as the experimental. Potential energy map of the phase transition between form I and II is also evaluated to demonstrate the dynamical behaviors of aspirin polymorph. It is indicated that activation energy required for the polymorphic transition is small enough to be able to overcome the energy barrier at room temperature.


Keywords: drug polymorphism, crystal structure analysis, phase transitions

P03.04.14


**Effects of initial conformations of small ligands on computational docking accuracies**

Akitumi Oda1, Ohgi Takashahi1, Noriyuki Yamaotsu2, Shuichi Hirino1

1Tohoku Pharmaceutical University, 4-4-1, Komatsushima, Aoba-ku, Sendai, Miyagi, 981-8558, Japan, 2Kitasato University, 5-9-1, Sirokane, Minato-ku, Tokyo, 108-8641, Japan, E-mail: oda@tohoku-pharm.ac.jp

Computational ligand docking is one of the most important techniques of Structure-Based Drug Design, which makes the most of 3D-structures of drug target proteins determined by experimental studies, such as NMR or crystallographic analyses for the drug discovery and development. In this study, the effects of initial conformations of ligands on computational docking were investigated, and appropriate settings of conditions for computational docking were determined. Five types of initial conformations were prepared, and docking calculations were carried out by using each conformation as inputs. Furthermore, several settings of docking parameters were used (default, accurate, high throughput, etc.), and robust settings for various initial structures were investigated. GOLD and eHiTS were used as docking software, and structurally known protein-ligand complexes were used as test set. Root mean square deviations between computational and experimental structures (RMSD) were adopted for criteria for evaluations, and the docking pose with RMSD < 2.0 Å were defined as “reasonable poses”.

When at least one of the generated poses by a docking trial was reasonable, the trial was defined as “success”, and when the top ranked pose, i.e. the pose with the lowest binding energy, was reasonable, the trial was defined as “top pose success”. The search abilities of docking were evaluated by “success rate” and “top pose success rate”. As the results, bad initial conformations, which were much different from crystal ligand structures, cause the worst success rate and the worst top pose success rate in all initial conformations. Comparing GOLD and eHiTS, eHiTS was better than GOLD to obtain reasonable poses regardless of rankings, but GOLD was better to obtain reasonable top poses.

Keywords: trypanosoma cruzi, energy metabolism, fumarate reductase, dihydroorototate dehydrogenase, drug design, parasite

P03.05.16


**First principles study of composition fluctuation and residual strain in InGaN/GaN MQW**

Kiichiro Mukose, Noriyuki Uehara, Akihiko Sakamoto, Yu Yoshioka, Masatoshi Sano

Tokyo University of Science, Faculty of Engineering, 1-3 Kagurazaka, Shinjuku-ku, Tokyo, 162-8601, Japan, E-mail: mukose@ee.kagu.tus.ac.jp

The quantitative relations between mechanical properties and the composition fluctuation in InGaN films are studied theoretically. In the ternary alloy InGaN, the indium composition has been known to show spatial inhomogeneity in various growth conditions. This composition fluctuation has been considered to form the quantum disk structures in InGaN quantum wells those influence the spontaneous emission rate in light emitting devices. To investigate the mechanical properties of the structures theoretically, a new method based on first principles calculation was used in this study. The simulation models of InGaN films contain triangular pillar-shaped cells, where the composition ratio, the strain and the stress in the each cell follow an equation of state which has been determined by ab initio electronic structure calculations. The quantitative