Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information for

Solvation of a chiral carboxylic acid: Effects of hydrogen bonding on the IR and VCD spectra of α-Methoxyphenylacetic acid

Karoline Bünnemann, Christian Merten*

Organic Chemistry 2, Ruhr-University Bochum, 44801 Bochum, Germany.

Contents

1. Concentration dependent IR spectra

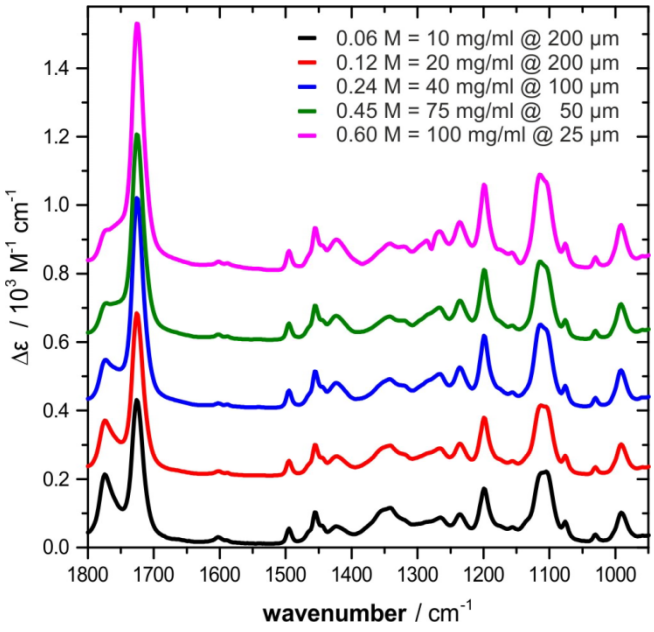


Figure S1. Concentration dependent IR spectra of MPAA in chloroform-d_1

2. Conformational analysis

2.1 Chloroform-d_1

Table S1. Geometries, zero-point-corrected electronic and Gibbs free energies and the corresponding Boltzmann populations of MPAA calculated within the **IEFPCM of chloroform**

	B3LYP / 6-311++G(2d,p) / IEFPCM						**B3LYP-GD3 / 6-311++G(2d,p) / IEFPCM**			
	α	**β**	**ΔE_{ZPC} [a)]**	**ΔG_{298K} [a)]**	**popΔE**	**popΔG**	**ΔE_{ZPC} [b)]**	**ΔG_{298K} [b)]**	**popΔE**	**popΔG**
	[deg]	[deg]	[kcal/mol]	[kcal/mol]	[%]	[%]	[kcal/mol]	[kcal/mol]	[%]	[%]
c1	166.2	99.0	0.00	0.00	44.1	45.7	0.00	0.14	37.2	29.1
c2	72.0	103.6	0.39	0.45	22.9	21.3	0.18	0.00	27.6	36.8
c3	167.7	-86.9	0.45	0.45	20.8	21.3	0.38	0.40	19.5	18.9
c4	72.9	-85.1	0.79	0.83	11.6	11.3	0.60	0.60	13.4	13.4
c5	-51.6	118.8	2.59	2.90	0.6	0.3	1.73	1.91	2.0	1.5
c6	-54.5	-47.2	3.58	3.63	0.1	0.1	2.78	2.76	0.3	0.3

[a)] Reference to E_h(c1)= -574.66133 hartree and G_h(c1) = -574.69993 hartree
[b)] Reference to E_h(c1)= -574.6792 hartree and G_h(c2) = -574.71761hartree

Table S2. Geometries, zero-point-corrected electronic and Gibbs free energies and the corresponding Boltzmann populations of the 10 most populated dimeric structures $(MPAA)_2$ calculated within the **IEFPCM of chloroform**

	B3LYP / 6-311++G(2d,p) / IEFPCM				**B3LYP-GD3 / 6-311++G(2d,p) / IEFPCM**			
	ΔE_{ZPC} [a)] [kcal/mol]	**ΔG_{298K} [a)]** [kcal/mol]	**popΔE** [%]	**popΔG** [%]	**ΔE_{ZPC} [b)]** [kcal/mol]	**ΔG_{298K} [b)]** [kcal/mol]	**popΔE** [%]	**popΔG** [%]
d11	0.00	0.00	24.8	23.1	0.00	0.00	20.67	19.44
d13	0.29	0.50	15.2	9.9	0.24	0.39	13.82	10.08
d12	0.32	0.33	14.4	13.2	0.20	0.24	14.72	12.99
d14	0.59	0.01	9.1	22.6	0.52	0.13	8.58	15.56
d22	0.65	0.75	8.3	6.5	0.43	0.41	10.05	9.76
d23	0.65	0.98	8.2	4.4	0.54	0.74	8.31	5.57
d33	0.68	0.47	7.9	10.4	0.63	0.80	7.09	5.01
d24	1.00	1.07	4.6	3.8	0.83	0.66	5.05	6.39
d34	1.03	1.04	4.4	4.0	0.83	0.77	5.09	5.26
d44	1.41	1.73	2.3	1.3	1.07	0.77	3.38	5.28

[a)] Reference to E_h(d11)= -1149.3405 hartree and G_h(d11) = -1149.39933 hartree
[b)] Reference to E_h(d11)= -1149.38127 hartree and G_h(d11) = -1149.43971 hartree

2.2 DMSO-d_6

Table S3. Geometries, zero-point-corrected electronic and Gibbs free energies and the corresponding Boltzmann populations of MPAA calculated within the **IEFPCM of DMSO**

	B3LYP / 6-311++G(2d,p) / IEFPCM						**B3LYP-GD3 / 6-311++G(2d,p) / IEFPCM**			
	α	**β**	**ΔE_{ZPC}** [a]	**ΔG_{298K}** [a]	**popΔE**	**popΔG**	**ΔE_{ZPC}** [b]	**ΔG_{298K}** [b]	**popΔE**	**popΔG**
	[deg]	[deg]	[kcal/mol]	[kcal/mol]	[%]	[%]	[kcal/mol]	[kcal/mol]	[%]	[%]
c1	166.2	99.0	0.00	0.00	44.7	42.4	0.00	0.00	37.24	38.40
c2	72.1	103.8	0.25	0.18	29.2	31.5	0.06	0.05	33.85	35.28
c3	167.7	-86.7	0.61	0.63	16.0	14.5	0.50	0.58	15.95	14.33
c4	72.9	-84.8	0.91	0.78	9.6	11.3	0.72	0.76	11.01	10.65
c5	-51.6	119.1	2.75	2.99	0.4	0.3	1.86	2.11	1.60	1.08
c6	-54.5	-47.1	3.57	3.56	0.1	0.1	2.77	2.97	0.34	0.25

[a] Reference to E_h(c1)= -574.66468 hartree and G_h(c1) = -574.70321 hartree
[b] Reference to E_h(c1)= -574.6825 hartree and G_h(c1) = -574.721 hartree

Table S4. Geometries, zero-point-corrected electronic and Gibbs free energies and the corresponding Boltzmann populations of **monosolvated MPAA-DMSO** calculated within the **IEFPCM of DMSO**

	B3LYP / 6-311++G(2d,p) / IEFPCM				**B3LYP-GD3 / 6-311++G(2d,p) / IEFPCM**			
	ΔE_{ZPC} [a]	**ΔG_{298K}** [a]	**popΔE**	**popΔG**	**ΔE_{ZPC}** [b]	**ΔG_{298K}** [b]	**popΔE**	**popΔG**
	[kcal/mol]	[kcal/mol]	[%]	[%]	[kcal/mol]	[kcal/mol]	[%]	[%]
bifurcated MPAA-DMSO					**bifurcated MPAA-DMSO**			
c1	0.00	0.26	28.29	16.92	0.04	0.00	19.99	38.64
c2	0.20	0.56	20.15	10.18	0.19	0.37	15.39	20.81
c3	0.53	0.91	11.49	5.68	0.55	0.69	8.50	11.99
c4	0.82	0.91	7.13	5.68	0.82	0.91	5.39	8.37
c5	2.90	3.55	0.21	0.07	2.11	2.73	0.61	0.39
c6	3.63	4.38	0.06	0.02	2.82	3.37	0.18	0.13
linear MPAA-DMSO					**angled MPAA-DMSO**			
c1	0.40	0.00	14.51	26.41	0.00	0.94	21.37	7.85
c2	0.62	0.04	9.91	24.52	0.13	1.04	17.29	6.70
c3	1.00	0.77	5.25	7.17	0.67	1.57	6.95	2.72
c4	1.36	1.26	2.84	3.14	0.97	1.77	4.18	1.94
c5	3.20	3.07	0.13	0.15	n/a [c]			
c6	3.98	3.58	0.03	0.06	2.99	2.62	0.14	0.46

[a] Reference to E_h(c1-bifurcated)= -1127.91603 hartree and G_h(c1-linear) = -1127.96747 hartree
[b] Reference to E_h(c1-angled)= -1127.9452 hartree and G_h(c1-bifurcated) = -1127.995704 hartree
[c] angled form of c3-DMSO does not exist due to steric reasons

2.3 ACN-d_3

Table S5. Geometries, zero-point-corrected electronic and Gibbs free energies and the corresponding Boltzmann populations of MPAA calculated within the **IEFPCM of acetonitrile**

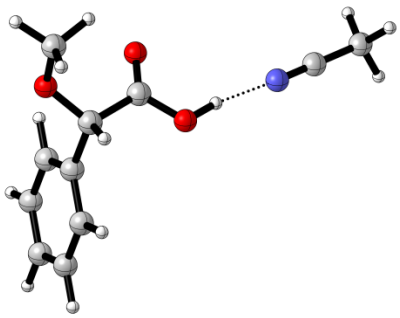
	B3LYP / 6-311++G(2d,p) / IEFPCM						B3LYP-GD3 / 6-311++G(2d,p) / IEFPCM			
	α [deg]	**β** [deg]	**ΔE_{ZPC}** [a)] [kcal/mol]	**ΔG_{298K}** [a)] [kcal/mol]	**popΔE** [%]	**popΔG** [%]	**ΔE_{ZPC}** [b)] [kcal/mol]	**ΔG_{298K}** [b)] [kcal/mol]	**popΔE** [%]	**popΔG** [%]
c1	166.2	99.0	0.00	0.00	44.6	42.2	0.00	0.00	37.4	39.4
c2	72.0	103.6	0.26	0.18	28.9	31.3	0.06	0.07	33.6	35.0
c3	167.7	-86.9	0.60	0.61	16.3	14.9	0.50	0.61	16.0	13.9
c4	72.9	-85.1	0.90	0.78	9.7	11.2	0.72	0.79	11.0	10.4
c5	-51.6	118.8	2.75	2.97	0.4	0.3	1.86	2.13	1.6	1.1
c6	-54.5	-47.2	3.57	3.56	0.1	0.1	2.78	3.01	0.3	0.2

[a)] Reference to E_h(c1)= -574.66454 hartree and G_h(c1) = -574.70306 hartree
[b)] Reference to E_h(c1)= -574.68237 hartree and G_h(c1) = -574.72091hartree

Table S6. Geometries, zero-point-corrected electronic and Gibbs free energies and the corresponding Boltzmann populations of **ACN-monosolvated** MPAA calculated within the **IEFPCM of acetonitrile**

	B3LYP / 6-311++G(2d,p) / IEFPCM				B3LYP-GD3 / 6-311++G(2d,p) / IEFPCM			
	ΔE_{ZPC} [a)] [kcal/mol]	**ΔG_{298K}** [a)] [kcal/mol]	**popΔE** [%]	**popΔG** [%]	**ΔE_{ZPC}** [b)] [kcal/mol]	**ΔG_{298K}** [b)] [kcal/mol]	**popΔE** [%]	**popΔG** [%]
c1	0.00	0.04	44.2	32.7	0.00	0.23	36.2	23.1
c2	0.26	0.21	28.6	24.6	0.06	0.00	32.9	34.2
c3	0.55	0.00	17.6	35.2	0.43	0.17	17.6	25.7
c4	0.94	0.95	9.0	7.1	0.69	0.51	11.3	14.5
c5	2.80	2.90	0.4	0.3	1.87	1.61	1.5	2.2
c6	3.56	3.12	0.1	0.2	2.76	2.98	0.3	0.2

[a)] Reference to E_h(c1)= -707.44385 hartree and G_h(c3) = -707.49366 hartree
[b)] Reference to E_h(c1)= -707.4647 hartree and G_h(c1) = -707.51453 hartree



2.4 Methanol-d_4

Table S7. Geometries, zero-point-corrected electronic and Gibbs free energies and the corresponding Boltzmann populations of MPAA calculated within the **IEFPCM of methanol**

	B3LYP / 6-311++G(2d,p) / IEFPCM						B3LYP-GD3 / 6-311++G(2d,p) / IEFPCM			
	α [deg]	β [deg]	ΔE_{ZPC} [a)] [kcal/mol]	ΔG_{298K} [a)] [kcal/mol]	popΔE [%]	popΔG [%]	ΔE_{ZPC} [b)] [kcal/mol]	ΔG_{298K} [b)] [kcal/mol]	popΔE [%]	popΔG [%]
c1	166.3	98.9	0.00	0.00	44.2	42.0	0.00	0.00	37.4	39.3
c2	72.0	103.5	0.25	0.18	28.9	31.2	0.07	0.07	33.3	34.9
c3	167.8	-86.9	0.58	0.60	16.5	15.2	0.50	0.61	16.2	14.0
c4	72.9	-85.2	0.88	0.78	9.9	11.3	0.72	0.78	11.2	10.4
c5	-51.6	118.7	2.75	2.97	0.4	0.3	1.86	2.13	1.6	1.1
c6	-54.5	-47.3	3.55	3.56	0.1	0.1	2.77	3.01	0.3	0.2

[a)] Reference to E_h(c1)= -574.66788 hartree and G_h(c1) = -574.70656 hartree
[b)] Reference to E_h(c1)= -574.68573 hartree and G_h(c1) = -574.72443 hartree

Table S8. Geometries, zero-point-corrected electronic and Gibbs free energies and the corresponding Boltzmann populations of **monosolvated MPAA-$(CD_3OD)_1$** calculated within the **IEFPCM of methanol**

		B3LYP / 6-311++G(2d,p) / IEFPCM				B3LYP-GD3 / 6-311++G(2d,p) / IEFPCM			
	OH[a)]	ΔE_{ZPC} [a)] [kcal/mol]	ΔG_{298K} [a)] [kcal/mol]	popΔE [%]	popΔG [%]	ΔE_{ZPC} [b)] [kcal/mol]	ΔG_{298K} [b)] [kcal/mol]	popΔE [%]	popΔG [%]
c1	proR	0.00	0.00	23.81	22.69	0.00	0.07	18.64	18.77
c1	proS	0.03	0.10	22.82	19.16	0.02	0.00	18.06	21.09
c2	proR	0.24	0.29	15.75	13.79	0.07	0.10	16.59	17.80
c2	proS	0.41	0.55	11.83	9.03	0.13	0.15	15.08	16.35
c3	proS	0.65	0.38	7.99	11.89	0.40	0.67	9.46	6.79
c3	proR	0.66	0.36	7.82	12.27	0.46	0.67	8.60	6.79
c4	proR	0.93	0.75	4.91	6.43	0.65	0.72	6.26	6.30
c4	proS	0.98	0.97	4.56	4.39	0.72	0.88	5.51	4.73
c5	proS	2.80	3.12	0.21	0.12	1.90	2.05	0.75	0.67
c5	proR	2.81	2.94	0.21	0.16	1.97	2.42	0.67	0.36
c6	proS	3.67	3.89	0.05	0.03	2.68	2.65	0.20	0.24
c6	proR	3.67	3.78	0.05	0.04	2.72	3.03	0.19	0.13

[a)] Configuration of OH-group considering the nomenclature shown in the Scheme S1 below this table.
[b)] Reference to E_h(c1-proR)= -690.4119 hartree and G_h(c1-proR) = -690.46001 hartree
[c)] Reference to E_h(c1-proR)= -690.4341 hartree and G_h(c1-proS) = -690.48137 hartree

Scheme S1. Definition of methanol-binding orientations with priorities CH_3 > H > Hbond > LP. Left: pro-S; right: pro-R.

Table S9. Geometries, zero-point-corrected electronic and Gibbs free energies and the corresponding Boltzmann populations of **twofold-solvated MPAA-$(CD_3OD)_2$** calculated within the **IEFPCM of methanol**

	B3LYP / 6-311++G(2d,p) / IEFPCM				**B3LYP-GD3 / 6-311++G(2d,p) / IEFPCM**			
	ΔE_{ZPC}[a)] [kcal/mol]	**ΔG_{298K}**[a)] [kcal/mol]	**popΔE** [%]	**popΔG** [%]	**ΔE_{ZPC}**[b)] [kcal/mol]	**ΔG_{298K}**[b)] [kcal/mol]	**popΔE** [%]	**popΔG** [%]
c1-proR-trans	0.00	0.00	12.58	16.20	0.03	0.57	9.65	7.25
c1-proS-trans	0.03	0.21	12.02	11.34	0.00	0.22	10.12	13.03
c1-proR-cis	0.19	0.47	9.09	7.30	0.01	0.49	10.02	8.23
c1-proS-cis	0.20	0.41	8.94	8.10	0.15	0.97	7.83	3.64
c2-proS-trans	0.29	0.40	7.76	8.29	0.17	0.00	7.57	18.86
c2-proR-trans	0.29	0.56	7.66	6.28	0.15	0.55	7.84	7.41
c2-proR-cis	0.43	0.54	6.05	6.55	0.18	0.83	7.41	4.61
c2-proS-cis	0.48	0.65	5.62	5.37	0.33	1.02	5.82	3.36
c3-proR-trans	0.49	0.70	5.48	4.93	0.39	0.82	5.28	4.76
c3-proS-trans	0.50	0.52	5.41	6.71	0.41	0.81	5.05	4.79
c3-proS-cis	0.59	0.60	4.61	5.86	0.38	0.67	5.34	6.04
c3-proR-cis	0.69	0.92	3.92	3.42	0.53	1.22	4.13	2.38
c4-proR-trans	0.85	1.11	3.01	2.50	0.67	0.94	3.25	3.84
c4-proS-trans	0.88	1.18	2.86	2.21	0.70	0.76	3.11	5.26
c4-proR-cis	1.01	1.14	2.30	2.36	0.80	1.27	2.62	2.22
c4-proS-cis	1.01	1.16	2.27	2.29	0.67	1.02	3.28	3.34
c5-proS-trans	2.89	3.20	0.10	0.07	2.06	3.13	0.31	0.10
c5-proR-trans	2.89	3.43	0.09	0.05	2.01	2.72	0.34	0.19
c5-proS-cis	3.02	3.52	0.08	0.04	2.07	2.59	0.31	0.24
c5-proR-cis	3.11	3.54	0.07	0.04	2.05	2.86	0.32	0.15
c6-proR-trans	3.57	4.14	0.03	0.01	2.70	3.89	0.11	0.03
c6-proS-trans	3.58	3.95	0.03	0.02	2.69	2.72	0.11	0.19
c6-proR-cis	3.71	4.02	0.02	0.02	2.77	3.31	0.09	0.07
c6-proS-cis	3.74	4.14	0.02	0.01	2.74	3.81	0.10	0.03

[a)] Reference to E_h(c1-proR-trans)= --806.157489 hartree and G_h(c1-proR-trans) = -806.21223 hartree
[b)] Reference to E_h(c1-proS-trans)= -806.185204 hartree and G_h(c2-proS-trans) = -806.24003 hartree

3. Calculated IR and VCD spectra

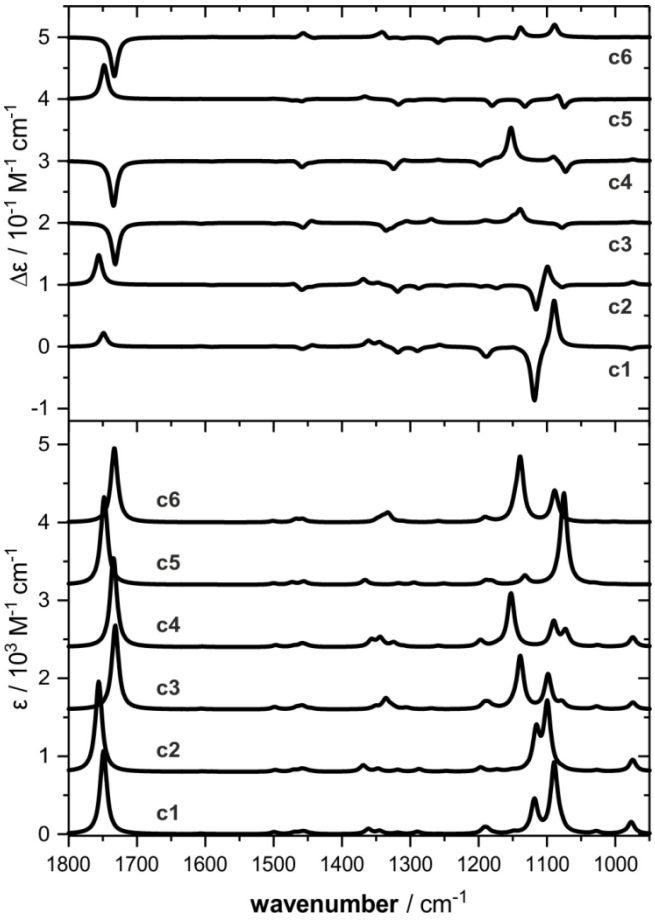


Figure S2. Single conformer IR and VCD spectra of MPAA calculated at the B3LYP/6-311++G(2d,p)/ IEFPCM(chloroform) level of theory.

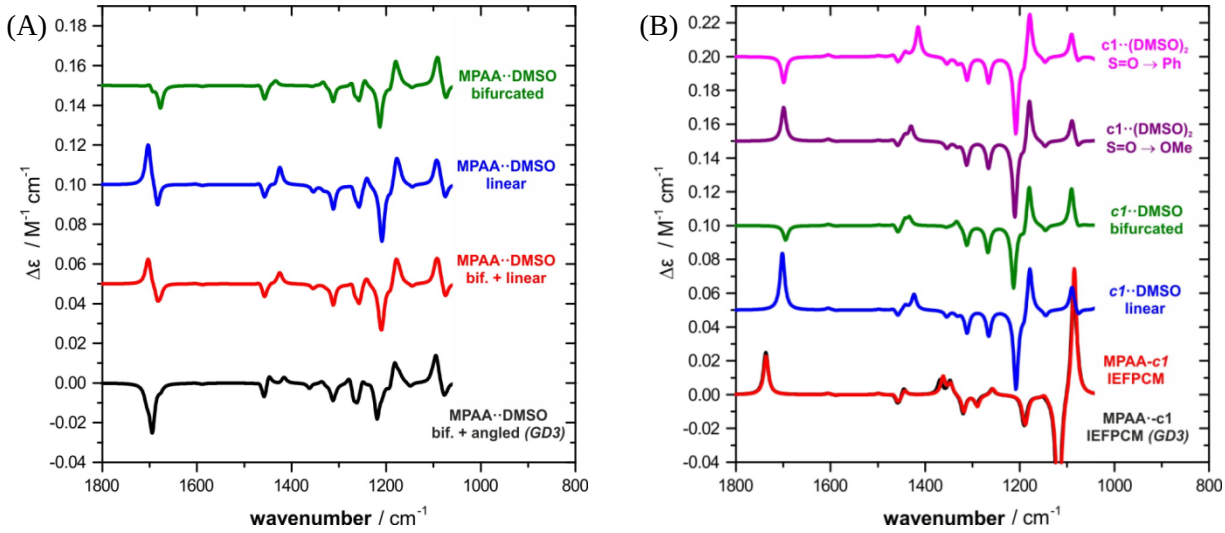


Figure S3. Comparison of calculated VCD spectra for MPAA··DMSO adducts: (A) Boltzmann weighted over all six conformers; (B) spectra for conformation c1

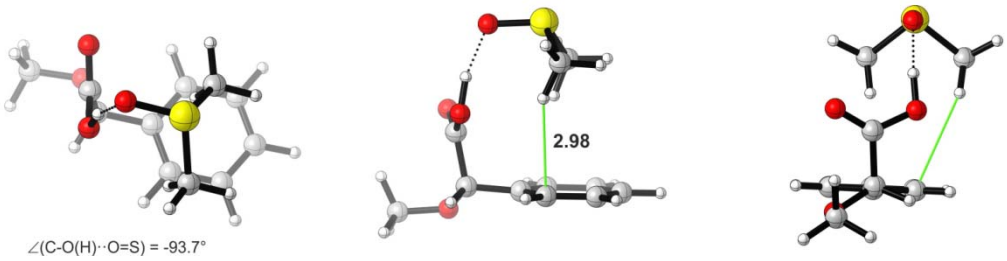


Figure S4. The structure of mono-solvated c1··$(DMSO)_1$ calculated by taking into account dispersion interactions with the B3LYP-GD3 functional under otherwise identical theoretical conditions.

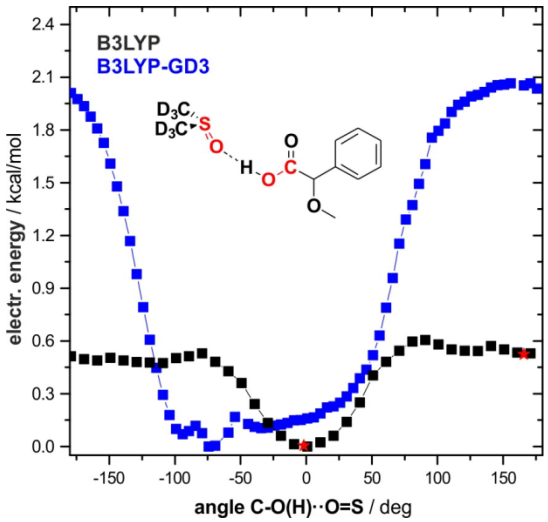


Figure S5. Potential energy surface for the rotation of the DMSO molecule bond to c1 (expressed as the angle C-O(H)··O=S). The black line corresponds to calculations using B3LYP, the blue line represents energies obtained with B3LYP-GD3.

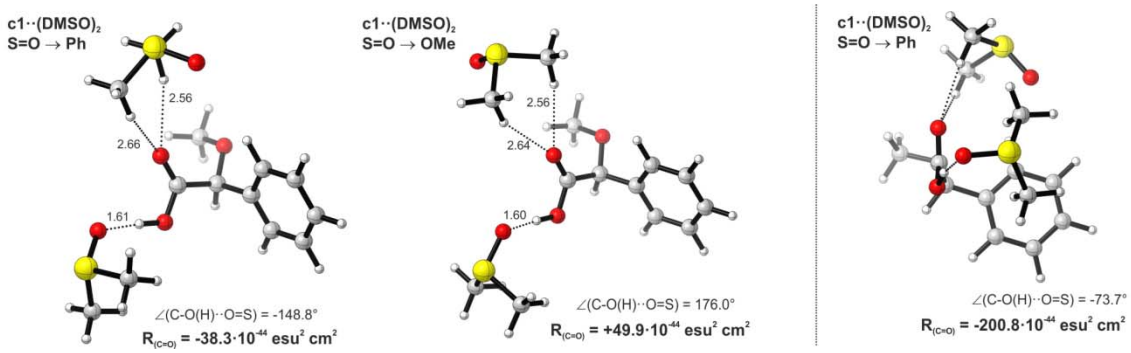


Figure S6. The structures of twofold-solvated c1··$(DMSO)_2$. Left: Structures obtained with the B3LYP functional; Right: Representative structure obtained after including dispersion corrections (B3LYP-GD3)

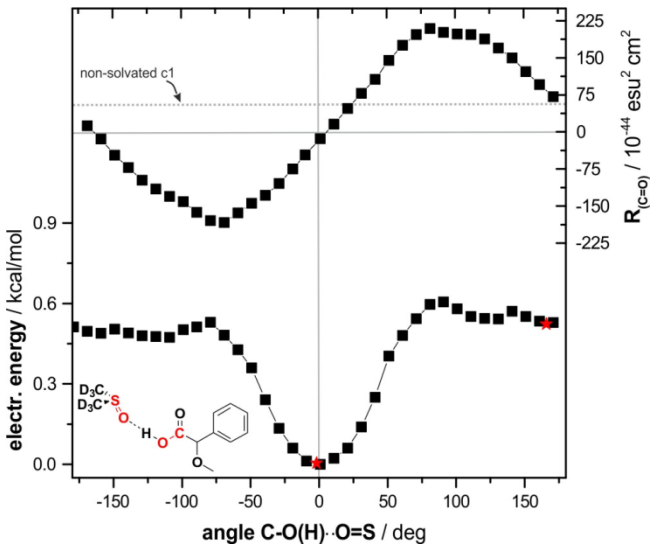


Figure S7. Dependence of the calculated rotational strength $R_{(C=O)}$ for the carbonyl stretching mode of c1··$(DMSO)_1$ on the spatial orientation of the DMSO molecules (expressed as the angle C-O(H)··O=S). The red stars mark the two localized minimum structures (B3LYP/6-311++G(2d,p)/IEFPCM(DMSO))

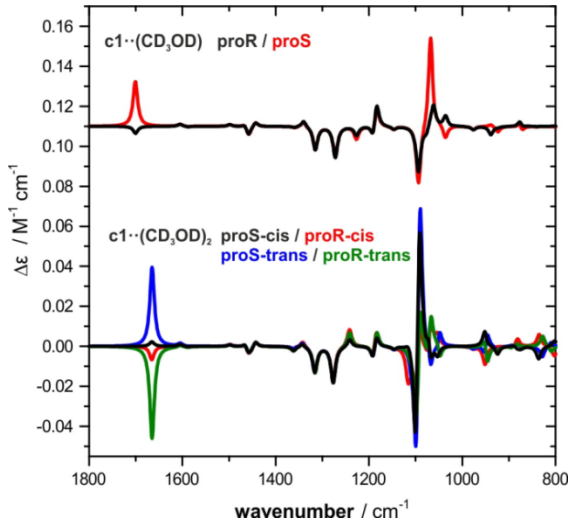


Figure S8. Calculated VCD spectra for conformer c1 of the MPAA··(CD_3OD) and MPAA··$(CD_3OD)_2$ adducts.

4. Vibrational energy distribution

In the vibrational analysis, the following atom numbering given below is used:

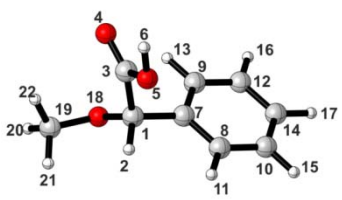


Table S10. Vibrational energy distribution analysis for c1 (B3LYP/6-311++G(2d,p)/IEFPCM(chloroform)). For better comparison, the range below 500 cm^{-1} is removed from the list. The color coding highlights the modes discussed in the main text, important vibrational contributions are printed in bold type.

ν_{scaled}	Contributing internal coordination and contribution in percentage					
3658	ν(OH) 100					
3129	ν(C_9-H_{13}) 62	ν(C_{12}-H_{16}) 22	ν(C_{14}-H_{17}) 10			
3123	ν(C_9-H_{13}) -24	ν(C_{10}-H_{15}) 37	ν(C_{14}-H_{17}) 30			
3113	ν(C_8-H_{11}) 20	ν(C_{10}-H_{15}) 24	ν(C_{12}-H_{16}) -29	ν(C_{14}-H_{17}) -17		
3105	ν(C_8-H_{11}) 38	ν(C_{12}-H_{16}) 36	ν(C_{14}-H_{17}) -20			
3099	ν(C_8-H_{11}) -34	ν(C_{10}-H_{15}) 31	ν(C_{12}-H_{16}) 12	ν(C_{14}-H_{17}) -22		
3064	ν(C_{19}-H_{20}) 91					
2999	ν(C_{19}-H_{21}) -31	ν(C_{19}-H_{22}) 67				
2952	ν(C_1-H_2) 99					
2940	ν(C_{19}-H_{21}) 65	ν(C_{19}-H_{22}) 27				
1749	ν(O_4-C_3) 87					
1606	ν(C_8-C_{10}) 10	ν(C9-C12) 29				
1590	ν(C_7-C_8) -18	ν(C14-C10) 27	δ(C7-C8-C10) 13			
1499	δ(H_{11}-C_8-C_{10}) 15	δ(H_{13}-C_9-C_{12}) 16	δ(H_{15}-C_{10}-C_{14}) 17	δ(H_{16}-C_{12}-C_{14}) 18		
1469	δ(H_{20}-C_{19}-H_{22}) -31	δ(H_{22}-C_9-C_{21}) 48	τ(H_{22}-C_{19}-O_{18}-C_1) 13			
1459	δ(H_{15}-C_{10}-C_{14}) -11	δ(H_{16}-C_{12}-C_{14}) 10	δ(H_{17}-C_{14}-C_{12}) -26			
1454	δ(H_{20}-C_{19}-H_{22}) -28	δ(H_{21}-C_{19}-H_{20}) 29	δ(H_{22}-C_{19}-H_{21}) -19	τ(H_{20}-C_{19}-O_{18}-C_1) -12	τ(H_{21}-C_{19}-O_{18}-C_1) 11	
1444	δ(H_{20}-C_{19}-H_{22}) 17	δ(H_{21}-C_{19}-H_{20}) 52	δ(H_{22}-C_{19}-H_{21}) 13			
1361	**δ(H_2-C_1-O_{18}) 57**					
1345	δ(H_{11}-C_8-C_{10}) -15	δ(H_{13}-C_9-C_{12}) 14	**τ(H_2-C_1-O_{18}-C_{19}) 23**			
1318	ν(C_8-C_{10}) -11	ν(C_9-C_{12}) 14	δ(H_{13}-C_9-C_{12}) -19	**τ(H_2-C_1-O_{18}-C_{19}) -11**		
1290	ν(C_7-C_8) 10	**δ(H_6-O_5-C_3) 25**	**δ(H_2-C_1-O_{18}) 16**			
1257	**δ(H_6-O_5-C_3) -12**	**τ(H_2-C_1-O_{18}-C_{19}) 33**				
1192	δ(H_{22}-C_{19}-H_{21}) 12	τ(H_{21}-C_{19}-O_{18}-C_1)-25	τ(H_{22}-C_{19}-O_{18}-C_1) 25			
1187	**ν(C_1-C_7) 30**					
1177	δ(H_{11}-C_8-C_{10}) 23	δ(H_{13}-C_9-C_{12}) 22	δ(H_{15}-C_{10}-C_{14}) -16	δ(H_{16}-C_{12}-C_{14}) -14		
1157	ν(C_{12}-C_{14}) 10	δ(H_{15}-C_{10}-C_{14}) -18	δ(H_{16}-C_{12}-C_{14}) 19	δ(H_{17}-C_{14}-C_{12}) 35		
1149	δ(H_{20}-C_{19}-H_{22}) 14	δ(H_{21}-C_{19}-H_{20}) -12	τ(H_{20}-C_{19}-O_{18}-C_1) 34	τ(H_{21}-C_{19}-O_{18}-C_1) -21	τ(H_{22}-C_{19}-O_{18}-C_1) -16	
1118	**ν(O_5-C_3) 27**	ν(O_{18}-C_1) 14	**δ(H_6-O_5-C_3) -17**			
1089	**ν(O_5-C_3) -25**	ν(O_{18}-C_1) 23	ν(O_{18}-C_{19}) -25	**δ(H_6-O_5-C_3) 10**		
1080	ν(C_8-C10) 20	ν(C_9-C_{12}) -14	δ(H_{13}-C_9-C_{12}) -13	δ(H_{17}-C_{14}-C_{17}) -13		
1028	ν(C_{12}-C_{14}) 18	ν(C_{14}-C_{10}) 16	δ(C_9-C_{12}-C_{14}) -18	δ(H_{15}-C_{10}-C_{14}) 10	δ(H_{16}-C_{12}-C_{14}) 11	δ(C_8-C_{10}-C_{14}) -10
1000	ν(C_{12}-C_{14}) 15	ν(C_{14}-C_{10}) 12	δ(C_9-C_{12}-C_{14}) 24	δ(C_8-C_{10}-C_{14}) 12	δ(C_{12}-C_{14}-C_{10}) -16	
988	τ(H_{15}-C_{10}-C_{14}-C_{10}) -13	τ(H_{16}-C_{12}-C_{14}-C_{10}) 24	τ(H_{17}-C_{14}-C_{12}-C_9) 28	τ(C_9-C_{12}-C_{14}-C_{10}) -13		
977	ν(O_{18}-C_1) 19	ν(O_{18}-C_{19}) 38	δ(O_{18}-C_1-C_7) -10			
967	τ(H_{11}-C_8-C_{10}-C_{14}) -17	τ(H_{13}-C_9-C_{12}-C_{14}) -20	τ(H_{15}-C_{10}-C_{14}-C_{10}) 31	τ(H_{16}-C_{12}-C_{14}-C_{10}) 21		
924	τ(H_{11}-C_8-C_{10}-C_{14}) -23	τ(H_{13}-C_9-C_{12}-C_{14}) 18	τ(H_{17}-C_{14}-C_{12}-C_9) 23			
878	ν(C_1-C_1) 25	δ(C_{12}-C_{14}-C_{10}) -10				
871	δ(C_{12}-C_{14}-C_{10}) 10	Θ(O_4-C_1-O_5-C_3) 20	Θ(C_3-C_7-O_{18}-C_1) 19			
839	τ(H_{11}-C_8-C_{10}-C_{14}) 27	τ(H_{13}-C_9-C_{12}-C_{14}) 25	τ(H_{15}-C_{10}-C_{14}-C_{10}) 23	τ(H_{16}-C_{12}-C_{14}-C_{10}) 25		
757	τ(H_{15}-C_{10}-C_{14}-C_{10}) 12	τ(H_{16}-C_{12}-C_{14}-C_{10}) -11	τ(C_7-C_8-C_{10}-C_{14}) -27			
717	δ(C_{12}-C_{14}-C_{10}) 18	Θ(O_4-C_1-O_5-C_3) -30				
696	τ(H_{11}-C_8-C_{10}-C_{14}) -11	τ(H_{13}-C_9-C_{12}-C_{14}) 11	τ(H_{17}-C_{14}-C_{12}-C_9) -17	τ(C_7-C_8-C_{10}-C_{14}) -35	τ(C_9-C_{12}-C_{14}-C_{10})-10	τ(C_{12}-C_{14}-C_{10}-C_8)10
650	ν(O_5-C_3) 15	δ(O_4-C_3-O_5) 40				
621	δ(C_9-C_{12}-C_{14}) -22	δ(C_8-C_{10}-C_{14}) 22	τ(H_6-O_5-C_3-C_1) -10			
617	δ(C_8-C_{10}-C_{14}) 16	τ(H_6-O_5-C_3-C_1) 27				
554	δ(O_{18}-C_1-C_7) 11	τ(H_6-O_5-C_3-C_1) 38				

Table S11. Vibrational energy distribution analysis for c1··ACN (B3LYP/6-311++G(2d,p)/IEFPCM($_{ACN}$)). For better comparison, modes involving ACN and the range below 500 cm^{-1} are removed from the list. The color coding highlights the modes discussed in the main text, important vibrational contributions are printed in bold type.

ν_{scaled}	Contributing internal coordination and contribution in percentage				
3252	ν(OH)97				
3128	ν(C_9-H_{13}) 40	ν(C_{10}-H_{15}) 12	ν(C_{12}-H_{16}) 26	ν(C_{14}-H_{17}) 20	
3122	n(C_9-H_{13}) -39	ν(C_{10}-H_{15}) 34	ν(C_{14}-H_{17}) 19		
3113	ν(C_8-H_{11}) -20	ν(C_9-H_{13}) -13	ν(C_{10}-H_{15}) -22	ν(C_{12}-H_{16}) 23	ν(C_{14}-H_{17}) 22
3105	ν(C_8-H_{11}) 37	ν(C_{12}-H_{15}) 37	ν(C_{14}-H_{17}) -17		
3100	ν(C_8-H_{11}) -33	ν(C_{10}-H_{15}) 30	ν(C_{12}-H_{16}) 13	ν(C_{14}-H_{17}) -22	
3062	ν(C_{19}-H_{20}) 90				
2999	ν(C_{19}-H_{21}) -33	ν(C_{19}-H_{22}) 65			
2957	ν(C_1-H_2) 98				
2941	ν(C_{19}-H_{21}) 62	ν(C_{19}-H_{22}) 29			
1715	ν(O_4-C_3) 86				
1605	ν(C_8-C_{10}) 10	ν(C_9-C_{12}) 30			
1589	n(C_7-C_8) -19	ν(C_{10}-C_{14}) 28	δ(C_9-C_{12}-C_{14}) 10		
1499	δ(H_{11}-C_8-H_{10}) -15	δ(H_{13}-C_9-C_{12}) -16	δ(H_{15}-C_{10}-C_8) 18	δ(H_{16}-C_{12}-C_{14}) -18	
1467	δ(H_{20}-C_{19}-H_{22}) -30	δ(H_{22}-C_{19}-H_{21}) 49	τ(H_{22}-C_{19}-O_{18}-C_1) 13		
1458	δ(H_{16}-C_{12}-C_{14}) -10	δ(H_{17}-C_{14}-C_{11}) 26			
1451	δ(H_{20}-C_{19}-H_{22}) -28	δ(H_{21}-C_{19}-H_{20}) 31	δ(H_{22}-C_{19}-H_{21}) -16	τ(H_{20}-C_{19}-O_{18}-C_1) -12	τ(H_{21}-C_{19}-O_{18}-C_1) 11
1442	δ(H_{20}-C_{19}-H_{22}) 18	δ(H_{21}-C_{19}-H_{20}) 49	δ(H_{22}-C_{19}-H_{21}) 16		
1382	**ν(O_5-C_3) 15**	**δ(H_6-O_5-C_3) 33**	**δ(H_2-C_1-O_{18}) -17**	**δ(O_4-C_3-O_5) -11**	
1351	δ(H_{11}-C_8-H_{10}) 14	δ(H_{15}-C_{10}-C_8) -10	**δ(H_2-C_1-O_{18}) 24**	**τ(H_2-C_1-O_{18}-C_{19}) 11**	
1326	δ(H_{11}-C_8-H_{10}) -12	δ(H_{13}-C_9-C_{12}) 16	**δ(H_2-C_1-O_{18}) 30**		
1306	ν(C_7-C_8) -12	ν(C_8-C_{10})11	ν(C_9-C_{12}) -11	ν(C_{12}-C_{14}) 10	**τ(H_2-C_1-O_{18}-C_{19}) 23**
1263	ν(C_7-C_8) 11	**τ(H_2-C_1-O_{18}-C_{19}) 27**			
1193	**ν(O_5-C_3) -12**	**ν(C_1-C_7) 24**			
1190	ν(O_{18}-C_1) 10	δ(H_{22}-C_{19}-H_{21}) 11	τ(H_{21}-C_{19}-O_{18}-C_1) -23	τ(H_{22}-C_{19}-O_{18}-C_1) 25	
1175	δ(H_{11}-C_8-H_{10}) 22	δ(H_{13}-C_9-C_{12}) 22	δ(H_{15}-C_{10}-C_8) 18	δ(H_{16}-C_{12}-C_{14}) -14	
1165	**ν(O_5-C_3) 35**	**τ(H_2-C_1-O_{18}-C_{19}) -13**			
1156	ν(C_{12}-C_{14}) 10	δ(H_{15}-C_{10}-C_8) 17	δ(H_{16}-C_{12}-C_{14}) 19	δ($_{H17}$.C_{14}-C_{11}) 36	
1145	δ(H_{20}-C_{19}-H_{22}) 14	δ(H_{21}-C_{19}-H_{20}) -12	τ(H_{20}-C_{19}-O_{18}-C_1) 33	τ(H_{22}-C_{19}-O_{18}-C_1) -18	τ(H_{21}-C_{19}-O_{18}-C_1) -16
1091	ν(O_{18}-C_1) 36	ν(O_{18}-C_{19}) -31			
1078	ν(C_8-C_{10}) 19	ν(C_9-C_{12}) -13	ν(O_{18}-C_{19}) 10	δ(H_{13}-C_9-C_{12}) -11	δ(H_{17}-C_{14}-C_{11}) -11
1027	ν(C_{10}-C_{14}) 17	ν(C_{12}-C_{14}) 19	δ(H_{16}-C_{12}-C_{14}) 11	δ(C_9-C_{12}-C_{14}) -18	δ(C_8-C_{10}-C_{14}) -12
999	ν(C_{10}-C_{14}) -13	ν(C_{12}-C_{14}) -15	δ(C_8-C_{10}-C_{14}) -12	δ(C_9-C_{12}-C_{14}) -24	δ(C_{12}-C_{14}-C_{10}) 17
990	τ(H_{15}-C_{10}-C_8-C_7) 14	τ(H_{16}-C_{12}-C_{14}-C_{10}) 16	τ(H_{17}-C_{14}-C_{12}-C_9) 21	τ(C_7-C_8-C_{10}-C_{14}) -12	τ(C_9-C_{12}-C_{14}-C_{10}) -11
976	ν(O_{18}-C_1) 18	ν(O_{18}-C_{19}) 38			
970	τ(H_{11}-C_8-C_7-C_1) 21	τ(H_{13}-C_9-C_7-C_1) 23	τ(H_{15}-C_{10}-C_8-C_7) -22	τ(H_{16}-C_{12}-C_{14}-C_{10}) 22	
925	τ(H_{11}-C_8-C_7-C_1) -22	τ(H_{13}-C_9-C_7-C_1) 19	τ(H_{17}-C_{14}-C_{12}-C_9) -17		
887	ν(C_3-C_1) 28				
873	δ(C_{12}-C_{14}-C_{10}) -14	τ(O_4-C_1-O_5-C_3) -22			
858	τ(H_6-O_5-C_3-C_1) 41	τ(N_{28}-H_6-O_5-C_3) 45			
840	τ(H_{11}-C_8-C_7-C_1) -26	τ(H_{13}-C_9-C_7-C_1) -26	τ(H_{15}-C_{10}-C_8-C_7) -23	τ(H_{16}-C_{12}-C_{14}-C_{10}) 24	
762	τ(H_{15}-C_{10}-C_8-C_7) -16	τ(H_{16}-C_{12}-C_{14}-C_{10}) -13	τ(C_7-C8-C_{10}-C_{14}) -14		
714	δ(C_{12}-C_{14}-C_{10}) 16	τ(O_4-C_1-O_5-C_3) -20			
697	τ(H_{17}-C_{14}-C_{12}-C_9) -28	τ(C_7-C_8-C_{10}-C_{14}) -23	τ(C_9-C_{12}-C_{14}-C_{10}) -10	τ(C_1-C_9-C_8-C_7) 12	
662	ν(O_5-C_3) 10	δ(O_4-C_3-O_5) 39	δ(O_{18}-C_1-C_3) 12		
620	δ(C_7-C_8-C_{10}) 18	δ(C_8-C_{10}-C_{14}) -35	δ(C_9-C_{12}-C_{14}) 25		
595	δ(C_7-C_8-C_{10}) 14	τ(O_4-C_1-O_5-C_3) -13	τ(O_{18}-C_3-C_7-C_1) 15		
514	δ(C_{19}-O_{18}-C_1) 11	τ(O_4-C_1-O_5-C_3) 13	τ(C_1-C_9-C_8-C_7) -19		

Table S12. Vibrational energy distribution analysis for $c1_l$··DMSO (B3LYP/6-311++G(2d,p)/IEFPCM($_{DMSO}$)). Modes involving DMSO and the range below 500 cm^{-1} are removed from the list. The color coding highlights the modes discussed in the main text, important vibrational contributions are printed in bold type.

ν_{scaled}	Contributing internal coordination and contribution in percentage					
3121	$\nu(C_9\text{-}H_{13})$ -44	$\nu(C_{10}\text{-}H_{15})$ 31	$\nu(C_{14}\text{-}H_{17})$ 14			
3113	$\nu(C_8\text{-}H_{11})$ -19	$\nu(C_9\text{-}H_{13})$ -16	$\nu(C_{10}\text{-}H_{15})$ -21	$\nu(C_{12}\text{-}H_{16})$ 19	$\nu(C_{14}\text{-}H_{17})$ 23	
3105	$\nu(C_8\text{-}H_{11})$ 35	$\nu(C_{12}\text{-}H_{16})$ 38	$\nu(C_{14}\text{-}H_{17})$ -16			
3099	$\nu(C_8\text{-}H_{11})$ 36	$\nu(C_{10}\text{-}H_{15})$ -30	$\nu(C_{12}\text{-}H_{16})$ -12	$\nu(C_{14}\text{-}H_{17})$ 20		
3060	$\nu(C_{19}\text{-}H_{20})$ 90					
2999	$\nu(C_{19}\text{-}H_{21})$ -32	$\nu(C_{19}\text{-}H_{22})$ 66				
2957	$\nu(C_1\text{-}H_2)$ 99					
2941	$\nu(C_{19}\text{-}H_{21})$ 64	$\nu(C_{19}\text{-}H_{22})$ 27				
2864	ν(OH) 92					
1702	$\nu(O_4\text{-}C_3)$ 85					
1605	$\nu(C_8\text{-}C_{10})$ 10	$\nu(C_9\text{-}C_{12})$ 30				
1588	$\nu(C_7\text{-}C_8)$ -18	$\nu(C_{14}\text{-}C_{10})$ 28	$\delta(C_7\text{-}C_8\text{-}C_{10})$ 11			
1498	$\delta(H_{11}\text{-}C_8\text{-}C_{10})$ 16	$\delta(H_{13}\text{-}C_9\text{-}C_{12})$ 16	$\delta(H_{15}\text{-}C_{10}\text{-}C_{14})$ 17	$\delta(H_{16}\text{-}C_{12}\text{-}C_{14})$ 18		
1467	$\delta(H_{20}\text{-}C_{19}\text{-}C_{22})$ -31	$\delta(H_{22}\text{-}C_{19}\text{-}C_{21})$ 48	$\tau(H_{22}\text{-}C_{19}\text{-}O_{18}\text{-}C_1)$ 13			
1458	$\delta(H_{15}\text{-}C_{10}\text{-}C_{14})$ -11	$\delta(H_{16}\text{-}C_{12}\text{-}C_{14})$ 10	$\delta(H_{17}\text{-}C_{14}\text{-}C_{10})$ 26			
1451	$\delta(H_{20}\text{-}C_{19}\text{-}C_{22})$ 28	$\delta(H_{21}\text{-}C_{19}\text{-}C_{20})$ -30	$\delta(H_{22}\text{-}C_{19}\text{-}C_{21})$ 17	$\tau(H_{20}\text{-}C_{19}\text{-}O_{18}\text{-}C_1)$ 12	$\tau(H_{21}\text{-}C_{19}\text{-}O_{18}\text{-}C_1)$ -11	
1442	$\delta(H_{20}\text{-}C_{19}\text{-}C_{22})$ 16	$\delta(H_{21}\text{-}C_{19}\text{-}C_{20})$ 50	$\delta(H_{22}\text{-}C_{19}\text{-}C_{21})$ 15			
1425	$\delta(O_{DMSO}\text{-}H_6\text{-}C_5)$ 14	**$\delta(H_6\text{-}O_5\text{-}C_3)$ 30**				
1354	$\delta(H_{11}\text{-}C_8\text{-}C_{10})$ 11	**$\delta(H_2\text{-}C_1\text{-}O_{18})$ 43**				
1332	$\delta(H_{11}\text{-}C_8\text{-}C_{10})$ -12	$\delta(H_{13}\text{-}C_9\text{-}C_{12})$ 14	$\delta(H_2\text{-}C_1\text{-}O_{18})$ 29	$\tau(H_2\text{-}C_1\text{-}O_{18}\text{-}C_{19})$ -11		
1311	$\nu(C_8\text{-}C_{10})$ 13	$\nu(C_9\text{-}C_{12})$ -15	$\nu(C_{12}\text{-}C_{14})$ 10	$\tau(H_2\text{-}C_1\text{-}O_{18}\text{-}C_{19})$ 24		
1266	$\nu(C_7\text{-}C_8)$ 12	**$\tau(H_2\text{-}C_1\text{-}O_{18}\text{-}C_{19})$ 20**				
1208	**$\nu(O_5\text{-}C_3)$ 40**	**$\nu(C_1\text{-}C_7)$ -12**	$\delta(H_2\text{-}C_1\text{-}O_{18})$ 11			
1191	$\delta(H_{22}\text{-}C_{19}\text{-}C_{21})$ 11	$\tau(H_{21}\text{-}C_{19}\text{-}O_{18}\text{-}C_1)$ -23	$\tau(H_{22}\text{-}C_{19}\text{-}O_{18}\text{-}C_1)$ 25			
1179	**$\nu(O_5\text{-}C_3)$ 13**	**$\nu(C_1\text{-}C_7)$ 20**	$\tau(H_2\text{-}C_1\text{-}O_{18}\text{-}C_{19})$ -13			
1174	$\delta(H_{11}\text{-}C_8\text{-}C_{10})$ -19	$\delta(H_{13}\text{-}C_9\text{-}C_{12})$ -20	$\delta(H_{15}\text{-}C_{10}\text{-}C_{14})$ 19	$\delta(H_{16}\text{-}C_{12}\text{-}C_{14})$ 15		
1155	$\nu(C_{12}\text{-}C_{14})$ -10	$\delta(H_{15}\text{-}C_{10}\text{-}C_{14})$ 17	$\delta(H_{16}\text{-}C_{12}\text{-}C_{14})$ -19	$\delta(H_{17}\text{-}C_{14}\text{-}C_{10})$ 36		
1145	$\delta(H_{20}\text{-}C_{19}\text{-}C_{22})$ 14	$\delta(H_{21}\text{-}C_{19}\text{-}C_{20})$ -12	$\tau(H_{20}\text{-}C_{19}\text{-}O_{18}\text{-}C_1)$ 34	$\tau(H_{21}\text{-}C_{19}\text{-}O_{18}\text{-}C_1)$ -18	$\tau(H_{22}\text{-}C_{19}\text{-}O_{18}\text{-}C_1)$ -18	
1090	$\nu(O_{18}\text{-}C_1)$ 37	$\nu(O_{18}\text{-}C_{19})$ -32				
1077	$\nu(C_8\text{-}C_{10})$ 19	$\nu(C_9\text{-}C_{12})$ -13	$\nu(O_{18}\text{-}C_{19})$ 10	$\delta(H_{13}\text{-}C_9\text{-}C_{12})$ -13	$\delta(H_{17}\text{-}C_{14}\text{-}C_{10})$ 11	
1026	$\nu(C_{12}\text{-}C_{14})$ 18	$\nu(C_{14}\text{-}C_{10})$ 15	$\delta(C_9\text{-}C_{12}\text{-}C_{14})$ -17	$\delta(H_{15}\text{-}C_{10}\text{-}C_{14})$ 11	$\delta(H_{16}\text{-}C_{12}\text{-}C_{14})$ 10	$\delta(C_8\text{-}C_{10}\text{-}C_{14})$ -10
999	$\nu(C_{12}\text{-}C_{14})$ -16	$\nu(C_{14}\text{-}C_{10})$ -13	$\delta(C_9\text{-}C_{12}\text{-}C_{14})$ -23	$\delta(C_8\text{-}C_{10}\text{-}C_{14})$ -12	$\delta(C_{12}\text{-}C_{14}\text{-}C_{10})$ 16	
990	$\tau(H_{15}\text{-}C_{10}\text{-}C_8\text{-}C_7)$ -13	$\tau(H_{17}\text{-}C_{14}\text{-}C_{10}\text{-}C_8)$ 18	$\tau(H_{17}\text{-}C_{14}\text{-}C_{10}\text{-}C_8)$ 22	$\tau(C_7\text{-}C_8\text{-}C_{10}\text{-}C_{14})$ 16		
977	$\nu(O_{18}\text{-}C_1)$ 17	$\nu(O_{18}\text{-}C_{19})$ 35				
970	$\tau(H_{11}\text{-}C_8\text{-}C_{10}\text{-}C_{14})$ 17	$\tau(H_{13}\text{-}C_9\text{-}C_7\text{-}C_1)$ -23	$\tau(H_{15}\text{-}C_{10}\text{-}C_8\text{-}C_7)$ 22	$\tau(H_{17}\text{-}C_{14}\text{-}C_{10}\text{-}C_8)$ 16		
963	$\tau(H_6\text{-}O_5\text{-}C_3\text{-}C_1)$ 31	$\tau(O_{DMSO}\text{-}H_6\text{-}O_5\text{-}C_3)$ 41	τ(S=O-H_6-O_5) -19			
924	$\tau(H_{11}\text{-}C_8\text{-}C_{10}\text{-}C_{14})$ 19	$\tau(H_{13}\text{-}C_9\text{-}C_7\text{-}C_1)$ 20	$\tau(H_{17}\text{-}C_{14}\text{-}C_{10}\text{-}C_8)$ 20			
891	$\nu(C_3\text{-}C_1)$ 28					
874	$\delta(C_{12}\text{-}C_{14}\text{-}C_{10})$ 15	$o(O_4\text{-}C_1\text{-}O_5\text{-}C_3)$ 19				
840	$\tau(H_{11}\text{-}C_8\text{-}C_{10}\text{-}C_{14})$ -26	$\tau(H_{13}\text{-}C_9\text{-}C_7\text{-}C_1)$ 27	$\tau(H_{15}\text{-}C_{10}\text{-}C_8\text{-}C_7)$ 23	$\tau(H_{17}\text{-}C_{14}\text{-}C_{10}\text{-}C_8)$ 24		
765	$\tau(H_{15}\text{-}C_{10}\text{-}C_8\text{-}C_7)$ -17	$\tau(H_{17}\text{-}C_{14}\text{-}C_{10}\text{-}C_8)$ 17	$\tau(H_{17}\text{-}C_{14}\text{-}C_{10}\text{-}C_8)$ -11	$o(C_1\text{-}C_8\text{-}C_9\text{-}C_7)$ -10		
720	$\delta(O_4\text{-}C_3\text{-}O_5)$ 12	$\delta(C_{12}\text{-}C_{14}\text{-}C_{10})$ 15	$o(O_4\text{-}C_1\text{-}O_5\text{-}C_3)$ -19			
697	$\tau(H_{11}\text{-}C_8\text{-}C_{10}\text{-}C_{14})$ -12	$\tau(H_{17}\text{-}C_{14}\text{-}C_{10}\text{-}C_8)$ 19	$\tau(C_7\text{-}C_8\text{-}C_{10}\text{-}C_{14})$ -23	$\tau(C_9\text{-}C_{12}\text{-}C_{14}\text{-}C_{10})$ -19	$\tau(C_{12}\text{-}C_{14}\text{-}C_{10}\text{-}C_8)$ 14	
670	$\delta(O_4\text{-}C_3\text{-}O_5)$ 35	$\delta(O_{18}\text{-}C_1\text{-}C_3)$ 13	$o(O_4\text{-}C_1\text{-}O_5\text{-}C_3)$ 11			
620	$\delta(C_9\text{-}C_{12}\text{-}C_{14})$ -25	$\delta(C_7\text{-}C_8\text{-}C_{10})$ -13	$\delta(C_8\text{-}C_{10}\text{-}C_{14})$ 37			
596	$\delta(C_7\text{-}C_8\text{-}C_{10})$ 14	$o(O_4\text{-}C_1\text{-}O_5\text{-}C_3)$ -13	$o(O_{18}\text{-}C_3\text{-}C_7\text{-}C_1)$ 16			
518	$\delta(O_5\text{-}C_3\text{-}C_1)$ 11	$\delta(C_{19}\text{-}O_{18}\text{-}C_1)$ -14	$o(O_4\text{-}C_1\text{-}O_5\text{-}C_3)$ -12	$o(C_1\text{-}C_8\text{-}C_9\text{-}C_7)$ -17		

5. Cartesian coordinates of selected structures

conformer c1

C	0.90122100	-0.15044500	-0.49631400
H	1.08504000	0.08207000	-1.55193700
C	1.56547800	0.95912700	0.33659000
O	2.12298100	0.80300600	1.39245300
O	1.42863300	2.15872600	-0.26133900
H	1.80975700	2.83317300	0.32505800
C	-0.59416400	-0.14043700	-0.24034600
C	-1.47198100	0.35000800	-1.20505200
C	-1.10151200	-0.61699600	0.96982000
C	-2.84316200	0.36519500	-0.96618700
H	-1.08491600	0.71837500	-2.14828200
C	-2.47161700	-0.60741000	1.20526200
H	-0.42337300	-1.00242200	1.72074600
C	-3.34545000	-0.11426600	0.23919200
H	-3.51725100	0.74555900	-1.72431600
H	-2.85791300	-0.98402500	2.14489800
H	-4.41288100	-0.10688400	0.42482000
O	1.41974600	-1.41712900	-0.16710400
C	2.75263600	-1.63218000	-0.62446200
H	3.01003400	-2.65606200	-0.36033400
H	2.81434700	-1.51271200	-1.71203500
H	3.45757700	-0.94947500	-0.14170700

dimer d11

C	-3.44736000	-1.04045800	-0.00451400
H	-3.78489100	-1.62561900	-0.86780400
C	-1.91376100	-1.13114900	0.02630000
O	-1.38403900	-1.15573000	-1.17925800
O	-4.02228300	-1.52589900	1.18498200
C	-3.94303900	-2.94180000	1.32772000
H	-2.90570600	-3.28044700	1.40556600
H	-4.46869200	-3.19134400	2.24738800
H	-4.42914400	-3.44563100	0.48484000
C	-3.84831200	0.41021400	-0.20029700
C	-4.29096500	0.85693900	-1.44388300
C	-3.76449300	1.31107900	0.86288900
C	-4.64762600	2.18984000	-1.62613700
H	-4.36108900	0.16198200	-2.27282800
C	-4.12685400	2.64096100	0.68136400
H	-3.42443100	0.96716700	1.83148300
C	-4.56679000	3.08405500	-0.56359500
H	-4.99362200	2.52639500	-2.59609300
H	-4.06378700	3.33312600	1.51256500
H	-4.84746400	4.12118000	-0.70329700
O	-1.26965900	-1.15468400	1.06500500
C	3.44735400	-1.04045800	0.00464300
H	3.78488100	-1.62551300	0.86800600
C	1.91375500	-1.13114700	-0.02616300
O	1.26965500	-1.15480500	-1.06486700
O	4.02227900	-1.52604700	-1.18479100
C	3.94303800	-2.94196500	-1.32735200
H	2.90570500	-3.28062300	-1.40516500
H	4.46870000	-3.19162500	-2.24698300
H	4.42913400	-3.44569000	-0.48440400
C	3.84831100	0.41023700	0.20024900
C	4.29101100	0.85710500	1.44376700
C	3.76445000	1.31098100	-0.86303800
C	4.64767800	2.19002600	1.62585500
H	4.36116600	0.16224200	2.27278800
C	4.12681900	2.64088400	-0.68167800
H	3.42435000	0.96695800	-1.83157800
C	4.56680200	3.08411900	0.56321400
H	4.99371100	2.52669200	2.59575900
H	4.06371900	3.33295300	-1.51295600
H	4.84748100	4.12126100	0.70278600
O	1.38403100	-1.15558300	1.17939600

H	0.38139200	-1.15405800	1.12691700
H	-0.38140000	-1.15419500	-1.12678000

Bifurcated c1-DMSO

C	-1.38911300	1.22621600	0.39081000
H	-1.50811400	1.57144900	1.42383800
C	0.07186400	0.76131500	0.23073500
O	0.72039800	0.91033200	-0.78484300
O	0.51465000	0.16343500	1.32570900
H	1.45767600	-0.18907700	1.20548200
C	-2.32138100	0.05478700	0.15083700
C	-3.02811800	-0.51369600	1.20946900
C	-2.47806400	-0.46964200	-1.13433700
C	-3.88031200	-1.59295600	0.99050000
H	-2.91590800	-0.11009300	2.20928600
C	-3.33415200	-1.54311000	-1.35444400
H	-1.93347100	-0.03302200	-1.96231000
C	-4.03583800	-2.10912700	-0.29213500
H	-4.42592000	-2.02473400	1.82102400
H	-3.45222000	-1.94026200	-2.35566800
H	-4.70133900	-2.94651400	-0.46474300
O	-1.71036200	2.26260600	-0.51410800
C	-1.10823100	3.51319100	-0.18600400
H	-1.46537500	4.23415800	-0.91921500
H	-1.40832400	3.83749200	0.81643700
H	-0.01712900	3.45875800	-0.23775400
S	3.98467600	-0.91891900	0.21843600
O	2.91397100	-0.83987600	1.31811500
C	4.21331100	0.77571100	-0.39234200
H(Iso=2)	4.64803500	1.34671200	0.42597000
H(Iso=2)	4.90743700	0.74042200	-1.23181300
H(Iso=2)	3.24597800	1.17849400	-0.68762000
C	3.16442300	-1.62060900	-1.24162300
H(Iso=2)	2.28129000	-1.02700200	-1.47184300
H(Iso=2)	3.87815900	-1.61314800	-2.06524800
H(Iso=2)	2.89881200	-2.64536800	-0.98858400

Linear c1-DMSO (only stable without GD3)

C	-1.56147200	1.09889500	0.48068000
H	-1.29903200	1.17355900	1.54196200
C	-0.24097600	1.06071500	-0.31419600
O	-0.08025400	1.60853100	-1.38354700
O	0.67842300	0.33853700	0.31207100
H	1.53388800	0.27071700	-0.22329200
C	-2.33133600	-0.18716800	0.25262000
C	-2.49391900	-1.10648100	1.28784700
C	-2.88544900	-0.46428600	-0.99937400
C	-3.19942400	-2.28862200	1.07805900
H	-2.07064000	-0.89773900	2.26378500
C	-3.59539000	-1.64165100	-1.20764200
H	-2.76415100	0.24458100	-1.80921200
C	-3.75240800	-2.55804700	-0.16985700
H	-3.32075600	-2.99432200	1.89119400
H	-4.02449800	-1.84582500	-2.18143600
H	-4.30447400	-3.47578600	-0.33380800
O	-2.37136000	2.19164600	0.09716500
C	-1.88302800	3.45247500	0.55135600
H	-2.60972600	4.20020100	0.23861000
H	-1.79816700	3.46522000	1.64353300
H	-0.91113500	3.68894800	0.10929100
S	4.26243600	-0.39676200	-0.41385400
O	2.93333800	0.10339400	-0.99685600
C	3.96509800	-2.09127000	0.16672200
H(Iso=2)	3.76788700	-2.69489400	-0.71709700
H(Iso=2)	4.86968800	-2.44108500	0.66389000
H(Iso=2)	3.11294800	-2.10278600	0.84461700
C	4.45239200	0.41054900	1.20136600
H(Iso=2)	3.56843900	0.22649900	1.81008700
H(Iso=2)	5.34743100	0.00935400	1.67599400
H(Iso=2)	4.57760800	1.47403800	1.00738400

Angled c1-DMSO (only stable with GD3)

C	-1.92585100	0.55752200	0.53656500
H	-2.04483400	0.73187200	1.61246900
C	-0.81787300	1.49882900	0.02534200
O	-0.81885600	2.00940800	-1.07312400
O	0.16451600	1.59944900	0.91104200
H	1.02790300	1.90913500	0.47233300
C	-1.41414000	-0.85087800	0.30138800
C	-0.71277500	-1.52010700	1.30415800
C	-1.55749700	-1.45012900	-0.95080700
C	-0.15736400	-2.77204200	1.05874500
H	-0.59333500	-1.05759300	2.27677500
C	-1.00855800	-2.70563600	-1.19307300
H	-2.09394700	-0.92824500	-1.73235200
C	-0.30309600	-3.36745900	-0.19130500
H	0.38868300	-3.28101800	1.84380200
H	-1.12442000	-3.16312800	-2.16829200
H	0.13066200	-4.34131500	-0.38373000
O	-3.14463700	0.74381300	-0.14200600
C	-3.78865300	1.97618800	0.17886900
H	-4.72499600	1.99380700	-0.37598000
H	-4.00211200	2.03617700	1.25213300
H	-3.17781200	2.83388500	-0.11759900
S	3.20635400	0.66572100	-0.32668400
O	2.48775400	2.01275900	-0.12763400
C	2.09455500	-0.37197800	-1.32339700
H(Iso=2)	1.97796400	0.12416700	-2.28471200
H(Iso=2)	2.57525400	-1.34108700	-1.45496500
H(Iso=2)	1.13567400	-0.48387900	-0.82142900
C	3.03627200	-0.23110700	1.24491700
H(Iso=2)	1.98372600	-0.26378100	1.52263600
H(Iso=2)	3.43782500	-1.23466300	1.10663900
H(Iso=2)	3.62177500	0.31148800	1.98458800

c1-ACN

C	0.97622000	1.11742700	-0.43676400
H	0.96090400	1.32040700	-1.51347500
C	-0.47916600	0.86816200	0.00181500
O	-0.94465900	1.22769900	1.05917200
O	-1.15170800	0.18653600	-0.92454100
H	-2.07147800	-0.01839100	-0.61603400
C	1.80105900	-0.12941900	-0.18099000
C	2.24279300	-0.91386600	-1.24528300
C	2.12039400	-0.50742000	1.12518800
C	2.99361300	-2.06279100	-1.01070400
H	2.00272400	-0.62561300	-2.26234000
C	2.87569000	-1.65129100	1.35920400
H	1.78262800	0.09746300	1.95754300
C	3.31228600	-2.43325600	0.29196900
H	3.33340000	-2.66320500	-1.84611100
H	3.12195100	-1.93422400	2.37574700
H	3.89945300	-3.32505100	0.47586500
O	1.54955200	2.20186300	0.26188400
C	1.04774100	3.47407700	-0.14392300
H	1.59336000	4.22182300	0.42874600
H	1.22341000	3.63752000	-1.21273300
H	-0.02109400	3.56969600	0.06707900
C	-6.22904000	-1.20597000	0.28087200
H(Iso=2)	-6.36181400	-2.27609500	0.11965000
H(Iso=2)	-6.43656600	-0.97181800	1.32544100
H(Iso=2)	-6.92518200	-0.65826800	-0.35488400
C	-4.86504500	-0.82631500	-0.04412000
N	-3.78663500	-0.52558000	-0.30002800

c1-(CD_3OD)$_1$

C	0.35502900	1.04583000	-0.48065600
H	0.18969600	1.12735700	-1.56084300
C	-0.95605300	0.53074500	0.14291500
O	-1.38949600	0.89284500	1.21465500

O	-1.53962500	-0.37744500	-0.63351100
H(Iso=2)	-2.36232600	-0.73531800	-0.18903400
C	1.46436200	0.04377100	-0.22505100
C	1.97236300	-0.72867700	-1.26831300
C	1.98402300	-0.11878400	1.06120200
C	2.98602400	-1.65371500	-1.03246800
H	1.57774300	-0.60573600	-2.27044200
C	3.00083900	-1.03788700	1.29565100
H	1.59614900	0.47914700	1.87656400
C	3.50278400	-1.80957300	0.24988000
H	3.37442800	-2.24675500	-1.85180500
H	3.40046300	-1.15402900	2.29608900
H	4.29391700	-2.52650800	0.43428400
O	0.73076600	2.29630300	0.05664700
C	-0.08528800	3.37880200	-0.38709800
H	0.32939400	4.28348400	0.05381600
H	-0.05821200	3.46304800	-1.47900100
H	-1.12147100	3.26100100	-0.05772500
C	-4.92413000	-1.47772700	-0.32927600
H(Iso=2)	-4.65397500	-1.98432900	-1.25329000
H(Iso=2)	-5.29029400	-0.47515300	-0.55849300
H(Iso=2)	-5.70197900	-2.04837800	0.18011400
O	-3.73146500	-1.42328500	0.47583900
H(Iso=2)	-3.93469800	-0.98189100	1.31000000

c1-($CD_3OD)_2$

C	1.04169700	1.07064700	-0.72553700
H	1.17399400	1.10380000	-1.81273900
C	-0.36812100	0.51213100	-0.45845900
O	-1.07272300	0.90134700	0.45668900
O	-0.69168400	-0.43501000	-1.31676900
H(Iso=2)	-1.59513900	-0.85360200	-1.11720600
C	2.07320000	0.13152600	-0.12941900
C	2.87610700	-0.65146900	-0.95718800
C	2.22431200	0.03921100	1.25606700
C	3.81945800	-1.51739000	-0.41039500
H	2.76783300	-0.58284100	-2.03354000
C	3.17075100	-0.82095900	1.80192000
H	1.60529800	0.64523100	1.90594600
C	3.96919200	-1.60307700	0.97017800
H	4.43985700	-2.11905600	-1.06379400
H	3.28394400	-0.88281400	2.87772400
H	4.70523600	-2.27383100	1.39700700
O	1.21021200	2.35534200	-0.16693800
C	0.50604500	3.38135600	-0.86473500
H	0.75640000	4.32023300	-0.37431700
H	0.82154800	3.42471100	-1.91273800
H	-0.57586400	3.22882700	-0.81717200
C	-3.01306600	-2.97648500	-0.69405500
H(Iso=2)	-2.55398000	-3.44173100	-1.56479400
H(Iso=2)	-4.03388500	-3.34919900	-0.58863700
H(Iso=2)	-2.43719000	-3.23733800	0.19735000
O	-3.01706800	-1.55891300	-0.91591000
H(Iso=2)	-3.40207600	-1.10214300	-0.13090400
C	-4.64211200	0.96270200	1.21627700
H(Iso=2)	-5.58491100	0.44103500	1.37357000
H(Iso=2)	-4.68216500	1.48817800	0.25824700
H(Iso=2)	-4.50074800	1.68929300	2.02011300
O	-3.60244300	-0.02263900	1.23026700
H(Iso=2)	-2.74327200	0.41108000	1.05925300