Supporting Information for Synthonic modelling of quercetin and its hydrates: explaining crystallization behaviour in terms of molecular conformation and crystal packing

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1. Optimisation of the Crystal Structures of Quercetin

The crystal structures of QA, QMH and QDH were optimised using the Forcite module in Materials Studio. The SMART algorithm was used and the convergence set to medium. All of the intra- and inter-molecular energies were calculated using the Dreiding forcefield with Gasteiger atomistic charges. The change in the unit cell lengths and angles are shown in Table S1.

Table S 1: Changes in unit cell lengths and angles for the three structures of quercetin when optimised using the Dreiding forcefield

	a	b	c	alpha	beta	gamma
QA	14.7998	11.2379	10.3512	90	90	90
QA opt	14.47376	11.27839	9.500386	90	90	90
%changes	*-2.20298*	*0.360254*	*-8.21947*	*0*	*0*	*0*
QMH	8.737	4.852	30.16	90	95.52	90
QMH opt	8.897072	4.874018	30.57541	90	96.12685	90
%changes	*1.832116*	*0.453792*	*1.377344*	*0*	*0.635312*	*0*
QDH	13.06	16.564	3.725	92.05	94.39	120.55
QDH opt	14.48199	17.21526	3.70578	82.59976	96.57497	124.8246
%changes	*10.88812*	*3.931768*	*-0.51597*	*-10.2664*	*2.314832*	*3.545948*

The maximum unit cell percentage changes were around 10%, suggesting that the Dreiding forcefield reasonably reproduce the experimental crystal structure.