

Tailored Supramolecular Gels for Isoniazid Crystallization – is Isoniazid Really Monomorphic?

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Supplementary Information

| Solvent | Initial | 30 mins | 1 hour | 1 day | 1 week |
|------------------|---------|---------|--------|-------|--------|
| 1,4-dioxane* | PG | G | G | CG | CG |
| 1-butanol* | G | G | G | G | G |
| 1-pentanol* | G | G | G | G | G |
| 1-propanol* | G | G | G | G | G |
| 2-butanol* | G | G | G | G | G |
| 2-ethylpyridine* | G | G | G | G | G |
| 2-picoline* | G | G | G | G | G |
| 2-propanol* | G | G | G | G | G |
| 3-picoline | G | G | G | G | G |
| 4-ethylpyridine | G | G | G | G | G |
| 4-picoline | G | G | G | G | G |
| Acetic acid | G | G | G | G | G |
| Cyclohexanone | G | G | G | G | G |
| Cyclopentanone | G | G | G | G | G |
| DMA | S | S | S | S | G |
| DMF | G | G | G | G | G |
| Ethanol* | G | G | G | G | G |
| Methanol* | G | G | G | G | G |
| Nitrobenzene | G | G | G | G | G |
| Pyridine | G | G | G | G | G |

Table S1. Gelation behaviour of **1** showing tests resulting in gelation (total 51 solvents examined). Key: G is gel, PG is partial gel, CG is collapsed gel and S is solution. The use of * highlight the samples in which the gels are opaque.

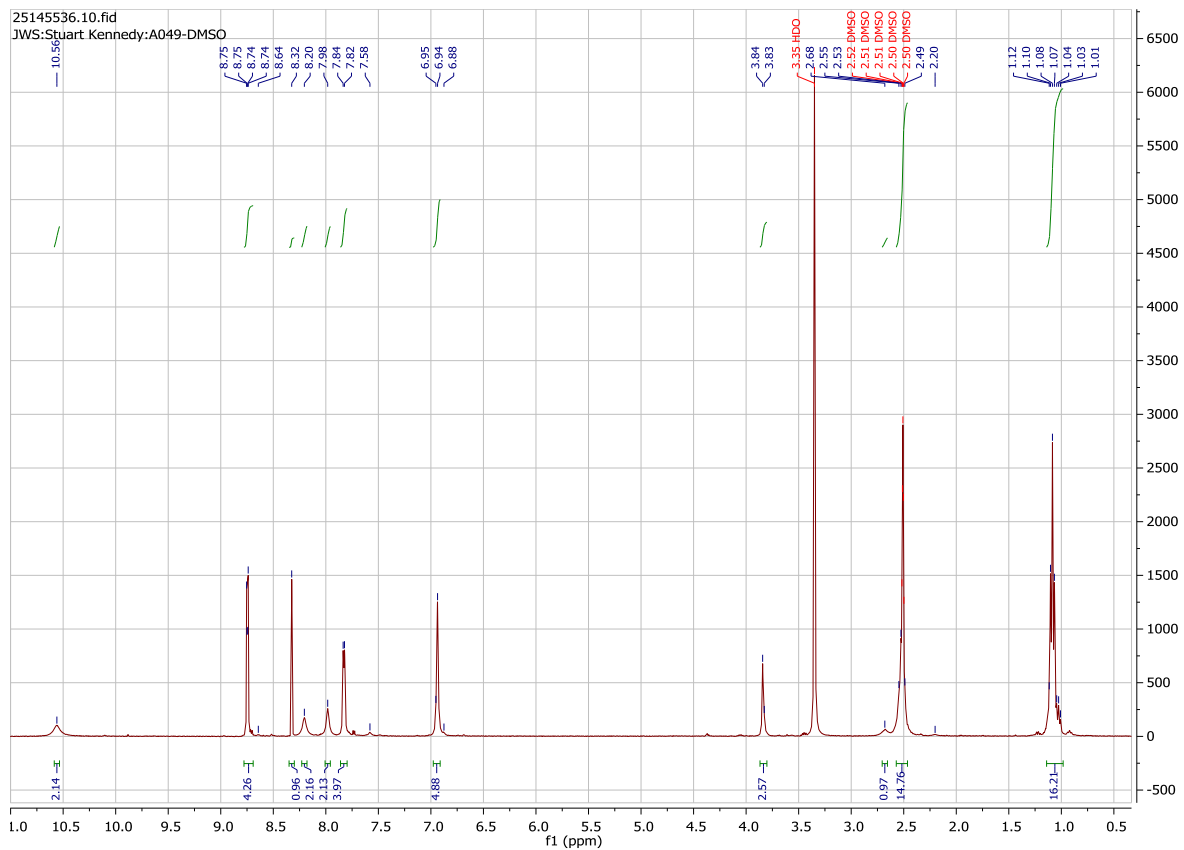


Figure S1 ^1H NMR spectrum of **1** in DMSO

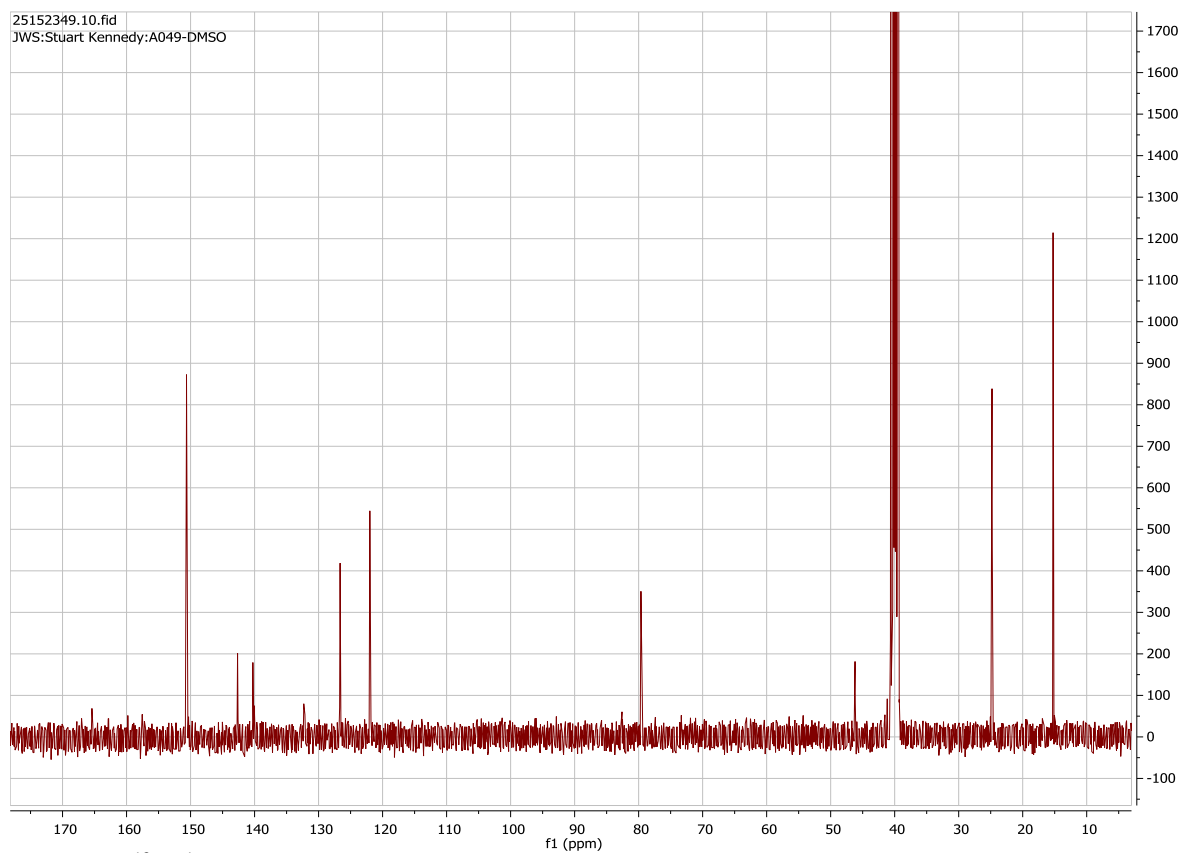


Figure S2 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2** in DMSO

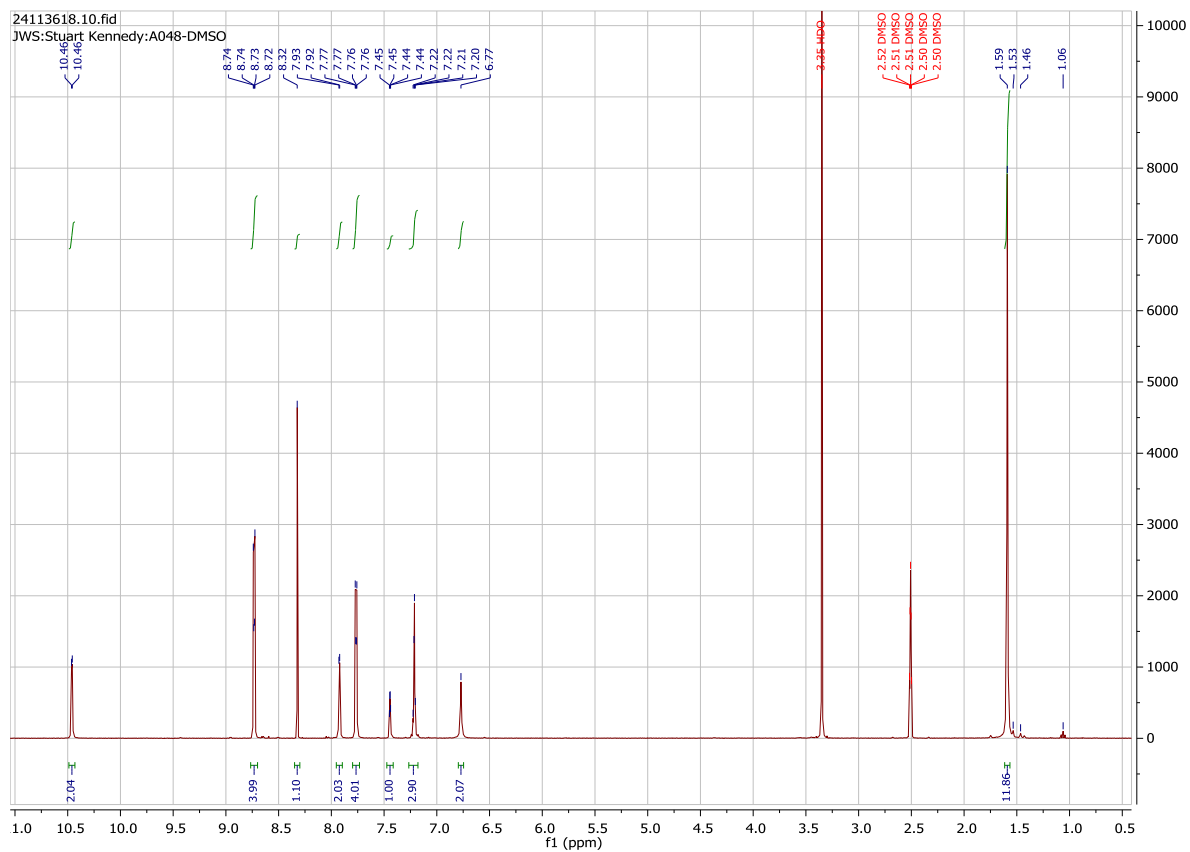


Figure S3 ^1H NMR spectrum of **2** in DMSO

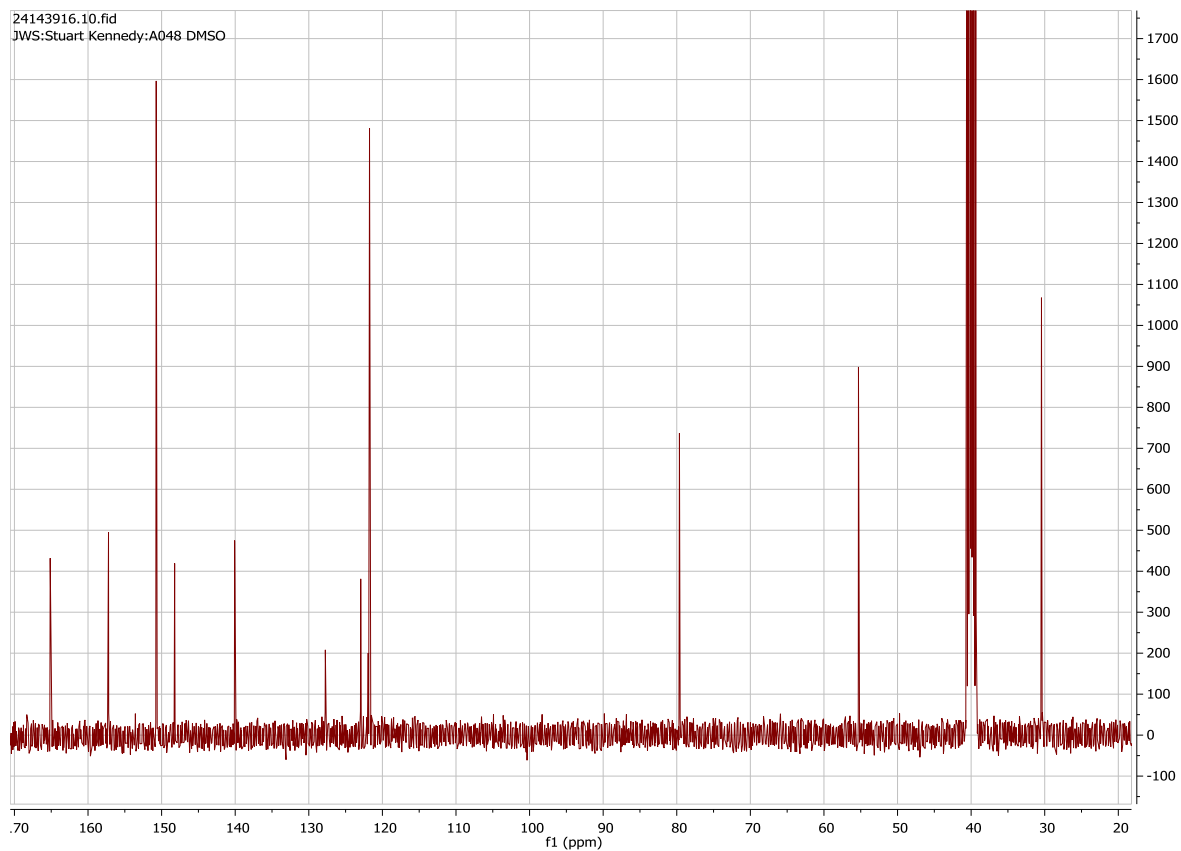


Figure S4 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2** in DMSO.

A097b, ESI - no column MeCN (TQD), RT 0.2350 mins, Scan# 27, NL 5.222E7, 28/01/2016 15:22, m/z [54.4-1972.4]

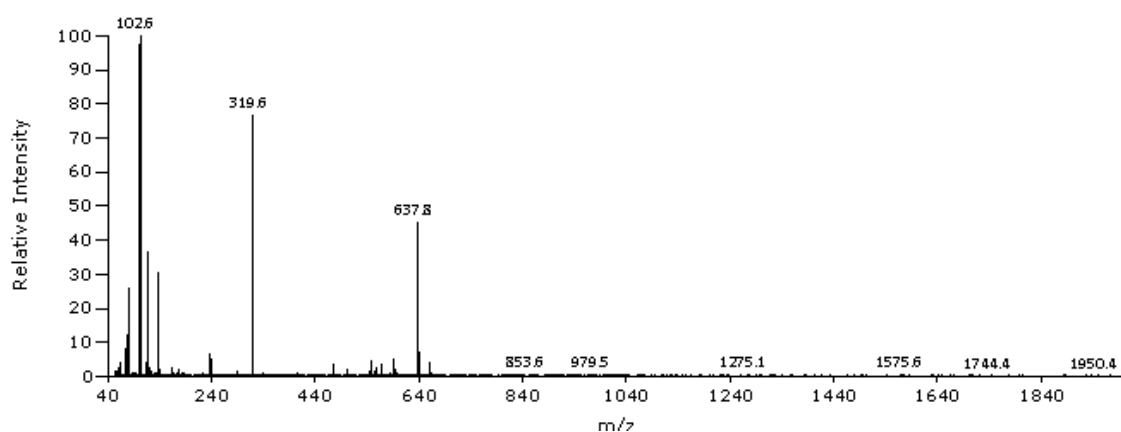


Figure S5 ESI-MS of 1.

A048, ESI - LC MeOH (TQD), RT 2.4187 mins, Scan# 278, NL 8.457E6, 14/05/2015 13:48, m/z [100.9-1980.2]

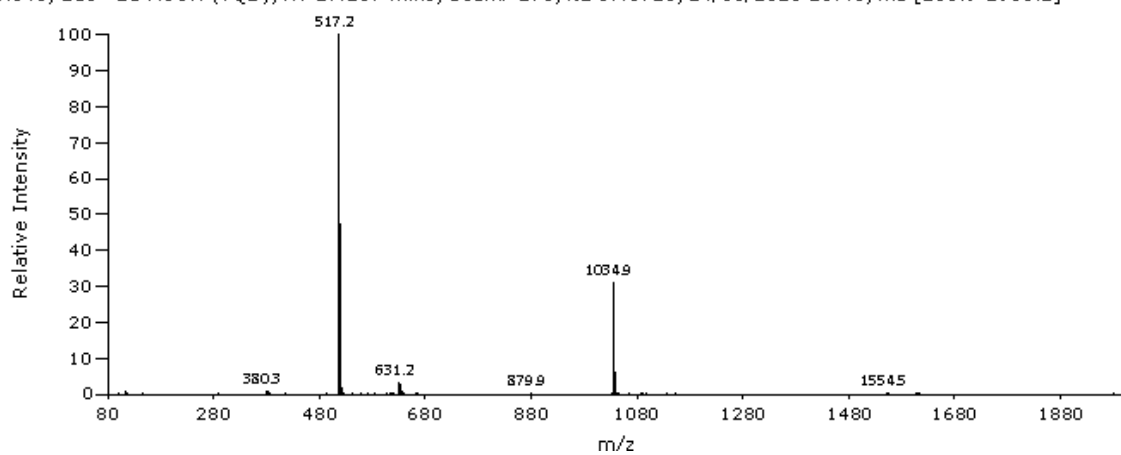


Figure S6 ESI-MS of 2.

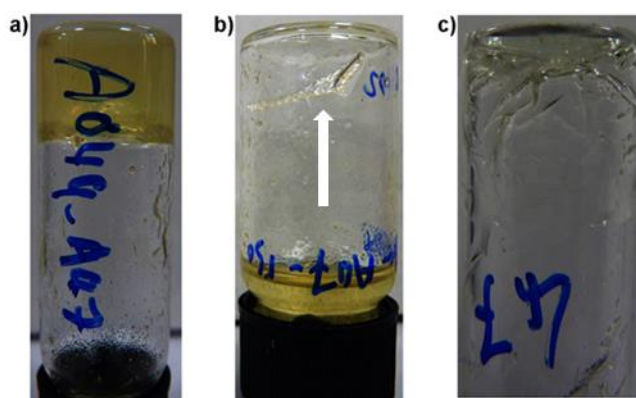


Figure S7. a) Nitrobenzene gel of 1 undergoing the inversion test. b) Single sample-spanning isoniazid crystal obtained after the collapse of a nitrobenzene gel. c) Relatively small needle-shaped crystals of isoniazid obtained from nitrobenzene.