Supplementary Information

Aromas: Lovely to Smell and Nice Solvents for Polyphenols? Curcumin Solubilisation Power of Fragrances and Flavours †

Michael Schmidt [1]*, Verena Huber [2], Didier Touraud [2]and Werner Kunz [2],*

[1] Institute of Materials Resource Management, University of Augsburg, Am Technologiezentrum 8, D-86159 Augsburg, Germany

[2] Institute of Physical and Theoretical Chemistry, University of Regensburg, D-93040 Regensburg, Germany; verena1.huber@chemie.uni-regensburg.de (V.H.); didier.touraud@chemie.uni-regensburg.de (D.T.)

* Correspondence: michael1.schmidt@uni-a.de (M.S.); werner.kunz@chemie.uni-regensburg.de (W.K.)

† This paper is dedicated to Farid Chemat, an outstanding scientist, colleague, and friend. Rest in peace, cher ami.
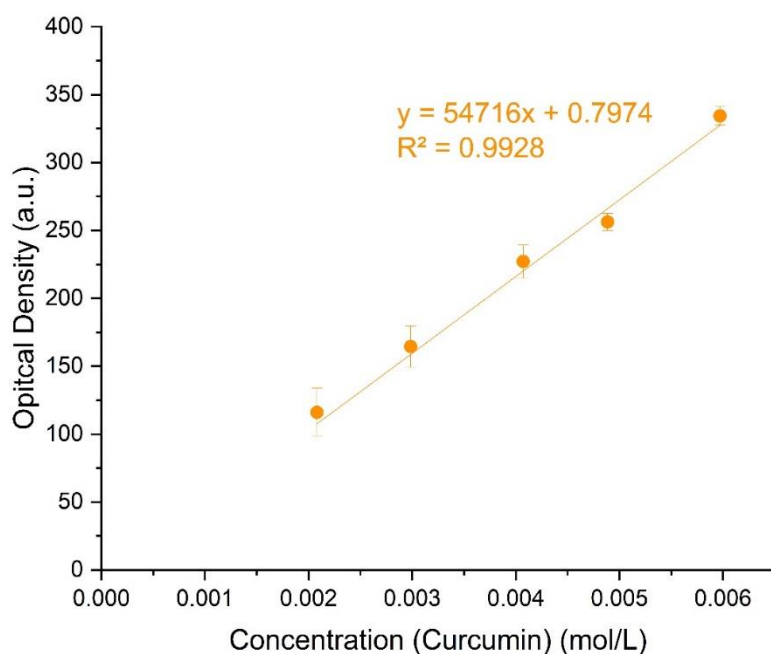
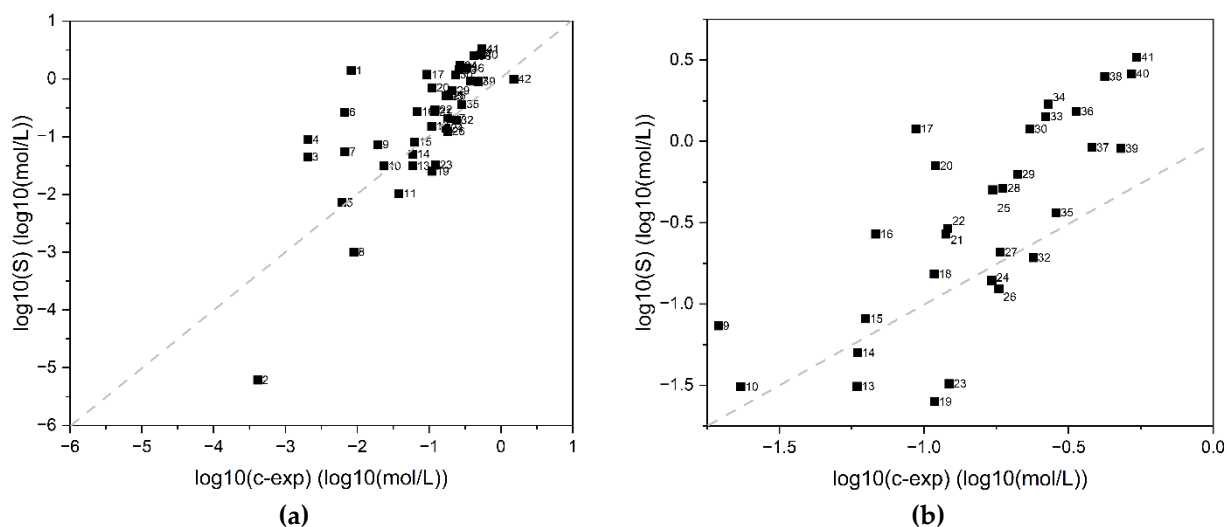**Figure S 1** Calibration curve of curcumin in ethanol at λ=425 nm.

(a)   **(b)**

Figure S 2 Calculated solubility of curcumin log10(S) vs the logarithmic curcumin concentration c(x) in the respective liquid solvents, (a) showing the whole graph, while (b) shows the section between -2<log10(c(x))<0 for better identification of the datapoints. The numbering of labels refers to the list in Table 1. Vanillin and veratraldehyde are excluded due to being solid compounds.
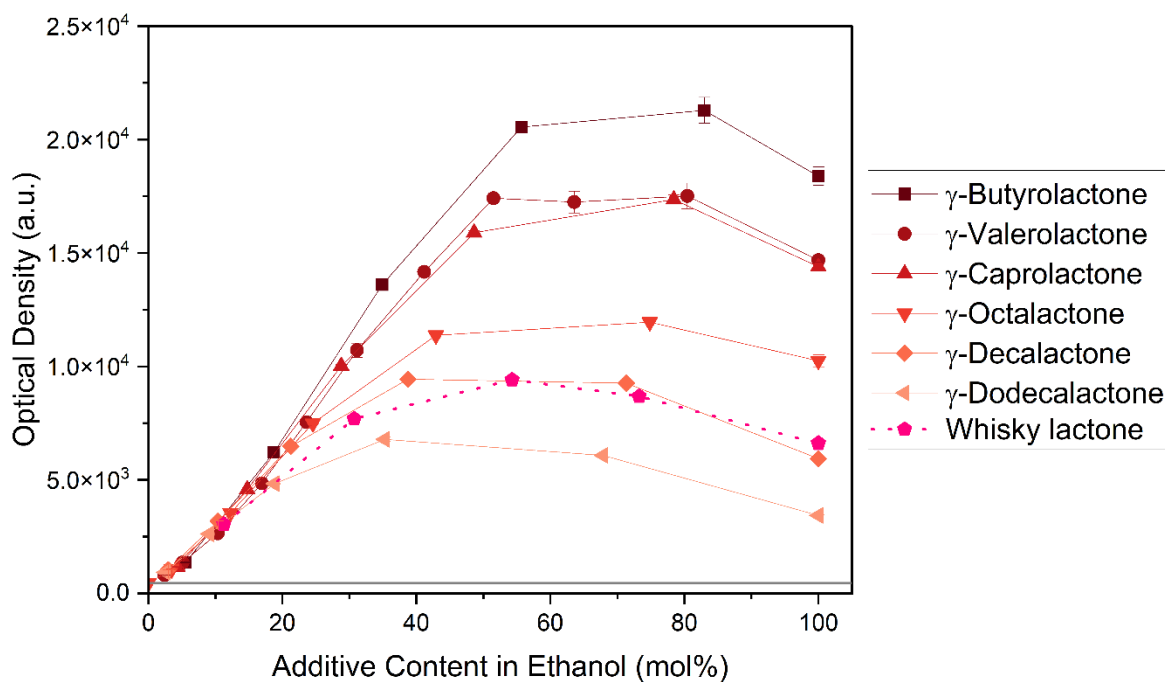

Figure S 3 Optical densities in arbitrary units (a.u.) of curcumin in binary ethanolic mixtures with γ-lactones.
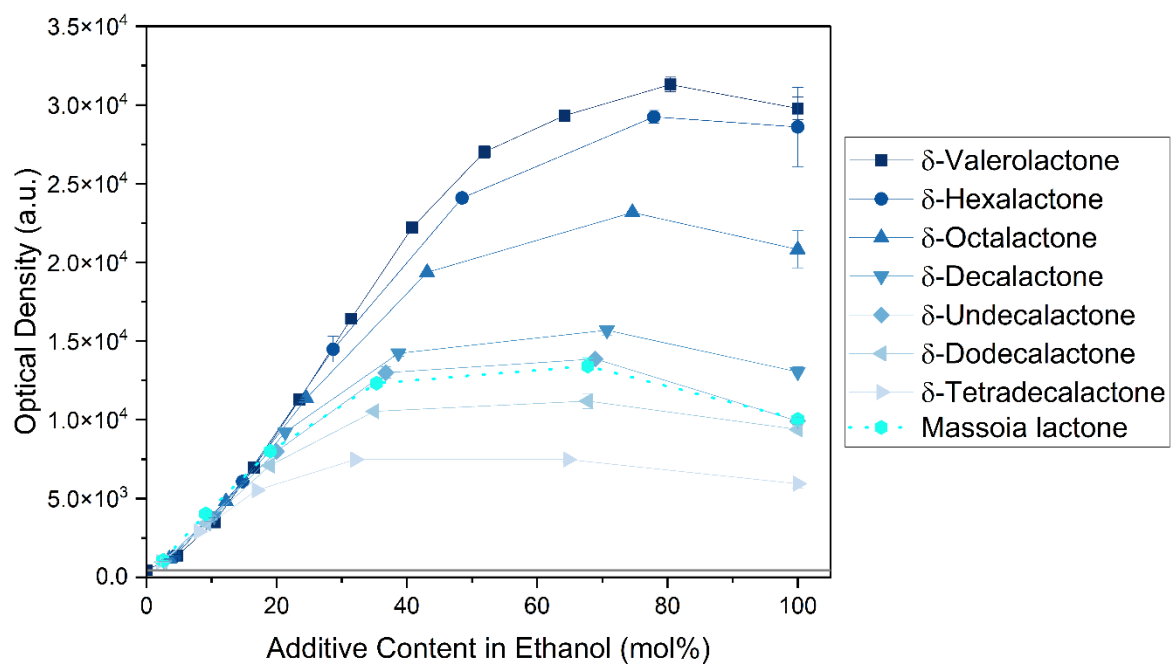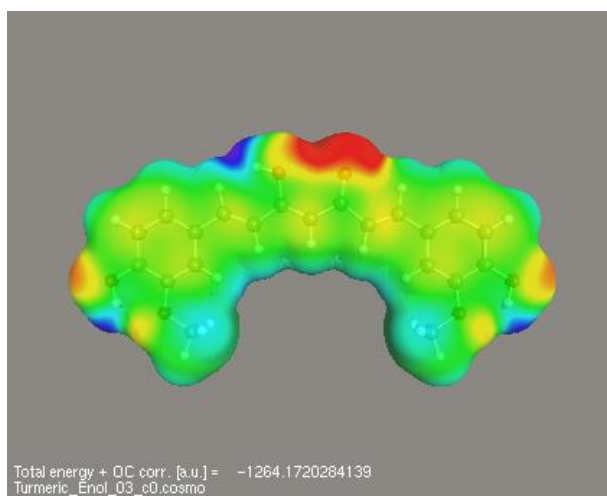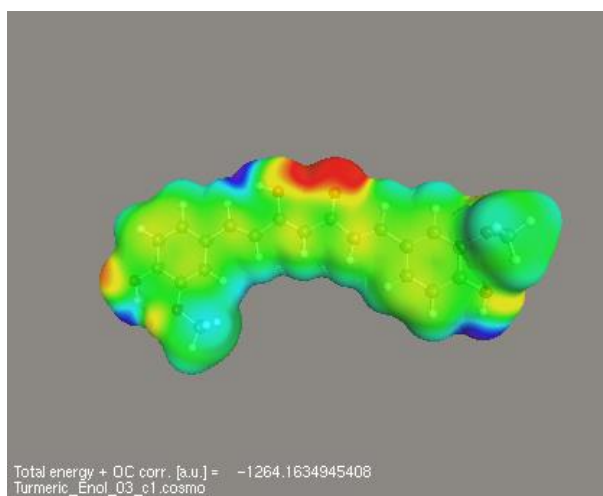
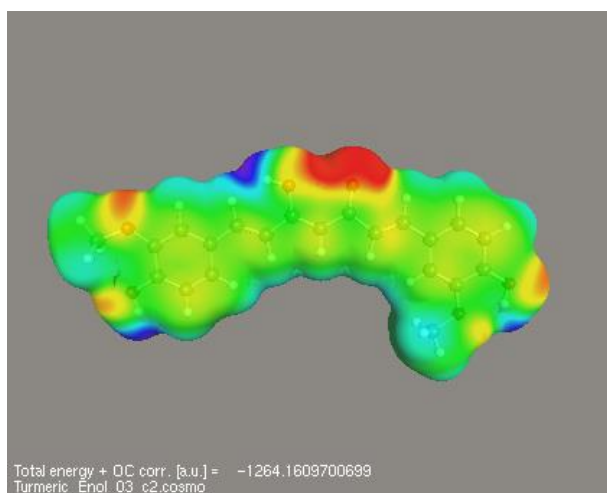**Figure S 4** Optical densities in arbitrary units (a.u.) of curcumin in binary ethanolic mixtures with δ-lactones.

(a)

(b)

Total energy + OC corr. [a.u.] = −1264.1720284139
Turmeric_Enol_03_c0.cosmo

Total energy + OC corr. [a.u.] = −1264.1634945408
Turmeric_Enol_03_c1.cosmo

(c)

(d)

Total energy + OC corr. [a.u.] = −1264.1609700699
Turmeric_Enol_03_c2.cosmo

Total energy + OC corr. [a.u.] = −1264.1550525821
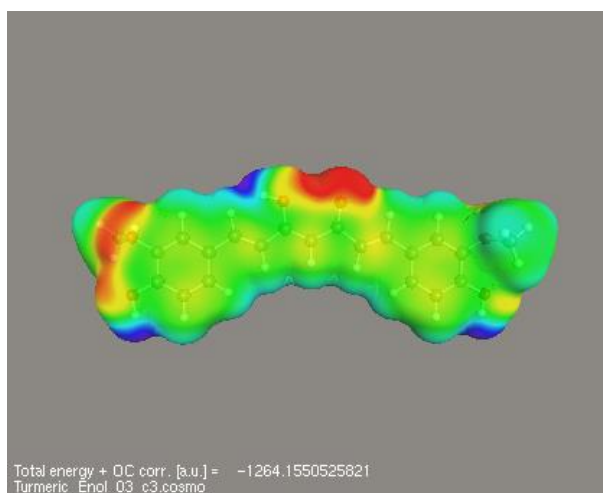Turmeric_Enol_03_c3.cosmo

Figure S 5 COSMO surfaces of the four keto-enol conformers of curcumin, (a) conformer 1, (b) conformer 2, (c) conformer 3, and (d) conformer 4.
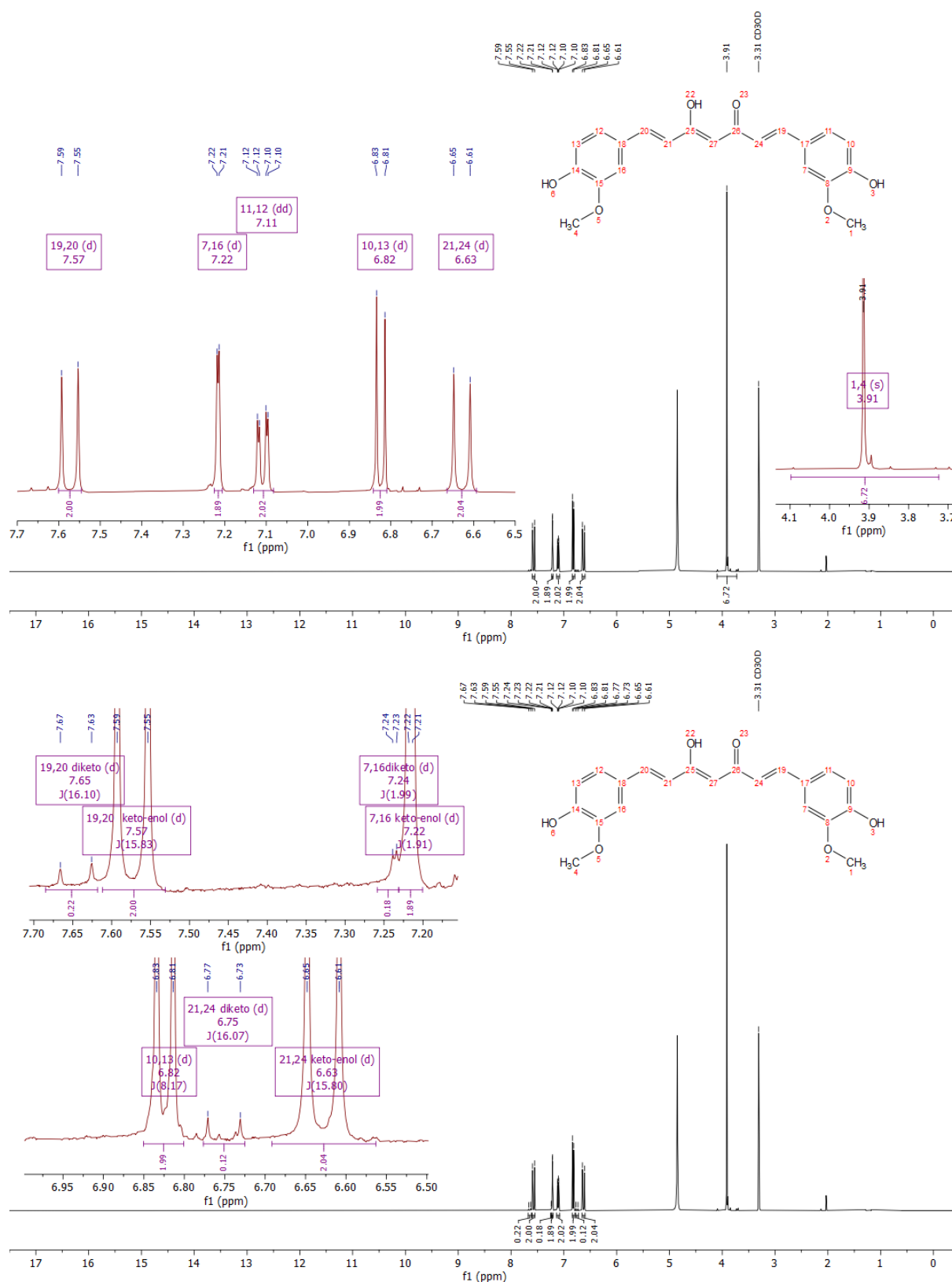
Figure S 6 ^{1}H-NMR spectrum of curcumin in methanol-d4 with assigned signals to the predominant conformer of curcumin (top) and of diketo/keto-enol groups of curcumin (bottom).

Signals of curcumin: δ H (400 MHz, methanol-d4) 3.91 (7 H, s), 6.63 (2 H, d, J 15.8), 6.82 (2 H, d, J 8.2), 7.11 (2 H, dd, J 8.2, 1.9), 7.22 (2 H, d, J 1.9), 7.57 (2 H, d, J 15.8).

Signals of diketo/keto-enol groups of curcumin: δ H (400 MHz, methanol-d4) 6.63 (2 H, d, J 15.8), 6.75 (0 H, d, J 16.1), 6.82 (2 H, d, J 8.2), 7.11 (2 H, dd, J 8.2, 1.9), 7.22 (2 H, d, J 1.9), 7.24 (0 H, d, J 2.0), 7.57 (2 H, d, J 15.8), 7.65 (0 H, d, J 16.1).
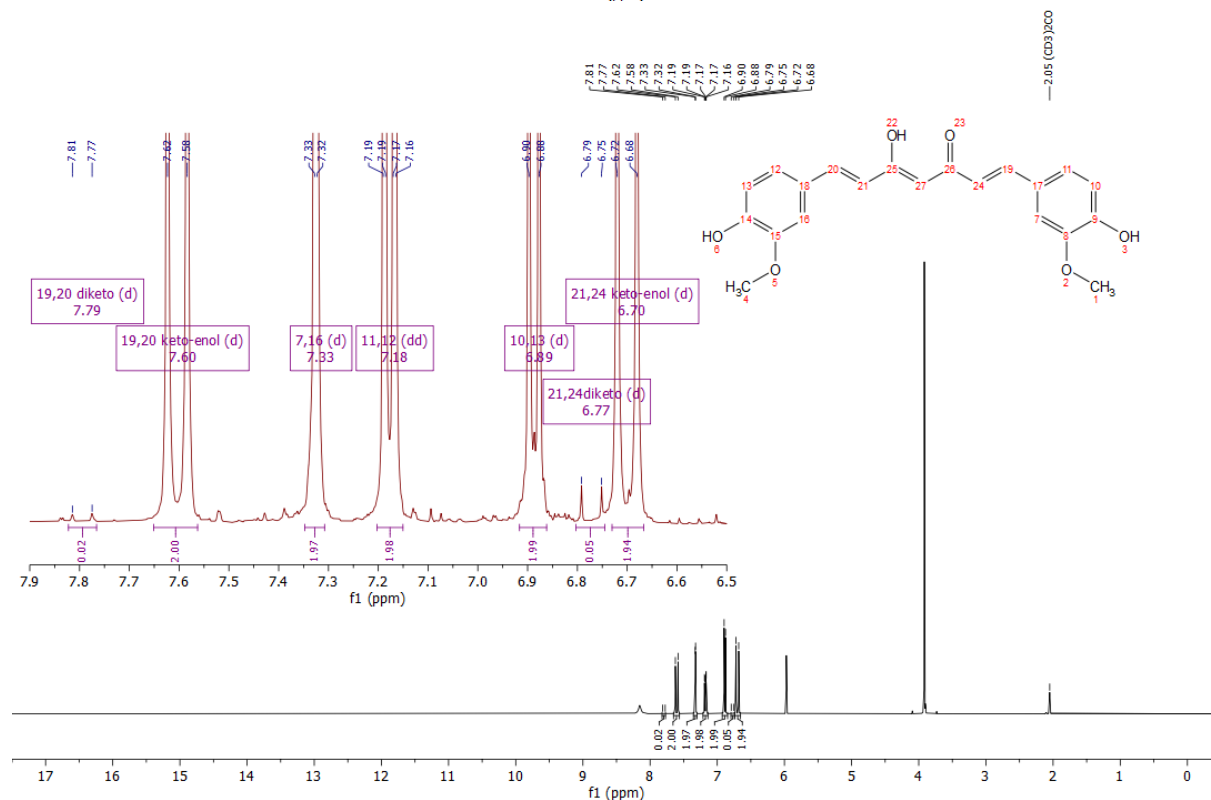

Figure S 7 ^{1}H-NMR spectrum of curcumin in acetone-d6 with assigned signals to the predominant conformer of curcumin (top) and of diketo/keto-enol groups of curcumin (bottom).

Signals of curcumin: δ H (400 MHz, acetone-d6) 3.92 (6 H, s), 5.97 (1 H, s), 6.70 (2 H, d, J 15.8), 6.89 (2 H, d, J 8.2), 7.14 – 7.21 (2 H, m), 7.33 (2 H, d, J 1.9), 7.60 (2 H, d, J 15.8), 8.15 (2 H, s), 16.42 (1 H, s).

Signals of diketo/keto-enol groups of curcumin: δ_H (400 MHz, acetone-d6) 3.92 (6 H, s), 5.97 (1 H, s), 6.70 (2 H, d, J 15.8), 6.77 (0 H, d, J 16.1), 6.89 (2 H, d, J 8.2), 7.18 (2 H, dd, J 8.2, 2.0), 7.33 (2 H, d, J 1.9), 7.60 (2 H, d, J 15.8), 7.79 (0 H, d, J 15.9), 8.15 (2 H, s), 16.42 (1 H, s).

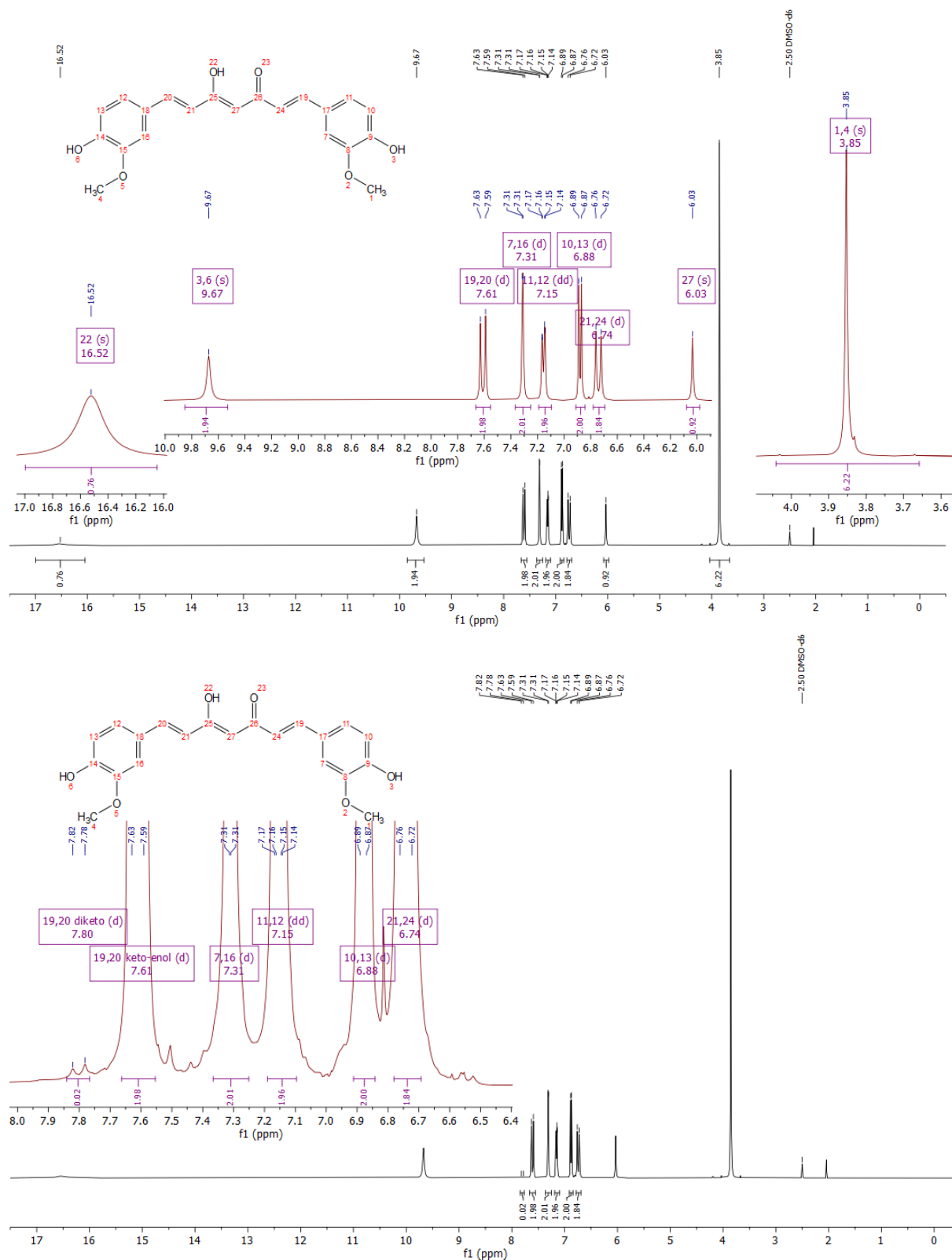**Figure S 8** ^{1}H-NMR spectrum of curcumin in DMSO-d6 with assigned signals to the predominant conformer of curcumin (top) and of diketo/keto-enol groups of curcumin (bottom).

Signals of curcumin: δ$_H$ (400 MHz, DMSO-d6) 3.85 (6 H, s), 6.03 (1 H, s), 6.74 (2 H, d, J 15.7), 6.88 (2 H, d, J 8.1), 7.15 (2 H, dd, J 8.4, 1.8), 7.31 (2 H, d, J 1.9), 7.61 (2 H, d, J 15.6), 9.67 (2 H, s), 16.52 (1 H, s).

Signals of diketo/keto-enol groups of curcumin: δ$_H$ (400 MHz, DMSO-d6) 6.74 (2 H, d, J 15.7), 6.88 (2 H, d, J 8.1), 7.15 (2 H, dd, J 8.4, 1.8), 7.31 (2 H, d, J 1.9), 7.61 (2 H, d, J 15.6), 7.80 (0 H, d, J 15.7).
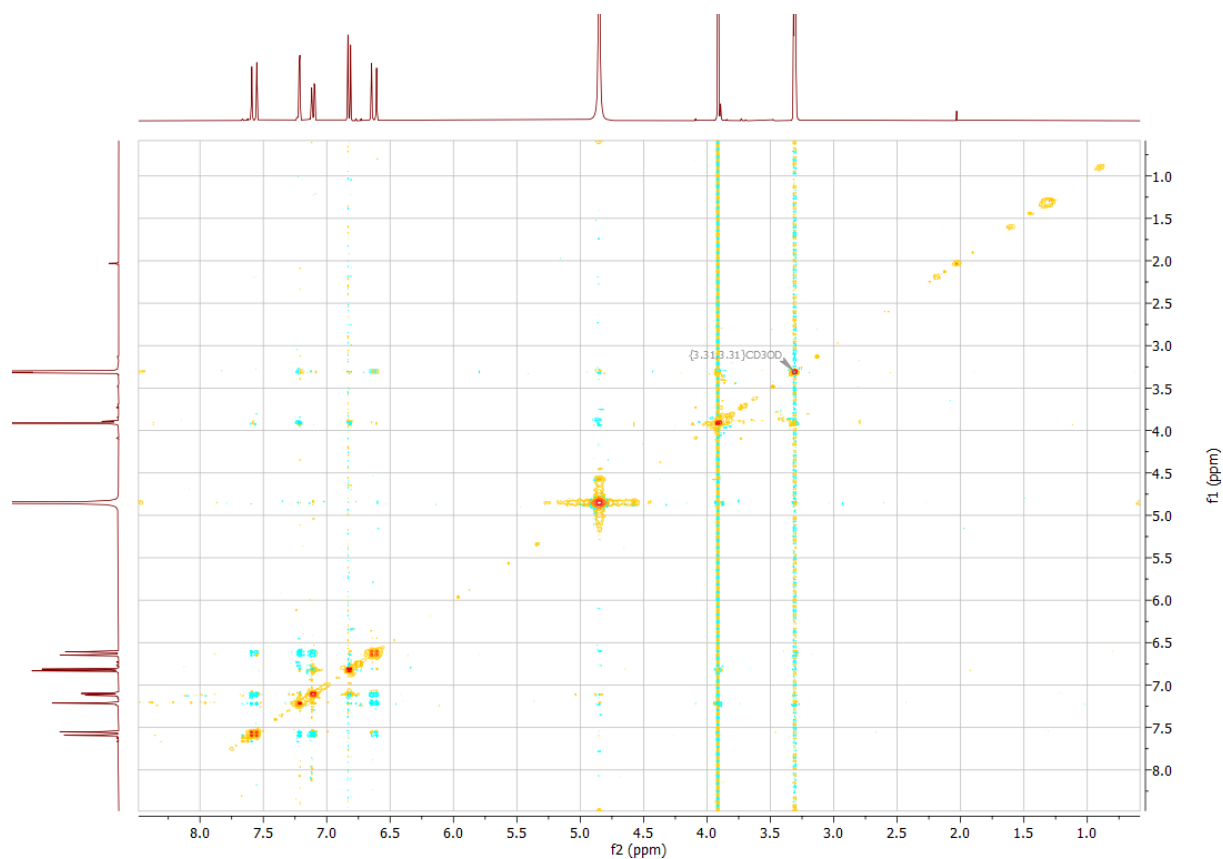

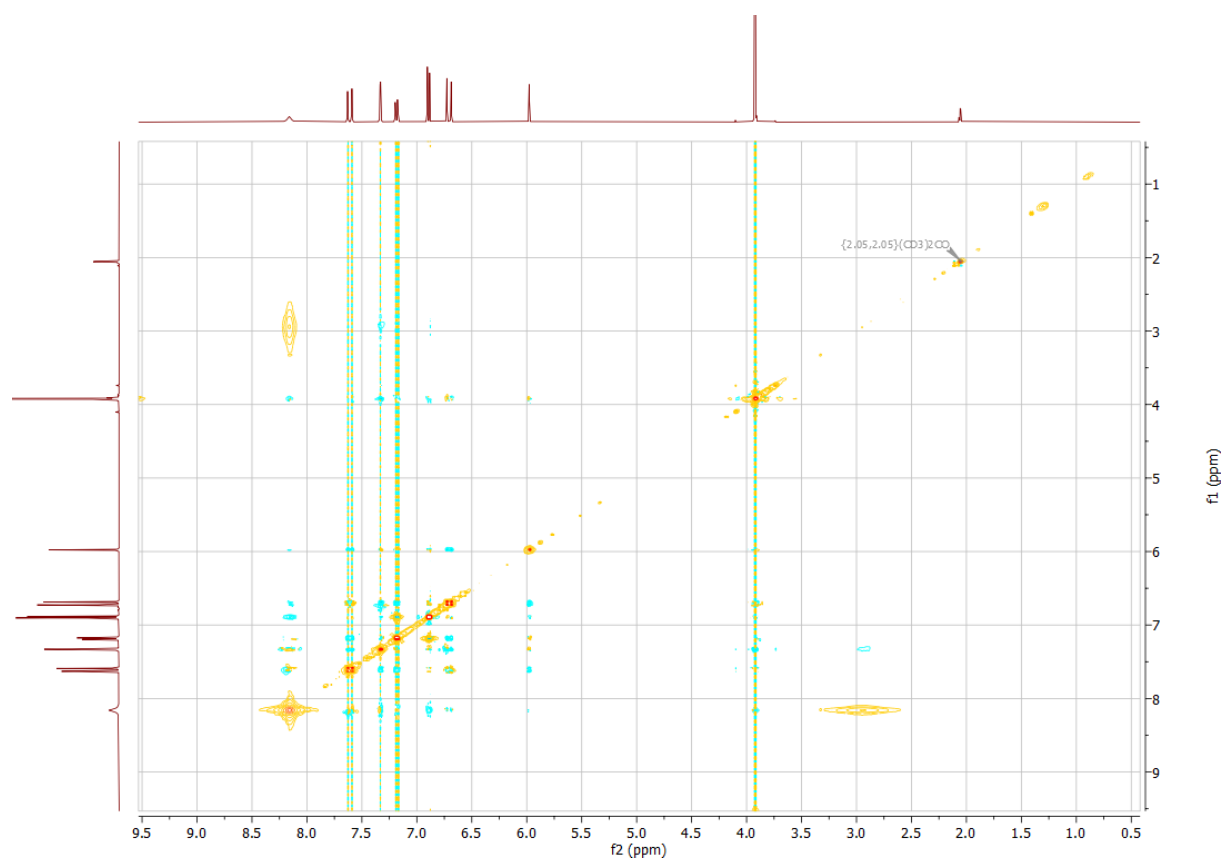**Figure S 9** [1]H-^{1}H NOESY spectrum of curcumin in methanol-d4.

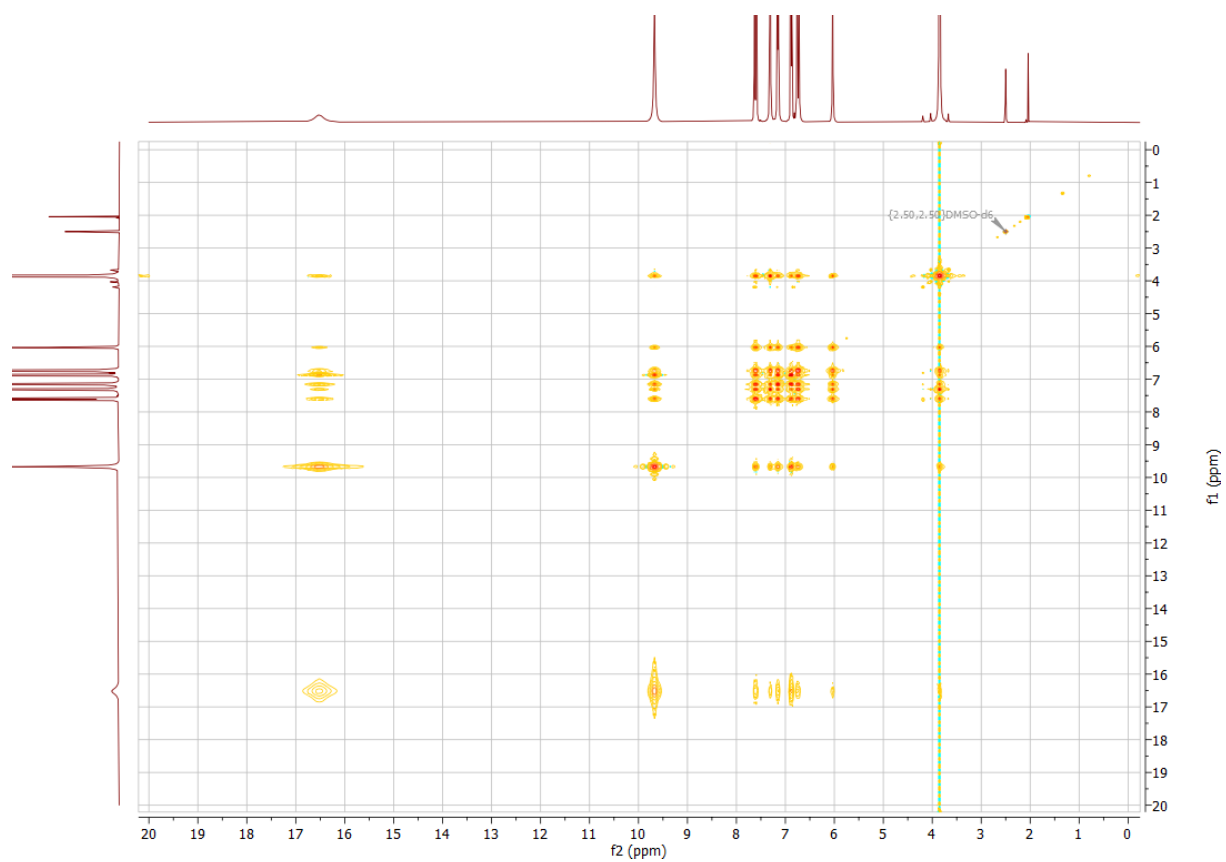**Figure S 10** ¹H-¹H NOESY spectrum of curcumin in acetone-d6.

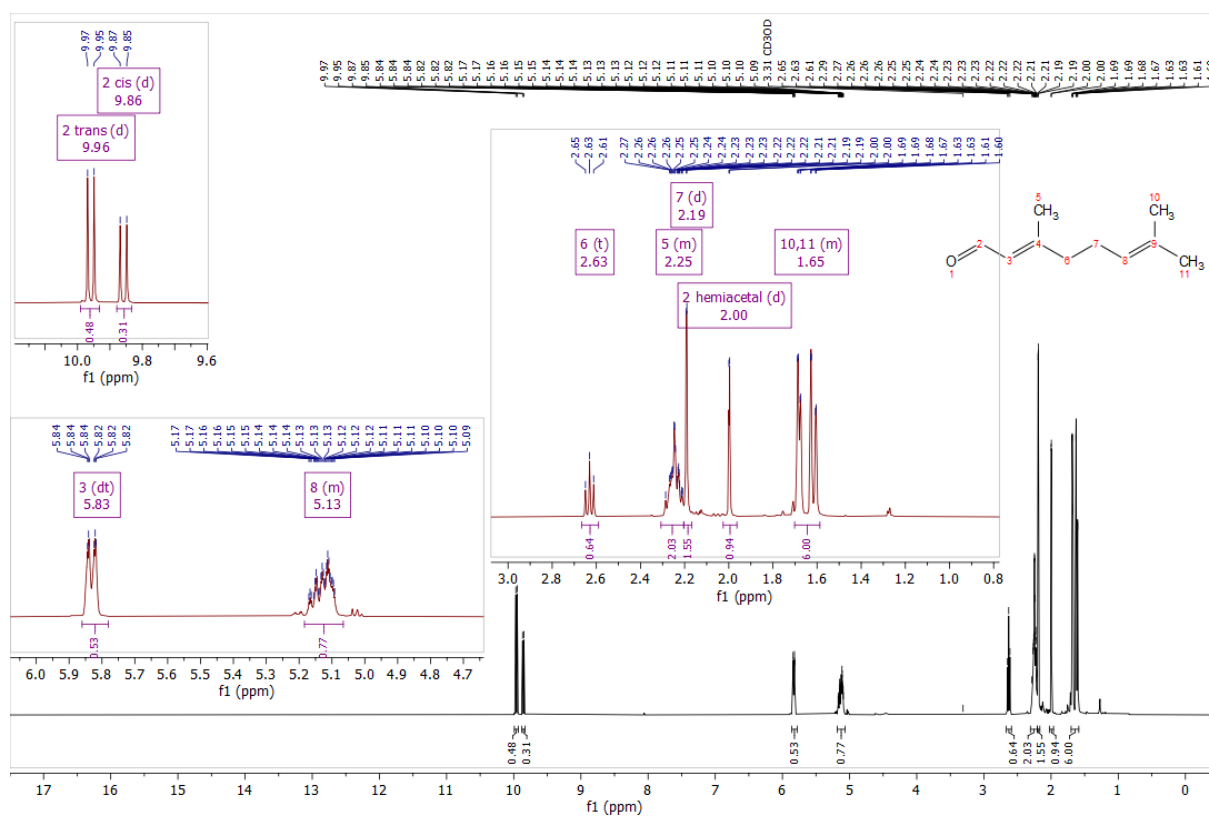**Figure S 11** ¹H-¹H NOESY spectrum of curcumin in DMSO-d6.

Figure S 12 ^{1}H NMR spectrum of citral in methanol-d4.

Signals of citral: δ_H (400 MHz, methanol-d4) 1.59 – 1.70 (6 H, m), 2.00 (1 H, d, J 1.4), 2.19 (2 H, d, J 1.4), 2.20 – 2.31 (2 H, m), 2.63 (1 H, t, J 7.4), 5.07 – 5.18 (1 H, m), 5.83 (1 H, dt, J 8.1, 1.3), 9.86 (0 H, d, J 8.2), 9.96 (0 H, d, J 8.0).
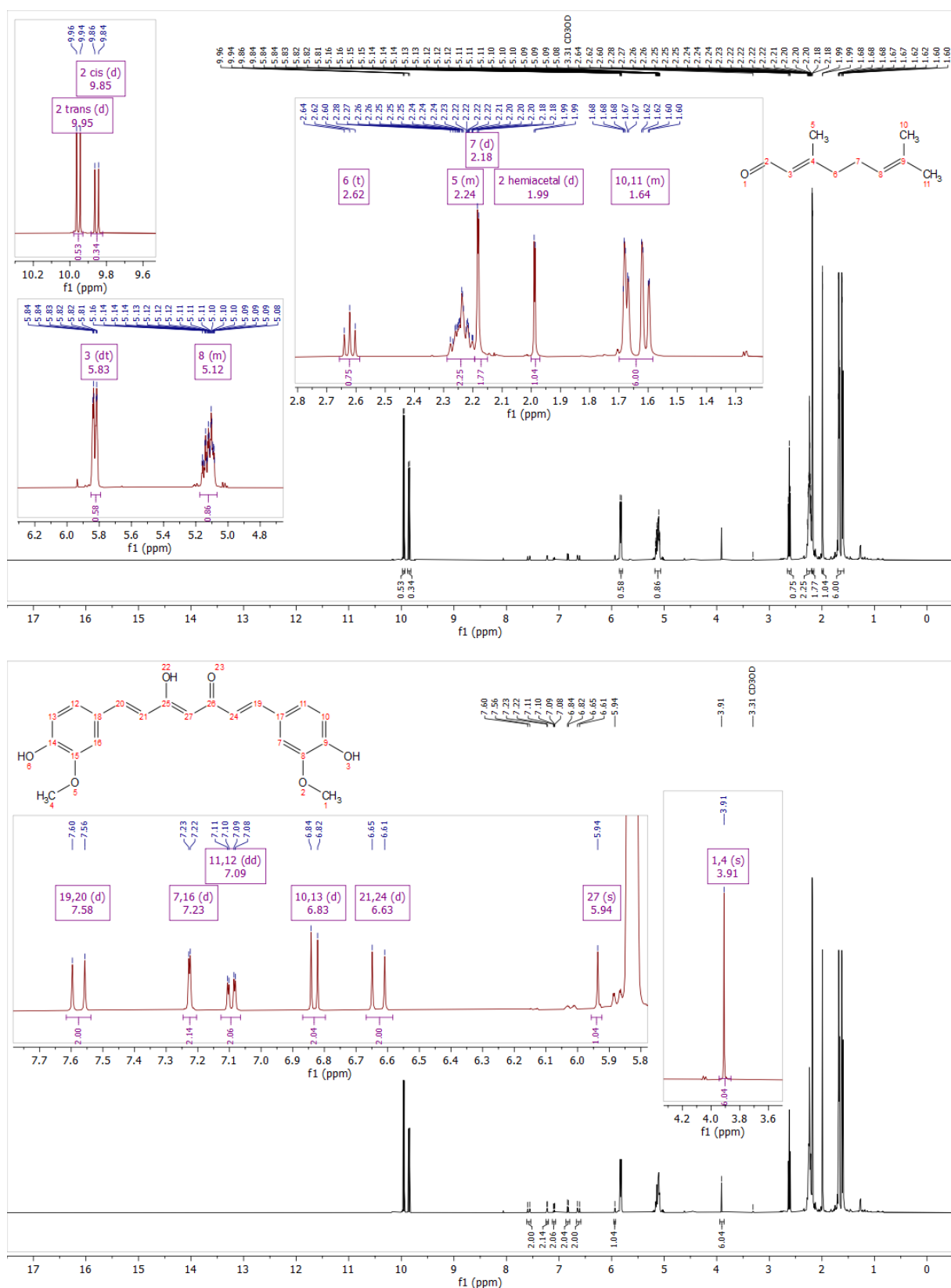
Figure S 13 ¹H NMR spectrum of curcumin in citral/methanol-d4 (30/70) (n/n) with assigned signals of citral (top) and of curcumin (bottom).

Signals of citral: δ ₕ (400 MHz, methanol-d4) 1.58 – 1.70 (6 H, m), 1.99 (1 H, d, J 1.4), 2.18 (2 H, d, J 1.5), 2.19 – 2.29 (2 H, m), 2.62 (1 H, t, J 7.4), 5.07 – 5.17 (1 H, m), 5.83 (1 H, dt, J 8.0, 1.3), 9.85 (0 H, d, J 8.1), 9.95 (1 H, d, J 8.0).

Signals of curcumin: δ H (400 MHz, methanol-d4) 3.91 (6 H, s), 5.94 (1 H, s), 6.63 (2 H, d, *J* 15.8), 6.83 (2 H, d, *J* 8.2), 7.09 (2 H, dd, *J* 8.3, 1.9), 7.23 (2 H, d, *J* 2.0), 7.58 (2 H, d, *J* 15.7).
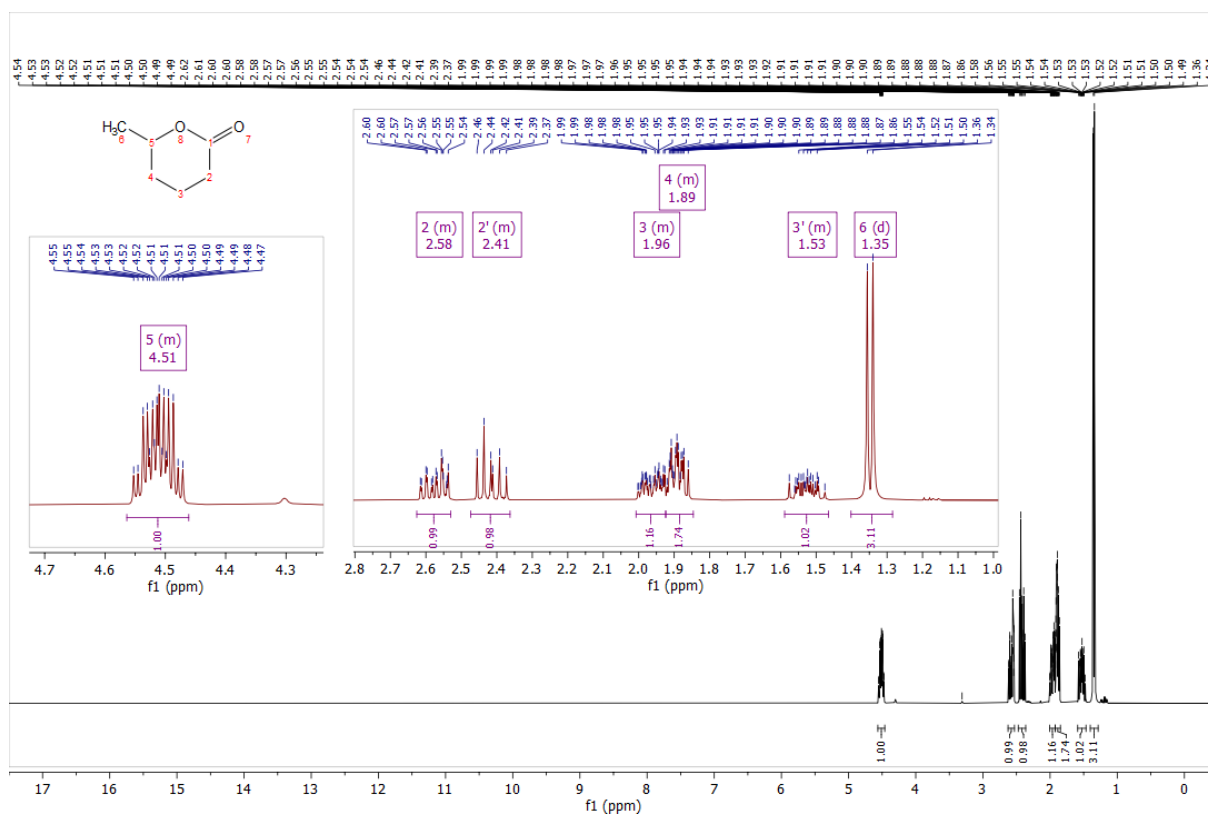

Figure S 14 ¹H NMR of delta-hexalactone in methanol-d4.

δ H (400 MHz, methanol-d4) 1.35 (3 H, d, *J* 6.4), 1.47 – 1.59 (1 H, m), 1.85 – 1.92 (2 H, m), 1.92 – 2.01 (1 H, m), 2.36 – 2.47 (1 H, m), 2.53 – 2.63 (1 H, m), 4.46 – 4.56 (1 H, m).
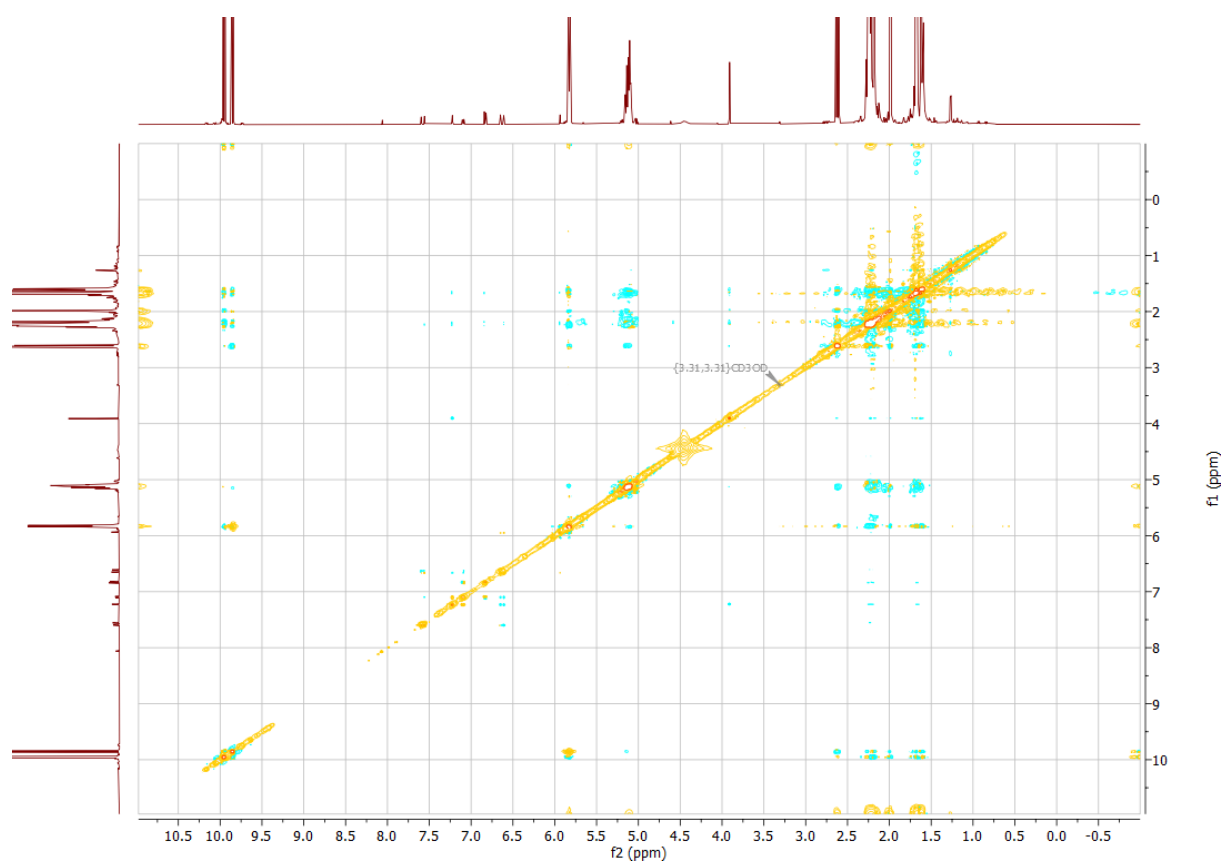
Figure S 15 ^{1}H spectrum of curcumin in delta-hexalactone/methanol-d4 (30/70) (n/n) with assigend signals of delta-hexalactone (top) and of curucmin (bottom).

δ H (400 MHz, methanol-d4) 1.32 (3 H, d, *J* 6.4), 1.42 – 1.55 (1 H, m), 1.80 – 1.90 (2 H, m), 1.90 – 1.96 (1 H, m), 2.32 – 2.45 (1 H, m), 2.49 – 2.61 (1 H, m), 4.40 – 4.52 (1 H, m).

δ H (400 MHz, methanol-d4) 3.93 (6 H, s), 6.03 (1 H, s), 6.72 (2 H, d, *J* 15.8), 6.86 (2 H, d, *J* 8.2), 7.16 (2 H, dd, *J* 8.3, 1.9), 7.29 (2 H, d, *J* 1.9), 7.61 (2 H, d, *J* 15.8), 9.07 (0 H, s).

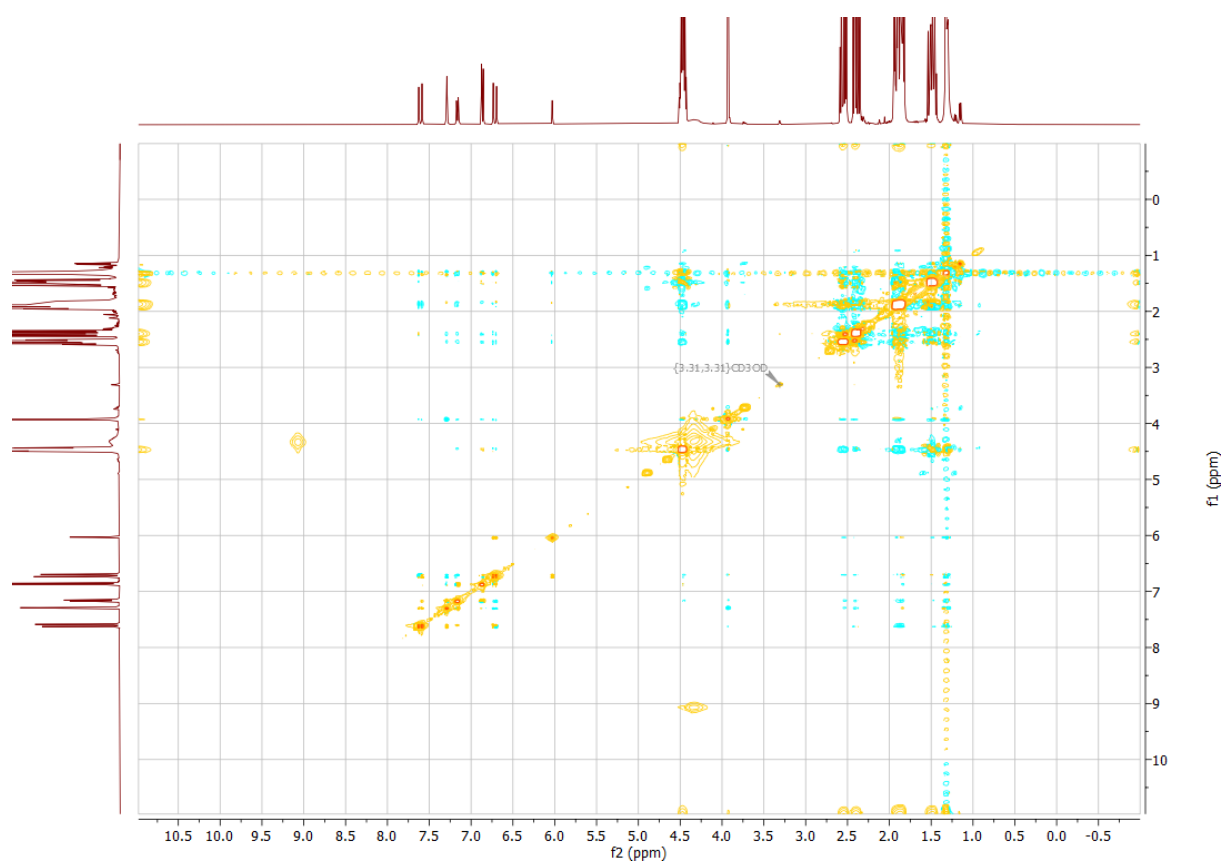**Figure S 16** ¹H-¹H NOESY spectrum of curcumin in citral/methanol-d4 (30/70) (n/n).

Figure S 17 ¹H-¹H NOESY spectrum of curcumin in delta-hexalactone/methanol-d4 (30/70) (n/n).