

Supporting Information

Investigation of Solid-State Hydrate-Anhydrous Phase Transformations of Dabigatran Etexilate Hemi-Edisylate

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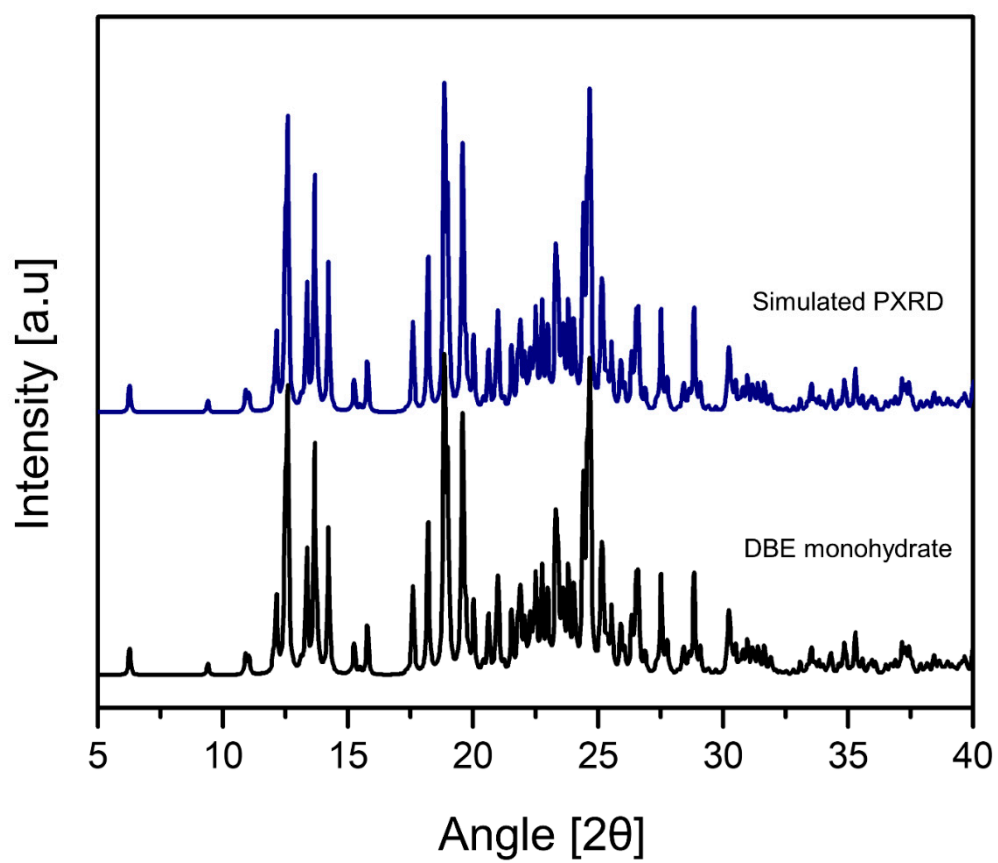
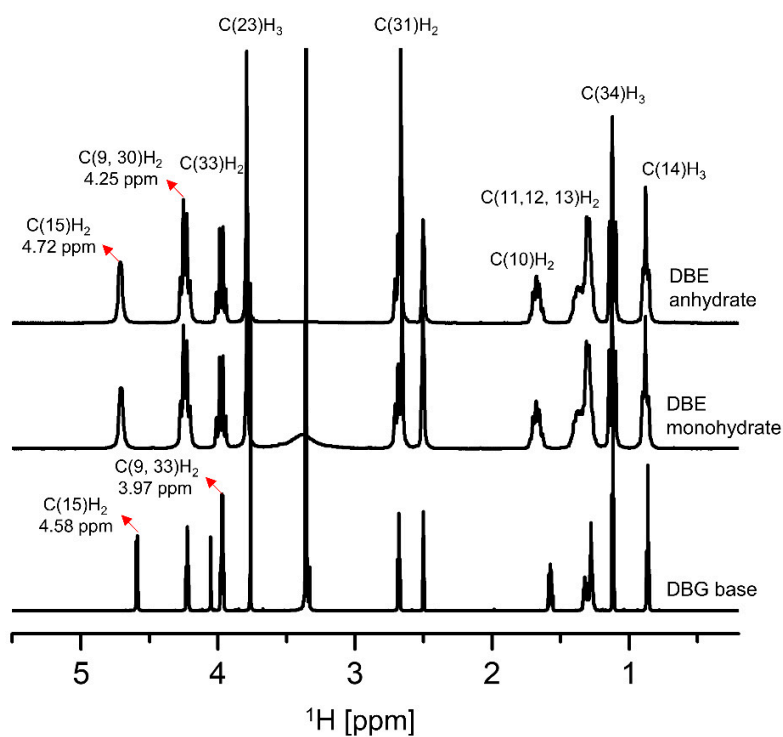
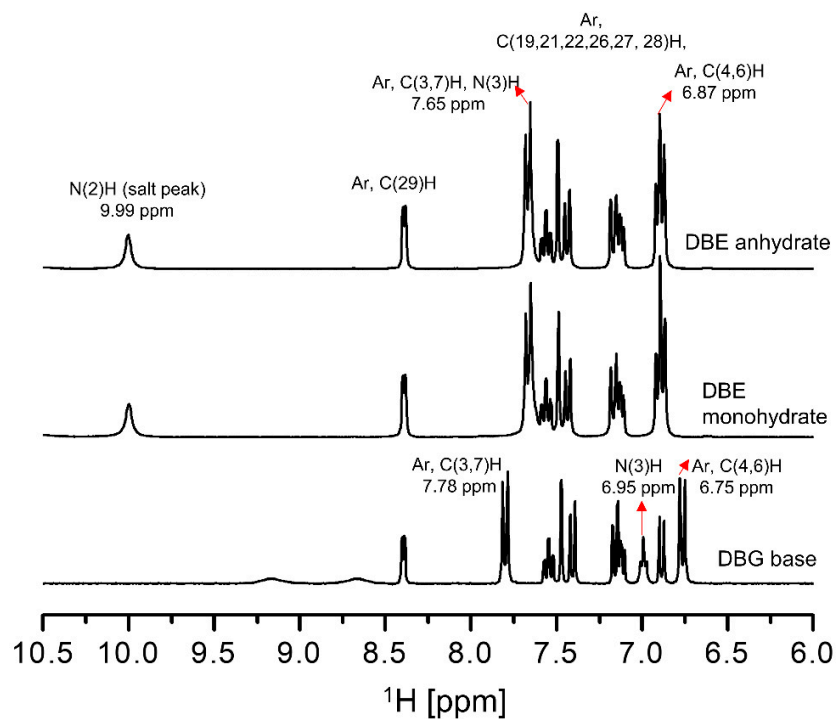


Figure S1. Simulated PXRD pattern and Powder PXRD pattern for DBE monohydrate.



(a)



(b)

Figure S2. Solution-state ^1H -NMR spectra of DBG and DBE (solvent: DMSO-d_6): (a) 1 ppm-5 ppm, (b) 6 ppm–10.5 ppm.

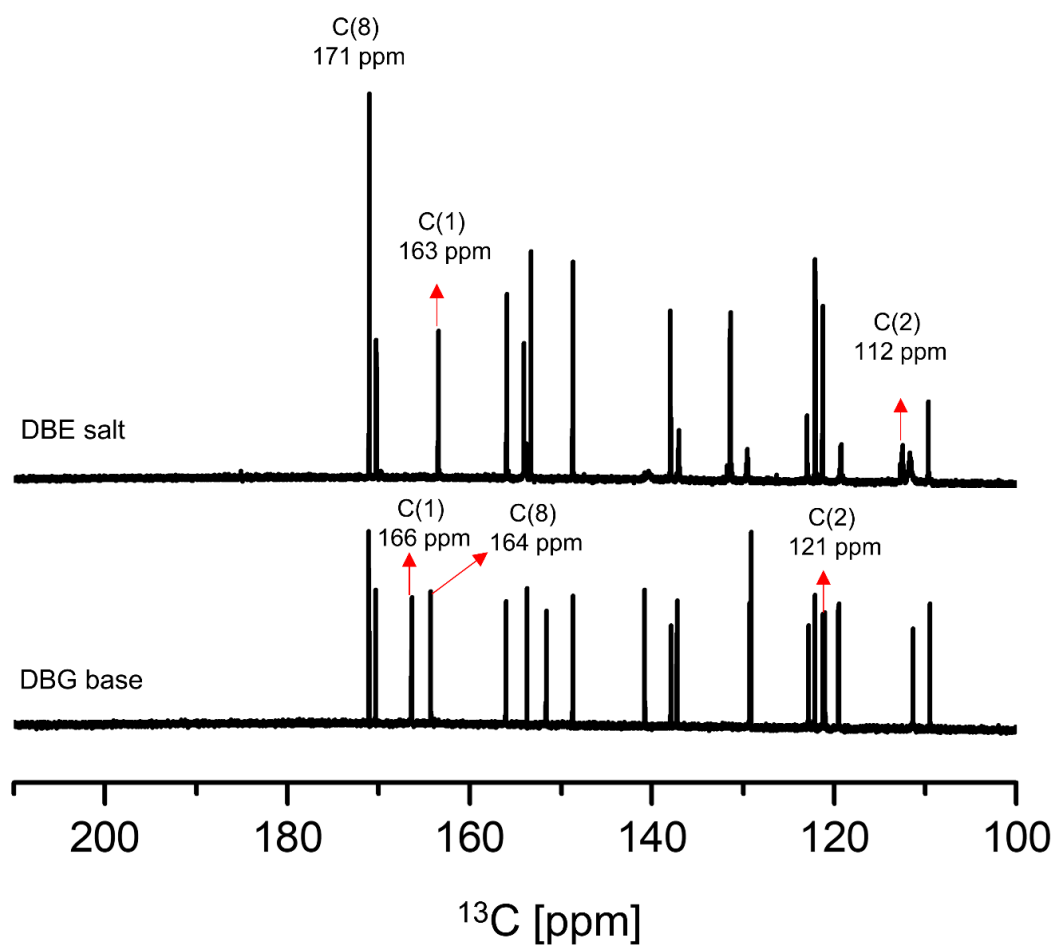


Figure S3. Solution-state ^{13}C -NMR spectra of DBG and DBE (solvent: DMSO-d_6).

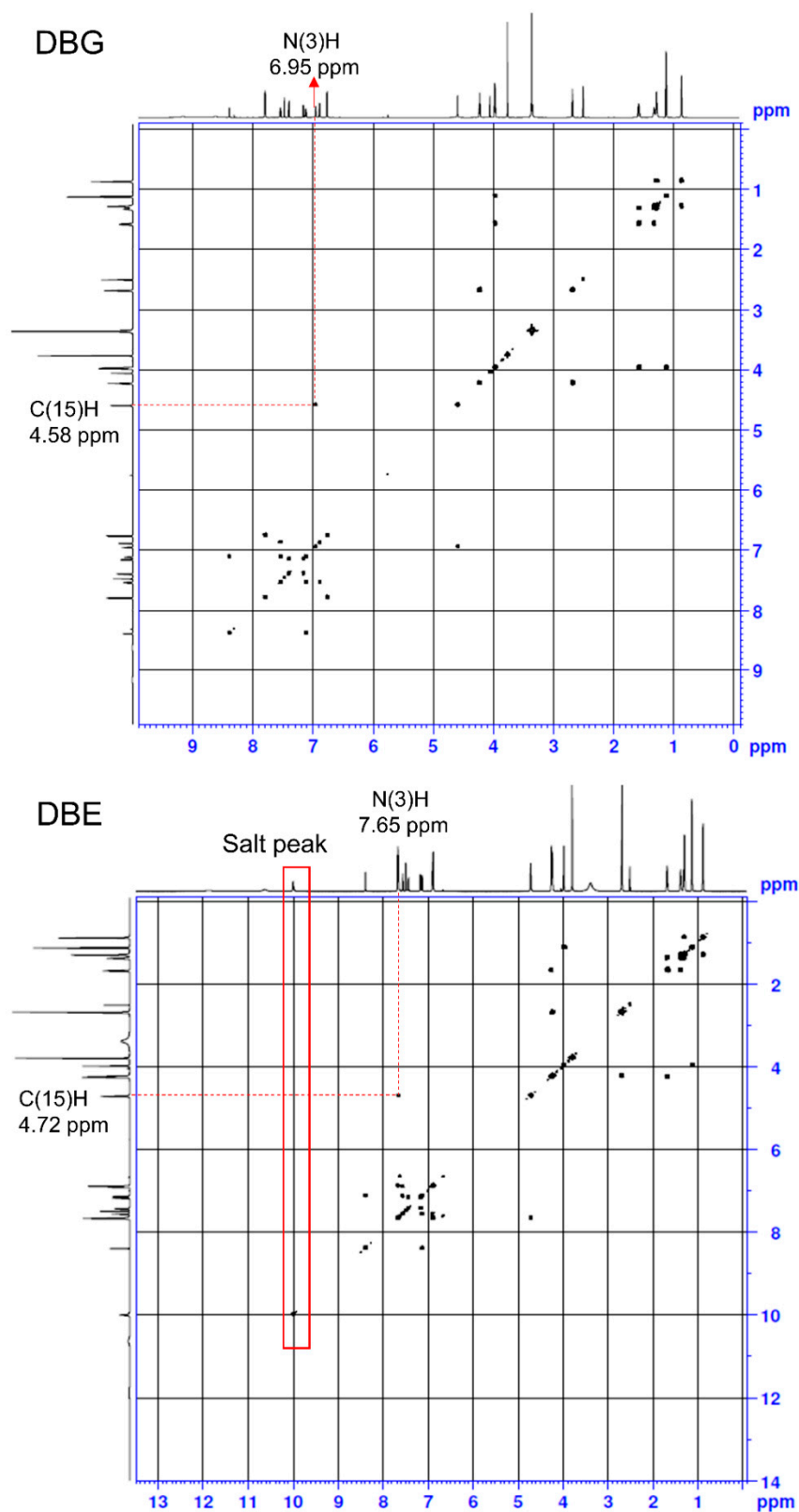


Figure S4. Solution-state 2D NMR ^1H - ^1H COSY spectra of DBG and DBE (solvent: DMSO- d_6).

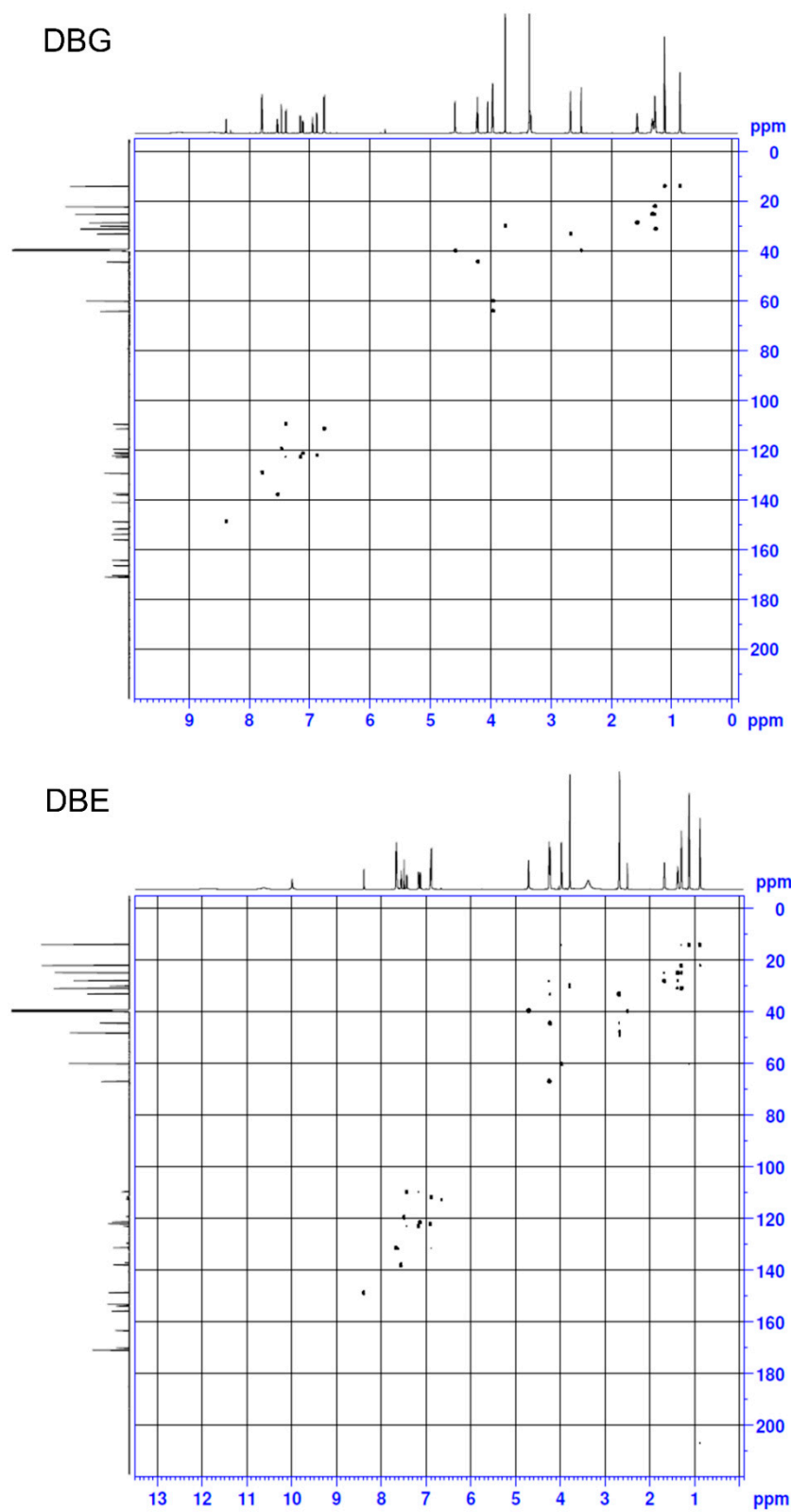


Figure S5. Solution-state 2D NMR ^1H - ^{13}C HSQC spectra of DBG and DBE (solvent: DMSO-d_6).

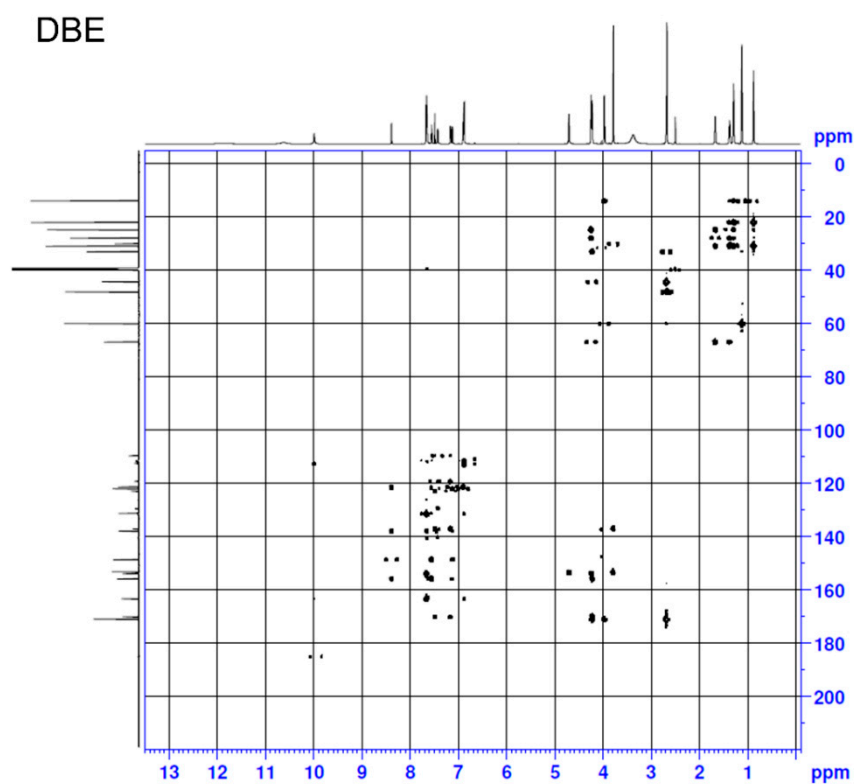
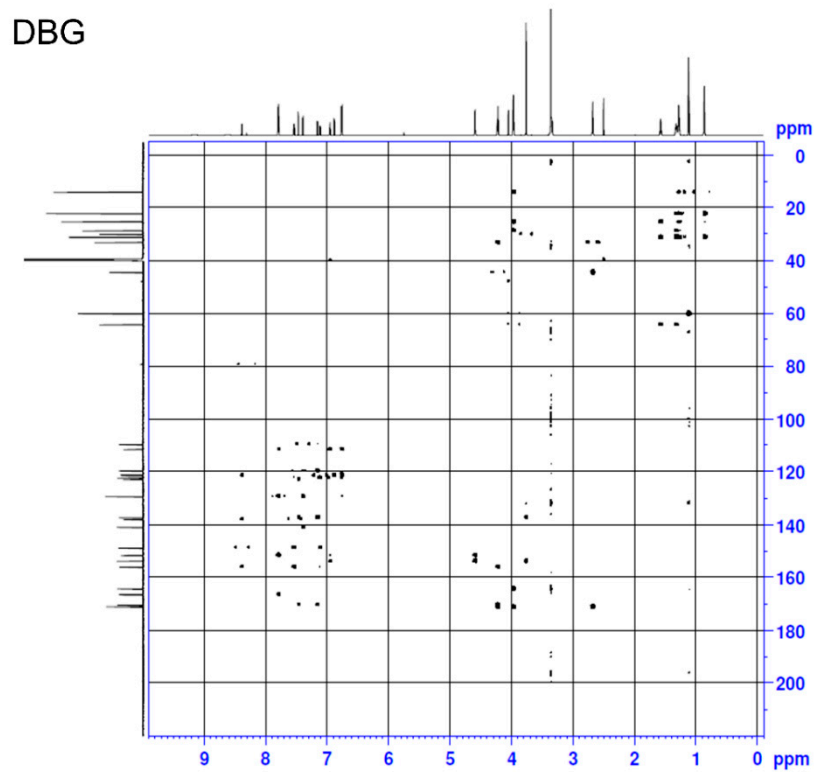


Figure S6. Solution-state 2D NMR ^1H - ^{13}C HMBC spectra of DBG and DBE (solvent: DMSO-d_6).

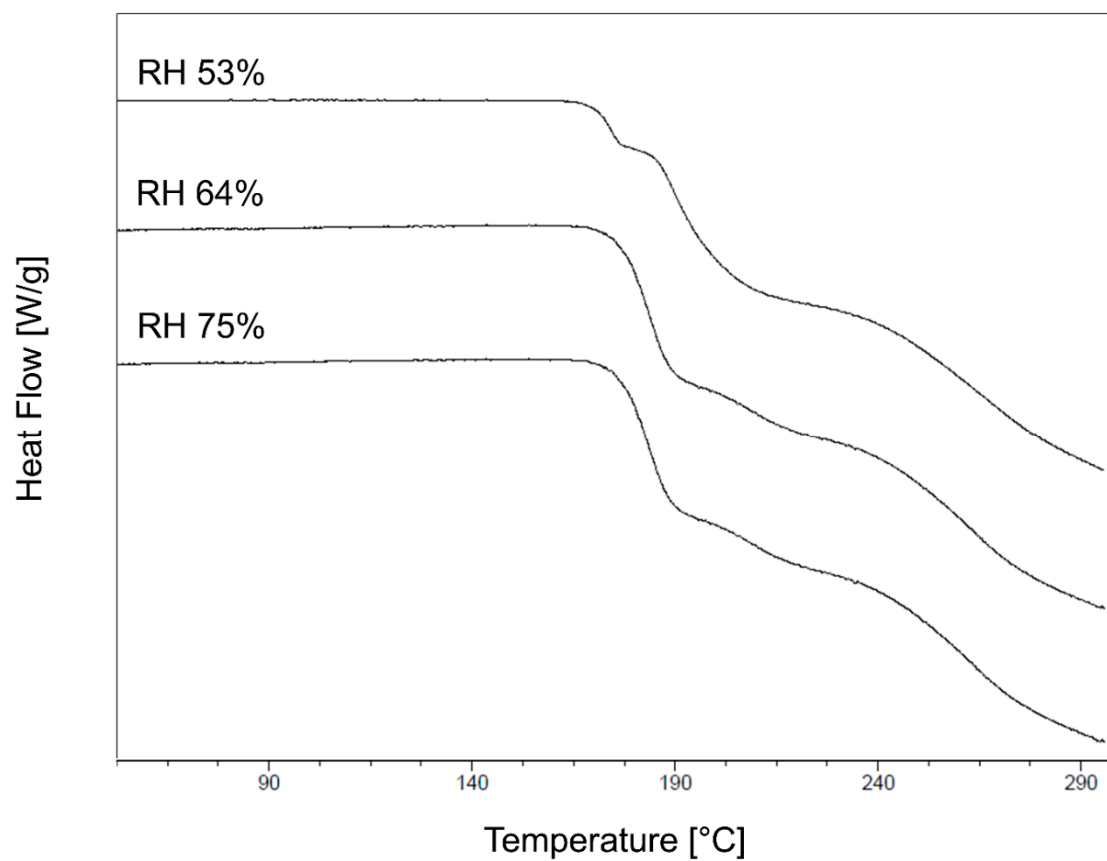


Figure S7. TGA curves of DBE anhydrate after 3 days storage at relative humidity (RH) 53%, 64%, 75% conditions (heating rate 10 °C/min, temperature range 30 °C–300 °C).

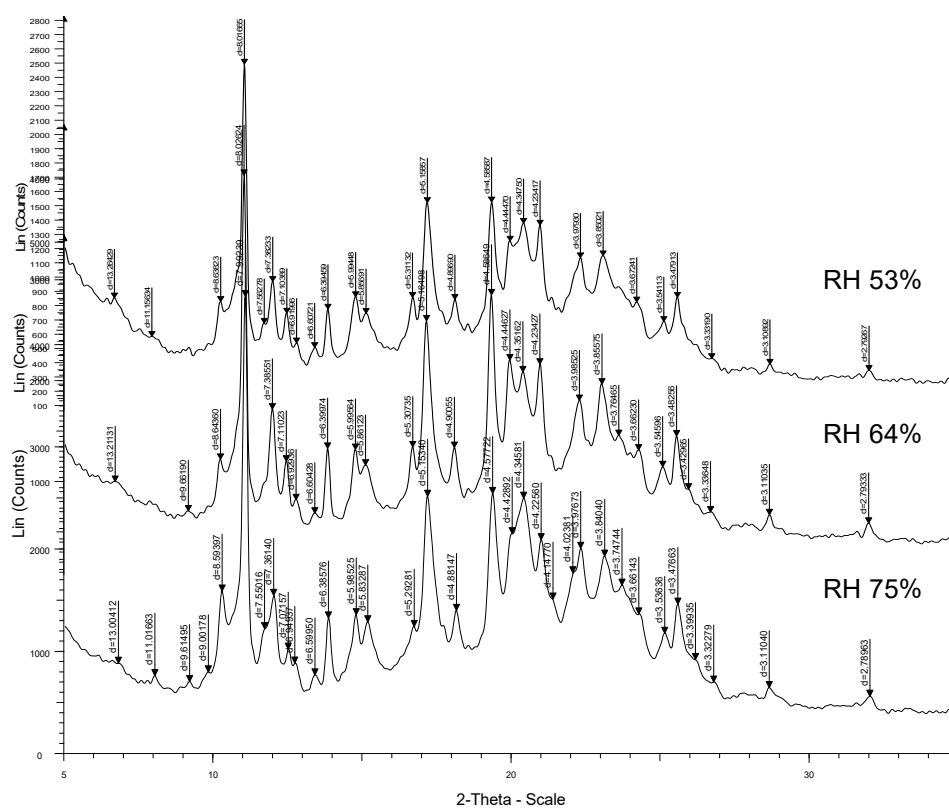


Figure S8. PXRD pattern of DBE anhydrate after 3 days of storage at relative humidity (RH) conditions of 53%, 64%, and 75%.