

Supporting Information

Racemic Conglomerate Formation via Crystallization of Metaxalone from Volatile Deep Eutectic Solvents

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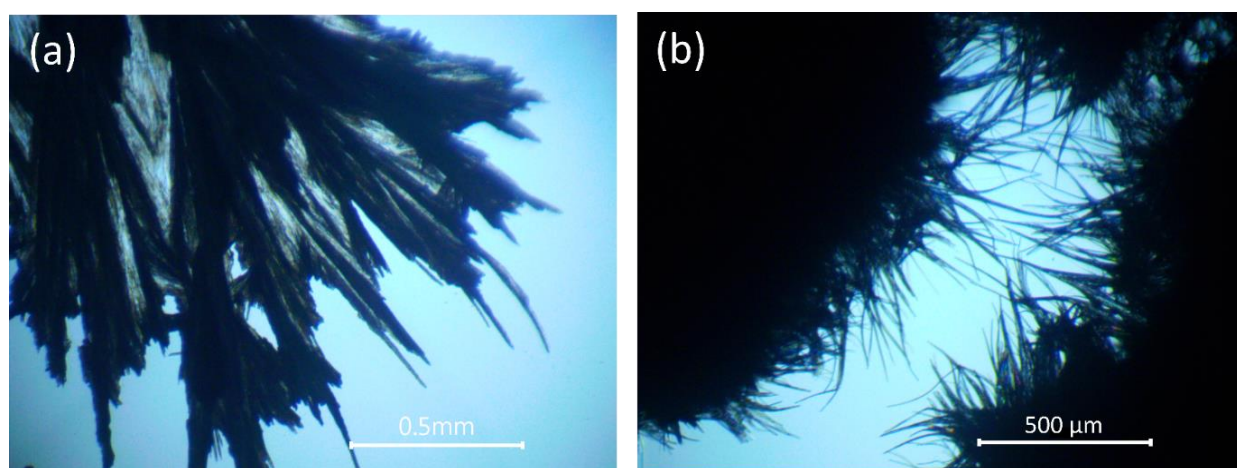


Figure S1. Unfiltered light microscopy images of the crystals shown in Figure 3 of (a) Form A-R/S and (b) Form A-rac metaxalone.

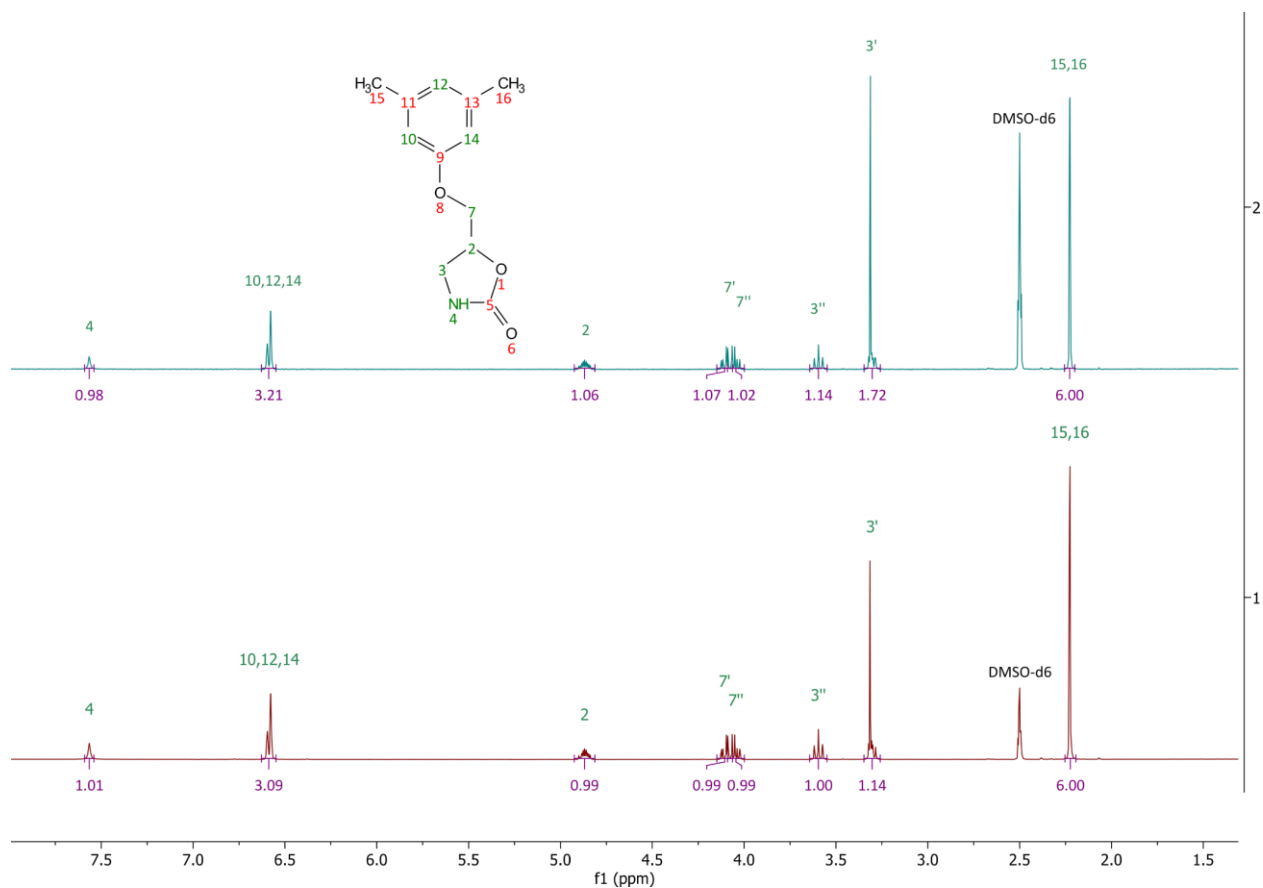


Figure S2. NMR data of metaxalone (1) Form A-rac and (2) Form A-R/S in DMSO-d (peak at 2.5 ppm), crystallized from volatile deep eutectic solvent crystallization with phenol. In pattern 2 the unexpected integration is likely due to the presence of a water peak integrated into the peak at 3.33 ppm from moisture in the solvent.

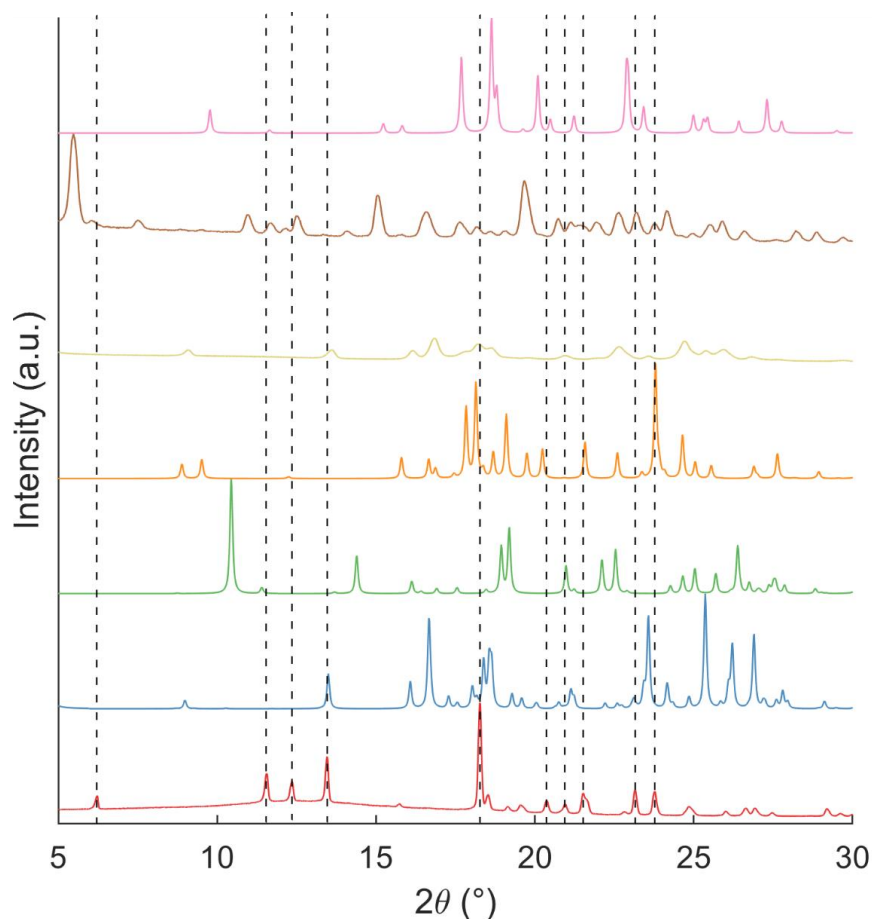


Figure S3. Powder X-ray diffraction pattern of an unknown metaxalone-phenol solvate (red), raw data with background not removed, with major peaks extended as dashed lines, compared to the powder patterns of Form A-rac (blue), Form B (green), Form A-S (orange), Form C-rac (yellow), Form C-S (brown) metaxalone and phenol (pink). Respective CCDC identifiers for Forms A-rac, B-rac and A-S: AXOGAW, AXOGAW01 and WISNEU, for phenol: PHENOL01.

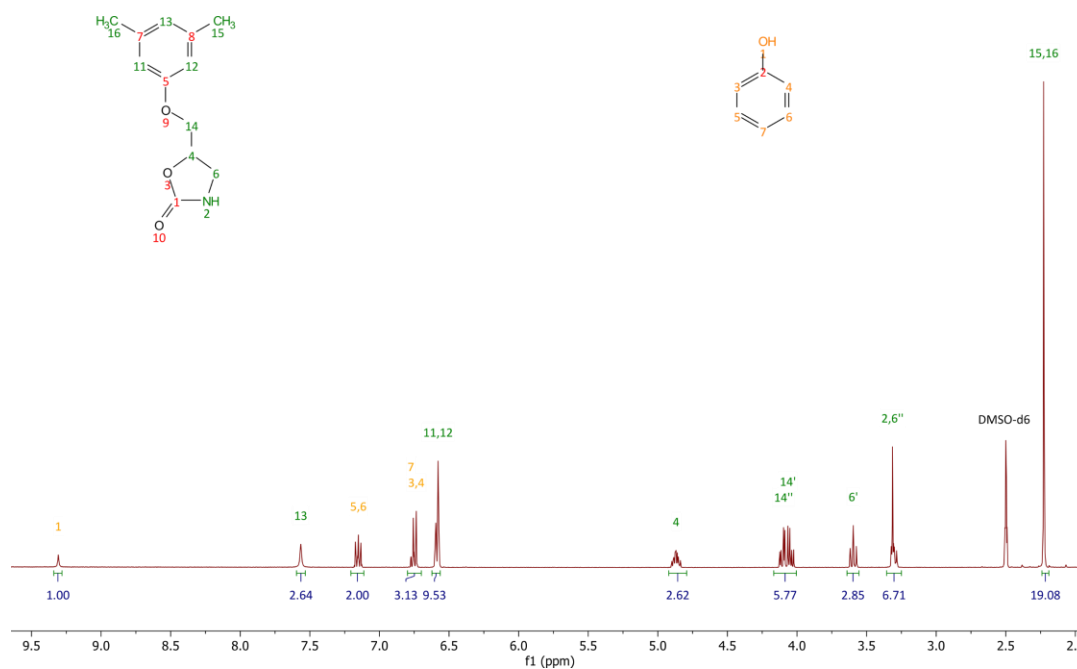


Figure S4. NMR data of a metaxalone-phenol solvate, crystallized from a ratio of 3:1 (phenol:metaxalone) volatile deep eutectic solvent, in DMSO-d (peak at 2.5 ppm).

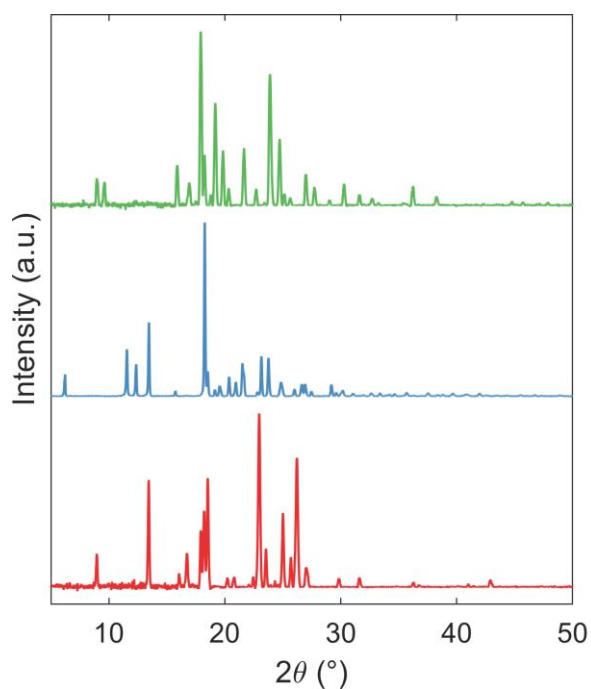


Figure S5. Powder X-ray diffraction patterns of metaxalone Form A-rac (red), an unknown MTX-phenol solvate (blue) and Form A-R/S (green), from 5° – 50°. All reflections for Form A-rac and A-R/S can be indexed to known forms Form A-rac and A-S with respective CCDC identifiers: AXOGAW and WISNEU.