

# 對結晶科學研究者的應用實例

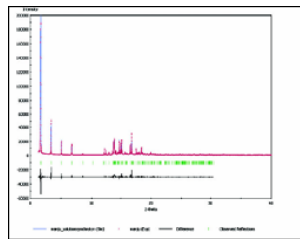
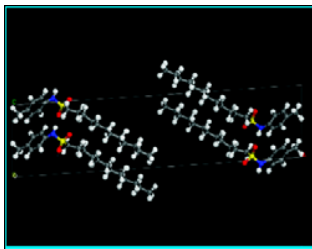
## Kodak 公司的 N-(p-Tolyl) -dodecylsulfonamide 的結晶構造的決定

Scientists at Kodak have successfully solved the crystal structure of N-(p-tolyl)-dodecylsulfonamide directly from powder diffraction data using Reflex Plus. Elucidation of the crystal structure from powder XRD data followed a systematic approach:

- Unit cell indexing using DICVOL91
  - Space group determination based on systematic absences and density considerations.
  - Pawley refinement.
  - Simulated annealing using PowderSolve (Reflex Plus)
  - Checking and connecting any close atom contacts using CVFF force field.
  - Final structure refinement using the Rietveld method
- Validation of the obtained structure was carried out by verifying that the solution was close to a minimum in energy.

*Crystal structure determination of N-(p-Tolyl)-Dodecylsulfonamide at Kodak*

*Reference:* M. Rajeswaran, T. N. Ianton, N. Zumbulyadis, D. I. Giesen, C. Conessa-Moratilla, S. T. Mistute, P. W. Stephens and A. Jaq, *J. Am. Chem. Soc.* 2002, 124, 14450-14459.



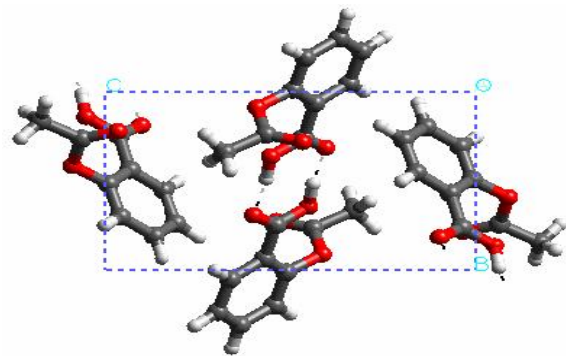
## 阿斯匹林的潛在多形

Scientists have used Polymorph Predictor to examine the potential for additional polymorphs of Aspirin.

Polymorph Predictor was successful in predicting the known crystal structure of aspirin, which contains a nonplanar conformer. Additional low-energy structures were also predicted that contained a planar conformer. While semiempirical and ab initio calculations indicated that the planar conformation is less stable than the nonplanar conformation, force field calculations suggested that the planar conformation is more stable. Several researchers proposed that additional polymorphs of aspirin might be found if experimental crystallization conditions could be developed that would stabilize the planar conformation. Such ideas will help researchers in their attempts to find additional experimental form of aspirin.

*Potential polymorphs of Aspirin*

*Reference:* R.S. Payne, R.C. Rowe, R.J. Roberts, M.H. Charlton, R. Docherty, *J. Comp. Chem.*, 1999, 20, 262-273



## 利用自我組合之硬性硫烴金膜所做的胺基酸結晶化控制-分子模型之研究

MS Modeling has been used to understand the self-assembled monolayers (SAMs) of rigid thiols on gold as heterogeneous nucleants to study the effects of interfacial molecular interaction on the nucleation and growth of L-alanine and DL-valanine crystals. Morphology for each amino acids was predicted using Morphology module. Faces that were slow growing had the greatest morphological importance, and hence were chosen for binding energy calculations by docking these dominant faces on various SAMs through molecular minimization and molecular dynamics simulation. The simulated binding energies between SAMs and the particular amino acid crystal faces were in good agreement with the observed nucleation planes of the amino acids, and could provide some insight into how crystal surfaces interact with the monolayer films and which faces will preferentially nucleate.

*Control of the crystallization of Amino Acids using self-assembled monolayers of rigid thiols on Gold – a Molecular modeling study.*

*Reference:* A. Y. Lee, A. Ulman, A.S. Myerson, *Langmuir*, 2002, 18, 5886-5898.

