

CSP: Paracetamol via Grid Search & PSO

Milan Kočí

FSNPE, Czech Technical University in Prague, Prague, Czech Republic;

kocimil1@fffi.cvut.cz

The greatest usage of paracetamol is in the pharmaceutical industry. Paracetamol shows a considerable tendency to polymorphism and the aim of this work was to predict the crystal structure of its most stable polymorph. We achieved the goal by generating a large number of structures by Grid Search and subsequent reducing of the number of structures using the global optimization algorithm Particle Swarm Optimization.

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