# Kenneth M Merz Jr

## List of Publications by Year in Descending Order



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|---|---|---|---|
| 330 papers | 36,221 citations | 71 h-index | 186 g-index |
| 489 ext. papers | 39,683 ext. citations | 7.6 avg, IF | 7.22 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 330 | Parameterization of a Dioxygen Binding Metal Site Using the MCPB.py Program. *Methods in Molecular Biology*, **2021**, 2199, 257-275 | 1.4 | |
| 329 | Parametrization of Trivalent and Tetravalent Metal Ions for the OPC3, OPC, TIP3P-FB, and TIP4P-FB Water Models. *Journal of Chemical Theory and Computation*, **2021**, 17, 2342-2354 | 6.4 | 10 |
| 328 | Open-Source Multi-GPU-Accelerated QM/MM Simulations with AMBER and QUICK. *Journal of Chemical Information and Modeling*, **2021**, 61, 2109-2115 | 6.1 | 3 |
| 327 | Quantum Chemistry Calculations for Metabolomics. *Chemical Reviews*, **2021**, 121, 5633-5670 | 68.1 | 18 |
| 326 | Harnessing the Power of Multi-GPU Acceleration into the Quantum Interaction Computational Kernel Program. *Journal of Chemical Theory and Computation*, **2021**, 17, 3955-3966 | 6.4 | 2 |
| 325 | Parameterization of Monovalent Ions for the OPC3, OPC, TIP3P-FB, and TIP4P-FB Water Models. *Journal of Chemical Information and Modeling*, **2021**, 61, 869-880 | 6.1 | 19 |
| 324 | AutoGraph: Autonomous Graph-Based Clustering of Small-Molecule Conformations. *Journal of Chemical Information and Modeling*, **2021**, 61, 1647-1656 | 6.1 | 1 |
| 323 | Formation of the Metal-Binding Core of the ZRT/IRT-like Protein (ZIP) Family Zinc Transporter. *Biochemistry*, **2021**, 60, 2727-2738 | 3.2 | 2 |
| 322 | FFENCODER-PL: Pair Wise Energy Descriptors for Protein-Ligand Pose Selection. *Journal of Chemical Theory and Computation*, **2021**, 17, 6647-6657 | 6.4 | 0 |
| 321 | A critical overview of computational approaches employed for COVID-19 drug discovery. *Chemical Society Reviews*, **2021**, 50, 9121-9151 | 58.5 | 36 |
| 320 | Refinement of pairwise potentials via logistic regression to score protein-protein interactions. *Proteins: Structure, Function and Bioinformatics*, **2020**, 88, 1559-1568 | 4.2 | 1 |
| 319 | Confronting Racism in Chemistry Journals. *ACS Applied Nano Materials*, **2020**, 3, 6131-6133 | 5.6 | |
| 318 | Confronting Racism in Chemistry Journals. *ACS Applied Polymer Materials*, **2020**, 2, 2496-2498 | 4.3 | |
| 317 | Systematic Parametrization of Divalent Metal Ions for the OPC3, OPC, TIP3P-FB, and TIP4P-FB Water Models. *Journal of Chemical Theory and Computation*, **2020**, 16, 4429-4442 | 6.4 | 18 |
| 316 | Validation of Free Energy Methods in AMBER. *Journal of Chemical Information and Modeling*, **2020**, 60, 5296-5300 | 6.1 | 7 |
| 315 | Parallel Implementation of Density Functional Theory Methods in the Quantum Interaction Computational Kernel Program. *Journal of Chemical Theory and Computation*, **2020**, 16, 4315-4326 | 6.4 | 10 |
| 314 | Confronting Racism in Chemistry Journals. *Organometallics*, **2020**, 39, 2331-2333 | 3.8 | |

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| 313 | Thermodynamics of Transition Metal Ion Binding to Proteins. *Journal of the American Chemical Society*, **2020**, 142, 6365-6374 | 16.4 | 13 |
| 312 | Metabolite Structure Assignment Using In Silico NMR Techniques. *Analytical Chemistry*, **2020**, 92, 10412-10419 | 7.4 | 7 |
| 311 | Pair Potentials as Machine Learning Features. *Journal of Chemical Theory and Computation*, **2020**, 16, 5385-5400 | 6.4 | 1 |
| 310 | Update to Our Reader, Reviewer, and Author Communities April 2020. *Energy & Fuels*, **2020**, 34, 5107-5108 | 4.1 | |
| 309 | Impact of the Special Issue on Women in Computational Chemistry. *Journal of Chemical Information and Modeling*, **2020**, 60, 3328-3330 | 6.1 | 2 |
| 308 | Update to Our Reader, Reviewer, and Author Communities April 2020. *Organometallics*, **2020**, 39, 1665-1666 | 3.8 | |
| 307 | Confronting Racism in Chemistry Journals. *Journal of Chemical Health and Safety*, **2020**, 27, 198-200 | 1.7 | |
| 306 | Converging Interests: Chemoinformatics, History, and Bibliometrics. *Journal of Chemical Information and Modeling*, **2020**, 60, 5870-5872 | 6.1 | 1 |
| 305 | MRP.py: A Parametrizer of Post-Translationally Modified Residues. *Journal of Chemical Information and Modeling*, **2020**, 60, 4424-4428 | 6.1 | 1 |
| 304 | ReaxFF/AMBER-A Framework for Hybrid Reactive/Nonreactive Force Field Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2020**, 16, 7645-7654 | 6.4 | 5 |
| 303 | Receptor-Ligand Binding Free Energies from a Consecutive Histograms Monte Carlo Sampling Method. *Journal of Chemical Theory and Computation*, **2020**, 16, 6645-6655 | 6.4 | 1 |
| 302 | Evolution of Alchemical Free Energy Methods in Drug Discovery. *Journal of Chemical Information and Modeling*, **2020**, 60, 5308-5318 | 6.1 | 24 |
| 301 | Random Forest Refinement of Pairwise Potentials for Protein-Ligand Decoy Detection. *Journal of Chemical Information and Modeling*, **2019**, 59, 3305-3315 | 6.1 | 11 |
| 300 | Using AMBER18 for Relative Free Energy Calculations. *Journal of Chemical Information and Modeling*, **2019**, 59, 3128-3135 | 6.1 | 62 |
| 299 | Random Forest Refinement of the KECSA2 Knowledge-Based Scoring Function for Protein Decoy Detection. *Journal of Chemical Information and Modeling*, **2019**, 59, 1919-1929 | 6.1 | 9 |
| 298 | Free-Energy-Based Protein Design: Re-Engineering Cellular Retinoic Acid Binding Protein II Assisted by the Moveable-Type Approach. *Journal of the American Chemical Society*, **2018**, 140, 3483-3486 | 16.4 | 2 |
| 297 | Quantum Crystallography: Current Developments and Future Perspectives. *Chemistry - A European Journal*, **2018**, 24, 10881-10905 | 4.8 | 77 |
| 296 | The Role of the Active Site Flap in Streptavidin/Biotin Complex Formation. *Journal of the American Chemical Society*, **2018**, 140, 5434-5446 | 16.4 | 12 |

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| 295 | Frontispiece: Quantum Crystallography: Current Developments and Future Perspectives. *Chemistry - A European Journal*, **2018**, 24, | 4.8 | 1 |
| 294 | Detailed potential of mean force studies on host-guest systems from the SAMPL6 challenge. *Journal of Computer-Aided Molecular Design*, **2018**, 32, 1013-1026 | 4.2 | 11 |
| 293 | Extended Zinc AMBER Force Field (EZAFF). *Journal of Chemical Theory and Computation*, **2018**, 14, 242-254 | 5.4 | 20 |
| 292 | Trapping intermediates in metal transfer reactions of the CusCBAF export pump of. *Communications Biology*, **2018**, 1, 192 | 6.7 | 10 |
| 291 | Simulating the Chelate Effect. *Journal of the American Chemical Society*, **2018**, 140, 15166-15169 | 16.4 | 18 |
| 290 | Generation of Pairwise Potentials Using Multidimensional Data Mining. *Journal of Chemical Theory and Computation*, **2018**, 14, 5045-5067 | 6.4 | 8 |
| 289 | Using Ligand-Induced Protein Chemical Shift Perturbations To Determine Protein-Ligand Structures. *Biochemistry*, **2017**, 56, 2349-2362 | 3.2 | 18 |
| 288 | Mechanism of Formation of the Nonstandard Product in the Prenyltransferase Reaction of the G115T Mutant of FtmPT1: A Case of Reaction Dynamics Calling the Shots?. *Biochemistry*, **2017**, 56, 2995-3007 | 3.2 | 2 |
| 287 | Metal Ion Modeling Using Classical Mechanics. *Chemical Reviews*, **2017**, 117, 1564-1686 | 68.1 | 189 |
| 286 | The BioFragment Database (BFDb): An open-data platform for computational chemistry analysis of noncovalent interactions. *Journal of Chemical Physics*, **2017**, 147, 161727 | 3.9 | 57 |
| 285 | On the fly estimation of host-guest binding free energies using the movable type method: participation in the SAMPL5 blind challenge. *Journal of Computer-Aided Molecular Design*, **2017**, 31, 47-60 | 4.2 | 9 |
| 284 | The Role of Molecular Dynamics Potential of Mean Force Calculations in the Investigation of Enzyme Catalysis. *Methods in Enzymology*, **2016**, 577, 1-29 | 1.7 | 5 |
| 283 | MCPB.py: A Python Based Metal Center Parameter Builder. *Journal of Chemical Information and Modeling*, **2016**, 56, 599-604 | 6.1 | 237 |
| 282 | Metal Ion Capture Mechanism of a Copper Metallochaperone. *Biochemistry*, **2016**, 55, 501-9 | 3.2 | 6 |
| 281 | Incorporation of side chain flexibility into protein binding pockets using MT. *Bioorganic and Medicinal Chemistry*, **2016**, 24, 4978-4987 | 3.4 | 4 |
| 280 | Acceleration of High Angular Momentum Electron Repulsion Integrals and Integral Derivatives on Graphics Processing Units. *Journal of Chemical Theory and Computation*, **2015**, 11, 1449-62 | 6.4 | 16 |
| 279 | Models for the Metal Transfer Complex of the N-Terminal Region of CusB and CusF. *Biochemistry*, **2015**, 54, 4226-35 | 3.2 | 8 |
| 278 | Effect of 10.5 M Aqueous Urea on Helicobacter pylori Urease: A Molecular Dynamics Study. *Biochemistry*, **2015**, 54, 4121-30 | 3.2 | 6 |

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| 277 | Intermolecular interaction of thiosemicarbazone derivatives to solvents and a potential Aedes aegypti target. *Journal of Molecular Structure*, **2015**, 1093, 219-227 | 3.4 | 5 |
| 276 | Implementation of Protocols To Enable Doctoral Training in Physical and Computational Chemistry of a Blind Graduate Student. *Journal of Chemical Education*, **2015**, 92, 1280-1283 | 2.4 | 7 |
| 275 | Free Energy-Based Conformational Search Algorithm Using the Movable Type Sampling Method. *Journal of Chemical Theory and Computation*, **2015**, 11, 5853-64 | 6.4 | 12 |
| 274 | Parameterization of highly charged metal ions using the 12-6-4 LJ-type nonbonded model in explicit water. *Journal of Physical Chemistry B*, **2015**, 119, 883-95 | 3.4 | 150 |
| 273 | N-Terminal Domain of the Cu(I)-Binding Protein CusB **2015**, 1-8 | | |
| 272 | Thiosemicarbazones as Aedes aegypti larvicidal. *European Journal of Medicinal Chemistry*, **2015**, 100, 162-75 | 6.8 | 25 |
| 271 | Role of substrate dynamics in protein prenylation reactions. *Accounts of Chemical Research*, **2015**, 48, 439-48 | 24.3 | 10 |
| 270 | KECSA-Movable Type Implicit Solvation Model (KMTISM). *Journal of Chemical Theory and Computation*, **2015**, 11, 667-82 | 6.4 | 16 |
| 269 | Reduction of urease activity by interaction with the flap covering the active site. *Journal of Chemical Information and Modeling*, **2015**, 55, 354-61 | 6.1 | 20 |
| 268 | Systematic Parameterization of Monovalent Ions Employing the Nonbonded Model. *Journal of Chemical Theory and Computation*, **2015**, 11, 1645-57 | 6.4 | 195 |
| 267 | Adenine formation without HCN. *Journal of Physical Chemistry A*, **2014**, 118, 3637-44 | 2.8 | 15 |
| 266 | Taking into Account the Ion-induced Dipole Interaction in the Nonbonded Model of Ions. *Journal of Chemical Theory and Computation*, **2014**, 10, 289-297 | 6.4 | 201 |
| 265 | Mechanistic insights into Mg2+-independent prenylation by CloQ from classical molecular mechanics and hybrid quantum mechanics/molecular mechanics molecular dynamics simulations. *Biochemistry*, **2014**, 53, 5034-41 | 3.2 | 8 |
| 264 | Bringing Clarity to the Prediction of Protein-Ligand Binding Free Energies via "Blurring". *Journal of Chemical Theory and Computation*, **2014**, 10, 1314-1325 | 6.4 | 15 |
| 263 | Origin of product selectivity in a prenyl transfer reaction from the same intermediate: exploration of multiple FtmPT1-catalyzed prenyl transfer pathways. *Biochemistry*, **2014**, 53, 6126-38 | 3.2 | 6 |
| 262 | Fragment-based error estimation in biomolecular modeling. *Drug Discovery Today*, **2014**, 19, 45-50 | 8.8 | 4 |
| 261 | Molecular Dynamics Study of Urease. *Journal of Chemical Theory and Computation*, **2014**, 10, 1852-1862 | 6.4 | 21 |
| 260 | Using quantum mechanical approaches to study biological systems. *Accounts of Chemical Research*, **2014**, 47, 2804-11 | 24.3 | 68 |

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| 259 | Studying allosteric regulation in metal sensor proteins using computational methods. *Advances in Protein Chemistry and Structural Biology*, **2014**, 96, 181-218 | 5.3 | 6 |
| 258 | Accurate macromolecular crystallographic refinement: incorporation of the linear scaling, semiempirical quantum-mechanics program DivCon into the PHENIX refinement package. *Acta Crystallographica Section D: Biological Crystallography*, **2014**, 70, 1233-47 | | 40 |
| 257 | Solution NMR refinement of a metal ion bound protein using metal ion inclusive restrained molecular dynamics methods. *Journal of Biomolecular NMR*, **2013**, 56, 125-37 | 3 | 19 |
| 256 | Computer-aided Drug Design: Using Numbers to your Advantage. *ACS Medicinal Chemistry Letters*, **2013**, 4, | 4.3 | 11 |
| 255 | Structure and dynamics of the N-terminal domain of the Cu(I) binding protein CusB. *Biochemistry*, **2013**, 52, 6911-23 | 3.2 | 23 |
| 254 | Development of the knowledge-based and empirical combined scoring algorithm (KECSA) to score protein-ligand interactions. *Journal of Chemical Information and Modeling*, **2013**, 53, 1073-83 | 6.1 | 41 |
| 253 | Calculation of Heats of Formation for Zn Complexes: Comparison of Density Functional Theory, Second Order Perturbation Theory, Coupled-Cluster and Complete Active Space Methods. *Journal of Chemical Theory and Computation*, **2013**, 9, | 6.4 | 21 |
| 252 | Quantum Mechanical Study of Vicinal J Spin-Spin Coupling Constants for the Protein Backbone. *Journal of Chemical Theory and Computation*, **2013**, 9, 4653-9 | 6.4 | 12 |
| 251 | Acceleration of Electron Repulsion Integral Evaluation on Graphics Processing Units via Use of Recurrence Relations. *Journal of Chemical Theory and Computation*, **2013**, 9, 965-76 | 6.4 | 40 |
| 250 | Conformational analysis and parallel QM/MM X-ray refinement of protein bound anti-Alzheimer drug donepezil. *Journal of Chemical Theory and Computation*, **2013**, 9, 1686-1693 | 6.4 | 21 |
| 249 | Rational Design of Particle Mesh Ewald Compatible Lennard-Jones Parameters for +2 Metal Cations in Explicit Solvent. *Journal of Chemical Theory and Computation*, **2013**, 9, 2733-2748 | 6.4 | 365 |
| 248 | The Movable Type Method Applied to Protein-Ligand Binding. *Journal of Chemical Theory and Computation*, **2013**, 9, 5526-5538 | 6.4 | 24 |
| 247 | Energetics of zinc-mediated interactions in the allosteric pathways of metal sensor proteins. *Journal of the American Chemical Society*, **2013**, 135, 30-3 | 16.4 | 18 |
| 246 | QM/MM refinement and analysis of protein bound retinoic acid. *Journal of Computational Chemistry* , **2012**, 33, 301-10 | 3.5 | 14 |
| 245 | Catalytic mechanism of aromatic prenylation by NphB. *Biochemistry*, **2012**, 51, 2606-18 | 3.2 | 28 |
| 244 | Insights into the mechanistic dichotomy of the protein farnesyltransferase peptide substrates CVIM and CVLS. *Journal of the American Chemical Society*, **2012**, 134, 820-3 | 16.4 | 15 |
| 243 | Wide-open flaps are key to urease activity. *Journal of the American Chemical Society*, **2012**, 134, 9934-7 | 16.4 | 38 |
| 242 | Solution structure of Mycobacterium tuberculosis NmtR in the apo state: insights into Ni(II)-mediated allostery. *Biochemistry*, **2012**, 51, 2619-29 | 3.2 | 37 |

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| 241 | The Effects of Computational Modeling Errors on the Estimation of Statistical Mechanical Variables. *Journal of Chemical Theory and Computation*, **2012**, 8, 3769-3776 | 6.4 | 22 |
| 240 | Conformational Analysis of Free and Bound Retinoic Acid. *Journal of Chemical Theory and Computation*, **2012**, 8, 1436-1448 | 6.4 | 17 |
| 239 | An Efficient Method to Evaluate Intermolecular Interaction Energies in Large Systems Using Overlapping Multicenter ONIOM and the Fragment Molecular Orbital Method. *Journal of Physical Chemistry Letters*, **2012**, 3, 2604-2610 | 6.4 | 19 |
| 238 | Simulations of allosteric motions in the zinc sensor CzrA. *Journal of the American Chemical Society*, **2012**, 134, 3367-76 | 16.4 | 36 |
| 237 | Statistics-based model for basis set superposition error correction in large biomolecules. *Physical Chemistry Chemical Physics*, **2012**, 14, 7795-9 | 3.6 | 9 |
| 236 | Comment on "A minimal implementation of the AMBER-GAUSSIAN interface for ab initio QM/MM-MD simulation". *Journal of Computational Chemistry*, **2012**, 33, 1643-4 | 3.5 | 2 |
| 235 | Prediction of trypsin/molecular fragment binding affinities by free energy decomposition and empirical scores. *Journal of Computer-Aided Molecular Design*, **2012**, 26, 647-59 | 4.2 | 10 |
| 234 | Insight into the cation-π interaction at the metal binding site of the copper metallochaperone CusF. *Journal of the American Chemical Society*, **2011**, 133, 19330-3 | 16.4 | 44 |
| 233 | Model for the fast estimation of basis set superposition error in biomolecular systems. *Journal of Chemical Physics*, **2011**, 135, 144110 | 3.9 | 28 |
| 232 | Electronic structure, chemical bonding, and oxidation numbers of first-row transition metals in [MePIm2] complexes and their cations. *International Journal of Quantum Chemistry*, **2011**, 111, 3630-3642 | 2.1 | 1 |
| 231 | Accurate assessment of the strain energy in a protein-bound drug using QM/MM X-ray refinement and converged quantum chemistry. *Journal of Computational Chemistry*, **2011**, 32, 2587-97 | 3.5 | 39 |
| 230 | Formal Estimation of Errors in Computed Absolute Interaction Energies of Protein-ligand Complexes. *Journal of Chemical Theory and Computation*, **2011**, 7, 790-797 | 6.4 | 116 |
| 229 | Ligand Identification Scoring Algorithm (LISA). *Journal of Chemical Information and Modeling*, **2011**, 51, 1296-306 | 6.1 | 23 |
| 228 | Pairwise additivity of energy components in protein-ligand binding: the HIV II protease-Indinavir case. *Journal of Chemical Physics*, **2011**, 135, 085101 | 3.9 | 14 |
| 227 | The energy computation paradox and ab initio protein folding. *PLoS ONE*, **2011**, 6, e18868 | 3.7 | 41 |
| 226 | Molecular recognition and drug-lead identification: what can molecular simulations tell us?. *Current Medicinal Chemistry*, **2010**, 17, 25-41 | 4.3 | 31 |
| 225 | Computational study of the resistance shown by the subtype B/HIV-1 protease to currently known inhibitors. *Biochemistry*, **2010**, 49, 4283-95 | 3.2 | 18 |
| 224 | The Utility of the HSAB Principle via the Fukui Function in Biological Systems. *Journal of Chemical Theory and Computation*, **2010**, 6, 548-559 | 6.4 | 34 |

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| 223 | Novel acyclic diaminocarbene ligands with increased steric demand and their application in gold catalysis. *Organic Letters*, **2010**, 12, 4860-3 | 6.2 | 63 |
| 222 | Finding a needle in the haystack: computational modeling of Mg2+ binding in the active site of protein farnesyltransferase. *Biochemistry*, **2010**, 49, 9658-66 | 3.2 | 15 |
| 221 | Limits of Free Energy Computation for Protein-Ligand Interactions. *Journal of Chemical Theory and Computation*, **2010**, 6, 1018-1027 | 6.4 | 72 |
| 220 | Divide-and-Conquer Hartree-Fock Calculations on Proteins. *Journal of Chemical Theory and Computation*, **2010**, 6, 405-411 | 6.4 | 117 |
| 219 | A Mixed QM/MM Scoring Function to Predict Protein-Ligand Binding Affinity. *Journal of Chemical Theory and Computation*, **2010**, 6, 3079-3091 | 6.4 | 63 |
| 218 | Importance of loop dynamics in the neocarzinostatin chromophore binding and release mechanisms. *Physical Chemistry Chemical Physics*, **2010**, 12, 3443-9 | 3.6 | 4 |
| 217 | Structural Survey of Zinc Containing Proteins and the Development of the Zinc AMBER Force Field (ZAFF). *Journal of Chemical Theory and Computation*, **2010**, 6, 2935-2947 | 6.4 | 275 |
| 216 | QM/MM X-ray refinement of zinc metalloenzymes. *Journal of Inorganic Biochemistry*, **2010**, 104, 512-22 | 4.2 | 46 |
| 215 | Further analysis and comparative study of intermolecular interactions using dimers from the S22 database. *Journal of Chemical Physics*, **2009**, 131, 065102 | 3.9 | 75 |
| 214 | Protein NMR chemical shift calculations based on the automated fragmentation QM/MM approach. *Journal of Physical Chemistry B*, **2009**, 113, 10380-8 | 3.4 | 79 |
| 213 | Conformational variability of benzamidinium-based inhibitors. *Journal of the American Chemical Society*, **2009**, 131, 7742-54 | 16.4 | 28 |
| 212 | Apo and nickel-bound forms of the Pyrococcus horikoshii species of the metalloregulatory protein: NikR characterized by molecular dynamics simulations. *Biochemistry*, **2009**, 48, 12024-33 | 3.2 | 13 |
| 211 | AM1 parameters for the prediction of 1H and 13C NMR chemical shifts in proteins. *Journal of Physical Chemistry A*, **2009**, 113, 11550-9 | 2.8 | 7 |
| 210 | Accurate benchmark calculations on the gas-phase basicities of small molecules. *Journal of Physical Chemistry A*, **2009**, 113, 10096-103 | 2.8 | 17 |
| 209 | Assessment of the CCSD and CCSD(T) coupled-cluster methods in calculating heats of formation for Zn complexes. *Journal of Physical Chemistry A*, **2009**, 113, 10081-8 | 2.8 | 12 |
| 208 | Explicitly representing the solvation shell in continuum solvent calculations. *Journal of Physical Chemistry A*, **2009**, 113, 6404-9 | 2.8 | 98 |
| 207 | Relative configuration of natural products using NMR chemical shifts. *Journal of Natural Products*, **2009**, 72, 709-13 | 4.9 | 38 |
| 206 | Assessment of the "6-31+G** + LANL2DZ" mixed basis set coupled with density functional theory methods and the effective core potential: prediction of heats of formation and ionization potentials for first-row-transition-metal complexes. *Journal of Physical Chemistry A*, **2009**, 113, 9843-51 | 2.8 | 234 |

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| 205 | Importance of dispersion and electron correlation in ab initio protein folding. *Journal of Physical Chemistry B*, **2009**, 113, 5290-300 | 3.4 | 61 |
| 204 | Assessment of the CCSD and CCSD(T) Coupled-Cluster Methods in Calculating Heats of Formation for Cu Complexes. *Molecular Physics*, **2009**, 107, 1251-1259 | 1.7 | 3 |
| 203 | Interpreting The Observed Substrate Selectivity And The Product Regioselectivity In Orf2-Catalyzed Prenylation From X-Ray Structures. *Challenges and Advances in Computational Chemistry and Physics*, **2009**, 351-375 | 0.7 | |
| 202 | The intrinsic dynamics and function of nickel-binding regulatory protein: insights from elastic network analysis. *Biophysical Journal*, **2008**, 94, 3769-78 | 2.9 | 15 |
| 201 | MNDO parameters for the prediction of 19F NMR chemical shifts in biologically relevant compounds. *Journal of Physical Chemistry A*, **2008**, 112, 8829-38 | 2.8 | 12 |
| 200 | A Combined QM/MM Poisson-Boltzmann Approach. *Journal of Chemical Theory and Computation*, **2008**, 4, 1200-7 | 6.4 | 15 |
| 199 | A Hylleraas functional based perturbative technique to relax the extremely localized molecular orbital wavefunction. *Journal of Chemical Physics*, **2008**, 129, 054101 | 3.9 | 10 |
| 198 | An efficient and accurate molecular alignment and docking technique using ab initio quality scoring. *Journal of Chemical Physics*, **2008**, 129, 025102 | 3.9 | 5 |
| 197 | Understanding the substrate selectivity and the product regioselectivity of Orf2-catalyzed aromatic prenylations. *Biochemistry*, **2007**, 46, 1303-11 | 3.2 | 21 |
| 196 | An ab initio investigation of the interactions involving the aromatic group of the set of fluorinated N-(4-sulfamylbenzoyl)benzylamine inhibitors and human carbonic anhydrase II. *Journal of Physical Chemistry B*, **2007**, 111, 5700-7 | 3.4 | 15 |
| 195 | A critical assessment of the performance of protein-ligand scoring functions based on NMR chemical shift perturbations. *Journal of Medicinal Chemistry*, **2007**, 50, 5128-34 | 8.3 | 32 |
| 194 | The hydrolysis of amides and the proficiency of amidohydrolases. The burden borne by kw. *Journal of Physical Chemistry B*, **2007**, 111, 6507-19 | 3.4 | 18 |
| 193 | Computational studies of the farnesyltransferase ternary complex part II: the conformational activation of farnesyldiphosphate. *Biochemistry*, **2007**, 46, 12375-81 | 3.2 | 25 |
| 192 | Assessment of density functional theory methods for the computation of heats of formation and ionization potentials of systems containing third row transition metals. *Journal of Physical Chemistry A*, **2007**, 111, 6044-53 | 2.8 | 85 |
| 191 | Interaction energy decomposition in protein-protein association: a quantum mechanical study of barnase-barstar complex. *Biophysical Chemistry*, **2007**, 125, 221-36 | 3.5 | 21 |
| 190 | An improved 6-31G basis set for atoms Ga through Kr. *International Journal of Quantum Chemistry*, **2007**, 107, 3028-3038 | 2.1 | 3 |
| 189 | The role of quantum mechanics in structure-based drug design. *Drug Discovery Today*, **2007**, 12, 725-31 | 8.8 | 193 |
| 188 | Haptic applications for molecular structure manipulation. *Journal of Molecular Graphics and Modelling*, **2007**, 25, 801-5 | 2.8 | 36 |

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| 187 | Insights into Cu(I) exchange in HAH1 using quantum mechanical and molecular simulations. *Biochemistry*, **2007**, 46, 8816-26 | 3.2 | 41 |
| 186 | Molecular dynamics study of ethanolamine as a pure liquid and in aqueous solution. *Journal of Physical Chemistry B*, **2007**, 111, 3695-703 | 3.4 | 71 |
| 185 | Critical Assessment of the Performance of Density Functional Methods for Several Atomic and Molecular Properties. *Journal of Chemical Theory and Computation*, **2007**, 3, 407-433 | 6.4 | 269 |
| 184 | Insights into the strength and origin of halogen bonding: the halobenzene-formaldehyde dimer. *Journal of Physical Chemistry A*, **2007**, 111, 1688-94 | 2.8 | 156 |
| 183 | Assessment of Semiempirical Quantum Mechanical Methods for the Evaluation of Protein Structures. *Journal of Chemical Theory and Computation*, **2007**, 3, 1609-1619 | 6.4 | 23 |
| 182 | Competitive hydrolytic and elimination mechanisms in the urease catalyzed decomposition of urea. *Journal of Physical Chemistry B*, **2007**, 111, 10263-74 | 3.4 | 46 |
| 181 | Quantum mechanical description of the interactions between DNA and water. *Journal of Molecular Graphics and Modelling*, **2006**, 24, 440-55 | 2.8 | 10 |
| 180 | Quantum mechanical and molecular dynamics simulations of ureases and Zn beta-lactamases. *Journal of Computational Chemistry*, **2006**, 27, 1240-62 | 3.5 | 52 |
| 179 | X-ray diffraction "fingerprinting" of DNA structure in solution for quantitative evaluation of molecular dynamics simulation. *Proceedings of the National Academy of Sciences of the United States of America*, **2006**, 103, 3534-9 | 11.5 | 84 |
| 178 | Assigning the protonation states of the key aspartates in β-Secretase using QM/MM X-ray structure refinement. *Journal of Chemical Theory and Computation*, **2006**, 2, 1057-1069 | 6.4 | 86 |
| 177 | Catalyzed decomposition of urea. Molecular dynamics simulations of the binding of urea to urease. *Biochemistry*, **2006**, 45, 4429-43 | 3.2 | 29 |
| 176 | A Fast QM/MM (Quantum Mechanical/Molecular Mechanical) Approach to Calculate Nuclear Magnetic Resonance Chemical Shifts for Macromolecules. *Journal of Chemical Theory and Computation*, **2006**, 2, 209-15 | 6.4 | 39 |
| 175 | Role of solvation in the energy stabilization inside the hydrophobic core of the protein rubredoxin. *Journal of Physical Chemistry B*, **2006**, 110, 15650-3 | 3.4 | 22 |
| 174 | Exploring the role of the active site cysteine in human muscle creatine kinase. *Biochemistry*, **2006**, 45, 11464-72 | 3.2 | 17 |
| 173 | Development of a Parametrized Force Field To Reproduce Semiempirical Geometries. *Journal of Chemical Theory and Computation*, **2006**, 2, 1070-7 | 6.4 | 9 |
| 172 | Semiempirical Comparative Binding Energy Analysis (SE-COMBINE) of a Series of Trypsin Inhibitors. *Journal of Chemical Theory and Computation*, **2006**, 2, 383-99 | 6.4 | 29 |
| 171 | Critical assessment of quantum mechanics based energy restraints in protein crystal structure refinement. *Protein Science*, **2006**, 15, 2773-84 | 6.3 | 38 |
| 170 | Quantum mechanics in structure-based drug design. *Current Opinion in Drug Discovery & Development*, **2006**, 9, 370-9 | | 19 |

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| 169 | Validation of the binding site structure of the cellular retinol-binding protein (CRBP) by ligand NMR chemical shift perturbations. *Journal of the American Chemical Society*, **2005**, 127, 5310-1 | 16.4 | 11 |
| 168 | Pairwise decomposition of residue interaction energies using semiempirical quantum mechanical methods in studies of protein-ligand interaction. *Journal of the American Chemical Society*, **2005**, 127, 6583-94 | 16.4 | 33 |
| 167 | Effects of fluorine substitution on the edge-to-face interaction of the benzene dimer. *Journal of Physical Chemistry B*, **2005**, 109, 17752-6 | 3.4 | 44 |
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