# Julio C Facelli

List of Publications by Year
in descending order

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| 193 | 5,761 | 109321 | 98798 |
|---|---|---|---|
| papers | citations | 35 h-index | 67 g-index |

| 220 | 220 | 220 | 4676 |
|---|---|---|---|
| all docs | docs citations | times ranked | 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. | 1.1 | 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 â€“ 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 â€“ 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. | 13.7 | 143 |
| 6 | Determination of molecular symmetry in crystalline naphthalene using solid-state NMR. Nature, 1993, 365, 325-327. | 27.8 | 109 |
| 7 | 15N Chemical Shift Principal Values in Nitrogen Heterocycles. Journal of the American Chemical Society, 1997, 119, 9804-9809. | 13.7 | 106 |
| 8 | Chemical shift tensors: Theory and application to molecular structural problems. Progress in Nuclear Magnetic Resonance Spectroscopy, 2011, 58, 176-201. | 7.5 | 106 |
| 9 | Advances in Theoretical and Physical Aspects of Spinâ€“Spin Coupling Constants. Annual Reports on NMR Spectroscopy, 2003, 51, 167-260. | 1.5 | 102 |
| 10 | Advances in theoretical and physical aspects of spin-spin coupling constants. Annual Reports on NMR Spectroscopy, 2000, 41, 55-184. | 1.5 | 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. | 5.1 | 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. | 4.7 | 89 |
| 14 | 15N Chemical Shift Tensors in Nucleic Acid Bases. Journal of the American Chemical Society, 1998, 120, 9863-9869. | 13.7 | 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. | 13.7 | 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. | 3.0 | 75 |
| 17 | 13C Dipolar NMR Spectrum of Matrix-Isolated o-Benzyne-1,2-13C2. Journal of the American Chemical Society, 1996, 118, 846-852. | 13.7 | 72 |
| 18 | Modified genetic algorithm to model crystal structures. I. Benzene, naphthalene and anthracene. Journal of Chemical Physics, 2002, 116, 5984-5991. | 3.0 | 69 |

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| 19 | Modeling NMR Chemical Shift:â€‰ A Survey of Density Functional Theory Approaches for Calculating Tensor Properties. Journal of Physical Chemistry A, 2005, 109, 1180-1187. | 2.5 | 67 |
| 20 | Effects of Hydrogen Bonding in the Calculation of15N Chemical Shift Tensors:Â Benzamide. Journal of the American Chemical Society, 1996, 118, 5488-5489. | 13.7 | 63 |
| 21 | Carbon-13 chemical shift tensors in polycyclic aromatic compounds. 2. Single-crystal study of naphthalene. Journal of the American Chemical Society, 1991, 113, 750-753. | 13.7 | 59 |
| 22 | Carbon-13 Chemical Shift Tensors in Polycyclic Aromatic Compounds. 5. Single-Crystal Study of Acenaphthene. Journal of the American Chemical Society, 1995, 117, 2336-2343. | 13.7 | 56 |
| 23 | Modified genetic algorithms to model cluster structures in medium-size silicon clusters. Physical Review A, 2004, 69, . | 2.5 | 54 |
| 24 | Density Functional Theory Calculations of the Structure and the15N and13C Chemical Shifts of Methyl Bacteriopheophorbideaand Bacteriochlorophylla. Journal of Physical Chemistry B, 1998, 102, 2111-2116. | 2.6 | 52 |
| 25 | A comparison of the IGLO and LORG methods for the calculations of nuclear magnetic shieldings. Journal of Computational Chemistry, 1990, 11, 32-44. | 3.3 | 47 |
| 26 | Carbon-13 Shift Tensors in Polycyclic Aromatic Compounds. 8.1A Low-Temperature NMR Study of Coronene and Corannulene. Journal of Physical Chemistry A, 2000, 104, 149-155. | 2.5 | 47 |
| 27 | Carbon-13 shielding tensors: experimental and theoretical determination. Accounts of Chemical Research, 1987, 20, 152-158. | 15.6 | 45 |
| 28 | The use of partially restricted molecular orbitals to investigate transmission mechanisms of spin-spin coupling constants. I. The? and? contributions within the FPT INDO method. Theoretica Chimica Acta, 1981, 59, 17-24. | 0.8 | 43 |
| 29 | Relationship of 13C NMR chemical shift tensors to diffraction structures. Acta Crystallographica Section B: Structural Science, 1995, 51, 540-546. | 1.8 | 43 |
| 30 | 13C NMR Investigation of Solid-State Polymorphism in 10-Deacetyl Baccatin III. Journal of the American Chemical Society, 2002, 124, 10589-10595. | 13.7 | 43 |
| 31 | Carbon-13 chemical-shift tensors in single-crystal methoxybenzenes. Journal of the Chemical Society Faraday Transactions I, 1988, 84, 3673. | 1.0 | 42 |
| 32 | Experimental and theoretical study of the methoxy group conformational effect on13C chemical shifts inortho-substituted anisoles. Magnetic Resonance in Chemistry, 1989, 27, 158-161. | 1.9 | 42 |
| 33 | Carbon-13 Chemical Shift Tensors in Polycyclic Aromatic Compounds. 6.1Single-Crystal Study of Perylene. Journal of the American Chemical Society, 1996, 118, 4880-4888. | 13.7 | 42 |
| 34 | Gene co-expression network analysis for identifying modules and functionally enriched pathways in SCA2. Human Molecular Genetics, 2017, 26, 3069-3080. | 2.9 | 40 |
| 35 | Low-temperature carbon-13 magnetic resonance in solids. 5. Chemical shielding anisotropy of the 13CH2 group. Journal of the American Chemical Society, 1985, 107, 6749-6754. | 13.7 | 38 |
| 36 | 15N Chemical Shift Tensors of Uracil Determined from 15N Powder Pattern and 15N-13C Dipolar NMR Spectroscopy. The Journal of Physical Chemistry, 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. Molecular Physics, 1995, 86, 865-872. | 1.7 | 37 |
| 38 | Low temperature 13C NMR magnetic resonance in solids 4. Cyclopropane, bicyclo[1.1.0]butane and [1.1.1] propellane. Theoretica Chimica Acta, 1985, 68, 421-430. | 0.8 | 36 |
| 39 | Effects of protonation on acetone: nuclear magnetic resonance and ab initio studies. Journal of the Chemical Society, Faraday Transactions, 1992, 88, 2459-2463. | 1.7 | 36 |
| 40 | Modeling NMR chemical shifts: a comparison of charge models for solid state effects on 15N chemical shift tensors. Solid State Nuclear Magnetic Resonance, 1998, 10, 185-189. | 2.3 | 36 |
| 41 | Modified genetic algorithms to model cluster structures in medium-sized silicon clusters:Si18â^'Si60. Physical Review A, 2006, 73, . | 2.5 | 35 |
| 42 | Low-temperature carbon-13 magnetic resonance in solids. 7. Methyl carbons. Journal of the American Chemical Society, 1986, 108, 6464-6470. | 13.7 | 34 |
| 43 | Carbon-13 chemical shielding tensors in polycyclic aromatic compounds. 1. Single-crystal study of pyrene. Journal of the American Chemical Society, 1987, 109, 2639-2644. | 13.7 | 34 |
| 44 | Solid State15N and13C NMR Study of Several Metal 5,10,15,20-Tetraphenylporphyrin Complexes. Journal of the American Chemical Society, 1997, 119, 7114-7120. | 13.7 | 34 |
| 45 | Low-temperature carbon-13 magnetic resonance. 8. Chemical shielding anisotropy of olefinic carbons. Journal of the American Chemical Society, 1988, 110, 3386-3392. | 13.7 | 33 |
| 46 | Transmission mechanisms of inter-proton long-range couplings in substituted anisoles. Magnetic Resonance in Chemistry, 1981, 17, 199-203. | 0.7 | 32 |
| 47 | Carbonates, Thiocarbonates, and the Corresponding Monoalkyl Derivatives: III. The 13C Chemical Shift Tensors in Potassium Carbonate, Bicarbonate and Related Monomethyl Derivatives. Solid State Nuclear Magnetic Resonance, 2002, 22, 29-49. | 2.3 | 32 |
| 48 | Ab initio study of the internal rotation barrier of formamide and the formamide-H2O complex. International Journal of Quantum Chemistry, 1993, 45, 123-132. | 2.0 | 30 |
| 49 | Carbon-13 Chemical Shift Tensors in Polycyclic Aromatic Compounds. 7.1 Symmetry Augmented Chemical Shiftâ^'Chemical Shift Correlation Spectroscopy and Single Crystal Study of Triphenylene. Journal of the American Chemical Society, 1998, 120, 9305-9311. | 13.7 | 30 |
| 50 | Predicting the start week of respiratory syncytial virus outbreaks using real time weather variables. BMC Medical Informatics and Decision Making, 2010, 10, 68. | 3.0 | 30 |
| 51 | Quantitative determination of different carbon types in fusinite and anthracite coals from carbon-13 nuclear magnetic resonance chemical shielding line-shape analysis. Analytical Chemistry, 1988, 60, 1574-1579. | 6.5 | 29 |
| 52 | Crystal structure prediction of flexible molecules using parallel genetic algorithms with a standard force field. Journal of Computational Chemistry, 2009, 30, 1973-1985. | 3.3 | 29 |
| 53 | Carbon-13 Chemical Shift Tensors and Molecular Conformation of Anisole. The Journal of Physical Chemistry, 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. Crystal Growth and Design, 2013, 13, 2181-2189. | 3.0 | 28 |

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| 55 | Iglo calculations of the antisymmetric components of nuclear magnetic shielding tensors. Chemical Physics Letters, 1984, 112, 147-149. | 2.6 | 27 |
| 56 | Low-temperature carbon-13 magnetic resonance in solids. 6. Methine carbons. Journal of the American Chemical Society, 1986, 108, 4268-4272. | 13.7 | 27 |
| 57 | Theoretical study of the in-plane components of the 13C shielding tensors in condensed aromatic hydrocarbons. Theoretica Chimica Acta, 1987, 71, 277-288. | 0.8 | 27 |
| 58 | A general framework to understand parallel performance in heterogeneous clusters: analysis of a new adaptive parallel genetic algorithm. Journal of Parallel and Distributed Computing, 2005, 65, 48-57. | 4.1 | 26 |
| 59 | Crystal structure prediction from first principles: The crystal structures of glycine. Chemical Physics Letters, 2015, 626, 20-24. | 2.6 | 26 |
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| 61 | Utility of gene-specific algorithms for predicting pathogenicity of uncertain gene variants. Journal of the American Medical Informatics Association: JAMIA, 2012, 19, 207-211. | 4.4 | 25 |
| 62 | Theoretical study of the adsorption of H on Sin clusters, (n=3â€“10). Journal of Chemical Physics, 2005, 123, 214302. | 3.0 | 24 |
| 63 | Molecular Structure and Carbon-13 Chemical Shielding Tensors Obtained from Nuclear Magnetic Resonance. Topics in Stereochemistry, 2007, , 1-61. | 2.0 | 24 |
| 64 | Alarm Settings of Continuous Glucose Monitoring Systems and Associations to Glucose Outcomes in Type 1 Diabetes. Journal of the Endocrine Society, 2020, 4, bvz005. | 0.2 | 24 |
| 65 | Effects of electronic resonance interaction on methoxy group NMR parameters: theoretical and experimental study of substituted 2-methoxypyridines. The Journal of Physical Chemistry, 1993, 97, 91-93. | 2.9 | 23 |
| 66 | A Nonsynonymous Variant in the GOLM1 Gene in Cutaneous Malignant Melanoma. Journal of the National Cancer Institute, 2018, 110, 1380-1385. | 6.3 | 23 |
| 67 | A theoretical study of the acetate 13C chemical shift tensor in cadmium acetate dihydrate. Chemical Physics Letters, 1999, 302, 499-504. | 2.6 | 22 |
| 68 | Modeling the13C chemical-shift tensor in organic single crystals by quantum mechanical methods: finite basis set effects. Magnetic Resonance in Chemistry, 2006, 44, 390-400. | 1.9 | 22 |
| 69 | Comparative pharmacokinetics of PAMAM-OH dendrimers and HPMA copolymers in ovarian tumor-bearing mice. Drug Delivery and Translational Research, 2013, 3, 260-271. | 5.8 | 22 |
| 70 | Molecular dynamics analysis of the aggregation propensity of polyglutamine segments. PLoS ONE, 2017, 12, e0178333. | 2.5 | 22 |
| 71 | Carbon-13 chemical shift tensors in aromatic compounds. 4. Substituted naphthalenes. Journal of the American Chemical Society, 1992, 114, 2832-2836. | 13.7 | 21 |
| 72 | NMR at Cryogenic Temperatures:Â A13C NMR Study of Ferrocene. Journal of Physical Chemistry A, 1998, 102, 7692-7697. | 2.5 | 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)]2- anions. Journal of the American Chemical Society, 1989, 111, 7619-7621. | 13.7 | 20 |
| 74 | Computational Science and Engineering Online (CSE-Online):Â A Cyber-Infrastructure for Scientific Computing. Journal of Chemical Information and Modeling, 2006, 46, 971-984. | 5.4 | 20 |
| 75 | Ring Current Effects in Crystals. Evidence from 13C Chemical Shift Tensors for Intermolecular Shielding in 4,7-Di-t-butylacenaphthene versus 4,7-Di-t-butylacenaphthylene. Journal of Physical Chemistry A, 2007, 111, 2020-2027. | 2.5 | 20 |
| 76 | Septo-hippocampal networks in chronic epilepsy. Experimental Neurology, 2010, 222, 86-92. | 4.1 | 20 |
| 77 | Characterization of uncertainty in the classification of multivariate assays: application to PAM50 centroid-based genomic predictors for breast cancer treatment plans. Journal of Clinical Bioinformatics, 2011, 1, 37. | 1.2 | 20 |
| 78 | Predicting cytotoxicity of PAMAM dendrimers using molecular descriptors. Beilstein Journal of Nanotechnology, 2015, 6, 1886-1896. | 2.8 | 20 |
| 79 | The use of partially restricted molecular orbitals to investigate transmission mechanisms of spin-spin coupling constants. IIIâ€”an INDO study of long-range Fï£¿H couplings in fluorinated derivatives of toluene. Magnetic Resonance in Chemistry, 1982, 19, 138-143. | 0.7 | 19 |
| 80 | A proton NMR analysis of the OCH3 group conformation in 2-methoxypyridines. Magnetic Resonance in Chemistry, 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. The Journal of Physical Chemistry, 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. The Journal of Physical Chemistry, 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. Journal of Chemical Physics, 2002, 116, 5992-5995. | 3.0 | 19 |
| 84 | Modeling solid-state effects on NMR chemical shifts using electrostatic models. Magnetic Resonance in Chemistry, 2004, 42, S41-S47. | 1.9 | 19 |
| 85 | Intermolecular shielding from molecular magnetic susceptibility. A new view of intermolecular ring current effects. Magnetic Resonance in Chemistry, 2006, 44, 401-408. | 1.9 | 19 |
| 86 | Health information technology adoption: Understanding research protocols and outcome measurements for IT interventions in health care. Journal of Biomedical Informatics, 2016, 63, 33-44. | 4.3 | 19 |
| 87 | Low-Temperature 13C Magnetic Resonance. 9.Steric Effects for Methyl Chemical Shift Tensors in Methylcyclohexanes. Journal of the American Chemical Society, 1995, 117, 8441-8446. | 13.7 | 18 |
| 88 | iBIOMES: Managing and Sharing Biomolecular Simulation Data in a Distributed Environment. Journal of Chemical Information and Modeling, 2013, 53, 726-736. | 5.4 | 18 |
| 89 | Modified genetic algorithm to model crystal structures: III. Determination of crystal structures allowing simultaneous molecular geometry relaxation. International Journal of Quantum Chemistry, 2004, 96, 312-320. | 2.0 | 17 |
| 90 | A Distributed Computing Method for Crystal Structure Prediction of Flexible Molecules:â€‰ An Application to N-(2-Dimethyl-4,5-dinitrophenyl) Acetamide. Journal of Chemical Theory and Computation, 2007, 3, 201-209. | 5.3 | 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. | 4.4 | 17 |
| 92 | Towards a content agnostic computable knowledge repository for data quality assessment. Computer Methods and Programs in Biomedicine, 2019, 177, 193-201. | 4.7 | 17 |
| 93 | Carbon-13 chemical shift tensors in aromatic compounds. 3. Phenanthrene and triphenylene. Journal of the American Chemical Society, 1992, 114, 2826-2832. | 13.7 | 16 |
| 94 | Cluster Analysis of 13C Chemical Shift Tensor Principal Values in Polycyclic Aromatic Hydrocarbons. Journal of Physical Chemistry A, 2001, 105, 7468-7472. | 2.5 | 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. | 4.4 | 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 on13C Chemical Shifts inOrtho-Substituted Phenetols. Magnetic Resonance in Chemistry, 1997, 35, 351-356. | 1.9 | 15 |
| 98 | Nitrogen-15 chemical shift in the pyridineâ€“methanol complex. Chemical Physics Letters, 2000, 322, 91-96. | 2.6 | 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. | 5.1 | 15 |
| 100 | Nanoinformatics: developing new computing applications for nanomedicine. Computing (Vienna/New) Tj ETQq0 0 0 rgBT /Overlock 10 T | 4.8 | 15 |
| 101 | A role for the MEGF6 gene in predisposition to osteoporosis. Annals of Human Genetics, 2021, 85, 58-72. | 0.8 | 15 |
| 102 | Human activity pattern implications for modeling SARS-CoV-2 transmission. Computer Methods and Programs in Biomedicine, 2021, 199, 105896. | 4.7 | 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. | 3.0 | 14 |
| 105 | Diblock copolymer bilayers as model for polymersomes: A coarse grain approach. Journal of Chemical Physics, 2017, 146, 244904. | 3.0 | 14 |
| 106 | Automatic Extraction of Nanoparticle Properties Using Natural Language Processing: NanoSifter an Application to Acquire PAMAM Dendrimer Properties. PLoS ONE, 2014, 9, e83932. | 2.5 | 14 |
| 107 | Temporal Pattern Detection to Predict Adverse Events in Critical Care: Case Study With Acute Kidney Injury. JMIR Medical Informatics, 2020, 8, e14272. | 2.6 | 14 |
| 108 | Solid-State 13C 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. International Journal of Molecular Sciences, 2002, 3, 858-872. | 4.1 | 13 |
| 110 | Modified genetic algorithms to model atomic cluster structures: CuSi clusters. Computational and Theoretical Chemistry, 2004, 681, 149-155. | 1.5 | 13 |
| 111 | STHAM: an agent based model for simulating human exposure across high resolution spatiotemporal domains. Journal of Exposure Science and Environmental Epidemiology, 2020, 30, 459-468. | 3.9 | 13 |
| 112 | Importance of multicenter integrals in semiempirical calculations of nuclear spin-spin coupling constants. 1. Isotropic coupling. Journal of the American Chemical Society, 1984, 106, 3407-3413. | 13.7 | 12 |
| 113 | Molecular dynamics simulations in drug delivery research: Calcium chelation of G3.5 PAMAM dendrimers. Cogent Chemistry, 2016, 2, 1229830. | 2.5 | 12 |
| 114 | Analysis of the IGLO bond contributions to the13C shielding tensors in the local bond frame. International Journal of Quantum Chemistry, 1987, 31, 45-55. | 2.0 | 11 |
| 115 | Solid-State 13C NMR Measurements in Methoxynaphthalenes:â€‰ Determination of the Substituent Chemical Shift Effects in the Principal Values. Journal of Physical Chemistry A, 1997, 101, 9169-9175. | 2.5 | 11 |
| 116 | Data model, dictionaries, and desiderata for biomolecular simulation data indexing and sharing. Journal of Cheminformatics, 2014, 6, 4. | 6.1 | 11 |
| 117 | Comprehensive methodology to monitor longitudinal change patterns during EHR implementations: a case study at a large health care delivery network. Journal of Biomedical Informatics, 2018, 83, 40-53. | 4.3 | 11 |
| 118 | Modeling NMR Chemical Shifts. , 2008, , 53-62. | | 10 |
| 119 | Consensus: a framework for evaluation of uncertain gene variants in laboratory test reporting. Genome Medicine, 2012, 4, 48. | 8.2 | 10 |
| 120 | Effects of the enlargement of polyglutamine segments on the structure and folding of ataxin-2 and ataxin-3 proteins. Journal of Biomolecular Structure and Dynamics, 2017, 35, 504-519. | 3.5 | 10 |
| 121 | Looking Behind the Curtain: Identifying Factors Contributing to Changes on Care Outcomes During a Large Commercial EHR Implementation. EGEMS (Washington, DC), 2019, 7, 21. | 2.0 | 10 |
| 122 | Ab initio study of cyclobutadiene and its aza-substituted derivatives. Ground state properties and vibrational frequencies. Computational and Theoretical Chemistry, 1991, 236, 119-133. | 1.5 | 9 |
| 123 | A parallel genetic algorithm to discover patterns in genetic markers that indicate predisposition to multifactorial disease. Computers in Biology and Medicine, 2008, 38, 826-836. | 7.0 | 9 |
| 124 | Calcium interactions with Cx26 hemmichannel: Spatial association between MD simulations biding sites and variant pathogenicity. Computational Biology and Chemistry, 2018, 77, 331-342. | 2.3 | 9 |
| 125 | Inclusion of hydrogenp orbitals in the semiempirical calculation ofNMR parameters. III:INDO CHF calculations of orbital and dipolar contributions to spin-spin coupling constants involving protons. International Journal of Quantum Chemistry, 1981, 20, 909-919. | 2.0 | 8 |
| 126 | The effect of transverse cross relaxation on nuclear magnetic resonance dipolar spectra. Journal of Chemical Physics, 1988, 89, 5542-5546. | 3.0 | 8 |

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| 127 | 13C Dipolar spectroscopy of nitromethane. Molecular Physics, 1988, 64, 1031-1040. | 1.7 | 8 |
| 128 | Proximity effects on the nuclear magnetic shielding tensor. Computational and Theoretical Chemistry, 1993, 281, 61-66. | 1.5 | 8 |
| 129 | A case for using grid architecture for state public health informatics: the Utah perspective. BMC Medical Informatics and Decision Making, 2009, 9, 32. | 3.0 | 8 |
| 130 | A domain analysis model for eIRB systems: Addressing the weak link in clinical research informatics. Journal of Biomedical Informatics, 2014, 52, 121-129. | 4.3 | 8 |
| 131 | The origin of the splitting of 13C and 15N NMR signals of 3(5)-phenyl-5(3)-methylpyrazolium chloride and bromide in the solid state: Quantum Espresso calculations. Journal of Molecular Structure, 2014, 1075, 551-558. | 3.6 | 8 |
| 132 | iBIOMES Lite: Summarizing Biomolecular Simulation Data in Limited Settings. Journal of Chemical Information and Modeling, 2014, 54, 1810-1819. | 5.4 | 8 |
| 133 | Using supervised machine learning classifiers to estimate likelihood of participating in clinical trials of a de-identified version of ResearchMatch. Journal of Clinical and Translational Science, 2021, 5, e42. | 0.6 | 8 |
| 134 | Nonplanarity of the methoxy groups in o-dimethoxybenzene: quantum chemical calculations of the 17O chemical shieldings. Computational and Theoretical Chemistry, 1992, 276, 307-313. | 1.5 | 7 |
| 135 | Nitrogen-15 Chemical Shifts in AT (Adenine-Thymine) and CG (Cytosine-Guanine) Nucleic Acid Base Pairs. Journal of Biomolecular Structure and Dynamics, 1998, 16, 619-629. | 3.5 | 7 |
| 136 | 13C Chemical-shift tensors in an analogous series of heterosubstituted polycyclic aromatic compounds. Magnetic Resonance in Chemistry, 2001, 39, 115-121. | 1.9 | 7 |
| 137 | Indirect (J) coupling of inequivalent 75As nuclei in crystalline and glassy As2Se3 and As2S3. Journal of Chemical Physics, 2003, 119, 8519-8525. | 3.0 | 7 |
| 138 | A novel <scp>CDKN</scp>2A variant (p16<sup>L117P</sup>) in a patient with familial and multiple primary melanomas. Pigment Cell and Melanoma Research, 2019, 32, 734-738. | 3.3 | 7 |
| 139 | An intronic variant in the CELF4 gene is associated with risk for colorectal cancer. Cancer Epidemiology, 2021, 72, 101941. | 1.9 | 7 |
| 140 | Generation and Classification of Activity Sequences for Spatiotemporal Modeling of Human Populations. Online Journal of Public Health Informatics, 2020, 12, e9. | 0.7 | 7 |
| 141 | Quantum mechanical calculations and experimental measurement of N-terminal charge effects on 1HN and 1HCÎ± chemical shifts in peptides. Biopolymers, 1998, 38, 573-581. | 2.4 | 6 |
| 142 | Ab initioglobal optimization of the structures ofSinH,n=4â€“10, using parallel genetic algorithms. Physical Review A, 2005, 72, . | 2.5 | 6 |
| 143 | Formation of one dimensional linear chains by Irâ€“Ir bonds in cis-dicarbonyldichloroiridate (I). Polyhedron, 2011, 30, 221-227. | 2.2 | 6 |
| 144 | Development and classification of a robust inventory of near real-time outcome measurements for assessing information technology interventions in health care. Journal of Biomedical Informatics, 2017, 73, 62-75. | 4.3 | 6 |

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| 145 | Mechanical properties of drug loaded diblock copolymer bilayers: A molecular dynamics study. Journal of Chemical Physics, 2018, 148, 214901. | 3.0 | 6 |
| 146 | SaTScan on a Cloud: On-Demand Large Scale Spatial Analysis of Epidemics. Online Journal of Public Health Informatics, 2010, 2, . | 0.7 | 6 |
| 147 | Structure and electronic properties of lithiumâ€“silicon clusters. Computational and Theoretical Chemistry, 2013, 1024, 61-68. | 2.5 | 5 |
| 148 | Understanding protein structural changes for oncogenic missense variants. Heliyon, 2021, 7, e06013. | 3.2 | 5 |
| 149 | Computational Feature Selection and Classification of RET Phenotypic Severity. Journal of Data Mining in Genomics & Proteomics, 2010, 01, . | 0.5 | 5 |
| 150 | Conformal Prediction in Clinical Medical Sciences. Journal of Healthcare Informatics Research, 2022, 6, 241-252. | 7.6 | 5 |
| 151 | Solid-state13C NMR and quantum chemical investigation of metal diene complexes. Magnetic Resonance in Chemistry, 2007, 45, 393-400. | 1.9 | 4 |
| 152 | From NMR spectra to structure. Concepts in Magnetic Resonance Part A: Bridging Education and Research, 2013, 42, 261-289. | 0.5 | 4 |
| 153 | Structure prediction of polyglutamine disease proteins: comparison of methods. BMC Bioinformatics, 2014, 15, S11. | 2.6 | 4 |
| 154 | A Rare Variant in ERF (rs144812092) Predisposes to Prostate and Bladder Cancers in an Extended Pedigree. Cancers, 2021, 13, 2399. | 3.7 | 4 |
| 155 | K-means cluster analysis of cooperative effects of CO, NO2, O3, PM2.5, PM10, and SO2 on incidence of type 2 diabetes mellitus in the US. Environmental Research, 2022, 212, 113259. | 7.5 | 4 |
| 156 | New theoretical results on the COâ€¦cyclobutadiene complex. Chemical Physics Letters, 1990, 173, 21-25. | 2.6 | 3 |
| 157 | Modeling of the 15N and 13C Chemical Shift Tensors in Purine. ACS Symposium Series, 1999, , 162-176. | 0.5 | 3 |
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