Supplementary ^{1}H ss-NMR data

1. Calculated ^{1}H chemical shifts on the geometrically optimized crystal structure models discussed in the paper: they are calculated from the computed chemical shielding as described in the text. For quercetin dihydrate, (w) denotes water, and the labeling scheme for their protons is included in the corresponding structure files (.cif)

H atom	*Quer1* δ^{calc} (^{1}H) [ppm]	*Quer2* δ^{calc} (^{1}H) [ppm]	*Quer3* δ^{calc} (^{1}H) [ppm]	*Quer dihydrate* δ^{calc} (^{1}H) [ppm]
(O5)H	11.0	12.8	13.0	13.2
(O7)H	2.4	6.8	6.9	7.8
(O3)H	6.7	7.2	7.4	7.0
(O3')H	5.7	5.6	5.7	8.9
(O4')H	7.5	7.8	8.0	9.9
(C6)H	4.9	5.1	5.3	4.7
(C8)H	3.6	4.3	4.5	5.0
(C2')H	5.9	6.2	6.4	5.4
(C5')H	4.7	4.8	5.0	5.1
(C6')H	5.1	5.3	5.5	6.6
(w1)H1	-	-	-	5.6
(w1)H2	-	-	-	4.4
(w2)H1	-	-	-	5.5
(w2)H2	-	-	-	5.2

2. Ultra-fast MAS ^{1}H ss-NMR spectra of the anhydrous (a), and dihydrate (b), forms of quercetin, recorded under homonuclear decoupling by e-DUMBO$_{1\text{-}22}$ pulse sequence, at 60 kHz sample spinning