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P2803 Modeling of Protein-Ligand Complexes Taking into Account the Induced Fit: Conformational and Positional Refinements Using Brownian Dynamics

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P2817 De novo peptide sequencing used by amino acid binding affinity for tandem mass spectrometry

<u>Mitsuhiro KANAZAWA</u>¹, Atsushi OGIWARA², Unpei NAGASHIMA¹ (Department of Chemistry, Graduate School of Pure and Applied Sciences, University of Tsukuba¹, Medical ProteoScope, Co. Ltd.²)

P2933 Implementation of MP2-correlation engine into ABINIT-MP/FMO program and emonstrative applications

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P2813 Development of the Total System ToMoCo for Molecular Design

<u>Masamoto ARAKAWA</u>¹, Soichiro MIZOBUCHI², Kimito FUNATSU¹ (The University of Tokyo¹, Toyohashi University of Technology²)

P2819 A Data-mining system for discovering drug-target proteins

Motoi TOBITA, Masashi NEMOTO, Ken HORIUCHI, Hiroyasu SHIMADA, and Tetsuo NISHIKAWA

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P2903 STUDY ON A BINDING AFFINITY DIFFERENCE BETWEEN CHITINASE-ARGADIN AND CHITINASE-ARGIFIN COMPLEXES USING MOLECULAR DYNAMICS SIMULATION

<u>Yuichi YANAI</u>¹, Hiroaki GOUDA¹, Shuichi HIRONO¹ (School of Pharmaceutical Sciences, Kitasato University¹)

P2906 Molecular Dynamics Simulations of liganded and unliganded proteins

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P2909 BioStation Dock: Application of protein-ligand docking to screen compounds (2)

<u>Toshiyuki SATO</u>¹, Kaori FUKUZAWA¹, Kozo AOKI³, Katsuki AMEMIYA², Kazuo KOYANO², Shinji AMARI³, Souichirou TANIMORI², and Tatsuya NAKANO⁴ (Fuji Research Institute Corporation¹, AdvanceSoft Corporation², University of Tokyo³, and National Institute of Health Sciences⁴)

P2926 QSAR Analysis of Human Placental Drug Transport

<u>Yuki HIBINO</u>, Takashi FUJIWARA, Shinichi KOBAYASHI, Kumiko SAKAMOTO, Masaru KIHARA, Aiko YAMAUCHI, Hiroshi CHUMAN (Graduate School of Pharmaceutical Sciences, The University of Tokushima)