

ELECTRONIC SUPPORTING INFORMATION:

Achieving molecular stability of racemic 4-*O*-benzyl-*myo*-inositol-1,3,5-orthoformate through crystal formation

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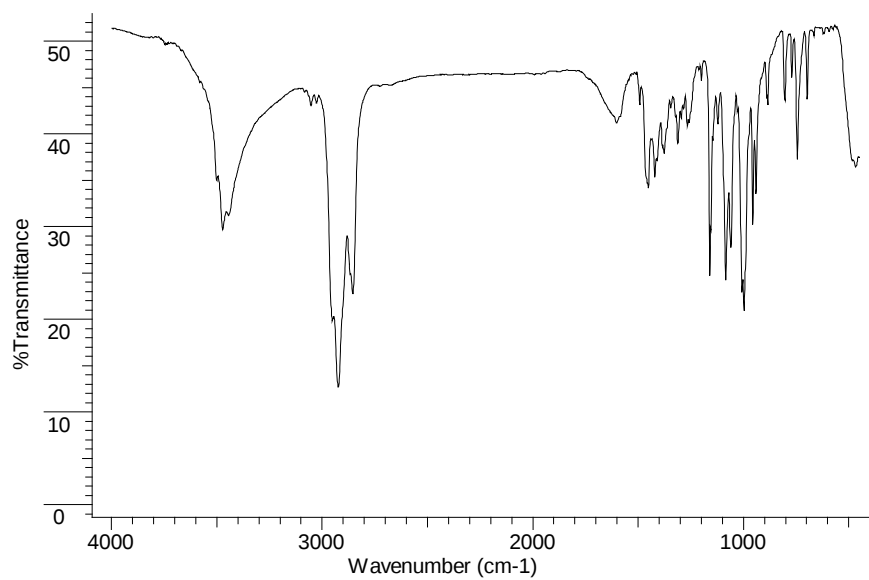
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Figure S1. IR spectra of racemic 4-*O*-benzyl-*myo*-inositol-1,3,5-orthoformate (**4**)

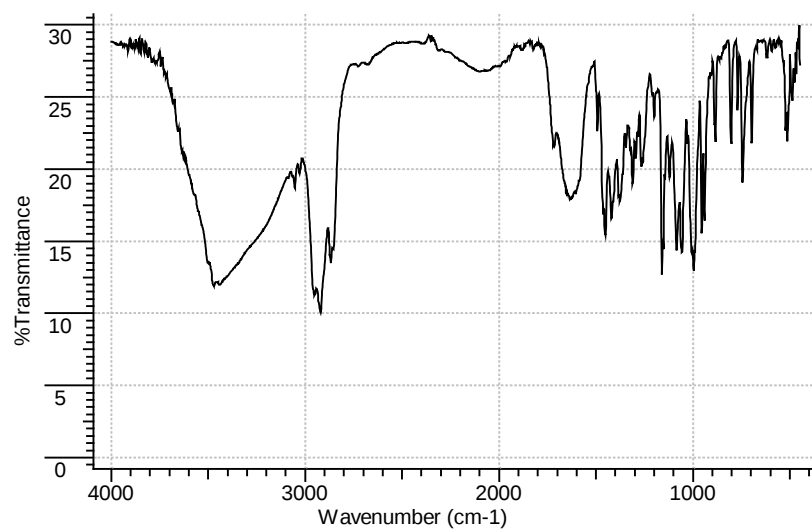
a) Form I crystals (nujol)



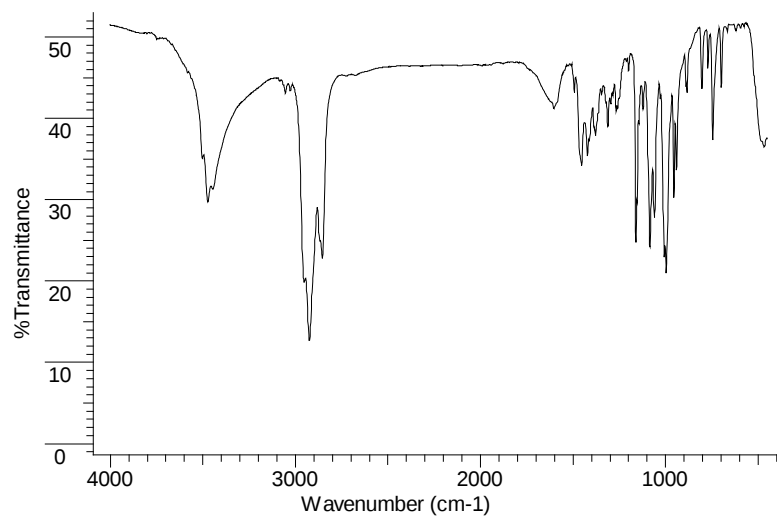
b) Gummy **4B** (neat)



c) Amorphous solid sample of **4C** (nujol)



d) Solid **4D**



e) Amorphous solid **4C** heated for 12 h at 130 °C (neat)

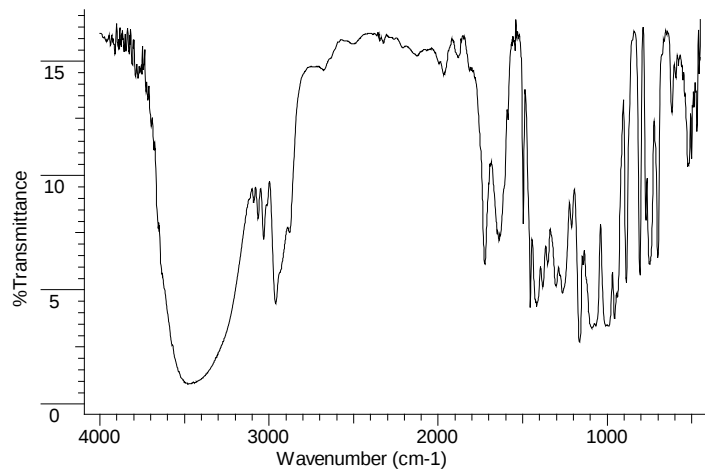
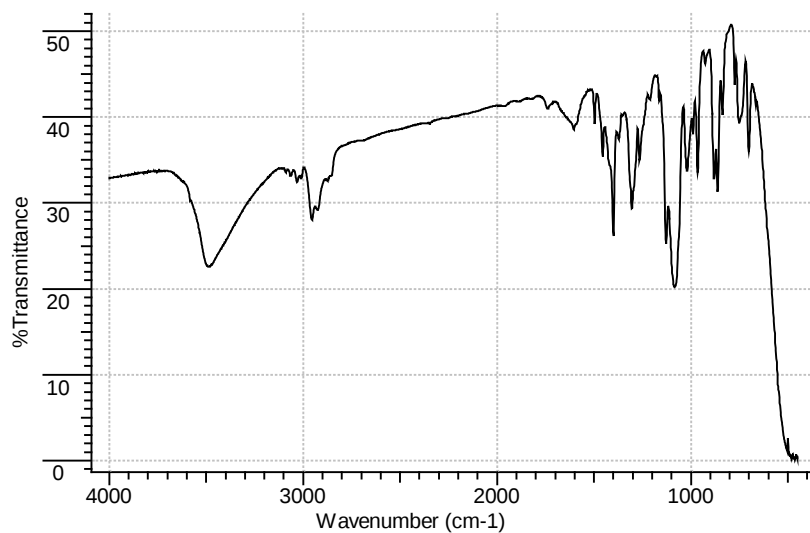
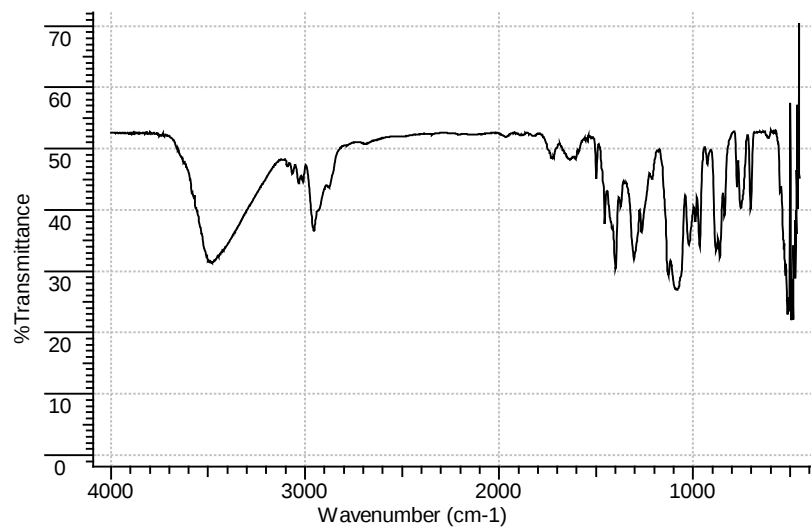


Figure S2. IR spectra of racemic 4-*O*-benzyl-*myo*-inositol-1,3,5-orthoacetate (**5**)

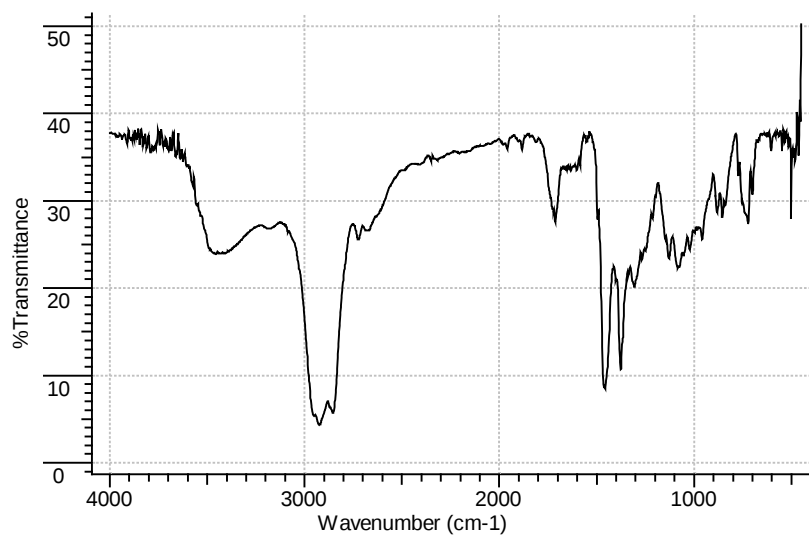
a) Freshly prepared **5** (CDCl₃)



b) **5** stored at ambient temperature for a month (neat)



c) Amorphous solid 5 (nujol):



d) 5 Heated at 120 °C for 6 hours (Nujol):

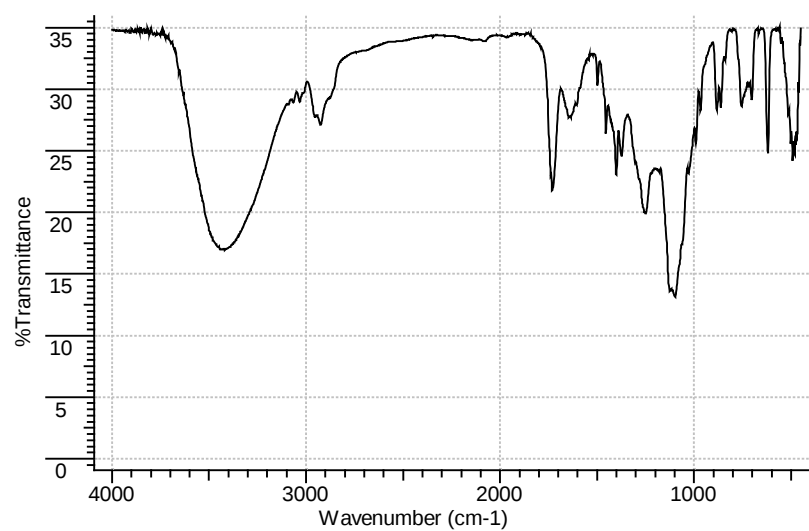
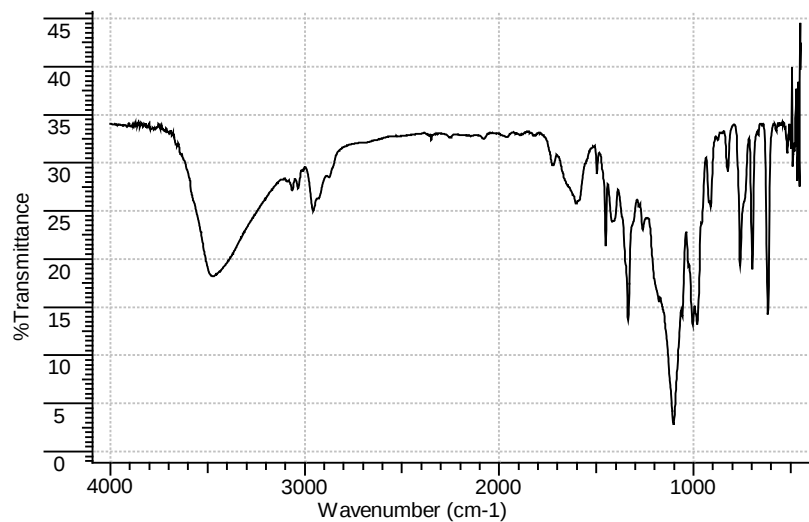
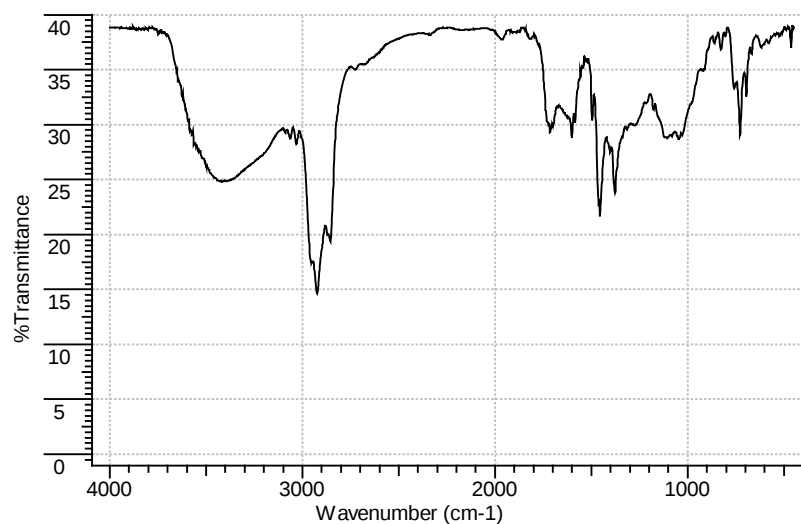


Figure S3. IR spectra of racemic 4-*O*-benzyl-*myo*-inositol-1,3,5-orthobenzoate (**6**)

a) Freshly prepared **6** (CDCl₃)



b) **6** stored at ambient temperature for a month (neat)



c) **6** Heated at 120°C for 6 hours (nujol)

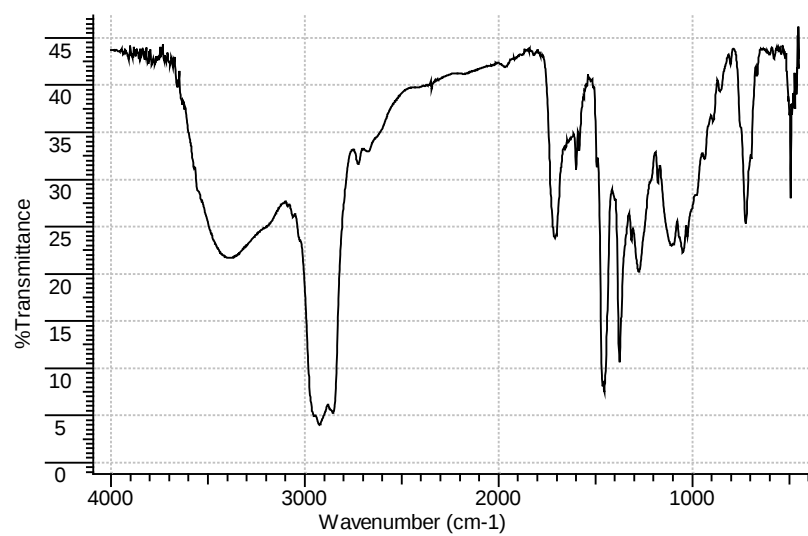
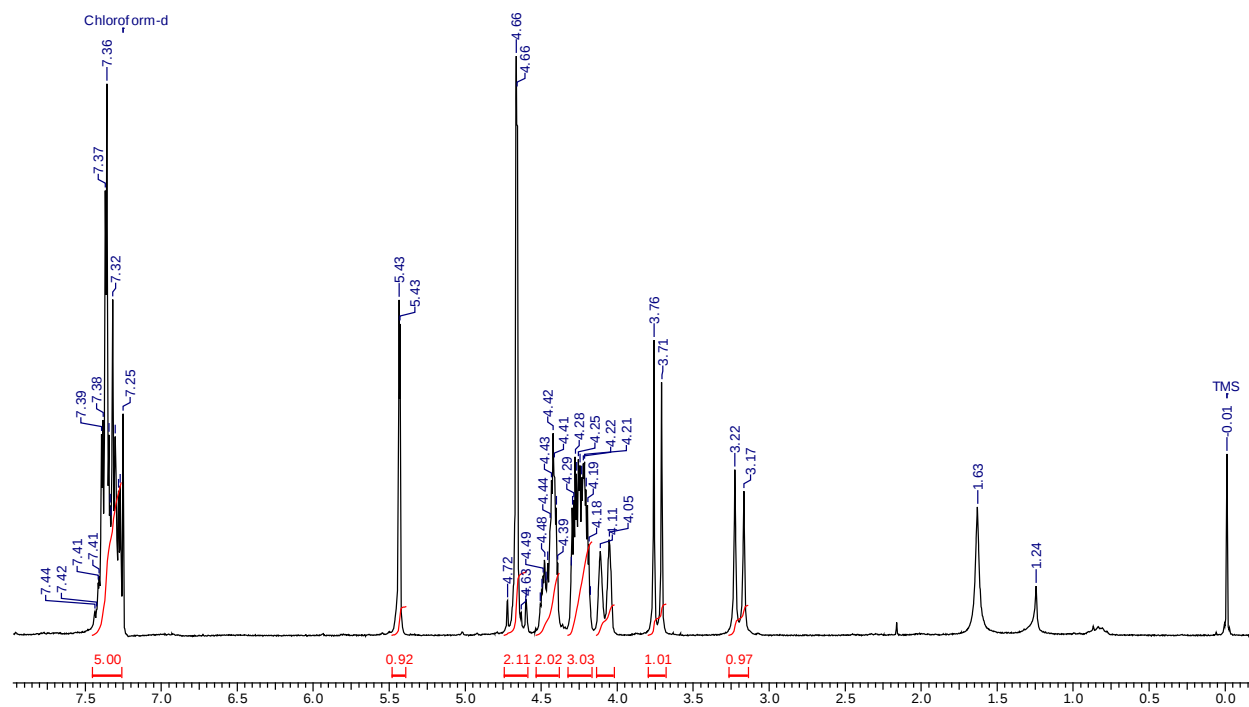
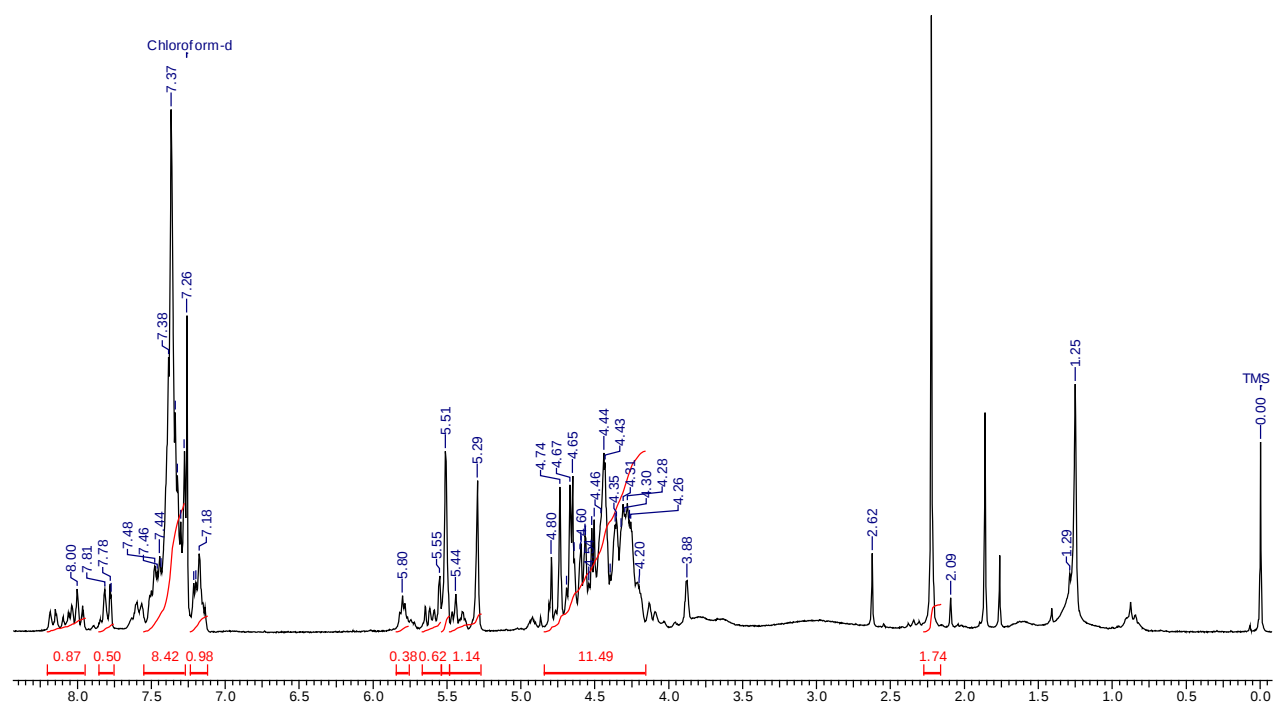


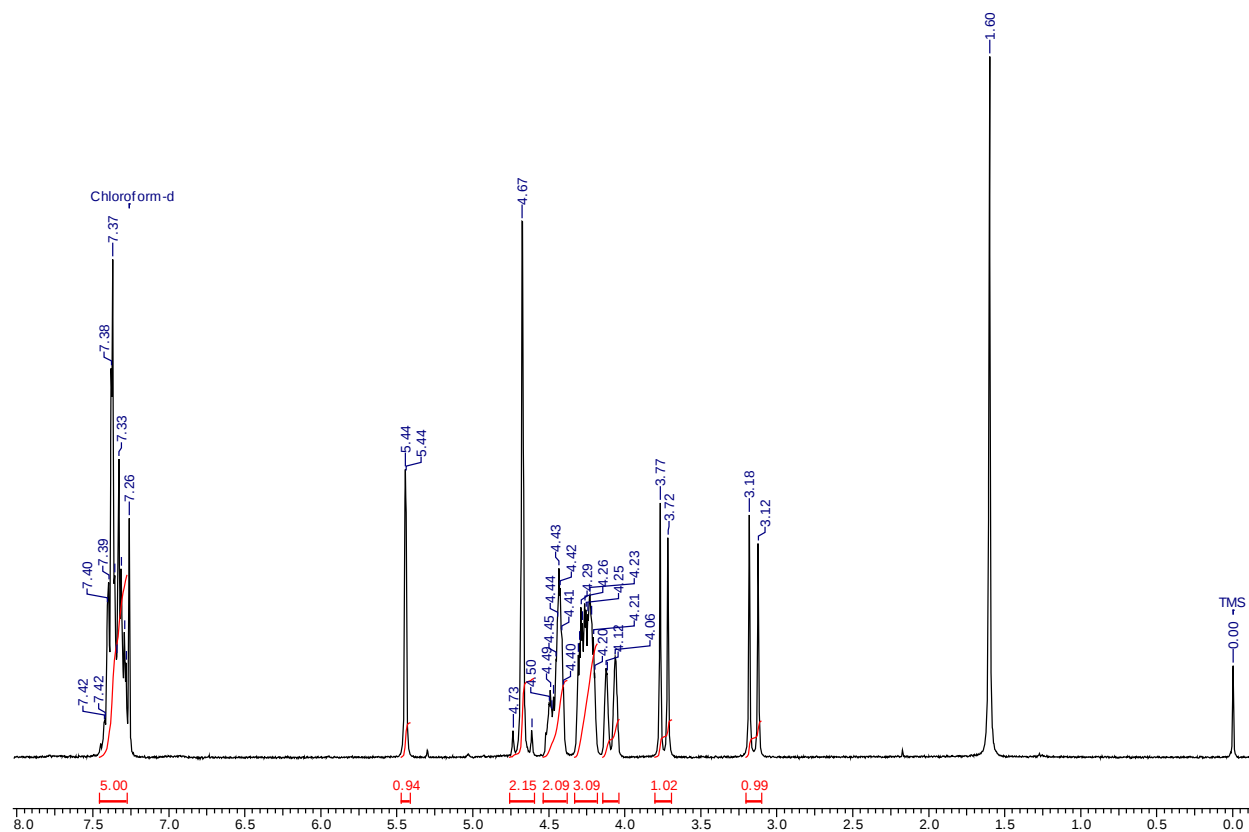
Figure S4. a) ^1H NMR spectrum (CDCl_3) of racemic 4-*O*-benzyl-*myo*-inositol-1,3,5-orthoformate (sample **4A**).



b) ^1H NMR spectrum (CDCl_3) of racemic 4-*O*-benzyl-*myo*-inositol-1,3,5-orthoformate (sample **4B**).



c) ^1H NMR spectrum (CDCl_3) of racemic 4-*O*-benzyl-*myo*-inositol-1,3,5-orthoformate (**4D**).



d) ^1H NMR spectrum (CDCl_3) of racemic 4-*O*-benzyl-*myo*-inositol-1,3,5-orthoformate (Form I crystals).

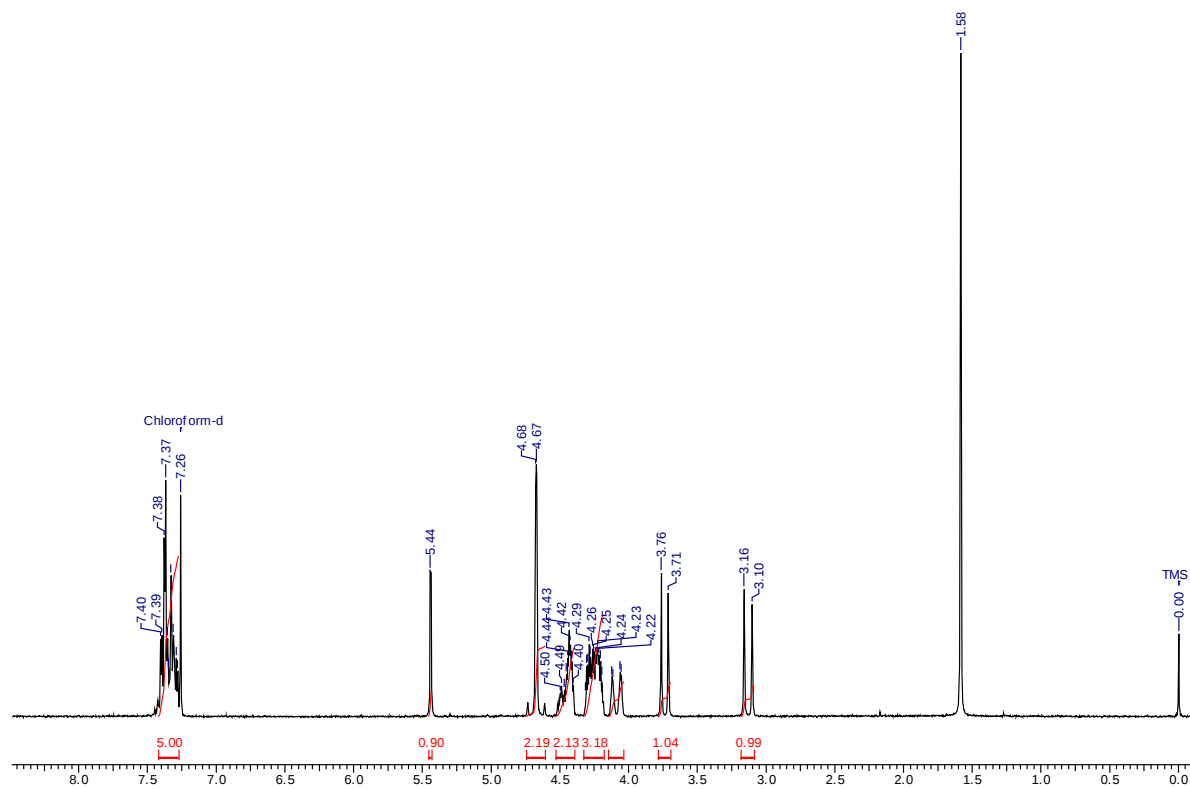


Figure S5. ^1H NMR spectrum (CDCl_3) of racemic 4-*O*-benzyl-*myo*-inositol-1,3,5-orthoacetate
(5)

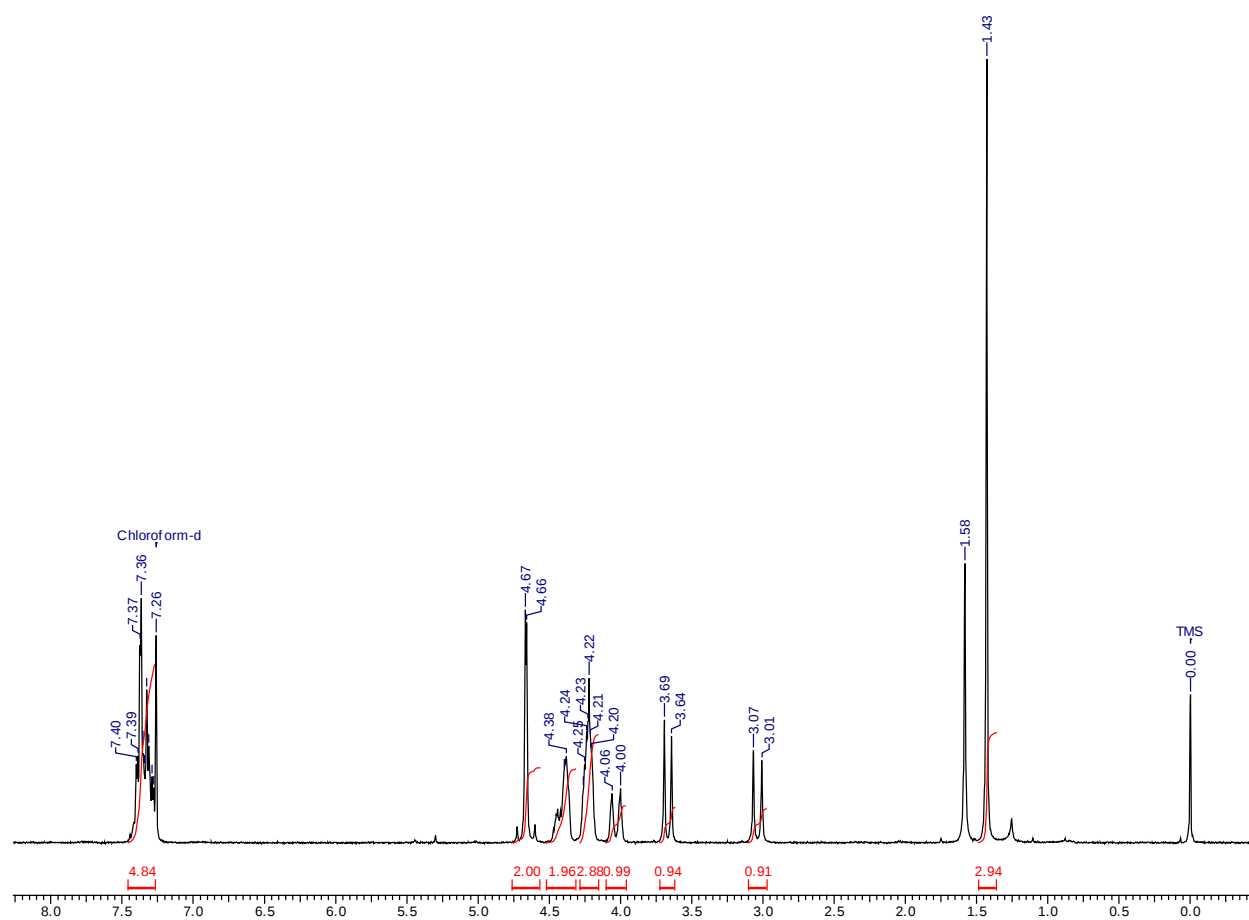


Figure S6. ^1H NMR spectrum (CDCl_3) of heated sample of racemic 4-*O*-benzyl-*myo*-inositol - 1,3,5-orthoacetate (**5**).

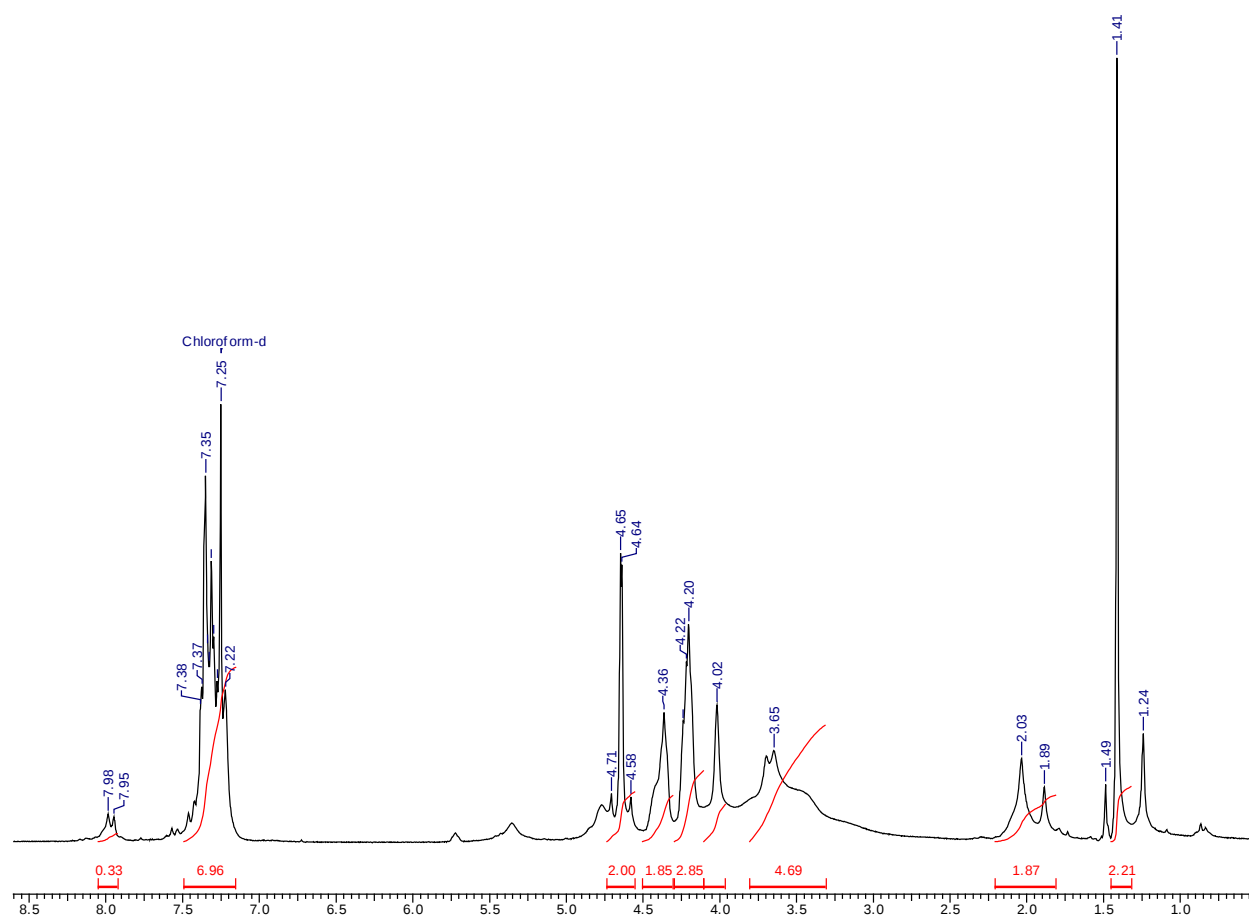


Figure S7. ^1H NMR spectrum (CDCl_3) of racemic 4-*O*-benzyl-*myo*-inositol-1,3,5-orthobenzoate
(6)

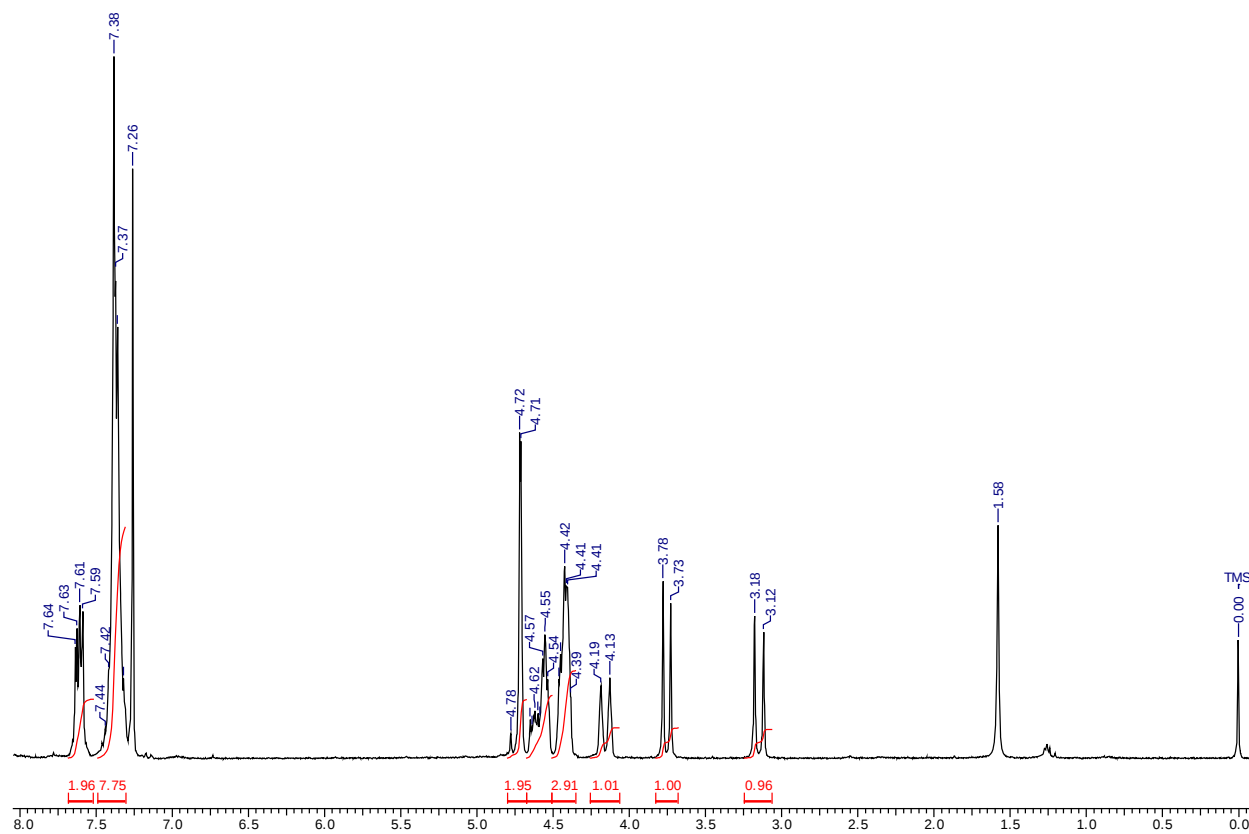


Figure S8. ^1H NMR spectrum (CDCl_3) of heated sample of racemic 4-*O*-benzyl-*myo*-inositol - 1,3,5-orthobenzoate (**6**).

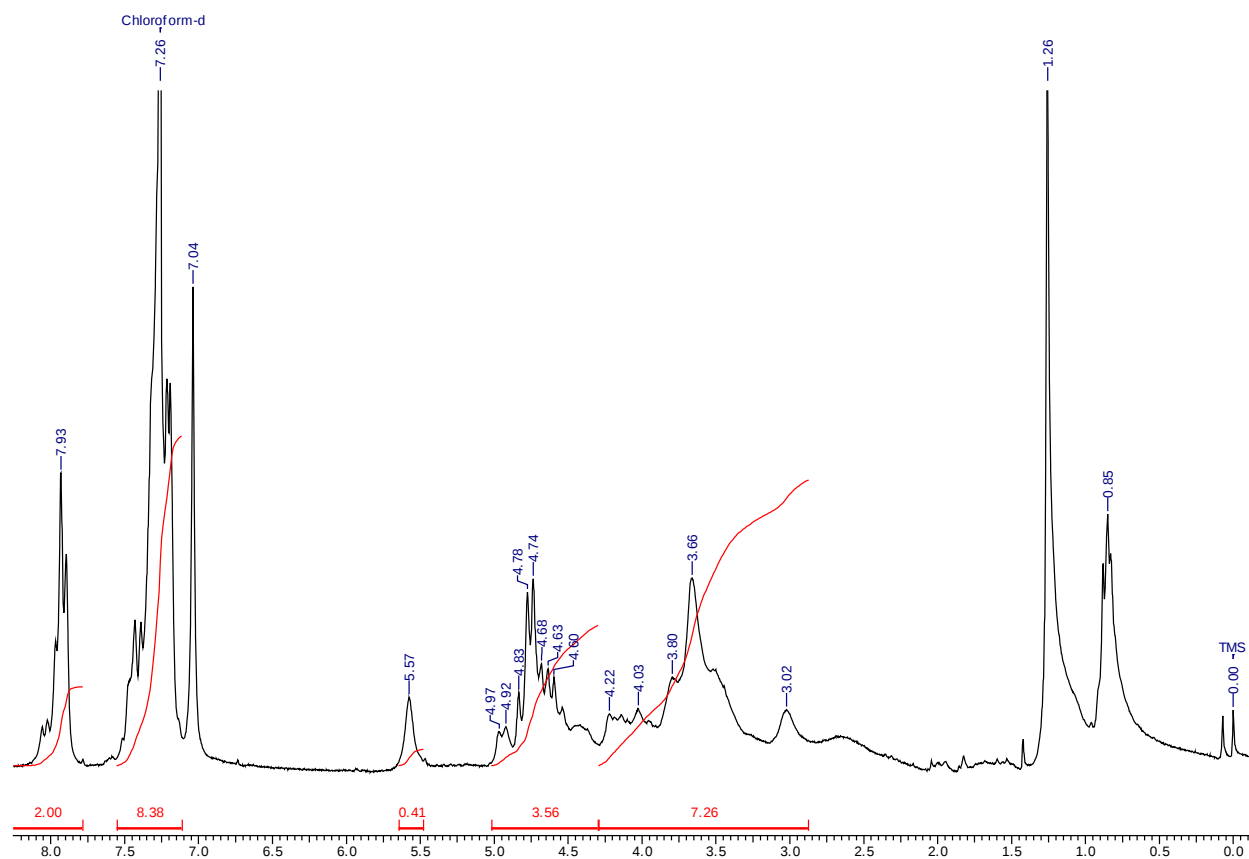


Figure S9. Simulated PXRD patterns for crystals of **4**.

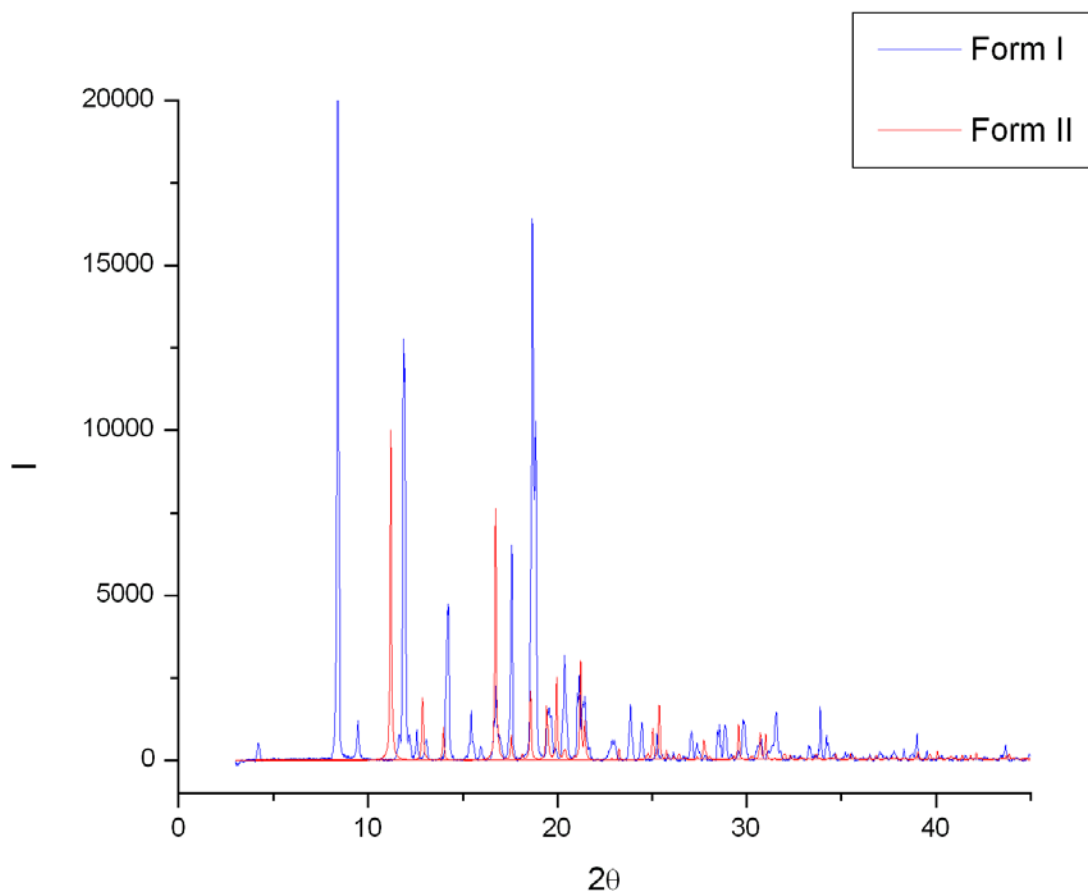


Figure S10. PXRD patterns for crystals of (a) black – sample **4D** and (b) blue - Form I.

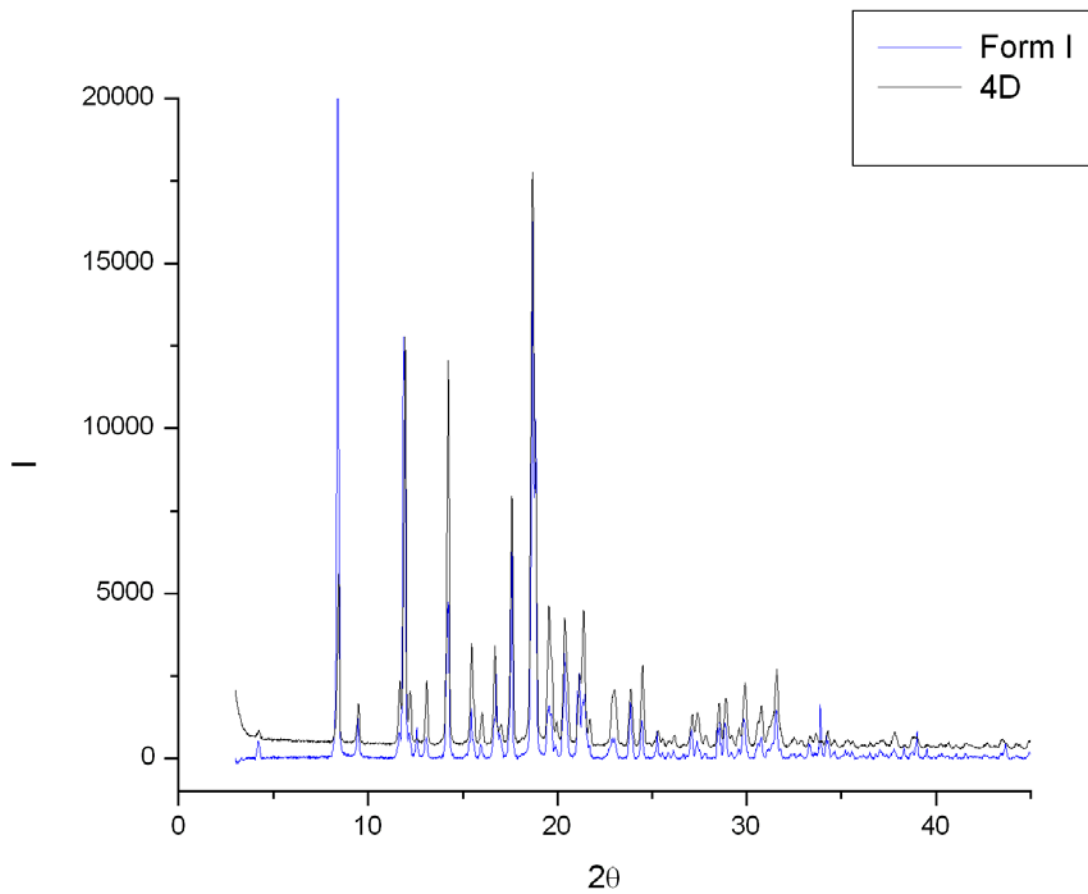


Figure S11. PXRD patterns for solid forms of **4**. (a) black – solid **4D** and (b) red – Form II.

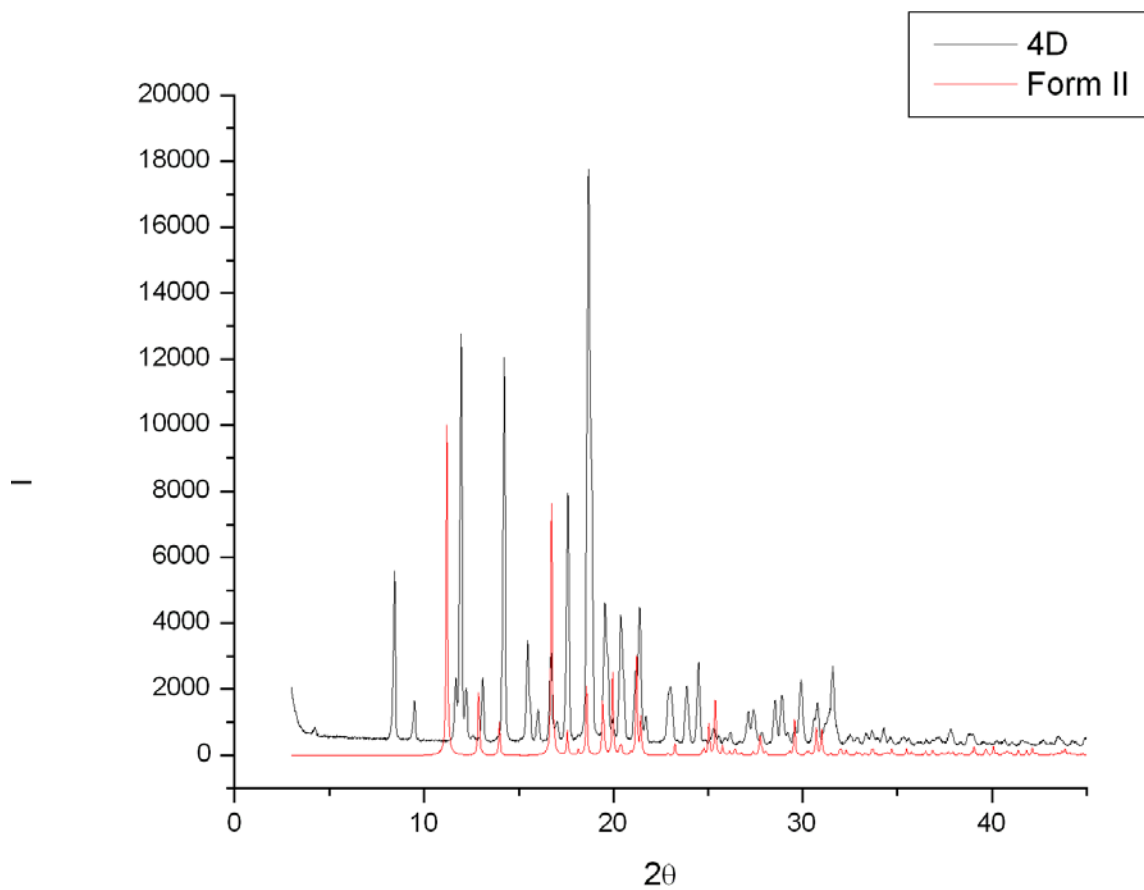


Figure S12. PXRD patterns of sample **4D**, Form I and Form II crystals

