Supporting information

Hydrogen Bonding Probes of Phenol –OH Groups: Shielding Ranges, Solvent Effects and Temperature Coefficients of ^{1}H NMR Shieldings and –OH Diffusion Coefficients

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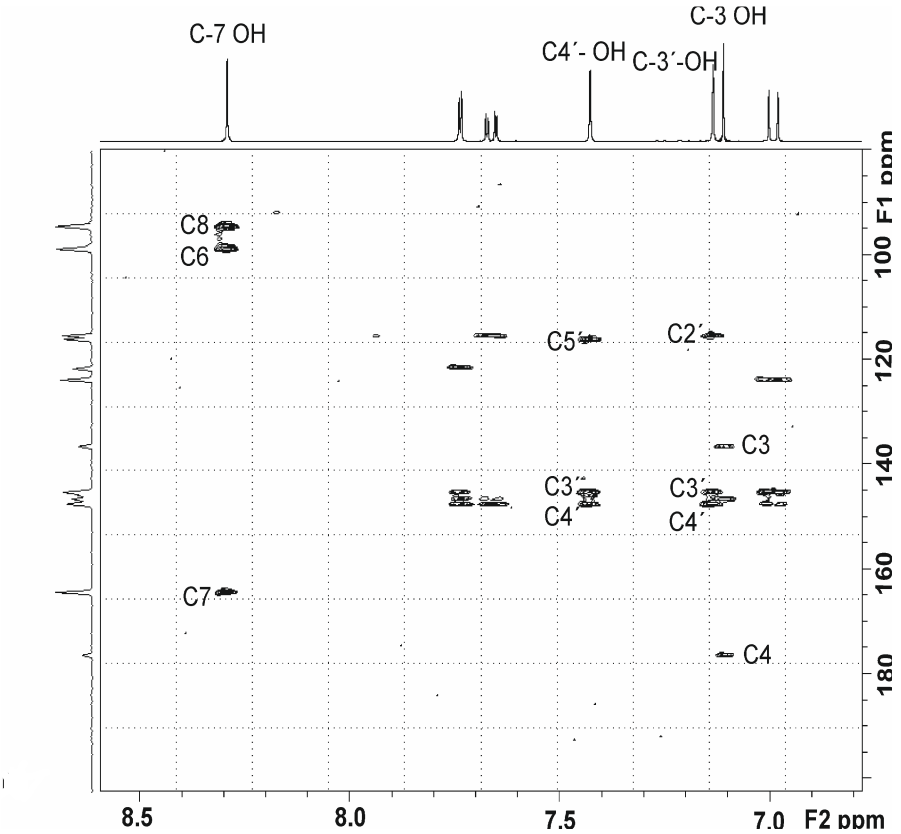
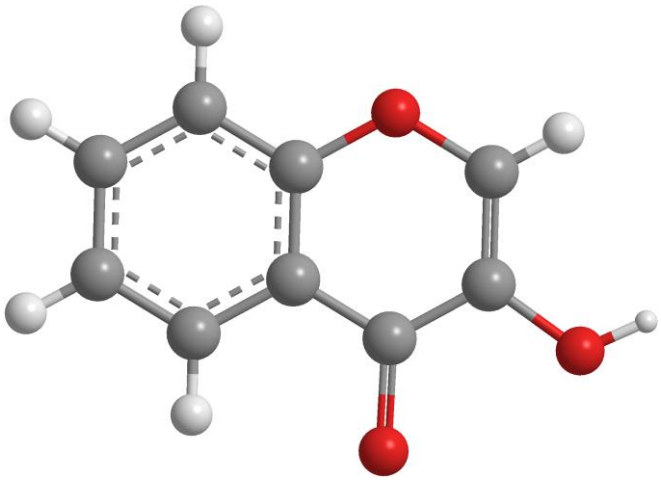


FIGURE S1. 2D ^{1}H - ^{13}C HMBC NMR spectrum (500 MHz) of quercetin, **1**, in CD_3CN, concentration 5 mM, with the presence of 2 μL picric acid, 8 mM in CD_3CN (number of scans = 12, experimental time = 3 h).



SCHEME S1. Structural CSD search query.

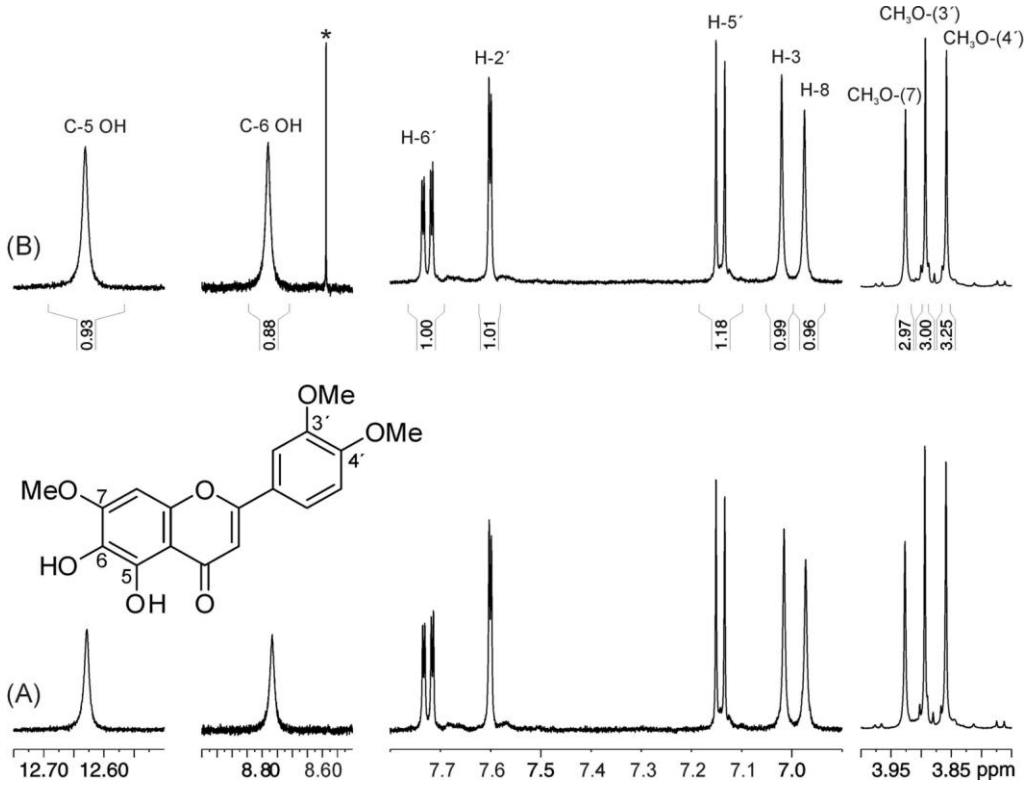


FIGURE S2. Selected regions of 500 MHz ^{1}H NMR of compound, **10**, in 0.5 mL DMSO-d_6 (T = 288 K, number of scans = 256, experimental time = 34 min). (A) without the addition of picric acid, (B) after the addition of 3 μL, 2 mM in DMSO-d_6, solution of picric acid. The peak with the asterisk denotes the absorption of picric acid.

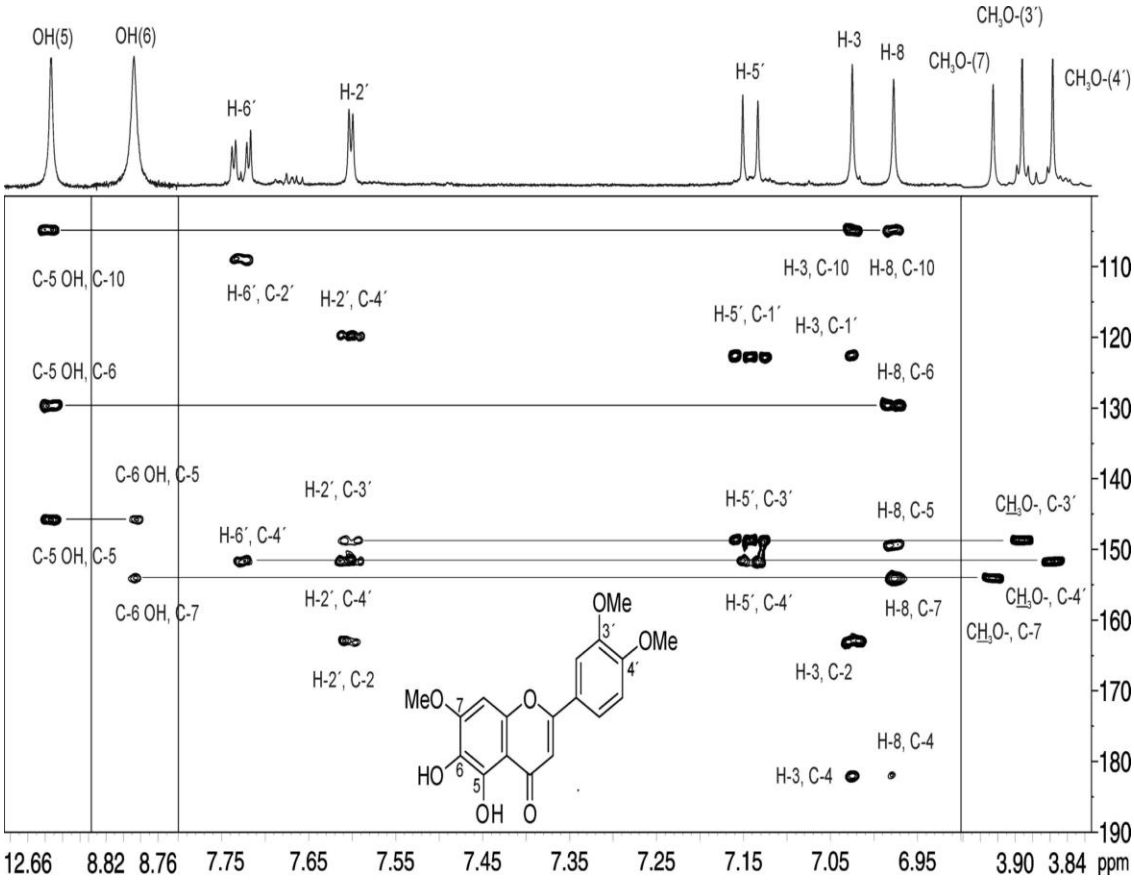


FIGURE S3. Selected regions of a 500 MHz 2D ^{1}H-^{13}C HMBC NMR (T = 288K, number of scans = 120, experimental time = 16 h) of compound, **10**, in 0.5 mL DMSO-d_6, after the addition of 3 μL, 2 mM in DMSO-d_6, solution of picric acid. The common cross-peaks of -OH groups, C-5 OH and C-6 OH, and of the methoxy groups, are demonstrated.

TABLE S1. NMR Spectroscopic Data (500 MHz, DMSO-d_6) for compound **10**.

notation	δ_C	δ_H (J in Hz)
2	163.2	–
3	103.2	7.02, s
4	181.98	–
5	145.69	12.63, s
6	129.62	8.79, s
7	154.04	–
8	90.99	6.97, s
9	149.62	–
10	104.74	–
OMe(7)	56.04	3.93, s
1′	122.5	–
2′	108.91	7.60, d (2.2)
3′	148.64	–
4′	151.64	–
5′	111.3	7.14, d (8.7)
6′	119.7	7.72, dd (2.1, 8.6)

OMe(3´)	55.58	3.89, s
OMe(4´)	55.45	3.89, s

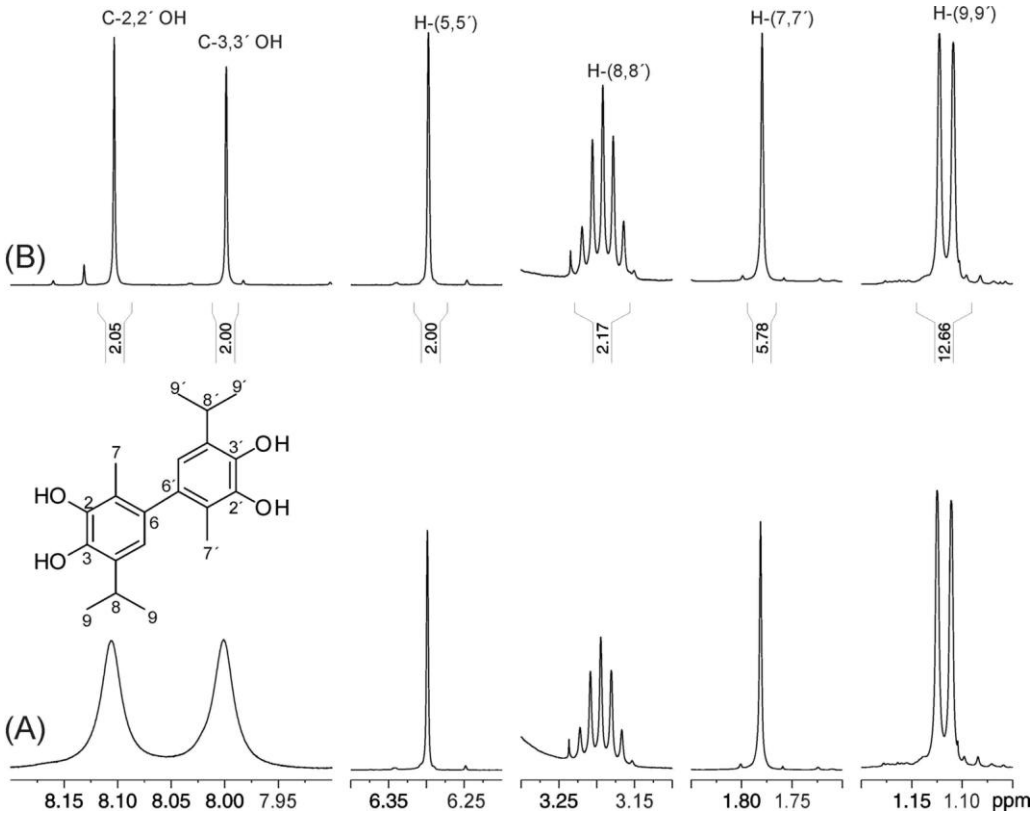


FIGURE S4. Selected regions of 500 MHz ^{1}H NMR of compound, **26**, in 0.5 mL DMSO-d_6 (T = 289 K, number of scans = 128, experimental time = 17 min). (A) without the addition of picric acid, (B) after the addition of 13 μL, 10 mM in DMSO-d_6, solution of picric acid.

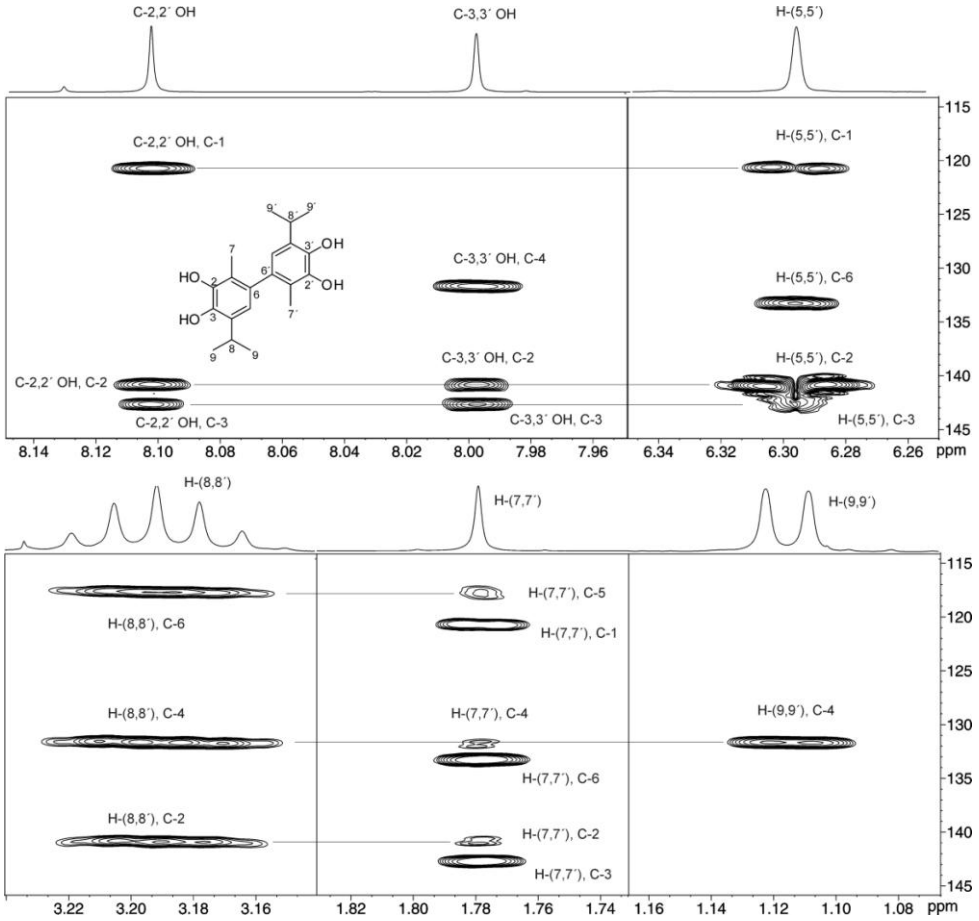


FIGURE S5. Selected areas of 500 MHz 2D ^{1}H-^{13}C HMBC NMR (T= 289 K, number of scans = 76, experimental time = 10 h) of compound, **26**, in 0.5 mL DMSO-d_6, with the addition of 13 μL, 10 mM in DMSO-d_6, solution of picric acid. The common cross-peaks between the OH groups are indicated.

TABLE S2. NMR Spectroscopic Data (500 MHz, DMSO-d_6) for compound **26**.

notation	δ_C	δ_H (J in Hz)
1, 1´	120.65	–
2, 2´	140.95	8.10, s
3, 3´	142.7	8.00, s
4, 4´	131.65	–
5, 5´	117.57	6.30, s
6, 6´	133.30	–
7, 7´	13.47	1.78, s
8, 8´	26.36	3.19, m
9, 9´	22.90	1.12, d (6.9)

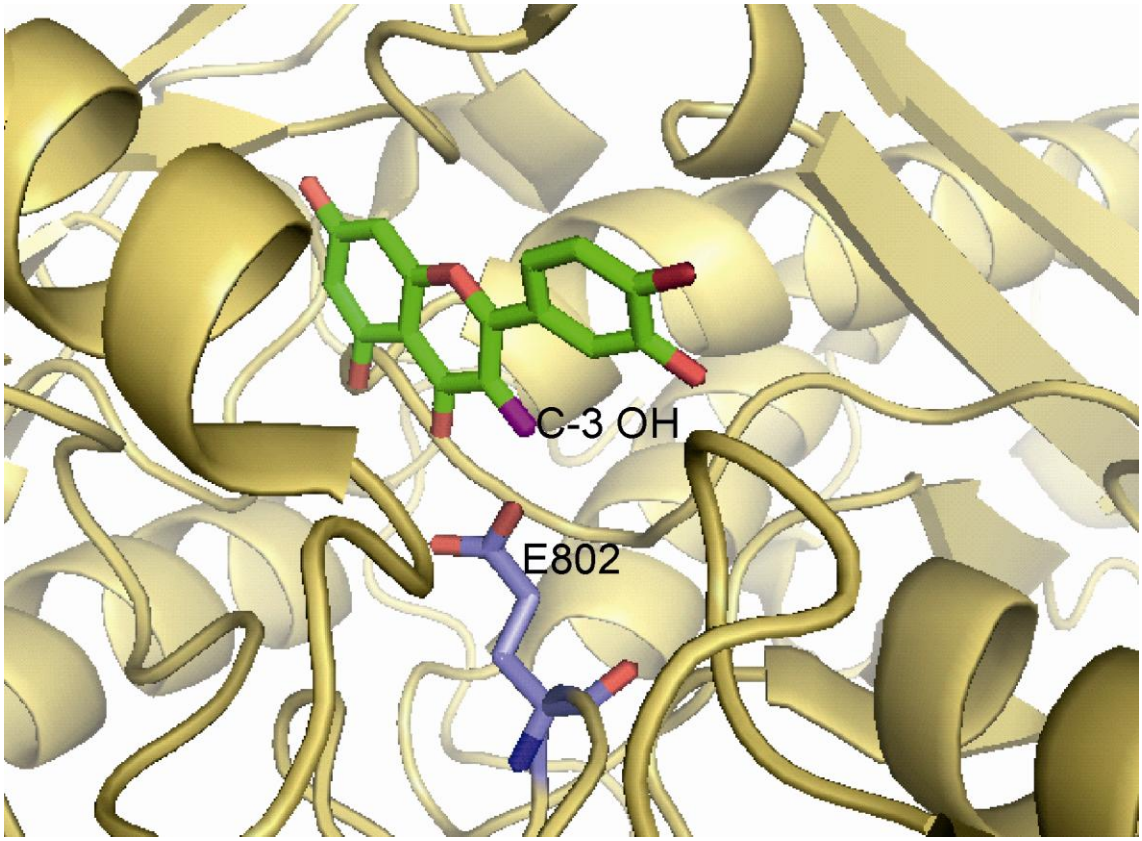


FIGURE S6. X-ray structure of xanthine oxidase in complex with quercetin (pdbid: 3NVY). The C-3 OH of quercetin interacts with the glutamate 802 (E802) of the protein (distance between OE1 of E802 and the C-3 OH was measured to 2.07 Å).