## A smooth particle mesh Ewald method

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**Citation Report** 

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5091 5092 5093 5094	Mechanism of Glutathione Transferase P1-1-Catalyzed Activation of the Prodrug Canfosfamide (TLK286,) Tj ETQq1         Using Multistate Reweighting to Rapidly and Efficiently Explore Molecular Simulation Parameters         Space for Nonbonded Interactions. Journal of Chemical Theory and Computation, 2013, 9, 4700-4717.         Porting ONETEP to graphical processing unitâ&based coprocessors. 1. FFT box operations. Journal of Computational Chemistry, 2013, 34, 2446-2459.         Comparative Computer Simulation Study of Cholesterol in Hydrated Unary and Binary Lipid Bilayers and in an Anhydrous Crystal. Journal of Physical Chemistry B, 2013, 117, 8758-8769.         Insight into î±-Synuclein Plasticity and Misfolding from Differential Micelle Binding. Journal of Physical Chemistry B, 2013, 117, 11448-11459.	1.0.7843 2.3 1.5 1.2 1.2	14 14 18 23 12
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<ul> <li>5091</li> <li>5092</li> <li>5093</li> <li>5094</li> <li>5095</li> <li>5096</li> <li>5097</li> <li>5098</li> </ul>	Mechanism of Glutathione Transferase P1-1-Catalyzed Activation of the Prodrug Canfosfamide (TLK286,) Tj ETQq1         Using Multistate Reweighting to Rapidly and Efficiently Explore Molecular Simulation Parameters         Space for Nonbonded Interactions. Journal of Chemical Theory and Computation, 2013, 9, 4700-4717.         Porting ONETEP to graphical processing unitâ€based coprocessors. 1. FFT box operations. Journal of         Computational Chemistry, 2013, 34, 2446-2459.         Comparative Computer Simulation Study of Cholesterol in Hydrated Unary and Binary Lipid Bilayers         and in an Anhydrous Crystal. Journal of Physical Chemistry B, 2013, 117, 8758-8769.         Insight into î±-Synuclein Plasticity and Misfolding from Differential Micelle Binding. Journal of Physical         Chemistry B, 2013, 117, 11448-11459.         Cationă <sup>-*</sup> ΀ Interactions As Lipid-Specific Anchors for Phosphatidylinositol-Specific Phospholipase C.         Journal of the American Chemical Society, 2013, 135, 5740-5750.         Toward Understanding the Outer Membrane Uptake of Small Molecules by Pseudomonas aeruginosa.         Molecular Dynamics Study of Oxidized Lipid Bilayers in NaCl Solution. Journal of Physical Chemistry B, 2013, 117, 8490-8501.	2.3 2.3 1.5 1.2 1.2 6.6 1.6 1.2	3129 rgBT / O 14 18 23 12 62 51 47

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111168 111169 111170 111171 111172 111173	De novo design of potent and selective mimics of IL-2 and IL-15. Nature, 2019, 565, 186-191.         Insight into the roles of two typical ion clusters and their second hydration shells: Implication for the nucleation mechanism in MgSO4 aqueous solution. Journal of Molecular Liquids, 2019, 278, 33-42.         Development of Polarizable Gaussian Model for Molecular Mechanical Calculations I: Atomic Polarizability Parameterization To Reproduce <i>ab Initio</i> Anisotropy. Journal of Chemical Theory and Computation, 2019, 15, 1146-1158.         EncoderMap: Dimensionality Reduction and Generation of Molecule Conformations. Journal of Chemical Theory and Computation, 2019, 15, 1209-1215.         Effect of Additives on Surfactant Micelle Shape Transformation: Rheology and Molecular Dynamics Studies. Journal of Physical Chemistry C, 2019, 123, 2922-2932.         Computational insights into the different catalytic activities of <scp>CYP</scp> 3A4 and <scp>CYP</scp> 3A5 toward <i>schisantherin E</i>	<ol> <li>13.7</li> <li>2.3</li> <li>2.3</li> <li>2.3</li> <li>1.5</li> <li>1.5</li> </ol>	<ul> <li>362</li> <li>12</li> <li>26</li> <li>72</li> <li>18</li> <li>9</li> </ul>
<ul> <li>11168</li> <li>11169</li> <li>11170</li> <li>11171</li> <li>11172</li> <li>11173</li> <li>11174</li> </ul>	De novo design of potent and selective mimics of IL-2 and IL-15. Nature, 2019, 565, 186-191.         Insight into the roles of two typical ion clusters and their second hydration shells: Implication for the nucleation mechanism in MgSO4 aqueous solution. Journal of Molecular Liquids, 2019, 278, 33-42.         Development of Polarizable Gaussian Model for Molecular Mechanical Calculations I: Atomic Polarizability Parameterization To Reproduce <i>&gt; ab Initio</i> > Anisotropy. Journal of Chemical Theory and Computation, 2019, 15, 1146-1158.         EncoderMap: Dimensionality Reduction and Generation of Molecule Conformations. Journal of Chemical Theory and Computation, 2019, 15, 1209-1215.         Effect of Additives on Surfactant Micelle Shape Transformation: Rheology and Molecular Dynamics Studies. Journal of Physical Chemistry C, 2019, 123, 2922-2932.         Computational insights into the different catalytic activities of <scp>CYP</scp> 3A4 and <scp>CYP</scp> 3A5 toward <i>schisantherin E</i> . Chemical Biology and Drug Design, 2019, 93, 854-864.         Molecular dynamics study of the molecular mobilities and side-chain terminal affinities of 2-methoxyethyl acrylate and 2-hydroxyethyl methacrylate. Polymer Journal, 2019, 51, 365-370.	<ol> <li>13.7</li> <li>2.3</li> <li>2.3</li> <li>1.5</li> <li>1.5</li> <li>1.3</li> </ol>	<ul> <li>362</li> <li>12</li> <li>26</li> <li>72</li> <li>18</li> <li>9</li> <li>8</li> </ul>
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11764 11765 11766 11767 11768	Structural Basis for GTP versus ATP Selectivity in the NMP Kinase AK3. Biochemistry, 2020, 59, 3570-3581.         Alchemical Binding Free Energy Calculations in AMBER20: Advances and Best Practices for Drug Discovery. Journal of Chemical Information and Modeling, 2020, 60, 5595-5623.         Transmembrane potential of physiologically relevant model membranes: Effects of membrane asymmetry. Journal of Chemical Physics, 2020, 153, 105103.         Morphing of Amphipathic Helices to Explore the Activity and Selectivity of Membranolytic Antimicrobial Peptides. Biochemistry, 2020, 59, 3772-3781.         Computational Insights into the Binding of Monolayer-Capped Gold Nanoparticles onto Amyloid-β Fibrils. ACS Chemical Neuroscience, 2020, 11, 3153-3160.         Drug repurposing for schistosomiasis: molecular docking and dynamics investigations. Journal of Biomolecular Structure and Dynamics, 2022, 40, 995-1009.	<ol> <li>1.2</li> <li>2.5</li> <li>1.2</li> <li>1.2</li> <li>1.2</li> <li>2.0</li> </ol>	<ul> <li>6</li> <li>177</li> <li>5</li> <li>4</li> <li>22</li> <li>3</li> </ul>
<ol> <li>11764</li> <li>11765</li> <li>11766</li> <li>11767</li> <li>11768</li> <li>11769</li> <li>11770</li> </ol>	Structural Basis for CTP versus ATP Selectivity in the NMP Kinase AK3. Biochemistry, 2020, 59, 3570-3581.         Alchemical Binding Free Energy Calculations in AMBER20: Advances and Best Practices for Drug Discovery. Journal of Chemical Information and Modeling, 2020, 60, 5595-5623.         Transmembrane potential of physiologically relevant model membranes: Effects of membrane asymmetry. Journal of Chemical Physics, 2020, 153, 105103.         Morphing of Amphipathic Helices to Explore the Activity and Selectivity of Membranolytic Antimicrobial Peptides. Biochemistry, 2020, 59, 3772-3781.         Computational Insights into the Binding of Monolayer-Capped Gold Nanoparticles onto Amyloid-Î <sup>2</sup> Fibrilis. ACS Chemical Neuroscience, 2020, 11, 3153-3160.         Drug repurposing for schistosomiasis: molecular docking and dynamics investigations. Journal of Biomolecular Structure and Dynamics, 2022, 40, 995-1009.         Methylation of EZH2 by PRMT1 regulates its stability and promotes breast cancer metastasis. Cell Death and Differentiation, 2020, 27, 3226-3242.	1.2 2.5 1.2 1.2 1.7 2.0	6 177 5 4 22 3
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13499	VPg Đ²Đ,руÑа PVY Đ, ĐºÑĐ;-ÑĐ²ÑĐ·Ñ‹Đ²Đ°ŇŽÑ‰Đ,е Ñ"Đ°ĐºÑ,Đ¾Ñ€Ñ‹ ÑĐµĐ¼ĐµĐ¹ŇŇ,Đ²Đ° elF4E ĐºĐ	⁰ <b>õl€</b> Ñ,Đ¾	Ñĵ,елÑ
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