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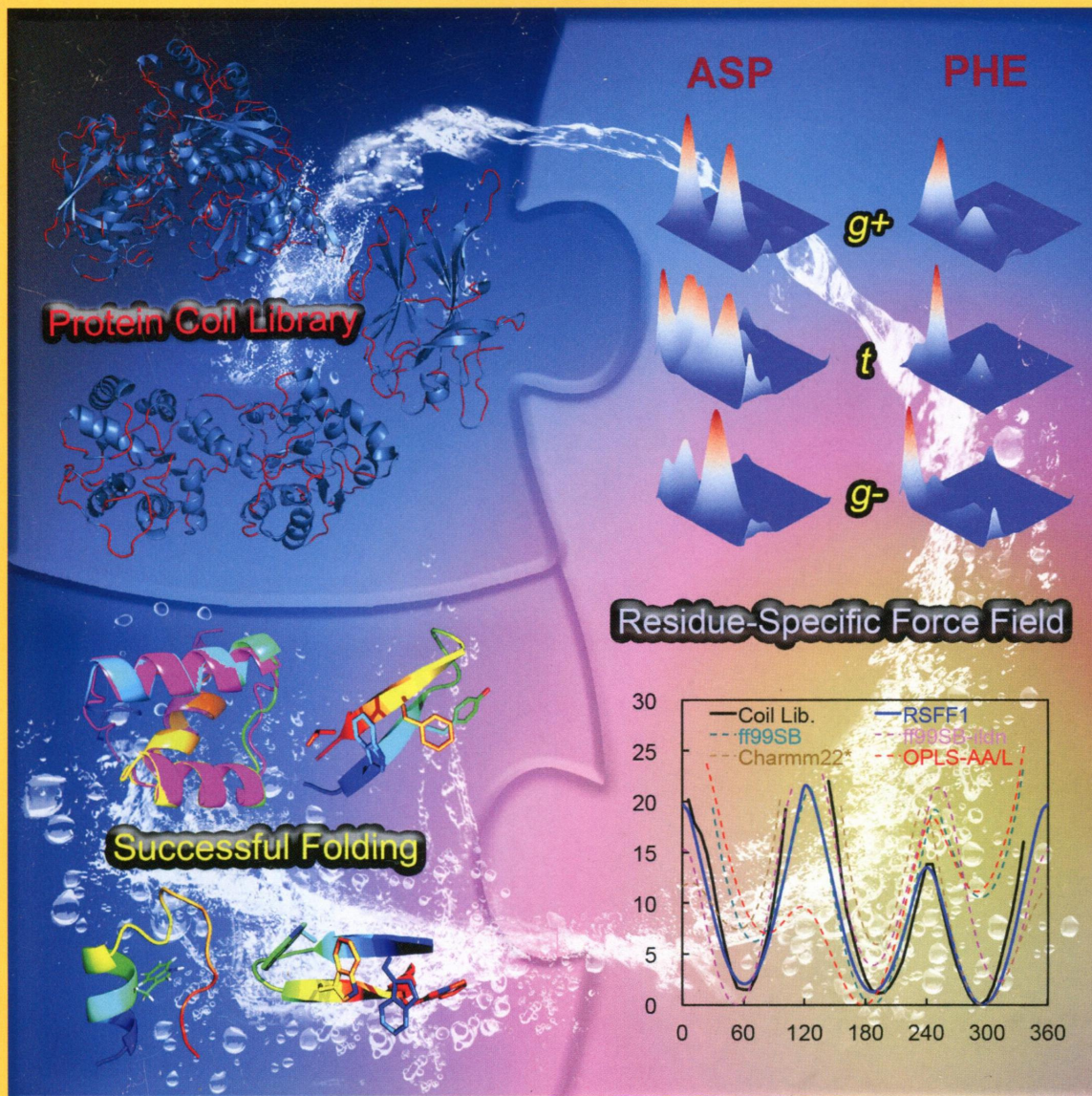
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B



Residue-Specific
Force Field Based on
Protein Coil Library
Potentials: RSFF1
(see page 6983)

BIOPHYSICAL CHEMISTRY, BIOMATERIALS, LIQUIDS, AND SOFT MATTER



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ON THE COVER: Residue-specific force field based on protein coil library potentials: RSFF1. The backbone and side-chain conformational features of the 20 amino acid residues from the coil regions of protein structures are incorporated into a new force field, RSFF1, using residue-specific parameters. The RSFF1 reproduces well the structural features of peptides and proteins. See page 6983.

Feature Article

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dx.doi.org/10.1021/jp5017449

Residue-Specific Force Field Based on the Protein Coil Library. RSFF1: Modification of OPLS-AA/L

Fan Jiang,* Chen-Yang Zhou, and Yun-Dong Wu*

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dx.doi.org/10.1021/jp412533b

Surface Adsorption and Bulk Aggregation of Cyclodextrins by Computational Molecular Dynamics Simulations as a Function of Temperature: α -CD vs β -CD

Edgar Mixcoha, José Campos-Terán, and Ángel Piñeiro*

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dx.doi.org/10.1021/jp501234p

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Debabrata Dey, Santosh Kumar, Rakesh Banerjee, Souvik Maiti, and Dibakar Dhara*

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dx.doi.org/10.1021/jp5022246

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dx.doi.org/10.1021/jp5030125

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dx.doi.org/10.1021/jp5031202

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Rong Zhang, Yuezhen Bin, Enyuan Dong, and Masaru Matsuo*

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[dx.doi.org/10.1021/jp503355h](https://doi.org/10.1021/jp503355h)

The Broken Ring: Reduced Aromaticity in Lys-Trp Cations and High pH Tautomer Correlates with Lower Quantum Yield and Shorter Lifetimes

Azaria Solomon Eisenberg and Laura J. Juszcak*

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[dx.doi.org/10.1021/jp503381r](https://doi.org/10.1021/jp503381r)

Lipid-Modified Polyethylenimine-Mediated DNA Attraction Evaluated by Molecular Dynamics Simulations

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[dx.doi.org/10.1021/jp503471j](https://doi.org/10.1021/jp503471j)

Ketoxime Coupling of *p*-Acetylphenylalanine at Neutral pH for Site-Directed Spin Labeling of Human Sulfite Oxidase

Aaron Hahn, Stefan Reschke, Silke Leimkühler, and Thomas Risse*

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[dx.doi.org/10.1021/jp503691n](https://doi.org/10.1021/jp503691n)

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Alexander D. Milov, Rimma I. Samoilova, Yuri D. Tsvetkov,* Cristina Peggion, Fernando Formaggio, and Claudio Toniolo

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[dx.doi.org/10.1021/jp503963z](https://doi.org/10.1021/jp503963z)

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