

# Quantum Mechanical Continuum Solvation Models

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Citation Report

#	ARTICLE	IF	CITATIONS
277	Molecular Modeling of Nucleic Acid Structure: Energy and Sampling. <i>Current Protocols in Nucleic Acid Chemistry</i> , 2001, 4, Unit 7.8.	0.5	4
279	Performance of ab initio and DFT PCM methods in calculating vibrational spectra in solution: Formaldehyde in acetonitrile as a test case. <i>Chemical Physics Letters</i> , 2005, 416, 206-211.	1.2	34
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1963	THEORETICAL STUDY ON CUI-CATALYZED LIGAND-FREE $\langle \text{N} \rangle$ -ARYLATION OF IMIDAZOLE WITH BROMOBENZENE. <i>Journal of Theoretical and Computational Chemistry</i> , 2012, 11, 1135-1147.	1.8	9
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2069	Vibrational circular dichroism spectroscopy of two chiral binaphthyl diphosphine ligands and their palladium complexes in solution. <i>Dalton Transactions</i> , 2012, 41, 10817.	1.6	18
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6290	Electrochemically Induced Synthesis of Triphenylamine-based Polyhydrazones. <i>Electrochimica Acta</i> , 2017, 230, 10-21.	2.6	29
6291	Catalytic Enantioselective Synthesis of Lactams through Formal [4+2] Cycloaddition of Imines with Homophthalic Anhydride. <i>Angewandte Chemie</i> , 2017, 129, 2714-2718.	1.6	10
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7950	Solvent effect on isomerization reaction of [( <i>i</i> -5-C <sub>5</sub> H <sub>5</sub> )(CO) <sub>2</sub> Re C(C <sub>2</sub> H <sub>5</sub> )(C <sub>6</sub> H <sub>5</sub> )] carbene complex to [( <i>i</i> -5-C <sub>5</sub> H <sub>5</sub> )(CO)(COC <sub>2</sub> H <sub>5</sub> )(C <sub>6</sub> H <sub>5</sub> )] carbyne complex: A computational investigation. <i>Journal of Molecular Liquids</i> , 2018, 265, 164-171.	2.3	14
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8882	Chemical forms of molybdenum ion in nitric acid solution studied using liquid-phase X-ray absorption fine structure, Ultraviolet–Visible absorption spectroscopy and first-principles calculations. <i>Chemical Physics Letters</i> , 2019, 723, 76-81.	1.2	7



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10276	Total Synthesis of (±)-Phyllanthidine: Development and Mechanistic Evaluation of a Ring Expansion for Installation of Embedded Nitrogen-Oxygen Bonds. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 9757-9766.	7.2	25
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11114	Synthesis and Characterization of Bis[( <i>R</i> or <i>T</i> ) <sub>2</sub> ETQq1] 0.784314 rgBT /Overlock 10 Tf 50 552 Td ( <i>S</i> )- <i>N</i> -1-( <i>X</i> -C<sub>3</sub>O, <i>p</i> -Br) with Symmetry- and Distance-Dependent Vibrational Circular Dichroism Enhancement and Sign Inversion. <i>Inorganic Chemistry</i> , 2021, 60, 14116-14131.	1.9	10
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11154	A binuclear copper(II) complex based on hydrazone ligand: Characterization, molecular docking, and theoretical and antimicrobial investigation. <i>Applied Organometallic Chemistry</i> , 2022, 36, e6461.	1.7	7
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11162	Insights into Paraben Adsorption by Metal-Organic Frameworks for Analytical Applications. <i>ACS Applied Materials &amp; Interfaces</i> , 2021, 13, 45639-45650.	4.0	9
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11187	How do arenediazonium salts behave in deep eutectic solvents? A combined experimental and computational approach. <i>Journal of Molecular Liquids</i> , 2021, 339, 116743.	2.3	13
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11214	Synthesis, spectroscopic characterization, DFT calculations, and molecular docking studies of new unsymmetric bishydrazone derivatives. <i>Journal of Molecular Structure</i> , 2021, 1244, 131224.	1.8	13
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11230	Molecular structure, spectroscopy and photochemistry of alprazolam. <i>Journal of Molecular Structure</i> , 2022, 1247, 131295.	1.8	3
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12230	New Two-Photon Absorbing Squaraine Derivative with Efficient Near-Infrared Fluorescence, Superluminescence, and High Photostability. <i>Journal of Physical Chemistry B</i> , 2022, 126, 3897-3907.	1.2	5
12232	Synergistic effects of side-functionalization and aza-substitution on the charge transport and optical properties of perylene-based organic materials: a DFT study. <i>New Journal of Chemistry</i> , 2022, 46, 10402-10414.	1.4	1
12233	Why does 2-(2-aminoethylamino)ethanol have superior CO <sub>2</sub> separation performance to monoethanolamine? A computational study. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 14172-14176.	1.3	5
12234	Copper(II) and zinc(II) complexation with N-ethylene hydroxycyclams and consequences on the macrocyclic backbone configuration. <i>Dalton Transactions</i> , 0, , .	1.6	5
12235	Donor-acceptor interactions of gold(III) porphyrins with cobalt(II) phthalocyanine: chemical structure of products, their spectral characterization and DFT study. <i>Dalton Transactions</i> , 0, , .	1.6	0
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12637	Investigations on photochemical behavior of antidepressant sertraline in water by DFT/TDDFT. <i>Journal of Environmental Chemical Engineering</i> , 2022, 10, 108657.	3.3	2
12638	Sum-frequency vibrational spectroscopy of methanol at interfaces due to Fermi resonance. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 27204-27211.	1.3	3
12639	Controlling the fluorescence quantum yields of benzothiazole-difluoroborates by optimal substitution. <i>Chemical Science</i> , 2022, 13, 13347-13360.	3.7	12
12640	One pot tandem dehydrogenative cross-coupling of primary and secondary alcohols by ruthenium amido-functionalized 1,2,4-triazole derived N-heterocyclic carbene complexes. <i>RSC Advances</i> , 2022, 12, 28961-28984.	1.7	6
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12642	Unravelling structures of radicals of kynurenic acid formed in the photoinduced reactions with tryptophan and N-acetyl tyrosine. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 27558-27565.	1.3	2

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12644	Formation and evolution of C-C, C-O, C=O and C-N bonds in chemical reactions of prebiotic interest. <i>RSC Advances</i> , 2022, 12, 28804-28817.	1.7	1
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12677	Synthesis and AIE properties of benzene fused cyclooctatrathiophenes. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2023, 436, 114362.	2.0	3
12678	Predicting Solvent Effects on $S_N2$ Reaction Rates: Comparison of QM/MM, Implicit, and MM Explicit Solvent Models. <i>Journal of Physical Chemistry B</i> , 2022, 126, 9047-9058.	1.2	9

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