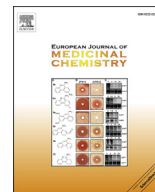




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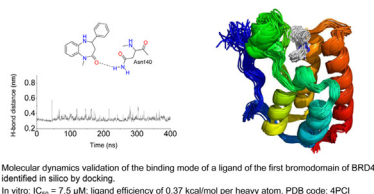
Molecular Dynamics: New Advances in Drug Discovery

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Molecular dynamics in drug design

Hongtao Zhao and Amedeo Caflisch*

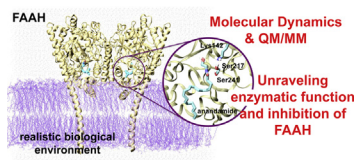
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Computational insights into function and inhibition of fatty acid amide hydrolase

Giulia Palermo, Ursula Rothlisberger, Andrea Cavalli and Marco De Vivo*

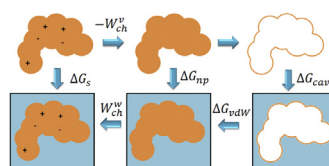
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Implicit solvent methods for free energy estimation

Sergio Decherchi, Matteo Masetti, Ivan Vyalov and Walter Rocchia*

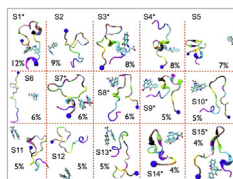
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Molecular structure of the NQTrp inhibitor with the Alzheimer Aβ1-28 monomer

Bogdan Tarus, Phuong H. Nguyen, Olivia Berthoumieu, Peter Faller, Andrew J. Doig and Philippe Derreumaux*

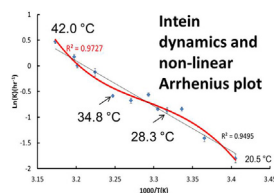
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Dynamics differentiate between active and inactive inteins

Melissa Cronin, Michael J. Coolbaugh, David Nellis, Jianwei Zhu, David W. Wood, Ruth Nussinov and Buyong Ma*

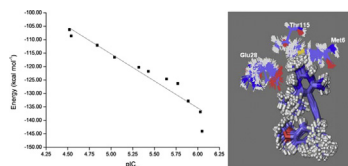
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Molecular modeling toward selective inhibitors of dihydrofolate reductase from the biological warfare agent *Bacillus anthracis*

Juliana O.S. Giacoppo, Daiana T. Mancini, Ana P. Guimarães, Arlan S. Gonçalves, Elaine F.F. da Cunha, Tanos C.C. França and Teodorico C. Ramalho*

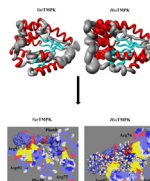
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Design of inhibitors of thymidylate kinase from *Variola virus* as new selective drugs against smallpox

Ana P. Guimarães, Felipe R. de Souza, Aline A. Oliveira, Arlan S. Gonçalves, Ricardo B. de Alencastro, Teodorico C. Ramalho and Tanos C.C. França*

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