Electronic Supplementary Material (ESI) for CrystEngComm

Temozolomide hydrochloride dihydrate†

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Electronic Supplementary Information†

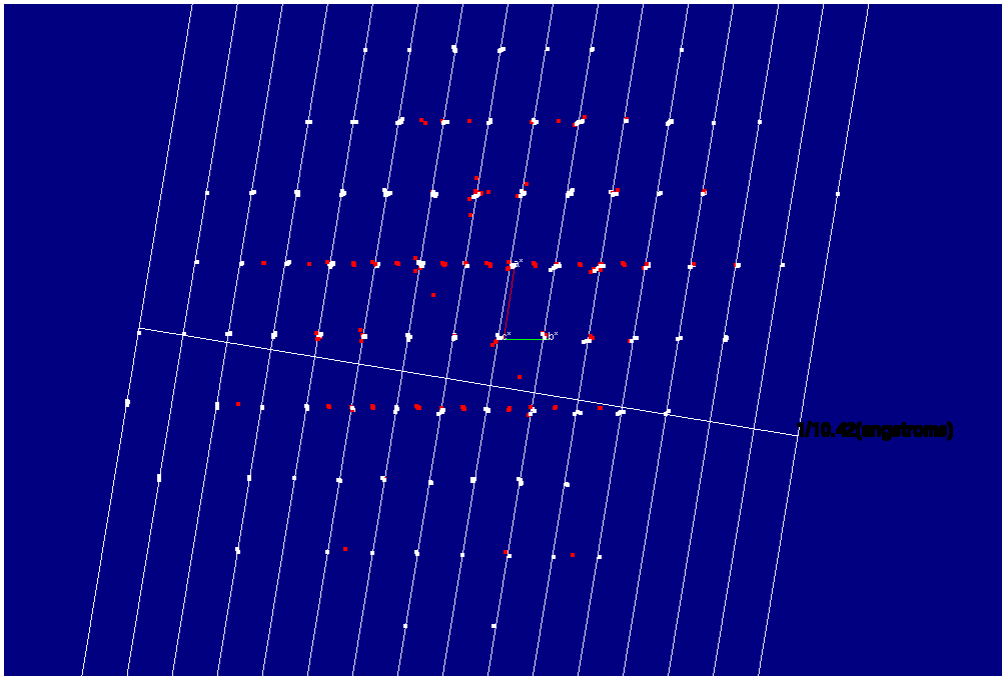

Figure S1 (a) Visualization of reflections in RLATT along *a*b** plane. Reflections are color coded. Major (white) and Twin (red)

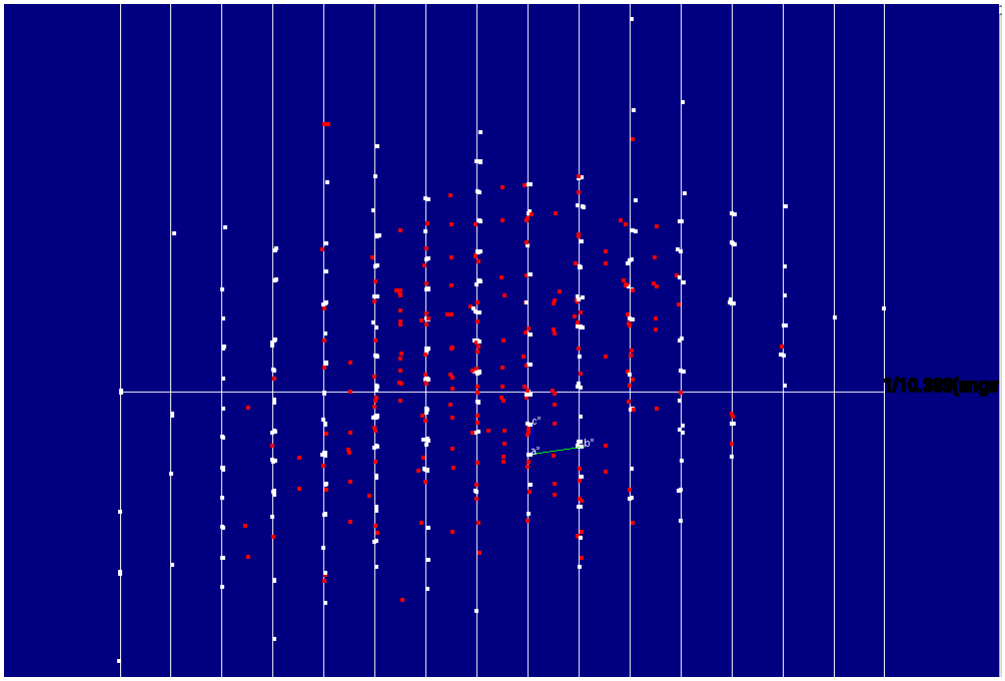

Figure S1 (b) Visualization of reflections in RLATT along *a*c** plane. This figure shows the many twinned spots.

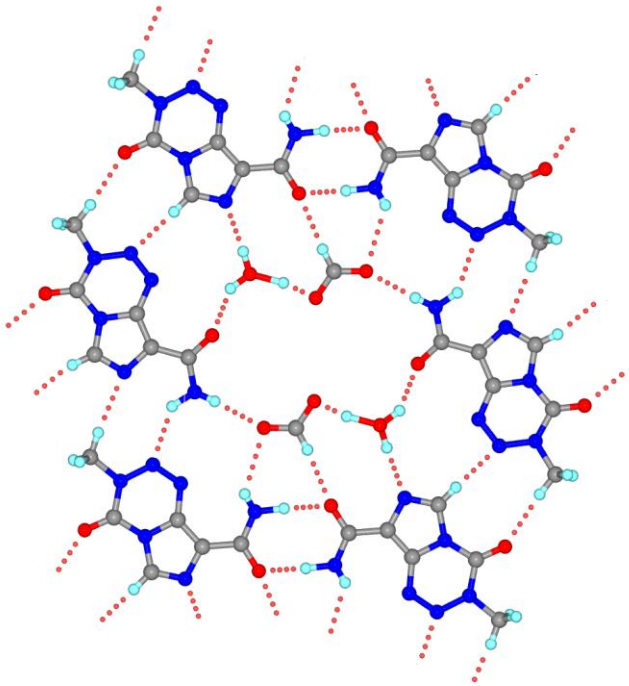

Figure S2 Crystal structure of temozolomide–formic acid monohydrate (2:1:1). Temozolomide exists in conformations A and B and are connected by amide dimer $R_2^2(8)$ synthon. The proton from formic acid is migrated to water forming a hydronium cation and a formate anion, and these two are linked by O–H···O hydrogen bonds. The imidazole N of TMZ is participates in N–H···O and C–H···O interactions.

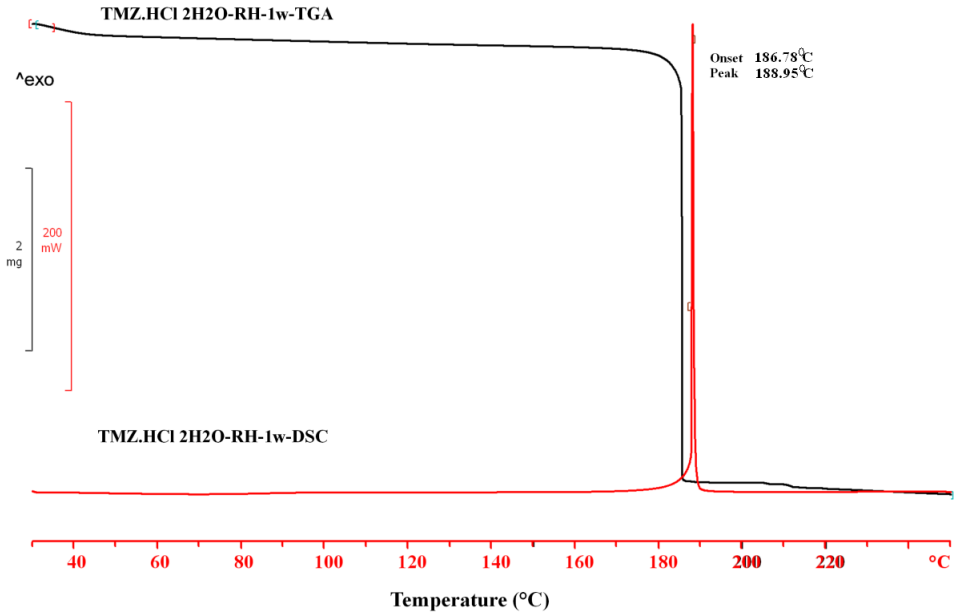

Figure S3 DSC and TGA comparisons of TMZ.HCl dihydrate after keeping the sample in accelerated stability chamber for 1 week gave PXRD pattern that matched with that of neutral temozolomide form 1 (commercial material). The product material has no water (TGA) and shows sharp melting endotherm at 189 ºC (DSC). The melting point of pure temozolomide is 194 ºC (sharp endotherm in DSC).

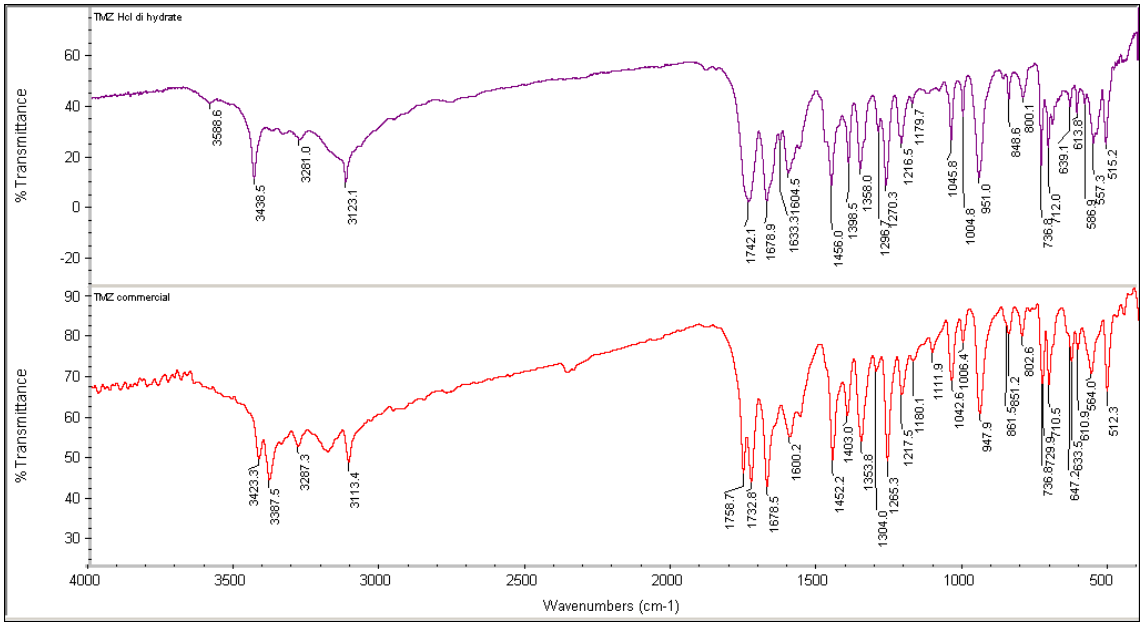

Figure S4 IR spectra (KBr) of TMZ.HCl dihydrate and temozolomide API.