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最優秀賞

201 SOLUTION STRUCTURE OF CHITINASE-ARGIFIN COMPLEX STUDIED BY MOLECULAR DYNAMICS

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111 BioStation Dock: Application of protein-ligand docking to screen

Toshiyuki Sato^{1,2}, Ikuo Okouchi^{1,2}, Kaori Fukuzawa^{1,2}, Kozo Aoki³, Kazuo Koyano¹, Shinji Amari³, Katsuki Amemiya¹, and Tatsuya Nakano⁴
(AdvanceSoft Corporation¹, Fuji Research Institute Corporation², University of Tokyo³, and National Institute of Health Sciences⁴)

110 Interaction analysis for SARS virus proteinase and its ligands with ab initio FMO method

Shinji Amari¹, Mayuko Takeda-Shitaka², Mitsuo Iwadate², Norio Yamamoto³, Nobutaka Fujii⁴, Naoki Yamamoto³, Hideaki Umeyama², Tatsuya Nakano⁵
(University of Tokyo¹, Kitasato University², Tokyo Medical and Dental University³, Kyoto University⁴, National Institute of Health Sciences⁵)

324 Analysis of transmembrane segment for membrane protein discrimination

Toshiyuki Tsuji¹, Shigeki Mitaku¹
(Division of Applied Physics Graduate School of Engineering Nagoya University¹)

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117 MD simulation of asymmetric phospholipid bilayers (POPC/POPE-POPS) with the physiological concentration of ions and cholesterols
Kenichi Mori, Masayuki Hata, Saburo Neya, Tyuji Hoshino
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204 Generation of a novel equation for logP estimation using a neural network

Sumie Tajima¹, Kenji Yamagishi², Makoto Haraguchi¹, Umpei Nagashima³
(Bestsystems Inc.¹, Rikkyo University², Grid Technology Research Center³)

311 Analysis of Similar Structural Protein with Low Sequence Identity by Coarse-Grained Charge Distribution in Sequence

Kenichiro Imai, Shigeki Mitaku
(Division of Applied Physics Graduate School of Engineering Nagoya University)

419 Automatic generation of cell-wide pathway model from complete genome

Kazuharu Arakawa^{1,2}, Yohei Yamada^{1,3}, Hiromi Komai^{1,3}, Kosaku Shinoda^{1,4}, Yoichi Nakayama^{1,3}, Masaru Tomita^{1,3}
(Institute for Advanced Biosciences, Keio University¹, Bioinformatics Program, Graduate School of Media and Governance², Department of Environmental Information³, Department of Policy Management⁴)

- 502** **Analysis and Prediction of Drug Excretion into Human Breast Milk (2nd)
- Additional Analysis Including Hydrophilic Compounds -**
Takashi Fujiwara, Yuki Hibino, Masaru Kihara, Aiko Yamauchi, Hiroshi Chuman
(Graduate School of Pharmaceutical Sciences, The University of Tokushima)
- 606** **An Electrophysiological Simulation Model of the Myocardial Cell Using E-
CELL System**
Sayaka Ishinabe^{1,2}, Yasuhiro Naito^{1,3}, Motohiro Yoneda^{1,2}, Katsuya Kawai^{1,2}, Shoko
Miyamoto^{1,2}, Shinobu Kuratomi⁴, Nobuaki Sarai⁴, Satoru Matsuoka⁴, Akinori Noma⁴, Masaru
(Institute for Advanced Biosciences, Keio University¹, Graduate School of Media and
Governance, Keio University², Department of Environmental Information, Keio University³,
Department of Physiology and Biophysics, Graduate School of Medicine, Kyoto University⁴)
- 710** **Development of a molecular memory system based on hairpin DNA**
Masahiro Takinoue¹, Akira Suyama^{1,2}
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