

Approaching Free Energy

Oliver Caldwell Ralston



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Guided Ligand and Drug Design Andrew M Davis and Simon J Teague and Gerard J Kleywegt 5 Dealing with Bound Waters in a Site Do they Leave or Stay Donald Hamelberg and J Andrew McCammon 6 Knowledge Based Methods in Structure Based Design Marcel L Verdonk and Wijnand T M Mooij 7 Combating Drug Resistance Identifying Resilient Molecular Targets and Robust Drugs Celia A Schiffer 8 Docking Algorithms and Scoring Functions State of the Art and Current Limitations Gregory L Warren and Catherine E Peishoff and Martha S Head 9 Application of Docking Methods to Structure Based Drug Design Demetri T Moustakas 10 Strength in Flexibility Modeling Side Chain Conformational Change in Docking and Screening Leslie A Kuhn 11 Avoiding the Rigid Receptor Side Chain Rotamers Amy C Anderson 12 Computational Prediction of Aqueous Solubility Oral Bioavailability P450 Activity and hERG Channel Blockade David E Clark 13 Shadows on Screens Brian K Shoichet and Brian Y Feng and Kristin E D Coan 14 Iterative Docking Strategies for Virtual Ligand Screening Albert E Beuscher IV and Arthur J Olson 15 Challenges and Progresses in Calculations of Binding Free Energies What Does it Take to Quantify Electrostatic Contributions to Protein Ligand Interactions Mitsunori Kato and Sonja Braun Sand and Arieh Warshel 16 Discovery and Extrapolation of Fragment Structures towards Drug Design Alessio Ciulli and Tom L Blundell and Chris Abell 17 A Link Means a Lot Disulfide Tethering in Structure Based Drug Design Jeanne A Hardy 18 The Impact of Protein Kinase Structures on Drug Discovery Chao Zhang and Sung Hou Kim

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Proceedings of the Section of Sciences Koninklijke Nederlandse Akademie van Wetenschappen. Afdeling Natuurkunde, 1914

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