology</i> , 2010, 222, 86-92.	2.0	20
77	Characterization of uncertainty in the classification of multivariate assays: application to PAM50 centroid-based genomic predictors for breast cancer treatment plans. <i>Journal of Clinical Bioinformatics</i> , 2011, 1, 37.	1.2	20
78	Predicting cytotoxicity of PAMAM dendrimers using molecular descriptors. <i>Beilstein Journal of Nanotechnology</i> , 2015, 6, 1886-1896.	1.5	20
79	The use of partially restricted molecular orbitals to investigate transmission mechanisms of spin-spin coupling constants. III. An INDO study of long-range F <sub>ij</sub> H couplings in fluorinated derivatives of toluene. <i>Magnetic Resonance in Chemistry</i> , 1982, 19, 138-143.	0.7	19
80	A proton NMR analysis of the OCH <sub>3</sub> group conformation in 2-methoxypyridines. <i>Magnetic Resonance in Chemistry</i> , 1982, 20, 40-41.	0.7	19
81	Ab initio and oxygen-17 NMR study of aromatic compounds with dicoordinate oxygen atoms. 1. Methoxy- and (methylenedioxy)benzene derivatives. <i>The Journal of Physical Chemistry</i> , 1990, 94, 7418-7423.	2.9	19
82	Ab initio and oxygen-17 NMR studies of the substituent effects on the tautomeric equilibrium in 6-X-(1H)-2-pyridones. <i>The Journal of Physical Chemistry</i> , 1992, 96, 7895-7898.	2.9	19
83	Modified genetic algorithm to model crystal structures. II. Determination of a polymorphic structure of benzene using enthalpy minimization. <i>Journal of Chemical Physics</i> , 2002, 116, 5992-5995.	1.2	19
84	Modeling solid-state effects on NMR chemical shifts using electrostatic models. <i>Magnetic Resonance in Chemistry</i> , 2004, 42, S41-S47.	1.1	19
85	Intermolecular shielding from molecular magnetic susceptibility. A new view of intermolecular ring current effects. <i>Magnetic Resonance in Chemistry</i> , 2006, 44, 401-408.	1.1	19
86	Health information technology adoption: Understanding research protocols and outcome measurements for IT interventions in health care. <i>Journal of Biomedical Informatics</i> , 2016, 63, 33-44.	2.5	19
87	Low-Temperature <sup>13</sup> C Magnetic Resonance. 9. Steric Effects for Methyl Chemical Shift Tensors in Methylcyclohexanes. <i>Journal of the American Chemical Society</i> , 1995, 117, 8441-8446.	6.6	18
88	iBIOMES: Managing and Sharing Biomolecular Simulation Data in a Distributed Environment. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 726-736.	2.5	18
89	Modified genetic algorithm to model crystal structures: III. Determination of crystal structures allowing simultaneous molecular geometry relaxation. <i>International Journal of Quantum Chemistry</i> , 2004, 96, 312-320.	1.0	17
90	A Distributed Computing Method for Crystal Structure Prediction of Flexible Molecules: An Application to N-(2-Dimethyl-4,5-dinitrophenyl) Acetamide. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 201-209.	2.3	17

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91	Development of a HIPAA-compliant environment for translational research data and analytics. Journal of the American Medical Informatics Association: JAMIA, 2014, 21, 185-189.	2.2	17
92	Towards a content agnostic computable knowledge repository for data quality assessment. Computer Methods and Programs in Biomedicine, 2019, 177, 193-201.	2.6	17
93	Carbon-13 chemical shift tensors in aromatic compounds. 3. Phenanthrene and triphenylene. Journal of the American Chemical Society, 1992, 114, 2826-2832.	6.6	16
94	Cluster Analysis of <sup>13</sup> C Chemical Shift Tensor Principal Values in Polycyclic Aromatic Hydrocarbons. Journal of Physical Chemistry A, 2001, 105, 7468-7472.	1.1	16
95	Associations Between the Time in Hypoglycemia and Hypoglycemia Awareness Status in Type 1 Diabetes Patients Using Continuous Glucose Monitoring Systems. Diabetes Technology and Therapeutics, 2020, 22, 787-793.	2.4	16
96	Nuclear magnetic resonance and PCILO study of the side-chain conformations in m-anisaldehyde and 2,5-dimethoxybenzaldehyde. The Journal of Physical Chemistry, 1983, 87, 2603-2607.	2.9	15
97	Experimental and Theoretical Study of the Ethoxy Group Conformational Effect on <sup>13</sup> C Chemical Shifts in Ortho-Substituted Phenetols. Magnetic Resonance in Chemistry, 1997, 35, 351-356.	1.1	15
98	Nitrogen-15 chemical shift in the pyridine-methanol complex. Chemical Physics Letters, 2000, 322, 91-96.	1.2	15
99	Modeling of Asphaltenes: Assessment of Sensitivity of <sup>13</sup> C Solid State NMR to Molecular Structure. Energy & Fuels, 2012, 26, 2161-2167.	2.5	15
100	Nanoinformatics: developing new computing applications for nanomedicine. Computing (Vienna/New) Tj ETQq0 0 0 rgBT /Overlock 10 T	3.2	15
101	A role for the <i>MEGF6</i> gene in predisposition to osteoporosis. Annals of Human Genetics, 2021, 85, 58-72.	0.3	15
102	Human activity pattern implications for modeling SARS-CoV-2 transmission. Computer Methods and Programs in Biomedicine, 2021, 199, 105896.	2.6	15
103	Influence of the INDO parameterization on the indirect spin-spin coupling constants as calculated by the FPT INDO method. Magnetic Resonance in Chemistry, 1980, 13, 137-142.	0.7	14
104	Identification of pneumonia and influenza deaths using the death certificate pipeline. BMC Medical Informatics and Decision Making, 2012, 12, 37.	1.5	14
105	Diblock copolymer bilayers as model for polymersomes: A coarse grain approach. Journal of Chemical Physics, 2017, 146, 244904.	1.2	14
106	Automatic Extraction of Nanoparticle Properties Using Natural Language Processing: NanoSifter an Application to Acquire PAMAM Dendrimer Properties. PLoS ONE, 2014, 9, e83932.	1.1	14
107	Temporal Pattern Detection to Predict Adverse Events in Critical Care: Case Study With Acute Kidney Injury. JMIR Medical Informatics, 2020, 8, e14272.	1.3	14
108	Solid-State <sup>13</sup> C NMR, X-ray, and Quantum Mechanical Studies of the Carbon Chemical Shifts Tensors of p-Tolyl Ether. The Journal of Physical Chemistry, 1994, 98, 12186-12190.	2.9	13

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109	15N Chemical Shifts in Energetic Materials: CP/MAS and ab Initio Studies of Aminonitropyridines, Aminonitropyrimidines, and Their N-Oxides. <i>International Journal of Molecular Sciences</i> , 2002, 3, 858-872.	1.8	13
110	Modified genetic algorithms to model atomic cluster structures: CuSi clusters. <i>Computational and Theoretical Chemistry</i> , 2004, 681, 149-155.	1.5	13
111	STHAM: an agent based model for simulating human exposure across high resolution spatiotemporal domains. <i>Journal of Exposure Science and Environmental Epidemiology</i> , 2020, 30, 459-468.	1.8	13
112	Importance of multicenter integrals in semiempirical calculations of nuclear spin-spin coupling constants. 1. Isotropic coupling. <i>Journal of the American Chemical Society</i> , 1984, 106, 3407-3413.	6.6	12
113	Molecular dynamics simulations in drug delivery research: Calcium chelation of G3.5 PAMAM dendrimers. <i>Cogent Chemistry</i> , 2016, 2, 1229830.	2.5	12
114	Analysis of the IGLO bond contributions to the <sup>13</sup> C shielding tensors in the local bond frame. <i>International Journal of Quantum Chemistry</i> , 1987, 31, 45-55.	1.0	11
115	Solid-State <sup>13</sup> C NMR Measurements in Methoxynaphthalenes: Determination of the Substituent Chemical Shift Effects in the Principal Values. <i>Journal of Physical Chemistry A</i> , 1997, 101, 9169-9175.	1.1	11
116	Data model, dictionaries, and desiderata for biomolecular simulation data indexing and sharing. <i>Journal of Cheminformatics</i> , 2014, 6, 4.	2.8	11
117	Comprehensive methodology to monitor longitudinal change patterns during EHR implementations: a case study at a large health care delivery network. <i>Journal of Biomedical Informatics</i> , 2018, 83, 40-53.	2.5	11
118	Modeling NMR Chemical Shifts. , 2008, , 53-62.		10
119	Consensus: a framework for evaluation of uncertain gene variants in laboratory test reporting. <i>Genome Medicine</i> , 2012, 4, 48.	3.6	10
120	Effects of the enlargement of polyglutamine segments on the structure and folding of ataxin-2 and ataxin-3 proteins. <i>Journal of Biomolecular Structure and Dynamics</i> , 2017, 35, 504-519.	2.0	10
121	Looking Behind the Curtain: Identifying Factors Contributing to Changes on Care Outcomes During a Large Commercial EHR Implementation. <i>EGEMS (Washington, DC)</i> , 2019, 7, 21.	2.0	10
122	Ab initio study of cyclobutadiene and its aza-substituted derivatives. Ground state properties and vibrational frequencies. <i>Computational and Theoretical Chemistry</i> , 1991, 236, 119-133.	1.5	9
123	A parallel genetic algorithm to discover patterns in genetic markers that indicate predisposition to multifactorial disease. <i>Computers in Biology and Medicine</i> , 2008, 38, 826-836.	3.9	9
124	Calcium interactions with Cx26 hemmichannel: Spatial association between MD simulations binding sites and variant pathogenicity. <i>Computational Biology and Chemistry</i> , 2018, 77, 331-342.	1.1	9
125	Inclusion of hydrogenp orbitals in the semiempirical calculation of NMR parameters. III: INDO CHF calculations of orbital and dipolar contributions to spin-spin coupling constants involving protons. <i>International Journal of Quantum Chemistry</i> , 1981, 20, 909-919.	1.0	8
126	The effect of transverse cross relaxation on nuclear magnetic resonance dipolar spectra. <i>Journal of Chemical Physics</i> , 1988, 89, 5542-5546.	1.2	8



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127	<sup>13</sup> C Dipolar spectroscopy of nitromethane. <i>Molecular Physics</i> , 1988, 64, 1031-1040.	0.8	8
128	Proximity effects on the nuclear magnetic shielding tensor. <i>Computational and Theoretical Chemistry</i> , 1993, 281, 61-66.	1.5	8
129	A case for using grid architecture for state public health informatics: the Utah perspective. <i>BMC Medical Informatics and Decision Making</i> , 2009, 9, 32.	1.5	8
130	A domain analysis model for eIRB systems: Addressing the weak link in clinical research informatics. <i>Journal of Biomedical Informatics</i> , 2014, 52, 121-129.	2.5	8
131	The origin of the splitting of <sup>13</sup> C and <sup>15</sup> N NMR signals of 3(5)-phenyl-5(3)-methylpyrazolium chloride and bromide in the solid state: Quantum Espresso calculations. <i>Journal of Molecular Structure</i> , 2014, 1075, 551-558.	1.8	8
132	iBIOMES Lite: Summarizing Biomolecular Simulation Data in Limited Settings. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 1810-1819.	2.5	8
133	Using supervised machine learning classifiers to estimate likelihood of participating in clinical trials of a de-identified version of ResearchMatch. <i>Journal of Clinical and Translational Science</i> , 2021, 5, e42.	0.3	8
134	Nonplanarity of the methoxy groups in o-dimethoxybenzene: quantum chemical calculations of the <sup>17</sup> O chemical shieldings. <i>Computational and Theoretical Chemistry</i> , 1992, 276, 307-313.	1.5	7
135	Nitrogen-15 Chemical Shifts in AT (Adenine-Thymine) and CG (Cytosine-Guanine) Nucleic Acid Base Pairs. <i>Journal of Biomolecular Structure and Dynamics</i> , 1998, 16, 619-629.	2.0	7
136	<sup>13</sup> C Chemical-shift tensors in an analogous series of heterosubstituted polycyclic aromatic compounds. <i>Magnetic Resonance in Chemistry</i> , 2001, 39, 115-121.	1.1	7
137	Indirect (J) coupling of inequivalent <sup>75</sup> As nuclei in crystalline and glassy As <sub>2</sub> Se <sub>3</sub> and As <sub>2</sub> S <sub>3</sub> . <i>Journal of Chemical Physics</i> , 2003, 119, 8519-8525.	1.2	7
138	A novel <i>CDKN2A</i> variant (p16 <sup>L117P</sup> ) in a patient with familial and multiple primary melanomas. <i>Pigment Cell and Melanoma Research</i> , 2019, 32, 734-738.	1.5	7
139	An intronic variant in the <i>CELF4</i> gene is associated with risk for colorectal cancer. <i>Cancer Epidemiology</i> , 2021, 72, 101941.	0.8	7
140	Generation and Classification of Activity Sequences for Spatiotemporal Modeling of Human Populations. <i>Online Journal of Public Health Informatics</i> , 2020, 12, e9.	0.4	7
141	Quantum mechanical calculations and experimental measurement of N-terminal charge effects on <sup>1</sup> HN and <sup>1</sup> H C $\alpha$ chemical shifts in peptides. <i>Biopolymers</i> , 1998, 38, 573-581.	1.2	6
142	Ab initio global optimization of the structures of Si <sub>n</sub> H <sub>n</sub> , n=4-10, using parallel genetic algorithms. <i>Physical Review A</i> , 2005, 72, .	1.0	6
143	Formation of one dimensional linear chains by Ir-Br bonds in cis-dicarbonyldichloroiridate (I). <i>Polyhedron</i> , 2011, 30, 221-227.	1.0	6
144	Development and classification of a robust inventory of near real-time outcome measurements for assessing information technology interventions in health care. <i>Journal of Biomedical Informatics</i> , 2017, 73, 62-75.	2.5	6

#	ARTICLE	IF	CITATIONS
145	Mechanical properties of drug loaded diblock copolymer bilayers: A molecular dynamics study. <i>Journal of Chemical Physics</i> , 2018, 148, 214901.	1.2	6
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