Solvates of an antifungal drug, griseofulvin: Structural, thermochemical and conformational analysis

Srinivasulu Aitipamula,*[,a] Pui Shan Chow,[a] and Reginald B.H. Tan*[,a,b]

[a]*Institute of Chemical and Engineering Sciences, A*STAR (Agency for Science, Technology and Research), 1, Pesek Road, Jurong Island, Singapore, 627833. Tel: (65) 6796 3858, Fax: (65) 6316 6183.*

Email: srinivasulu_aitipamula@ices.a-star.edu.sg

[b]*Department of Chemical & Biomolecular Engineering, National University of Singapore, 4 Engineering Drive 4, Singapore 117576.*

Email: reginald_tan@ices.a-star.edu.sg

Electronic Supplementary Information

(5 Pages)

Contents

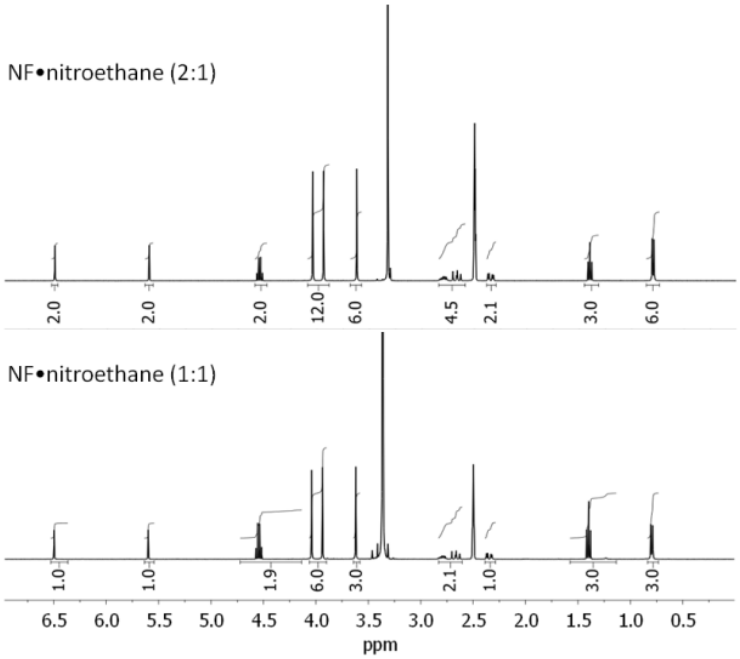

Fig. S1 Comparison of the ^{1}H NMR (in DMSO-d_6) spectra of the 2:1 and 1:1 solvates of GF•nitroethane. Notice the peak integration for peaks corresponding to nitroethane at 1.35 and 4.65 ppm.

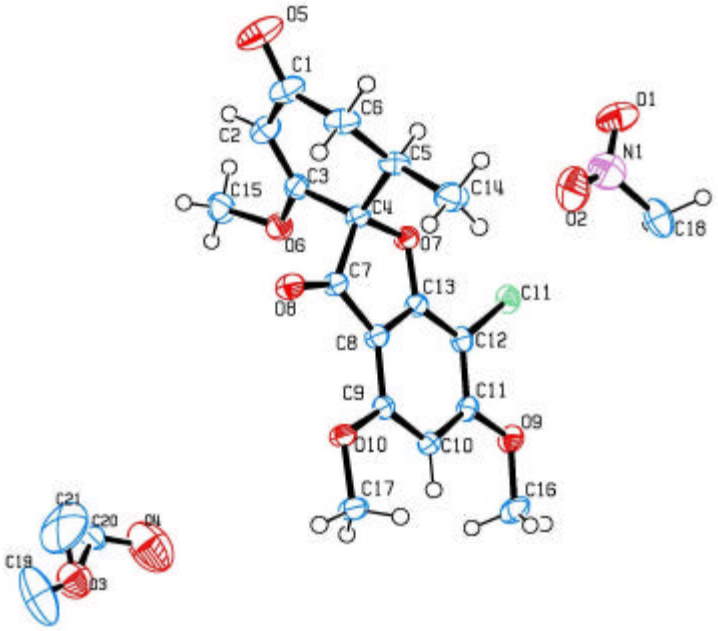

Fig. S2 An ORTEP plot of the asymmetric unit of the crystal structure of GF•nitroethane (1:1). Notice that the nitroethane molecule is disordered and could not be modelled accurately.

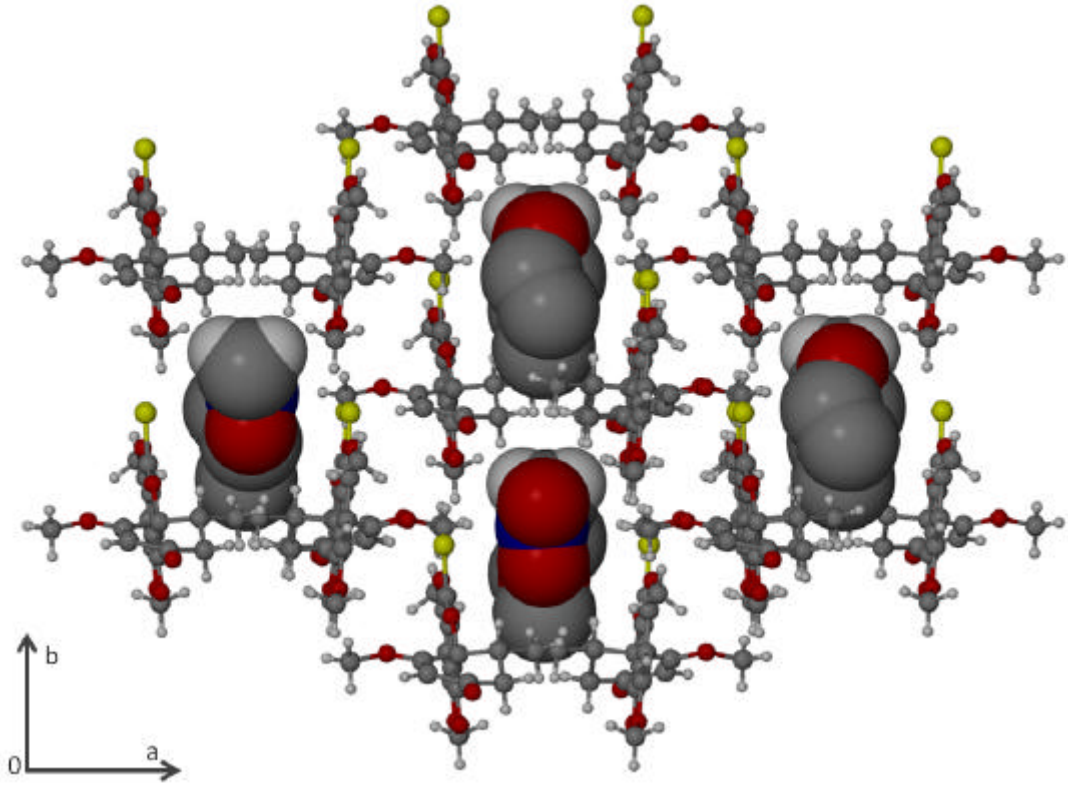

Fig. S3 Crystal structure of the GF•nitroethane (1:1) showing the disordered nitroethane molecules located in the channels formed by the GF molecules.

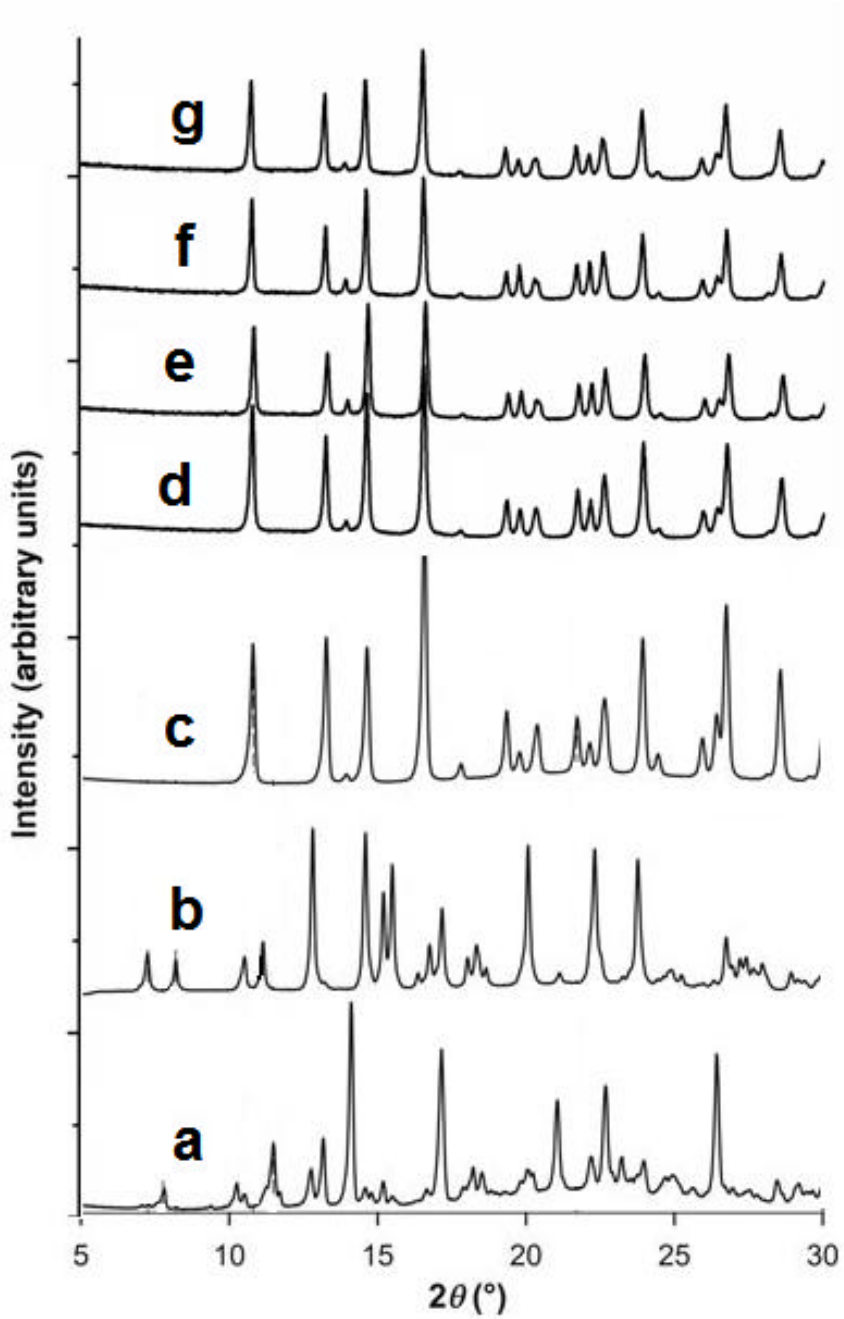

Fig. S4 Comparison of the PXRD patterns of the polymorphs of GF with samples obtained in the desolvation experiments: (a) Form III, (b) Form II, (c) Form I, (d) desolvation product of GF•acetonitrile, (e) desolvation product of GF•nitromethane, (f) desolvation product of GF•nitroethane (2:1), and (g) desolvation product of GF•nitroethane (1:1).

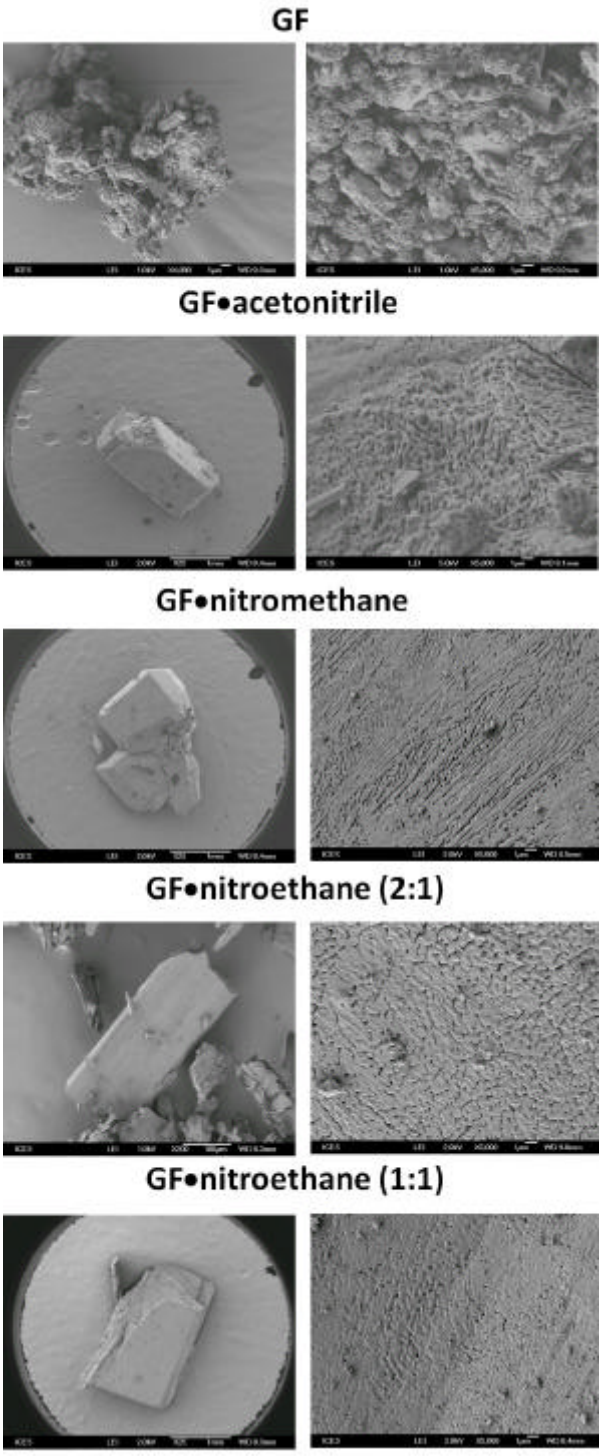

Fig. S5 SEM images of the GF and desolvation products of GF solvates.