Supporting Information

Bile Acid Derivatives as Novel Co-adsorbents for Enhanced Performance of Blue Dye-Sensitized Solar Cells

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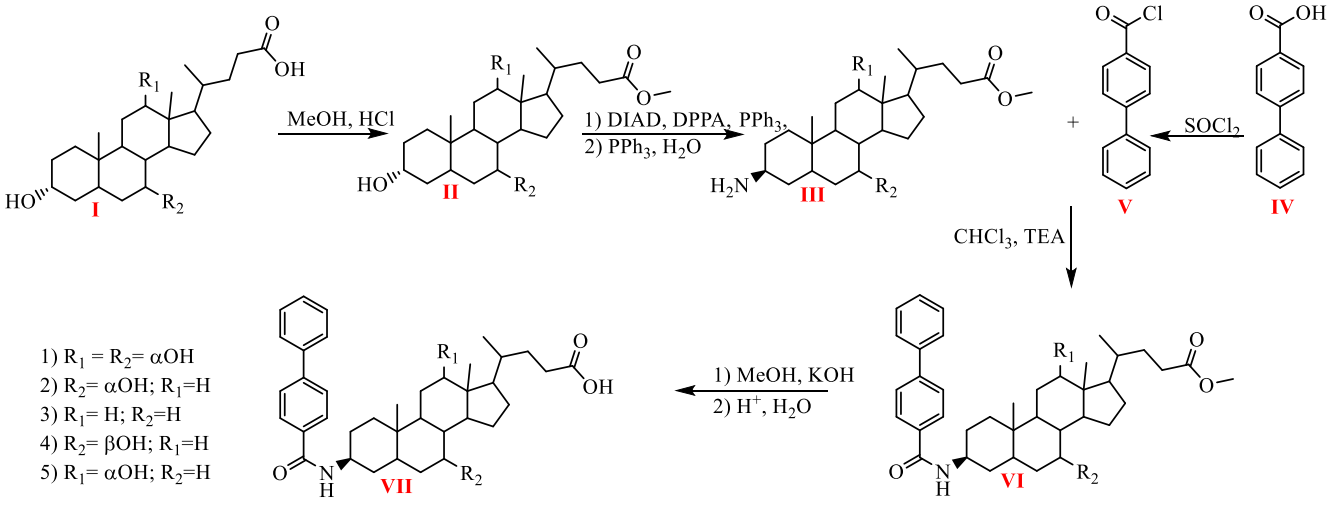
1 Synthesis of coadsorbers

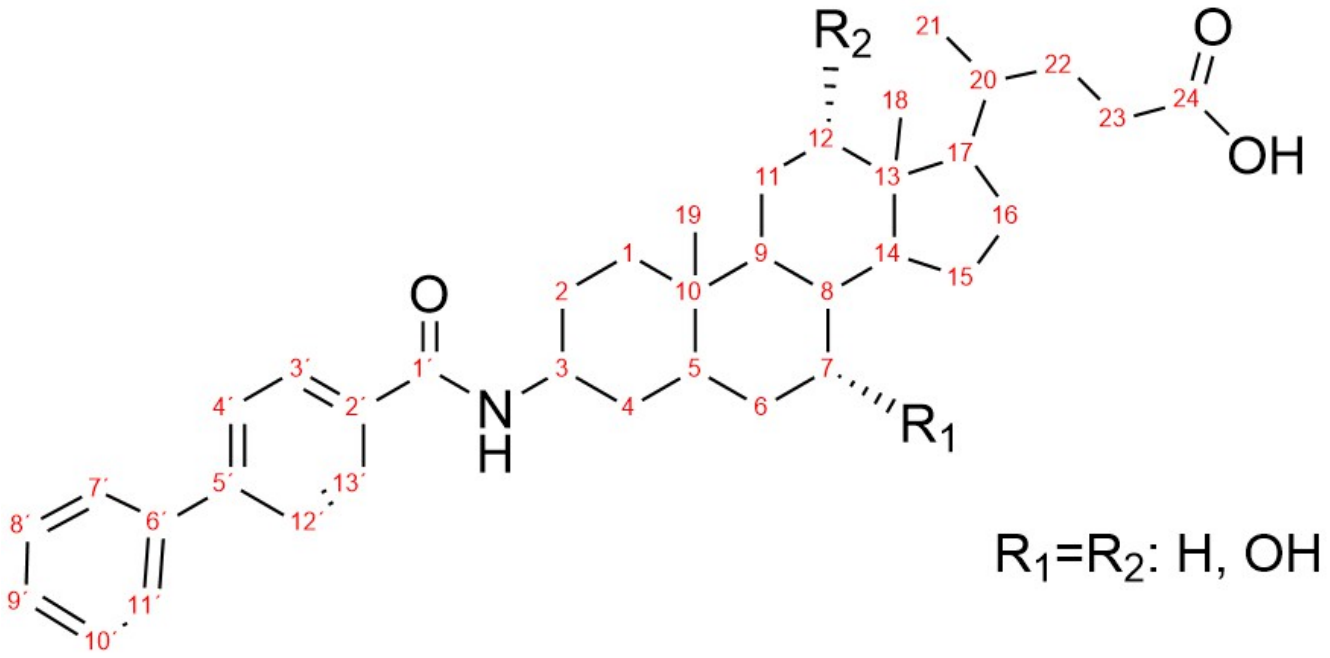


Scheme S1. Schematic of synthesis of the new compounds

2 Structural Information

NMR spectra

NMR Samples were dissolved in DMSO-D6 and measured in a Brucker 600 MHz, data were collected using Topspin version and analyzed with MestreNova version:



Scheme S2. Structure of the new compounds

H:	δ-H: Cholic	δ-H: Deoxycholic	δ-H: Chenodeoxycholic	δ-H: Ursodeoxycholic	δ-H: Litocholic
1	1.43; 1.33	1.14; 1.34	1.49; 1.36	1.47; 1.40	1.48; 1.37
2	1.63; 1.57	1.62; 1.56	1.57; 1.54	1.56	1.58
3	4.08	4.19	4.08	4.12	4.18
4	2.60; 1.49	2.03; 1.38	2.56; 1.50	1.87; 1.50	2.03; 1.37
5	1.73	1.77	1.73	1.32	1.77
6	1.85; 1.34	1.83; 1.13	1.87; 1.37	1.70; 1.38	1.85; 1.13
7	3.65	1.36; 1.08	3.66	3.33	1.37; 1.07
8	1.38	1.37	1.38	1.41	1.37
9	2.19	1.85	1.80	1.82	2.08
10	-	-	-	-	-
11	1.43	1.40	1.41; 1.24	1.38; 1.23	1.37; 1.20
12	3.80	3.80	1.92; 1.15	1.94; 1.16	1.93; 1.19
13	-	-	-	-	-
14	2.00	1.59	1.44	1.18	1.42
15	1.66; 0.99	1.53; 1.01	1.68; 1.01	1.86; 1.36	1.80; 1.25
16	1.73; 1.18	1.75; 1.18	1.80; 1.25	1.75; 1.21	1.55; 1.03
17	1.81	1.79	1.10	1.03	1.09
18	0.61	0.62	0.63	0.64	0.63
19	0.90	0.93	0.93	0.96	0.96
20	1.30	1.31	1.39	1.36	1.37
21	0.94	0.93	0.84	0.89	0.89
22	1.67; 1.22	1.66; 1.21	1.69; 1.20	1.69; 1.21	1.68; 1.20
23	2.23; 2.11	2.23; 2.11	2.23; 2.12	2.23; 2.11	2.23; 2.11
24	-	-	-	-	-

Table S1. Chemicals shift of protons in the sinthetized derivatives (δ: ppm)

C:	δ-C: Cholic	δ-C: Deoxycholic	δ-C: Chenodeoxycholic	δ-C: Ursodeoxycholic	δ-C: Litocholic
1	31.1	31.1	31.3	31.0	31.2
2	24.8	24.8	24.8	24.8	24.8
3	46.3	46.2	46.3	45.9	46.1
4	33.6	30.5	33.5	31.6	30.6
5	36.9	37.0	36.8	43.5	37.0
6	34.8	26.9	34.8	37.7	26.9
7	66.9	26.2	66.8	71.1	26.3
8	40.0	36.0	39.5	38.8	35.3
9	26.3	32.9	32.4	37.8	31.4
10	35.2	34.6	35.4	34.6	35.1
11	29.2	29.2	21.0	21.6	21.3
12	71.6	71.7	39.9	40.3	40.2
13	46.3	46.5	42.4	43.6	42.7
14	41.9	48.0	50.5	56.3	39.8
15	23.2	24.0	23.6	27.2	27.9
16	27.7	27.6	28.2	28.6	24.3
17	46.7	46.7	56.0	55.3	56.0
18	12.9	12.9	12.2	12.6	12.4
19	23.2	23.8	23.5	24.0	24.0
20	35.5	35.5	35.6	35.4	35.7
21	17.5	17.4	18.7	18.8	18.7
22	31.1	31.2	31.3	31.2	31.2
23	31.1	31.3	31.3	31.3	31.2
24	175.4	175.4	175.4	175.4	175.8

Table S2. Chemicals shift of carbons in the sinthetized derivatives (δ: ppm)

H:	δ-H: Cholic	δ-H: Deoxycholic	δ-H: Chenodeoxycholic	δ-H: Ursodeoxycholic	δ-H: Litocholic
1´	-	-	-	-	-
2´	-	-	-	-	-
3´	7.91	7.91	7.90	7.91	7.91
4´	7.74	7.75	7.74	7.75	7.74
5´	-	-	-	-	-
6´	-	-	-	-	-
7´	7.72	7.72	7.72	7.72	7.72
8´	7.50	7.50	7.50	7.50	7.50
9´	7.41	7.42	7.41	7.41	7.41
10´	7.50	7.50	7.50	7.50	7.50
11´	7.72	7.72	7.72	7.72	7.72
12´	7.74	7.75	7.74	7.75	7.74
13´	7.91	7.91	7.90	7.91	7.91
N-H	7.95	8.03	7.96	8.03	8.06

Table S3. Chemicals shift of protons in the biphenyl moiety of the sinthetized derivatives (δ: ppm)

C:	δ-C: Cholic	δ-C: Deoxycholic	δ-C: Chenodeoxycholic	δ-C: Ursodeoxycholic	δ-C: Litocholic
1´	166.7	166.8	166.6	166.6	166.9
2´	134.6	134.6	134.8	134.6	134.5
3´	128.6	128.8	128.7	128.8	128.8
4´	126.7	126.7	126.7	126.7	126.7
5´	142.9	142.9	143.0	145.0	142.9
6´	139.8	139.9	140.0	139.8	139.8
7´	127.5	127.3	127.3	127.3	126.3
8´	129.5	129.4	129.5	128.5	129.5
9´	128.7	128.4	128.7	128.4	128.5
10´	129.5	129.4	129.5	129.5	129.5
11´	127.5	127.3	127.3	127.3	126.3
12´	126.7	126.7	126.7	126.7	126.7
13´	128.6	128.8	128.7	128.8	128.8

Table S4. Chemicals shift of carbons in the biphenyl moiety of the sinthetized derivatives (δ: ppm)

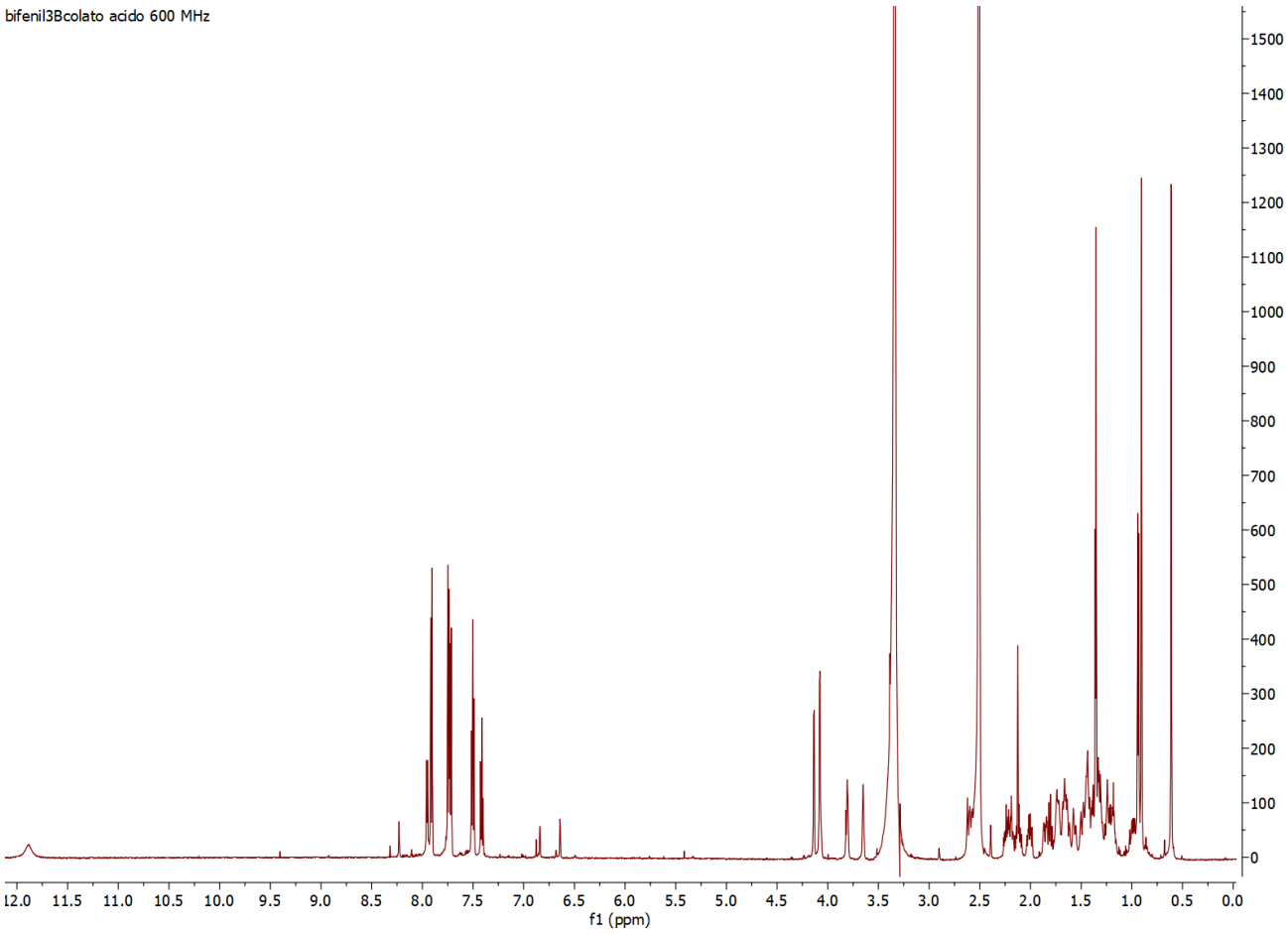


Figure S1. 1H-NMR spectrum of Cholic acid/Biphenyl in DMSO-D6 (600 MHz).

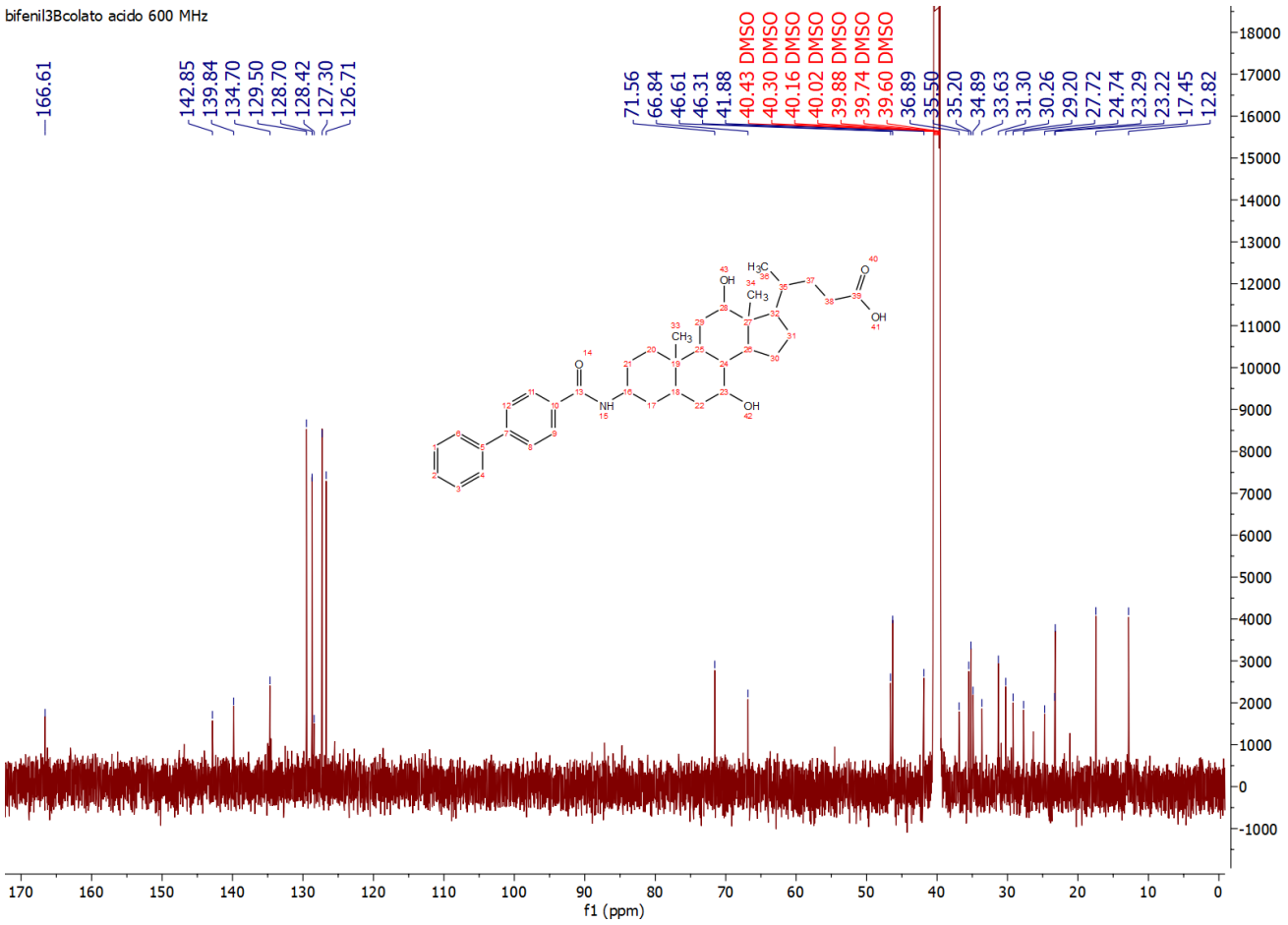


Figure S2. 13C-NMR spectrum of Cholic acid/Biphenyl in DMSO-D6 (600 MHz)

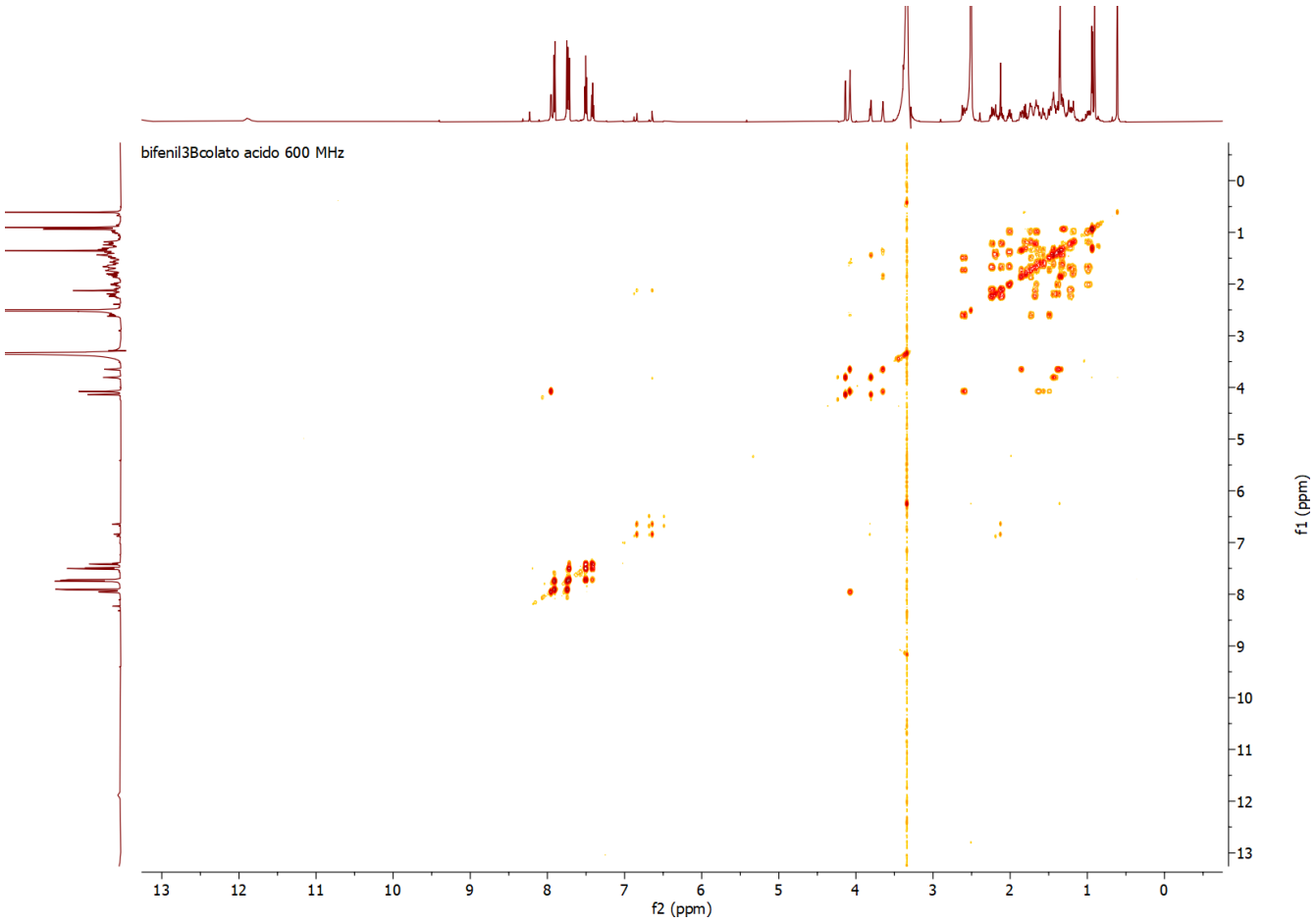


Figure S3. COSY NMR spectrum of Cholic acid/Biphenyl in DMSO-D6 (600 MHz)

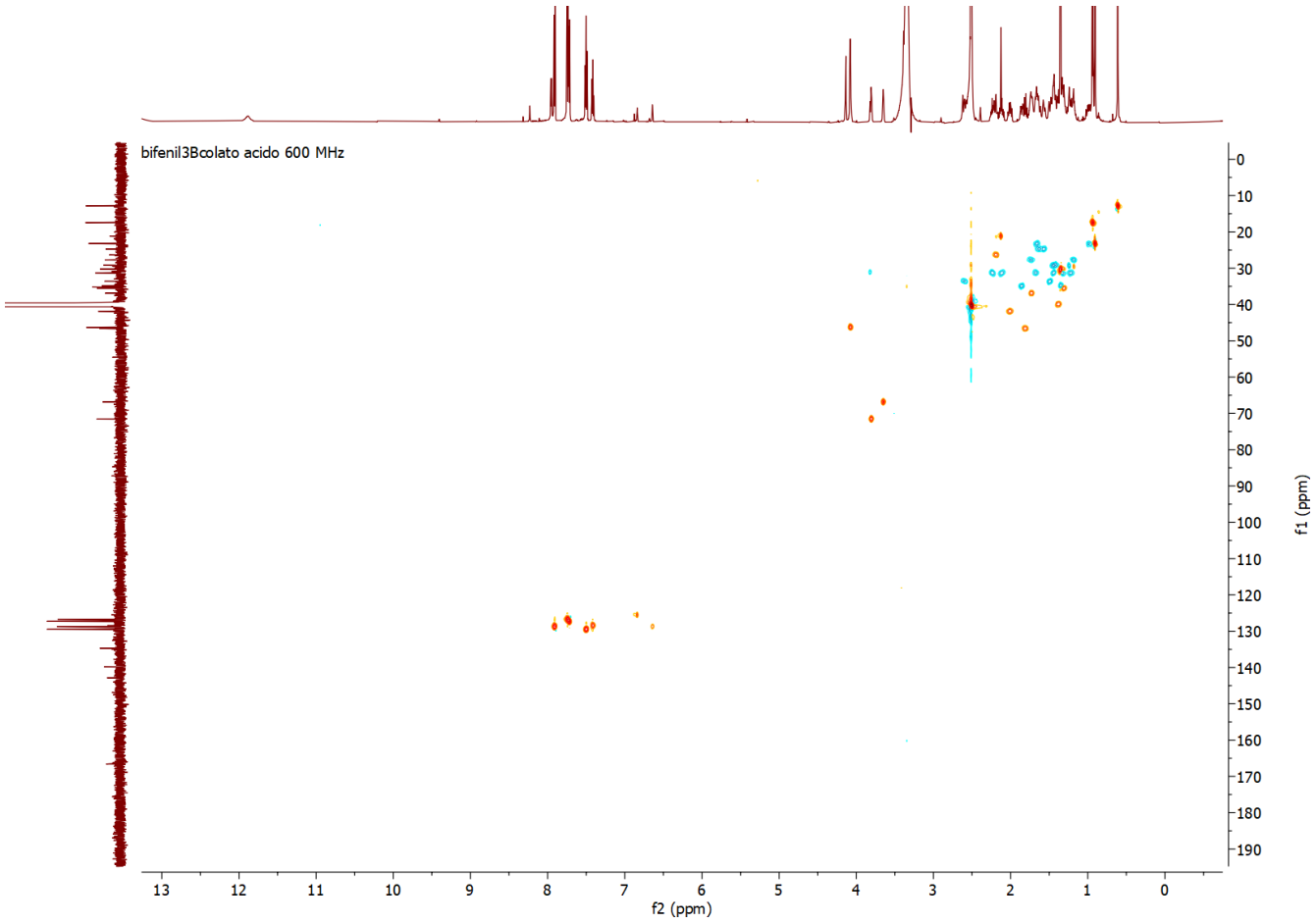


Figure S4. HSQC NMR spectrum of Cholic acid/Biphenyl in DMSO-D6 (600 MHz)

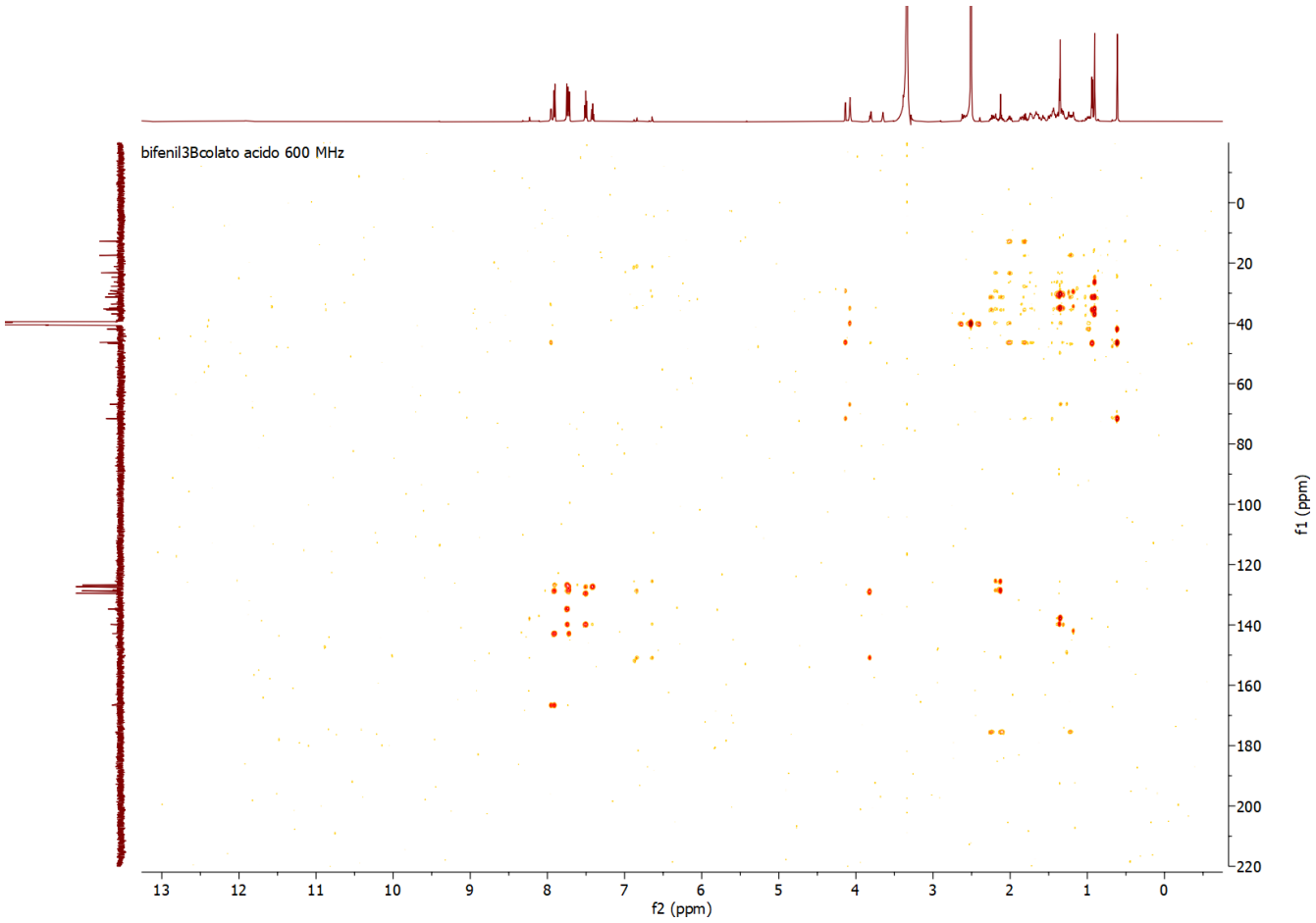


Figure S5. HMBC NMR spectrum of Cholic acid/Biphenyl in DMSO-D6 (600 MHz)

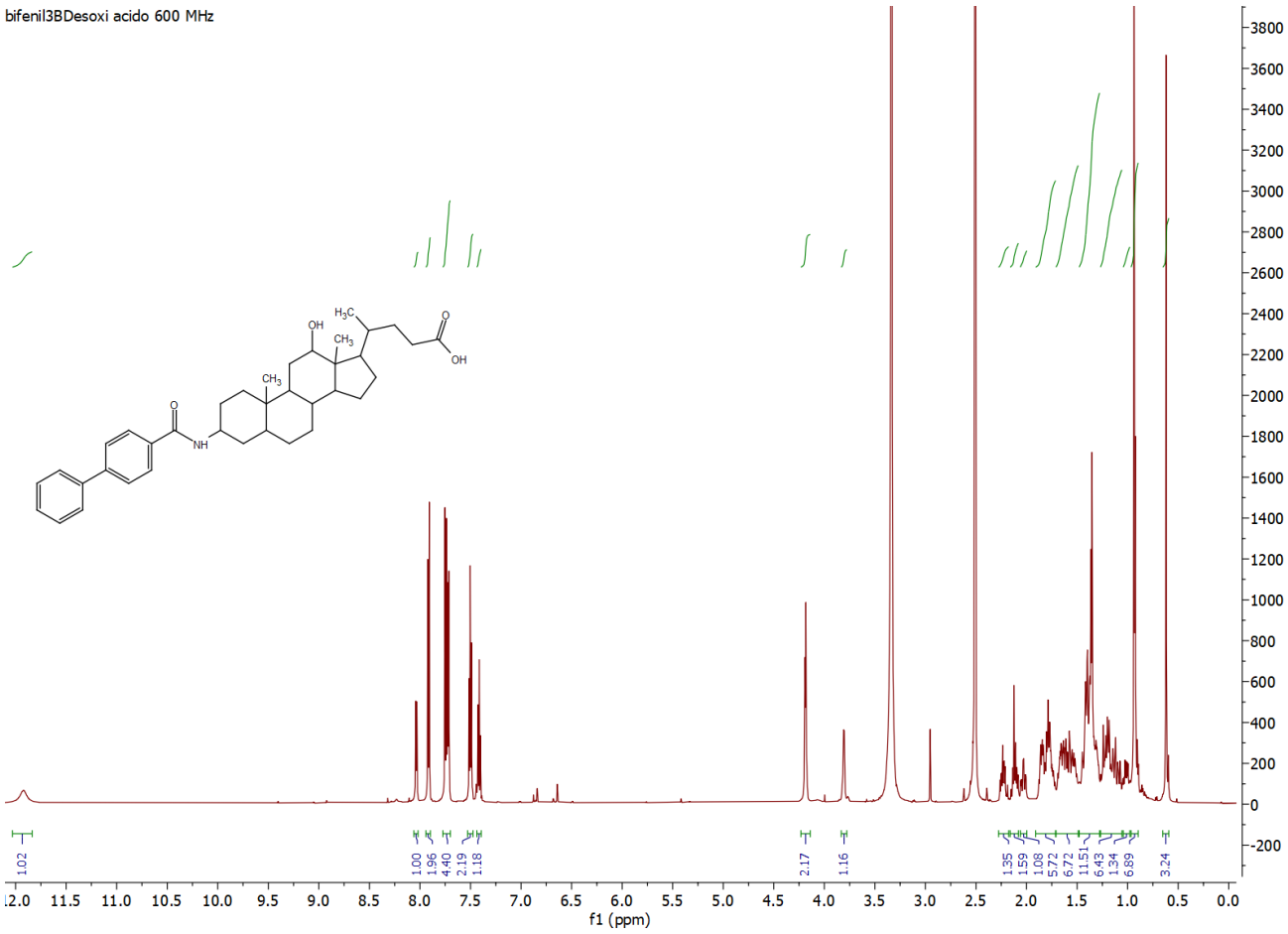


Figure S6. 1H-NMR spectrum of Desoxycholic acid/Biphenyl in DMSO-D6 (600 MHz).

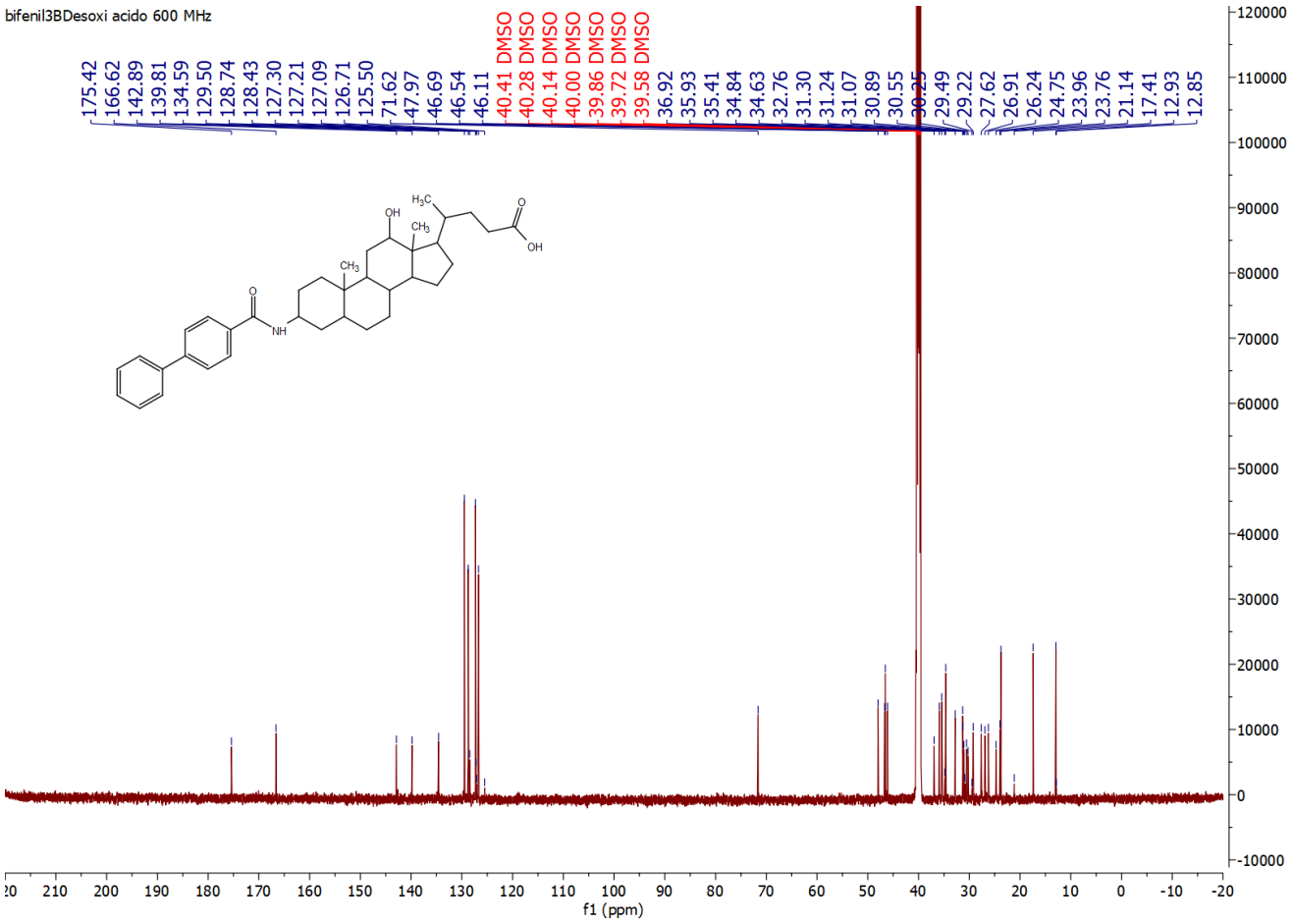


Figure S7. 13C-NMR spectrum of Desoxycholic acid/Biphenyl in DMSO-D6 (600 MHz).

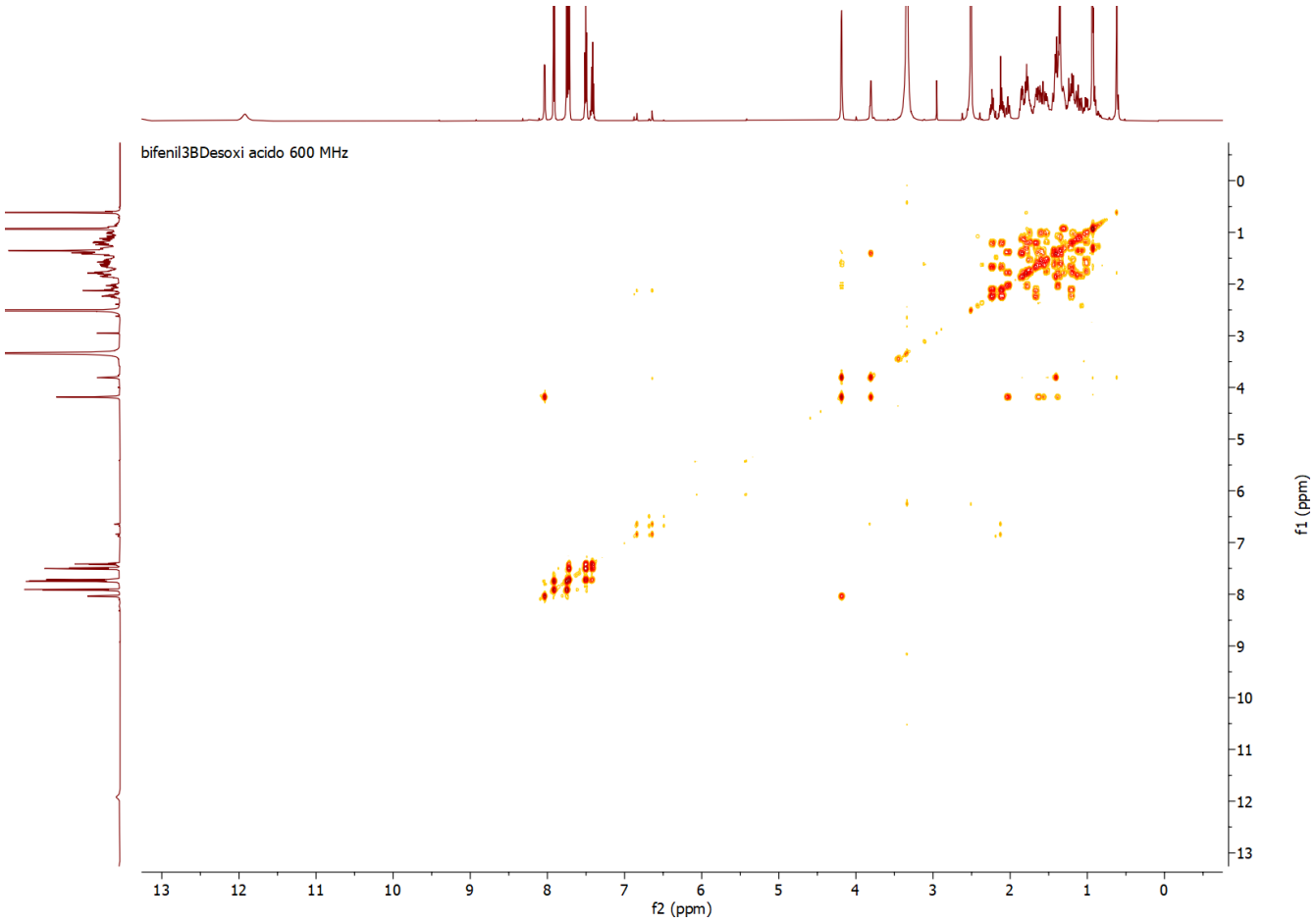


Figure S8. COSY NMR spectrum of Desoxycholic acid/Biphenyl in DMSO-D6 (600 MHz).

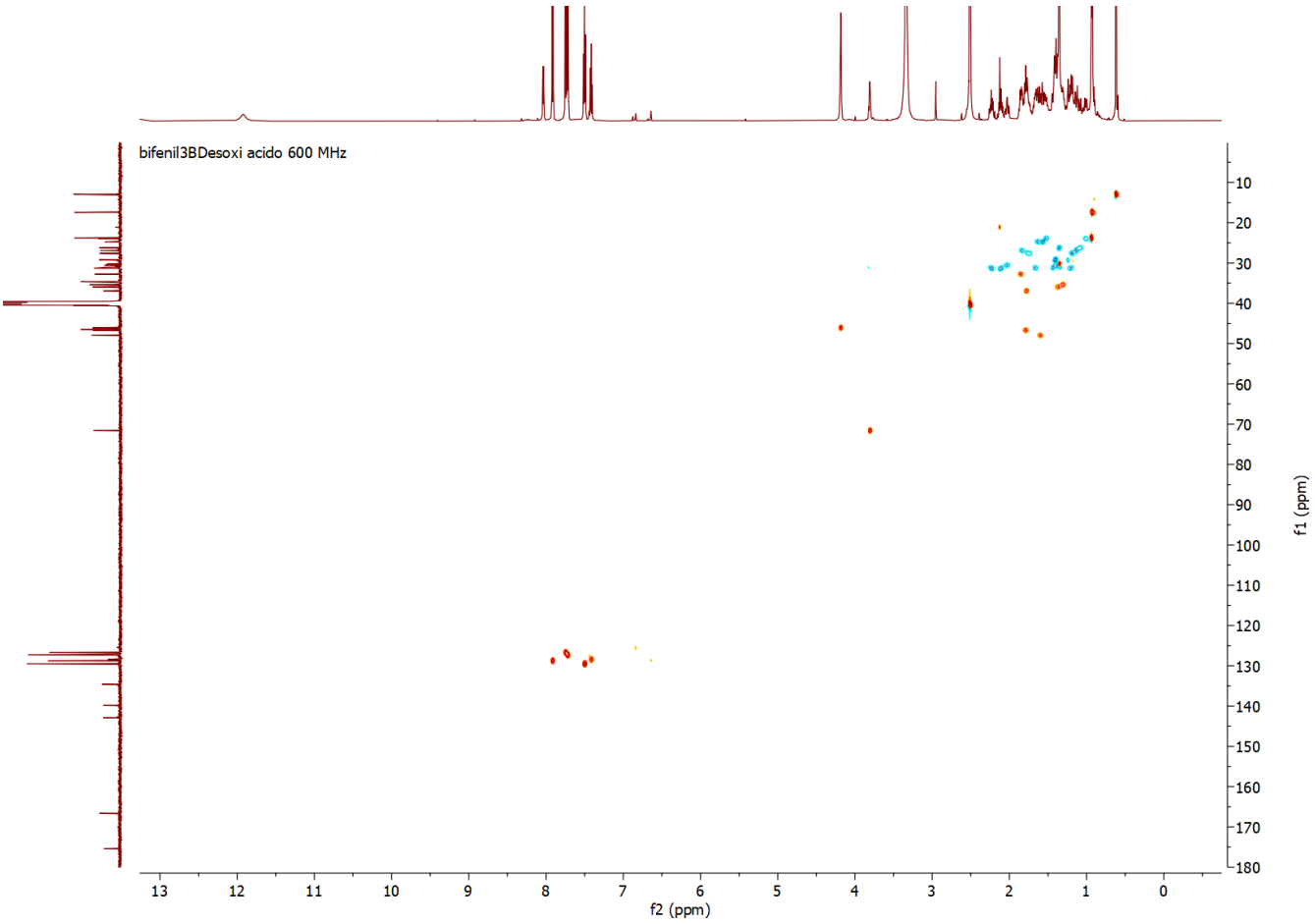


Figure S9. HSQC NMR spectrum of Desoxycholic acid/Biphenyl in DMSO-D6 (600 MHz).

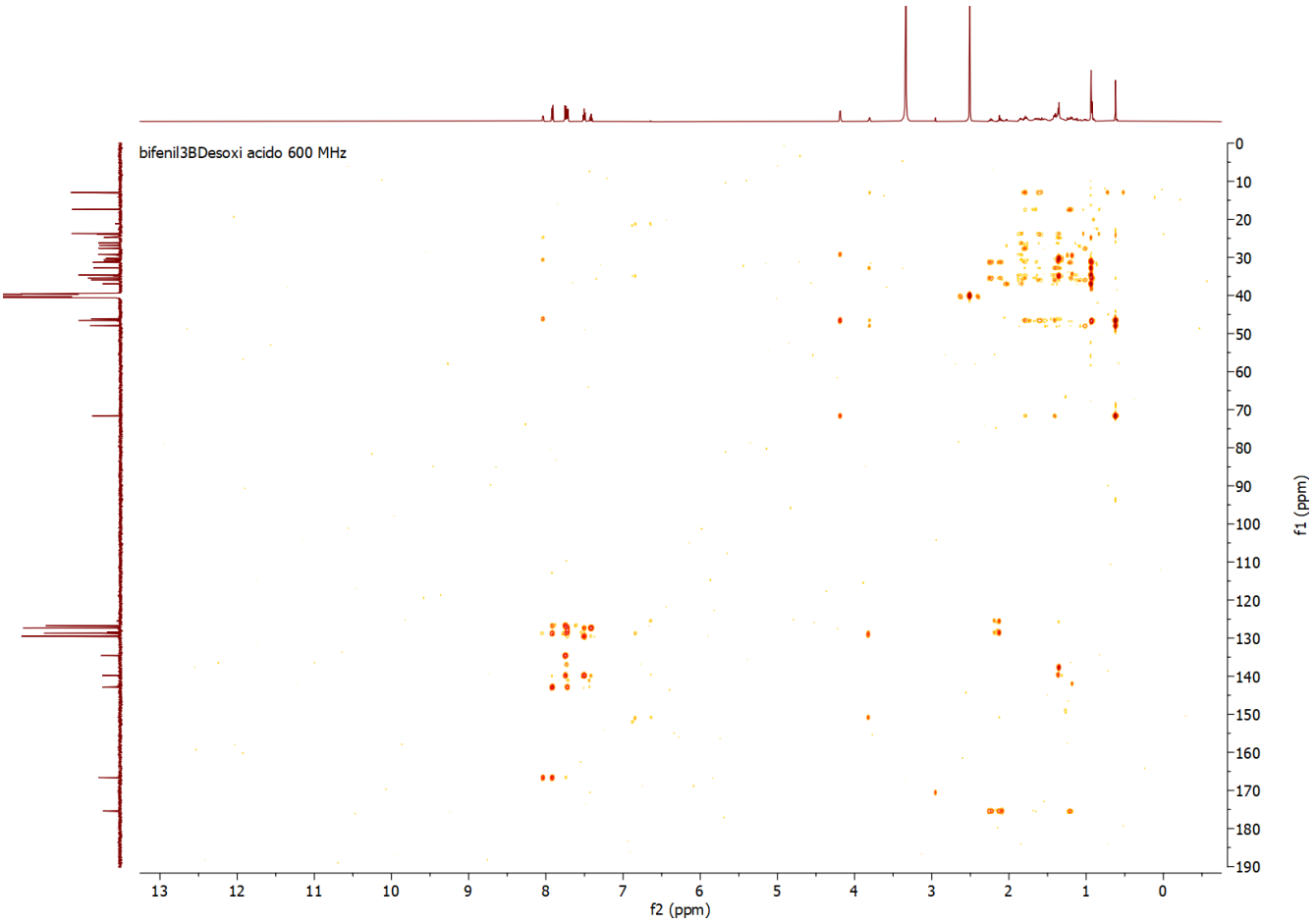


Figure S10. HMBC NMR spectrum of Desoxycholic acid/Biphenyl in DMSO-D6 (600 MHz).

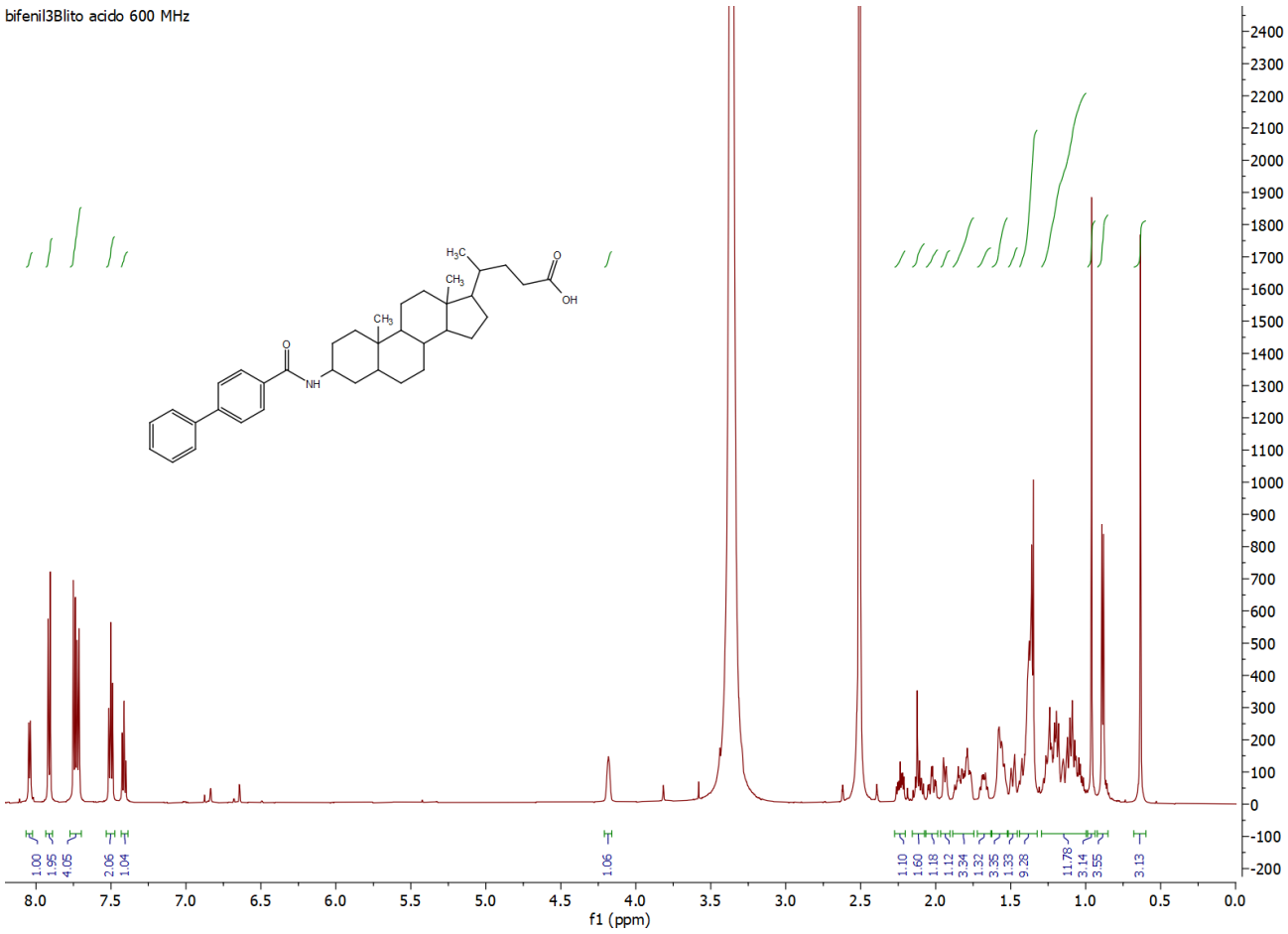


Figure S11. 1H-NMR spectrum of lithocholic acid/Biphenyl in DMSO-D6 (600 MHz).

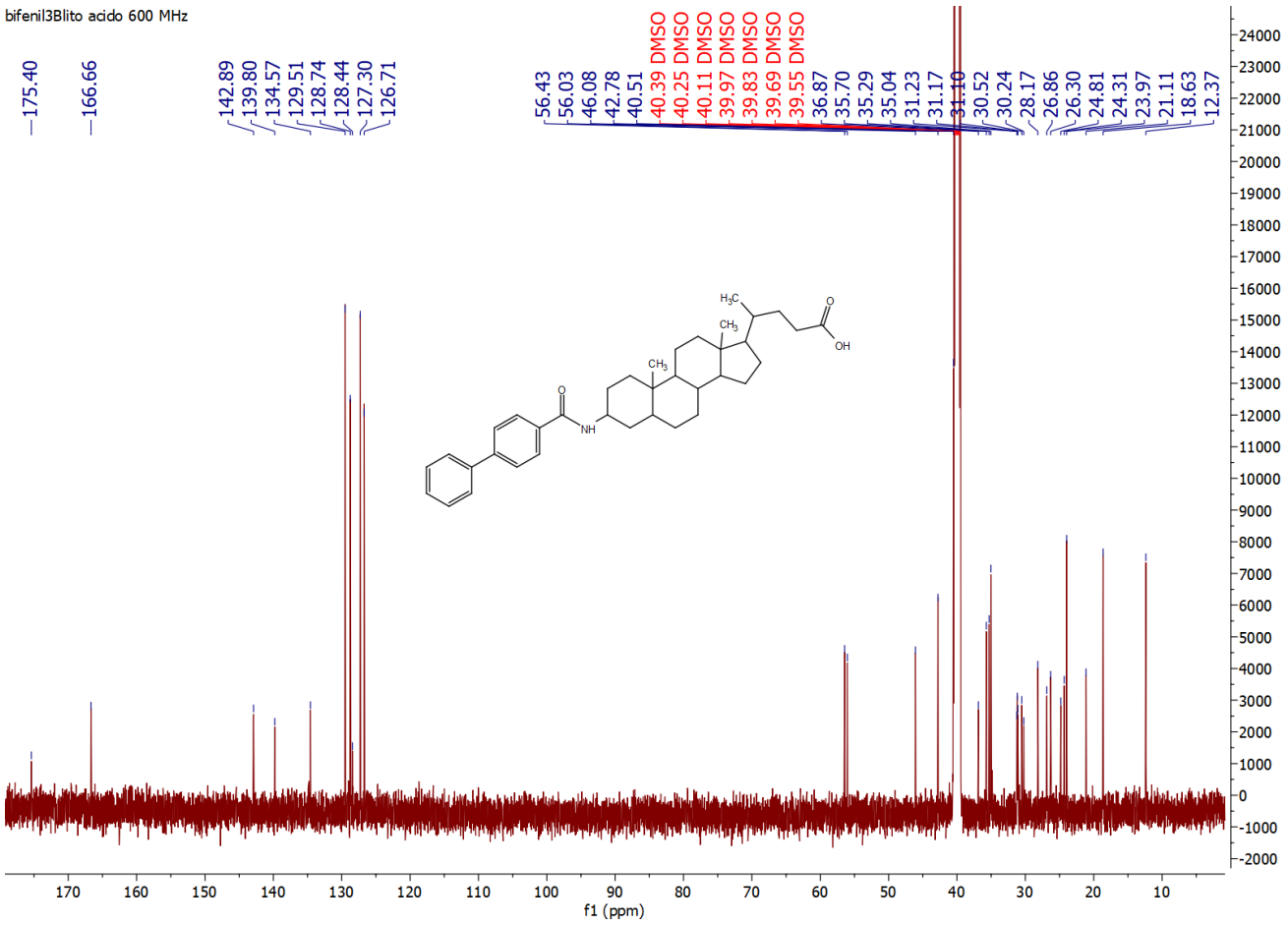


Figure S12. 13C-NMR spectrum of lithocholic acid/Biphenyl in DMSO-D6 (600 MHz).

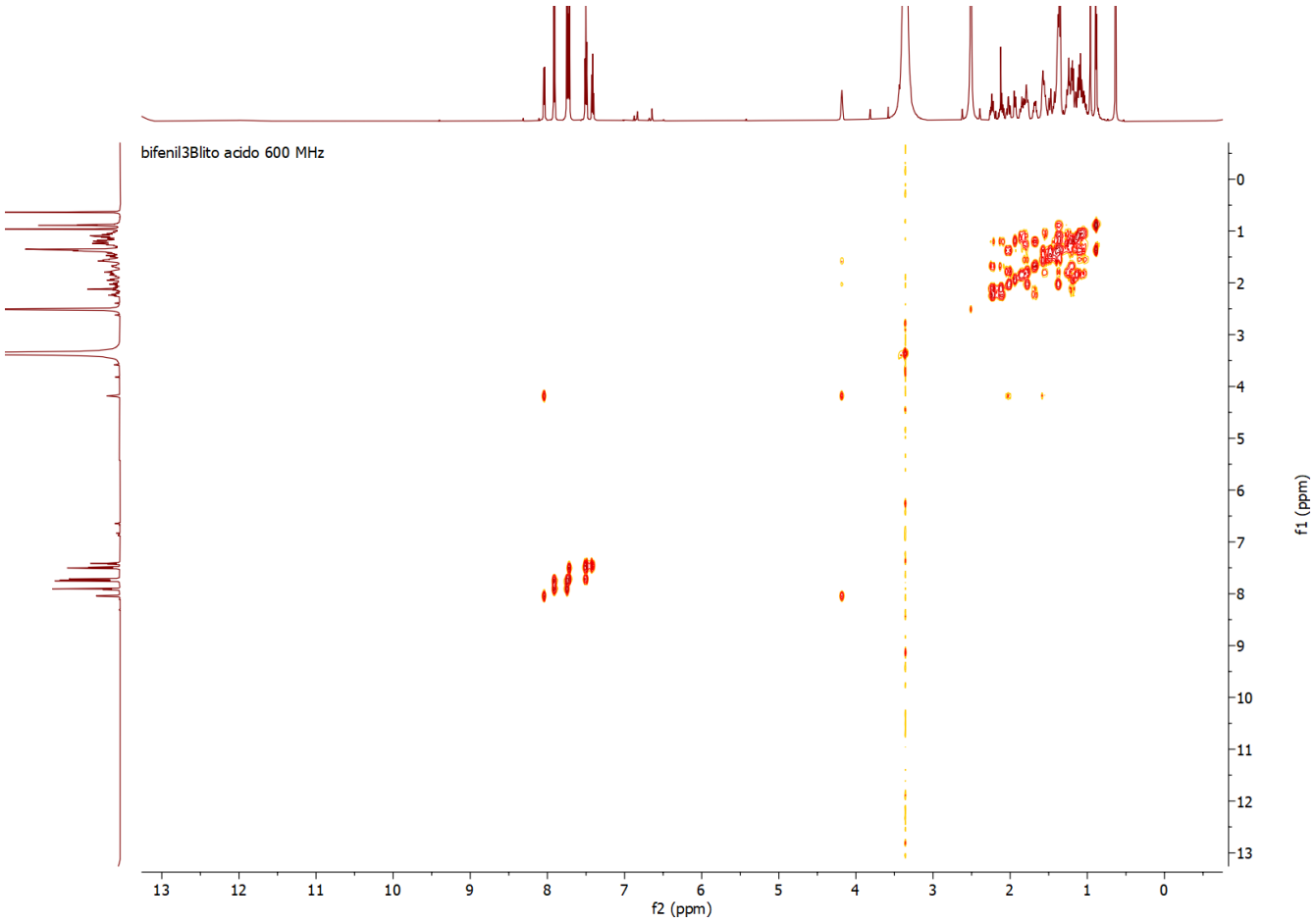


Figure S13. COSY NMR spectrum of lithocholic acid/Biphenyl in DMSO-D6 (600 MHz).

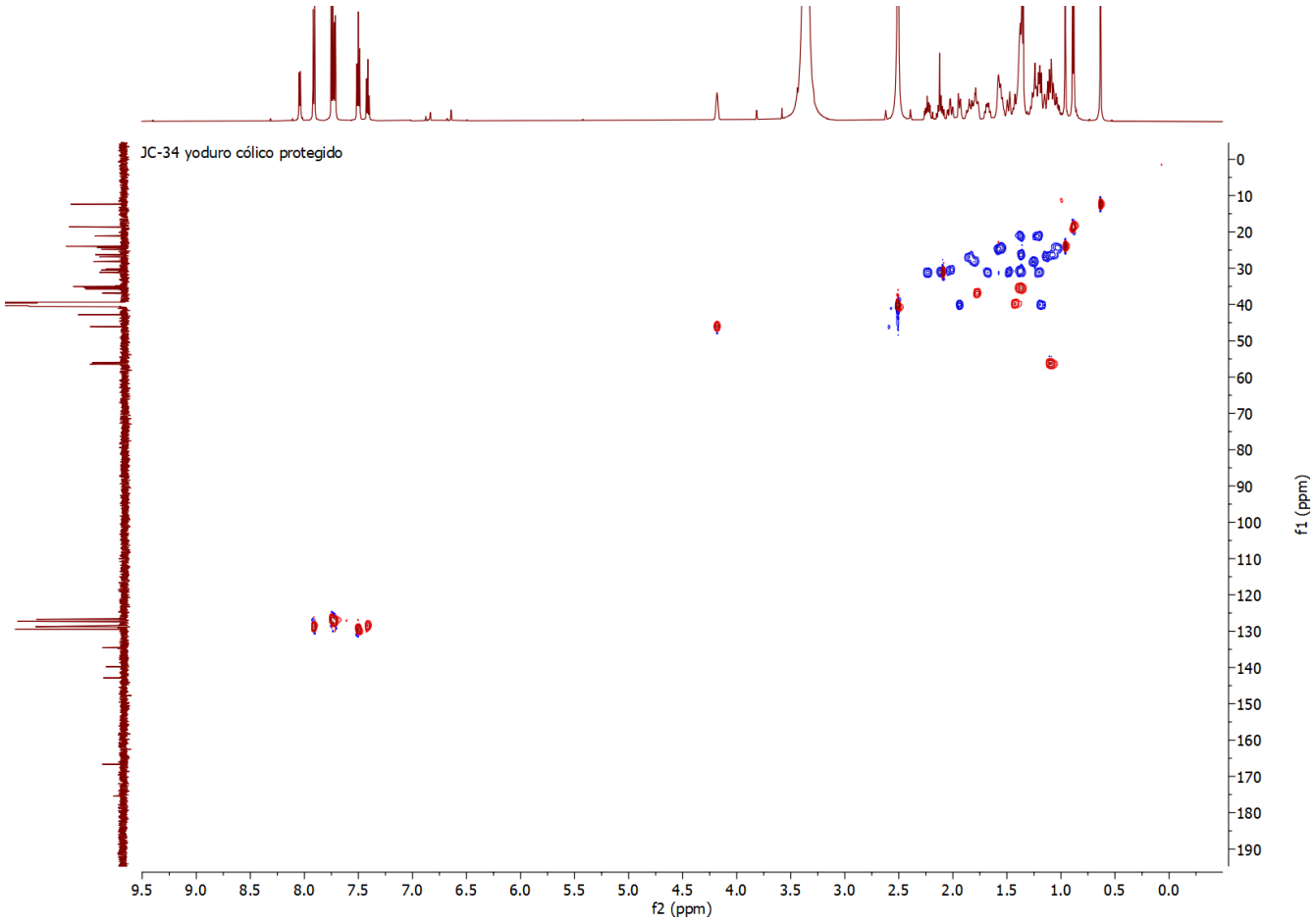


Figure S14. HSQC NMR spectrum of lithocholic acid/Biphenyl in DMSO-D6 (600 MHz).

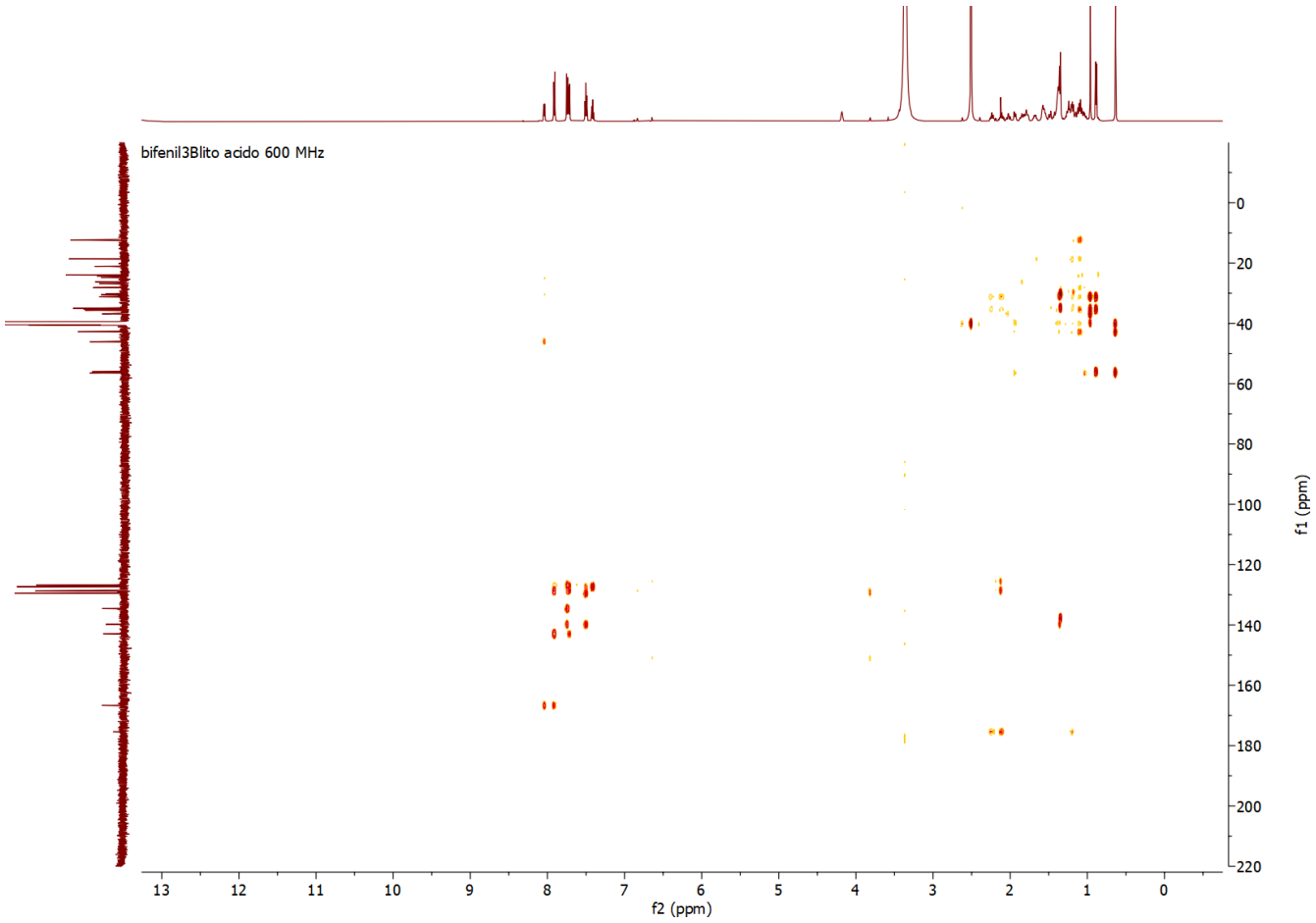


Figure S15. HMBC NMR spectrum of lithocholic acid/Biphenyl in DMSO-D6 (600 MHz).

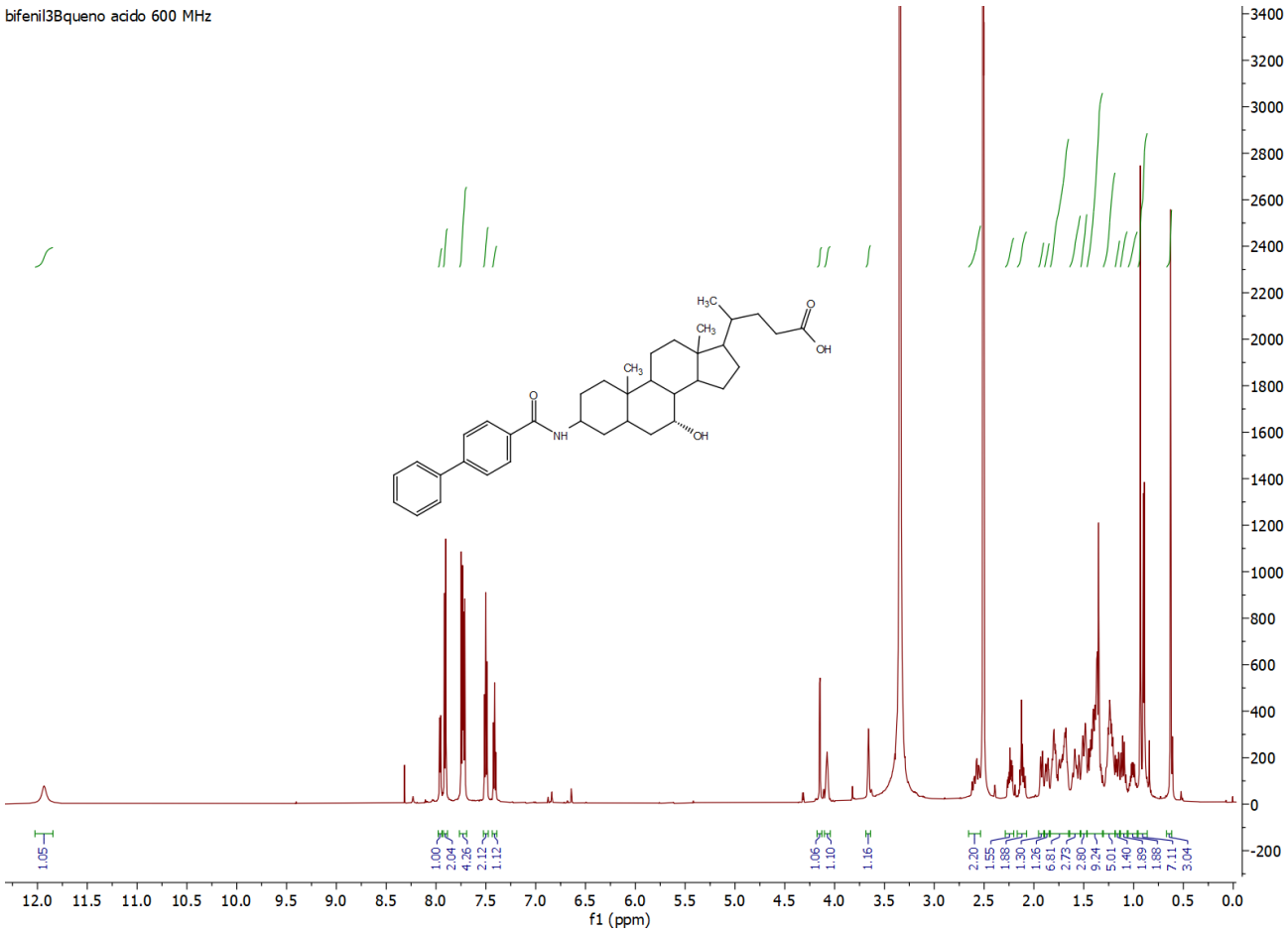


Figure S16. 1H-NMR spectrum of chenodesoxycholic acid/Biphenyl in DMSO-D6 (600 MHz).

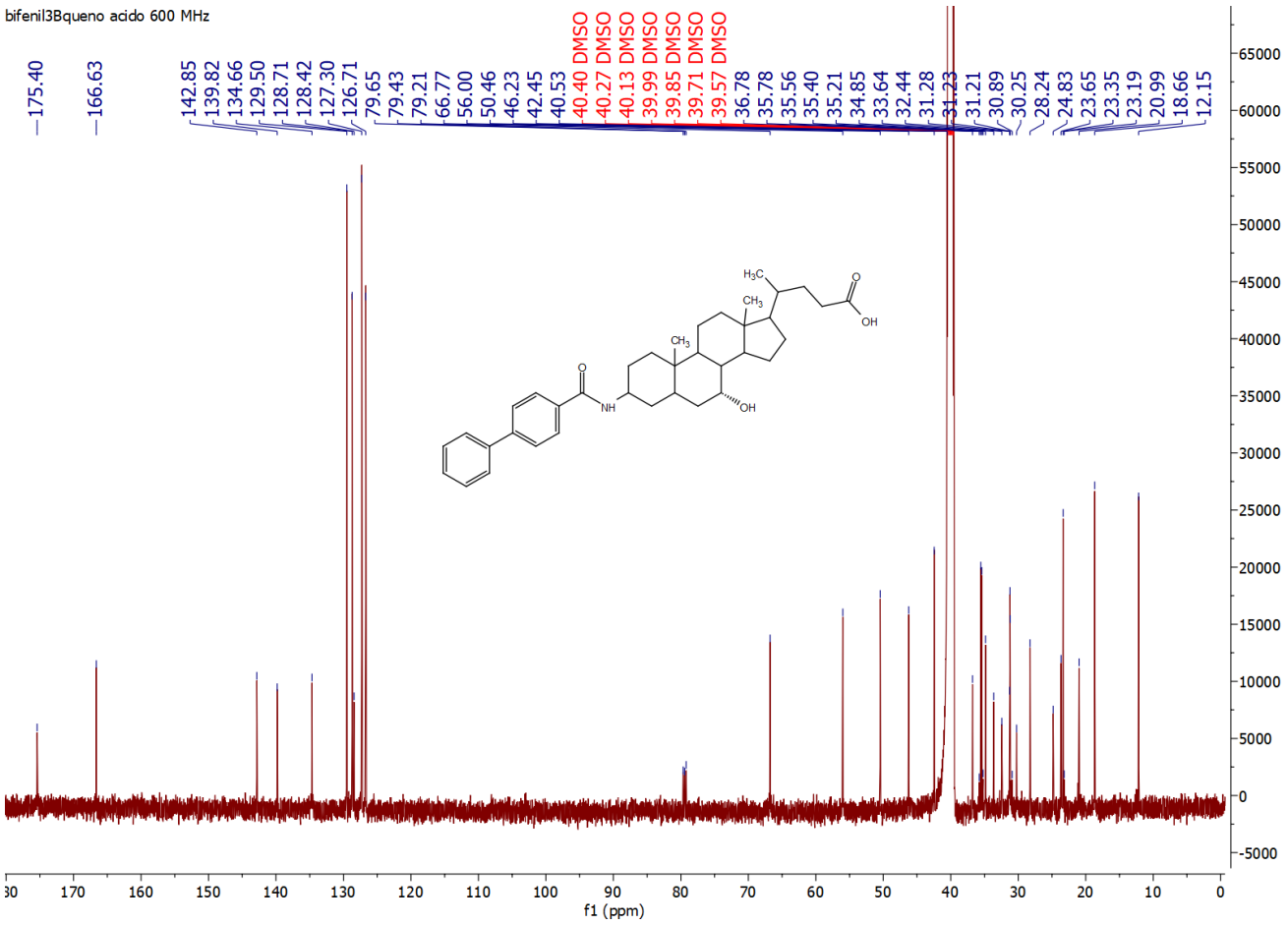


Figure S17. 13C-NMR spectrum of chenodesoxycholic acid/Biphenyl in DMSO-D6 (600 MHz)

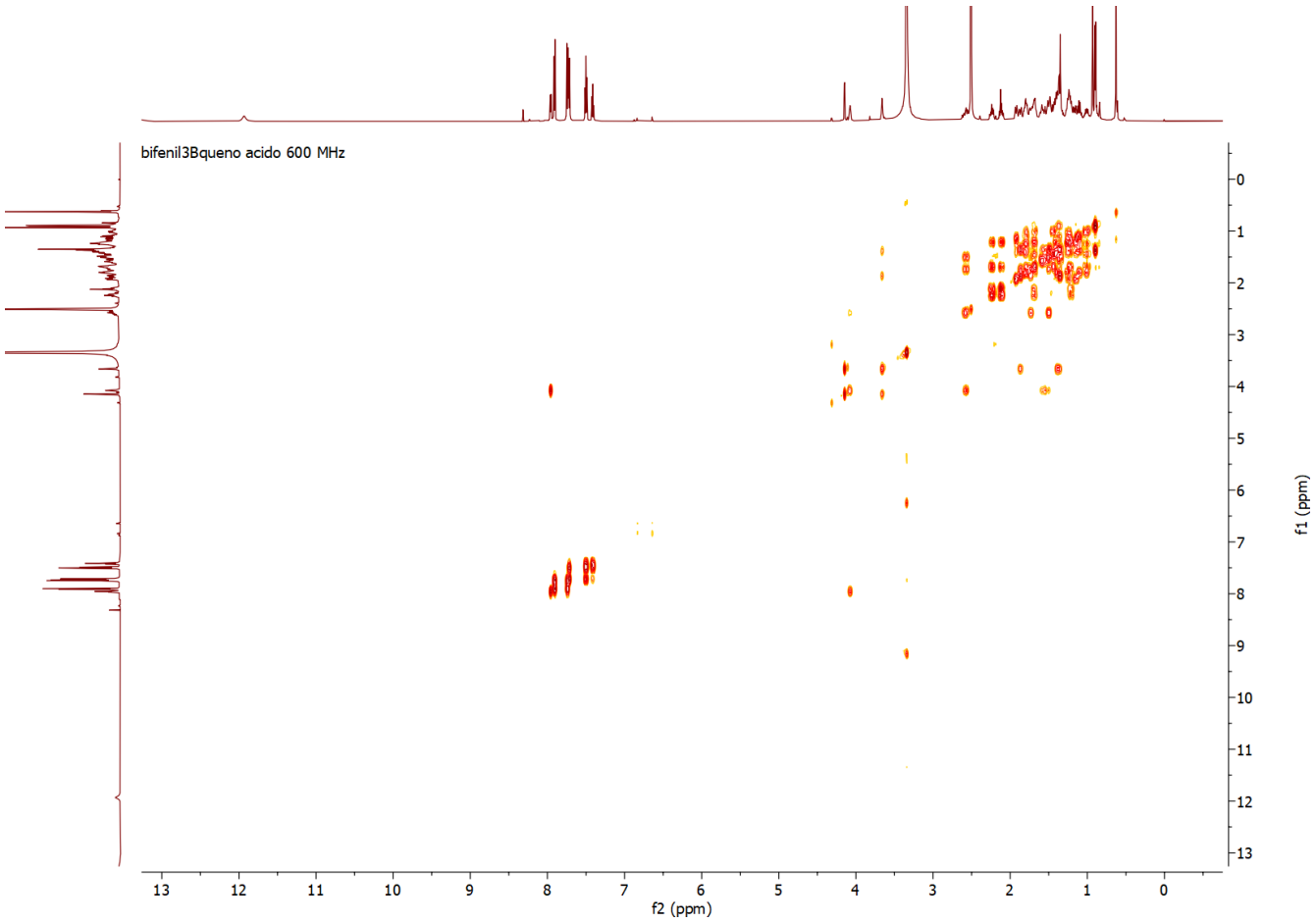


Figure S18. COSY-NMR spectrum of chenodesoxycholic acid/Biphenyl in DMSO-D6 (600 MHz)

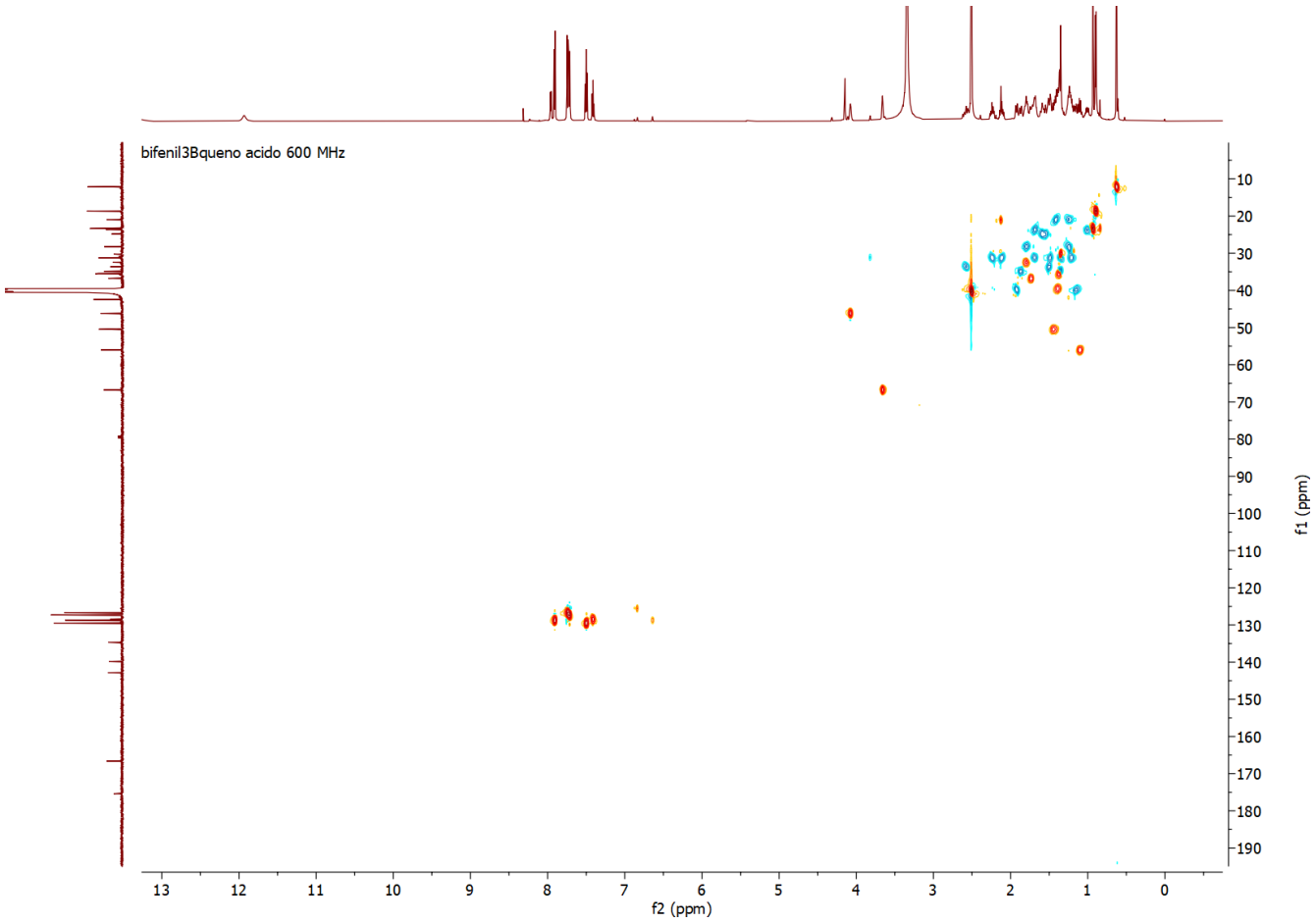


Figure S19. HSQC NMR spectrum of chenodesoxycholic acid/Biphenyl in DMSO-D6 (600 MHz)

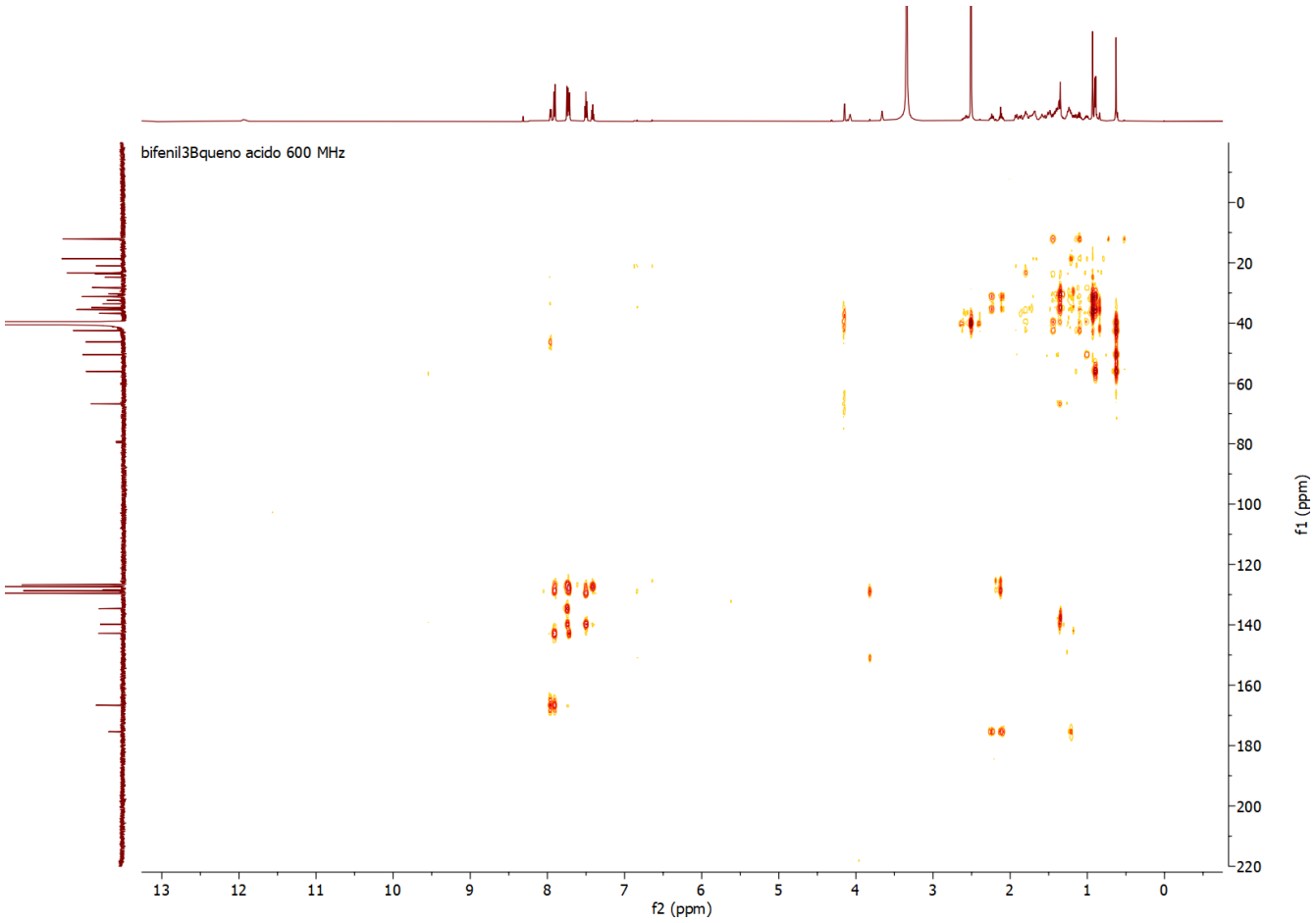


Figure S20. HMBC NMR spectrum of chenodesoxycholic acid/Biphenyl in DMSO-D6 (600 MHz)

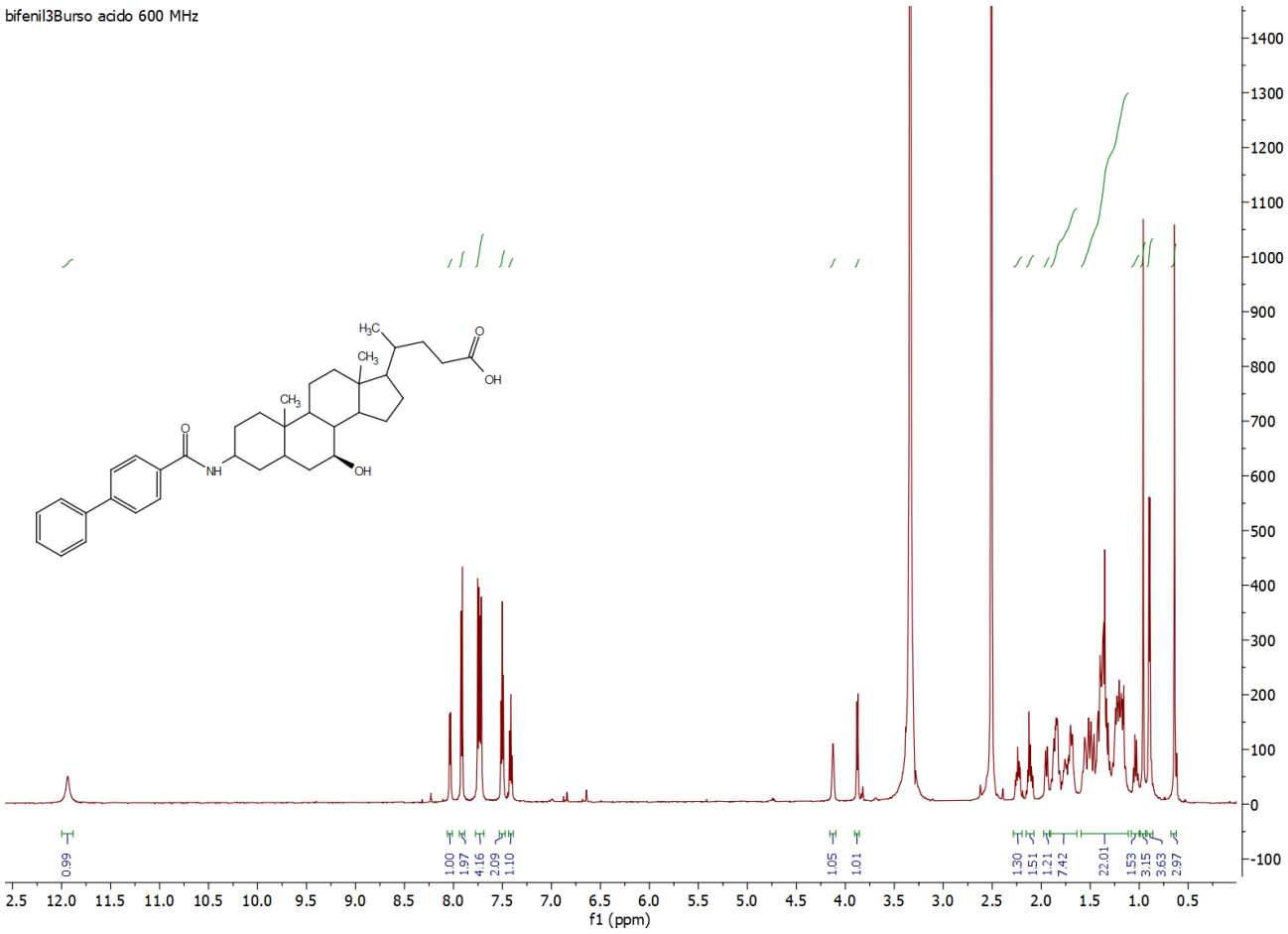


Figure S21. 1H-NMR spectrum of Ursodesoxycholic acid/Biphenyl in DMSO-D6 (600 MHz)

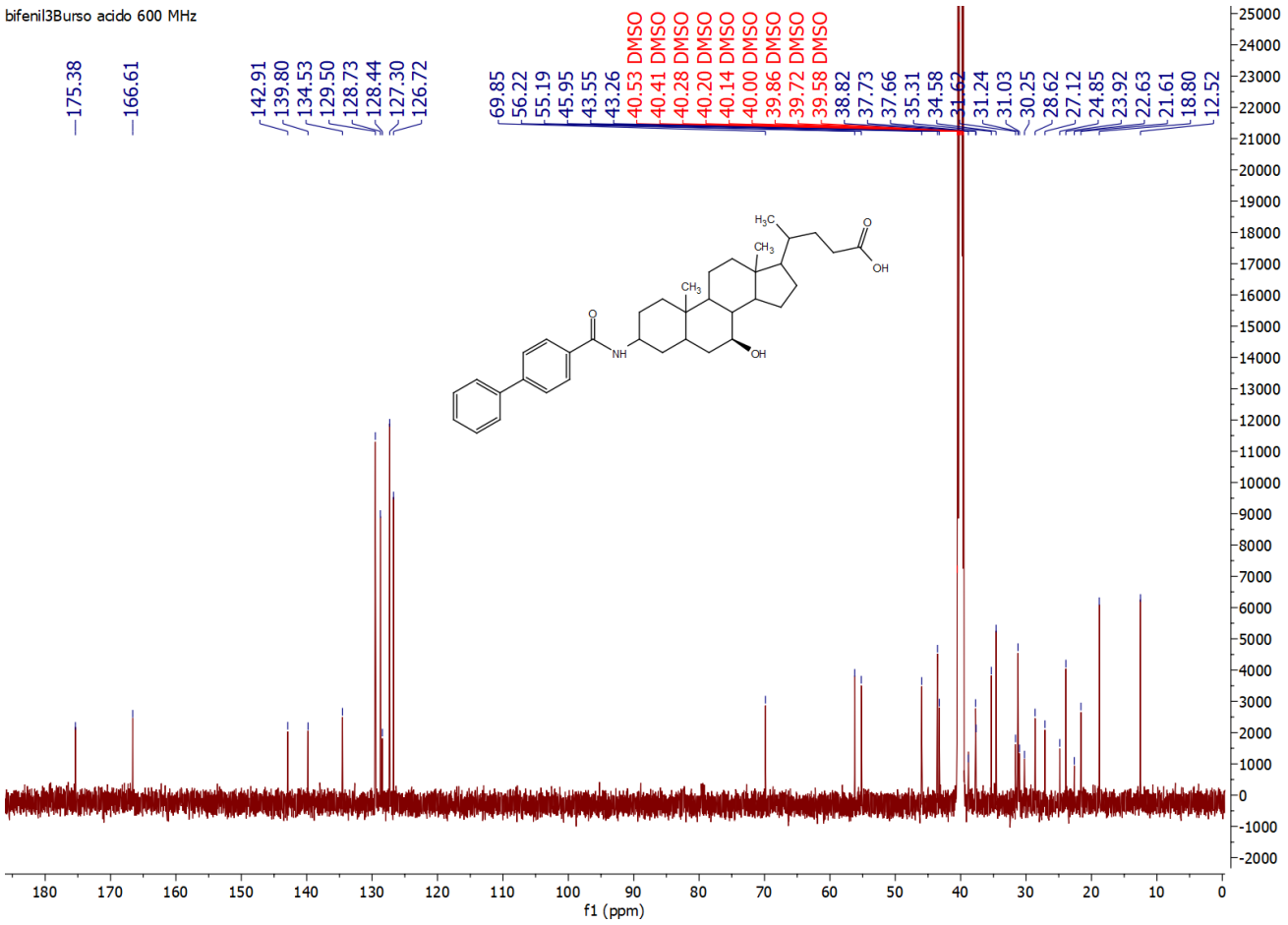


Figure S22. 13C-NMR spectrum of Ursodesoxycholic acid/Biphenyl in DMSO-D6 (600 MHz)

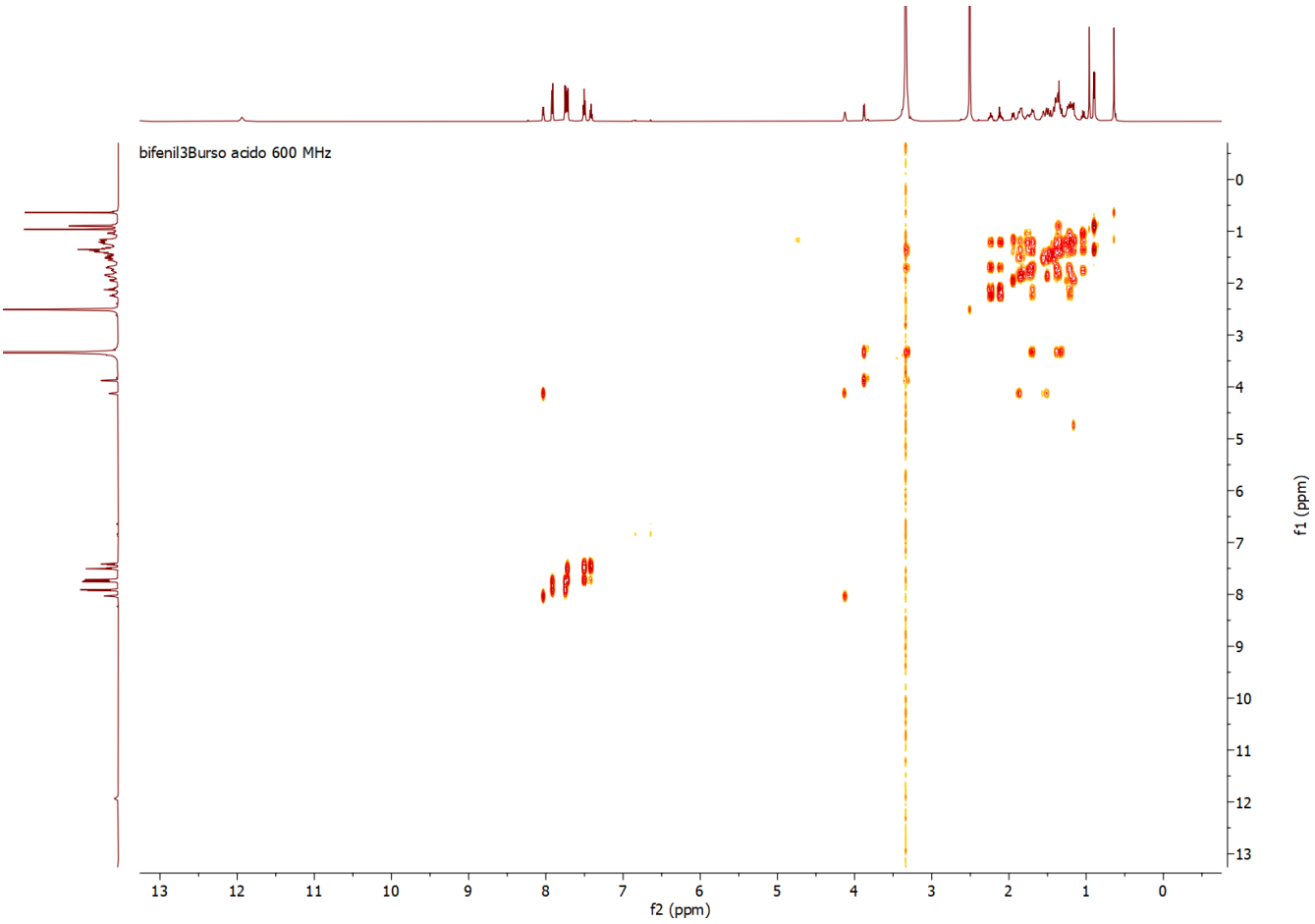


Figure S23. COSY NMR spectrum of Ursodesoxycholic acid/Biphenyl in DMSO-D6 (600 MHz)

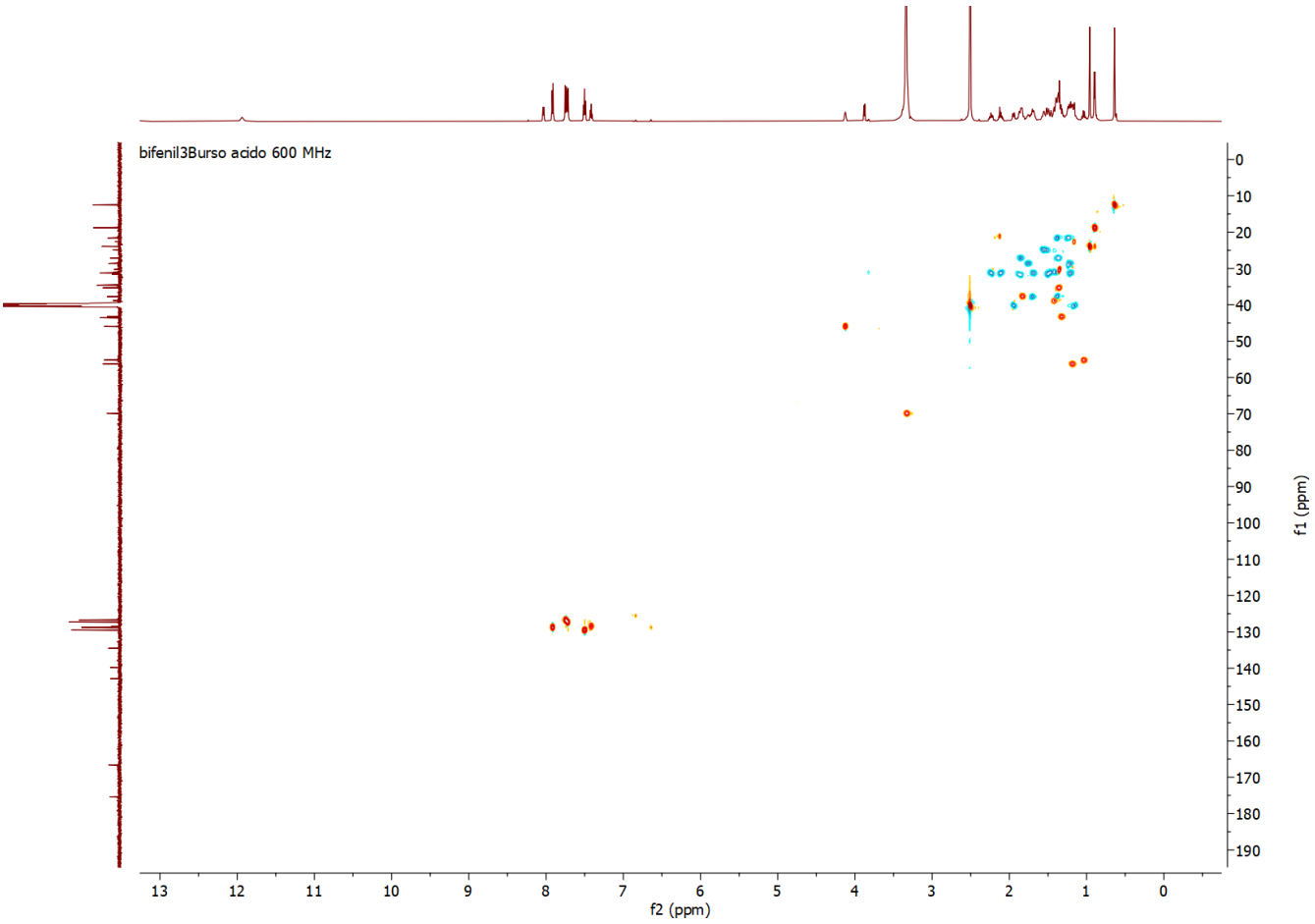


Figure S24. HSQC NMR spectrum of Ursodesoxycholic acid/Biphenyl in DMSO-D6 (600 MHz)

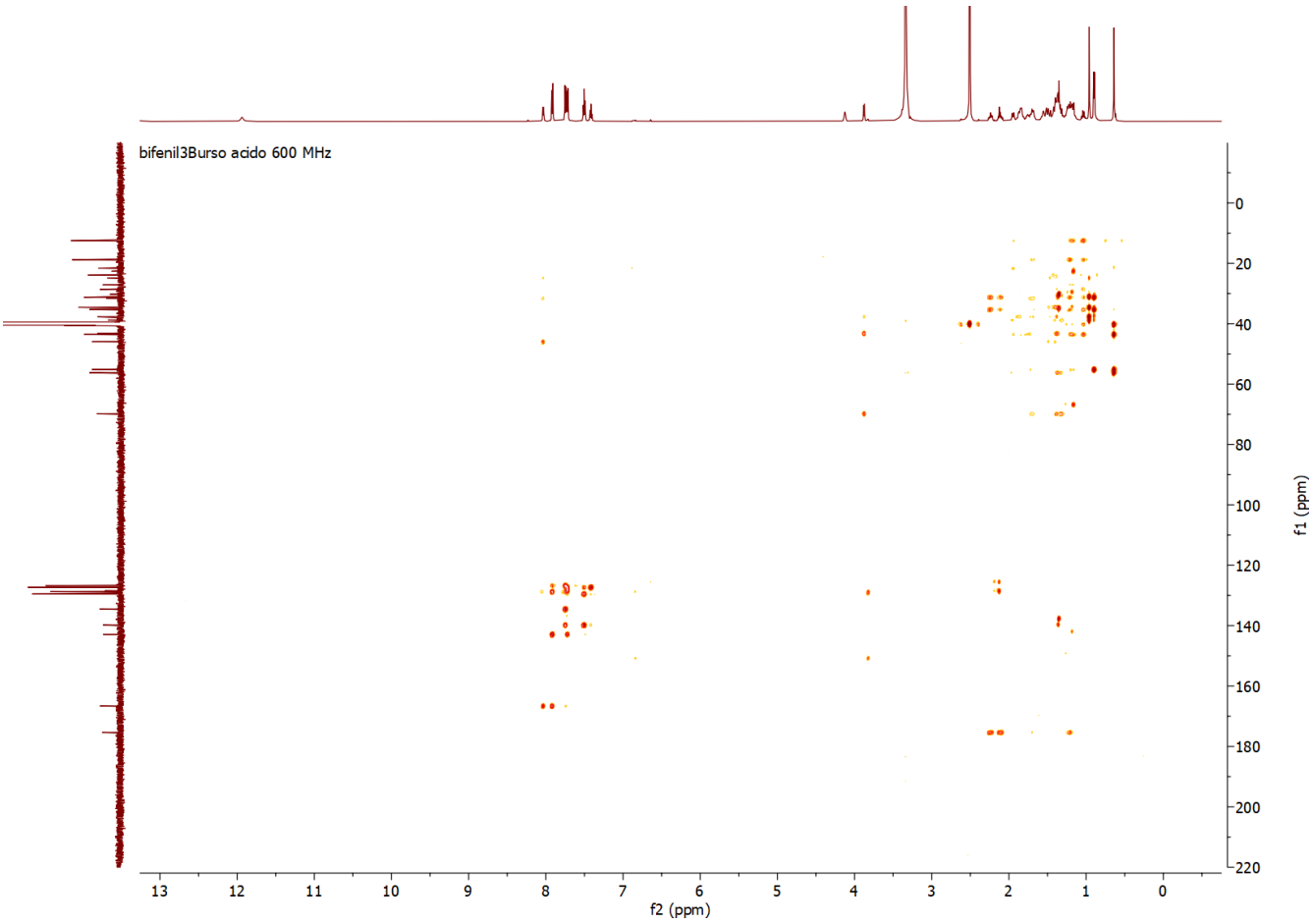


Figure S25. HMBC NMR spectrum of Ursodesoxycholic acid/Biphenyl in DMSO-D6 (600 MHz)

ESI-Orbitrap-MS analysis

Samples were dissolved in methanol and measured in a Orbitrap Exploris 120, data were analyzed with Thermo Scientific Xcalibur version: 4.5.474.0

Compound	[M+H]	Calculated Mass	Current mass
BI-AC-01-C	$C_{37}H_{50}O_5N^+$	588.36890	588.3686
BI-AC-02-D	$C_{37}H_{50}O_4N^+$	572.37398	572.3738
BI-AC-03-L	$C_{37}H_{50}O_3N^+$	556.37907	556.3781
BI-AC-04-U	$C_{37}H_{50}O_4N^+$	572.37398	572.3727
BI-AC-05-Q	$C_{37}H_{50}O_4N^+$	572.37398	572.3733

Table S5. HR-ESI-MS data of the synthesized compounds.

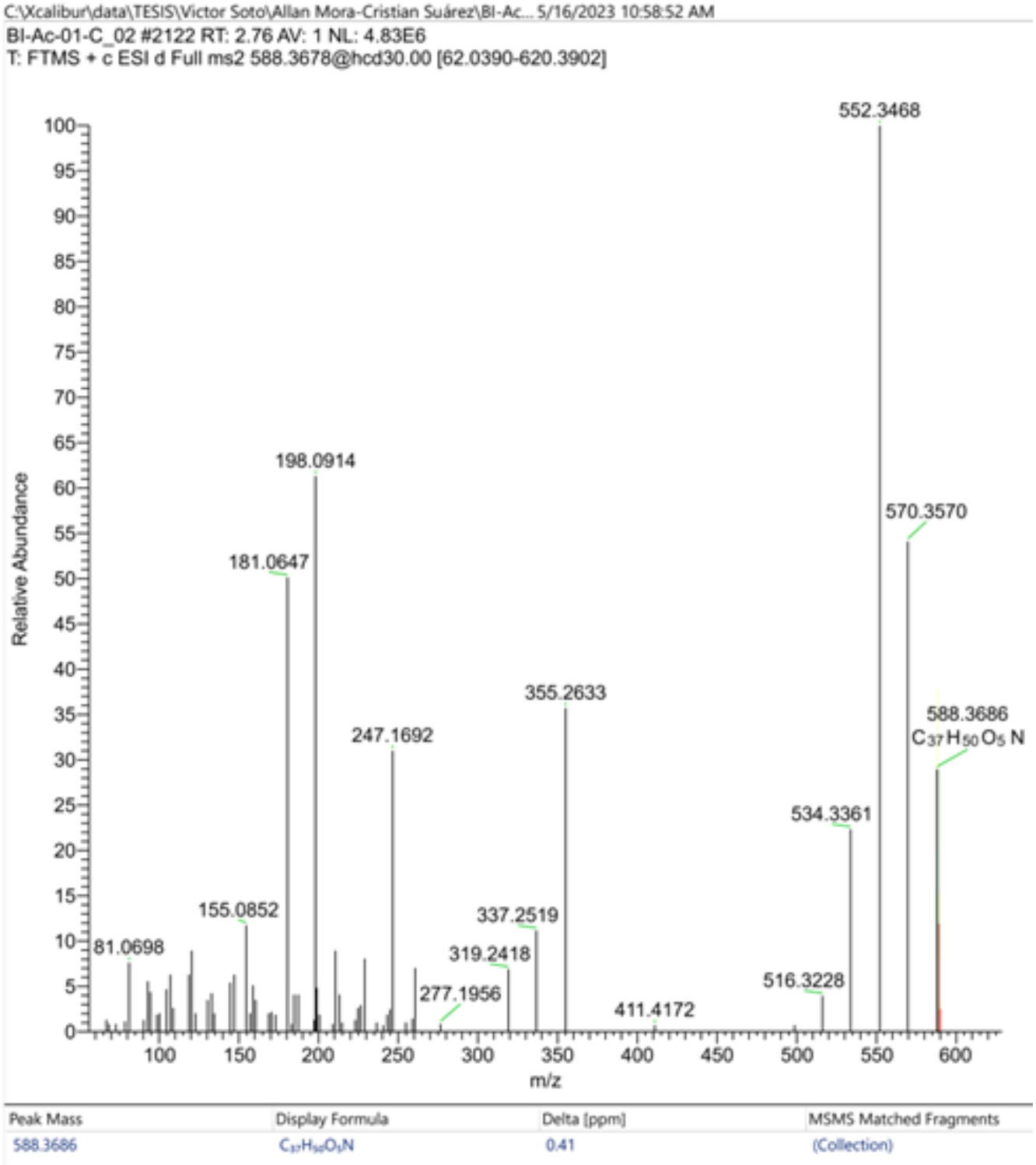


Figure S26. ESI-Orbitrap-MS of the Biphenyl Cholic acid derivative.

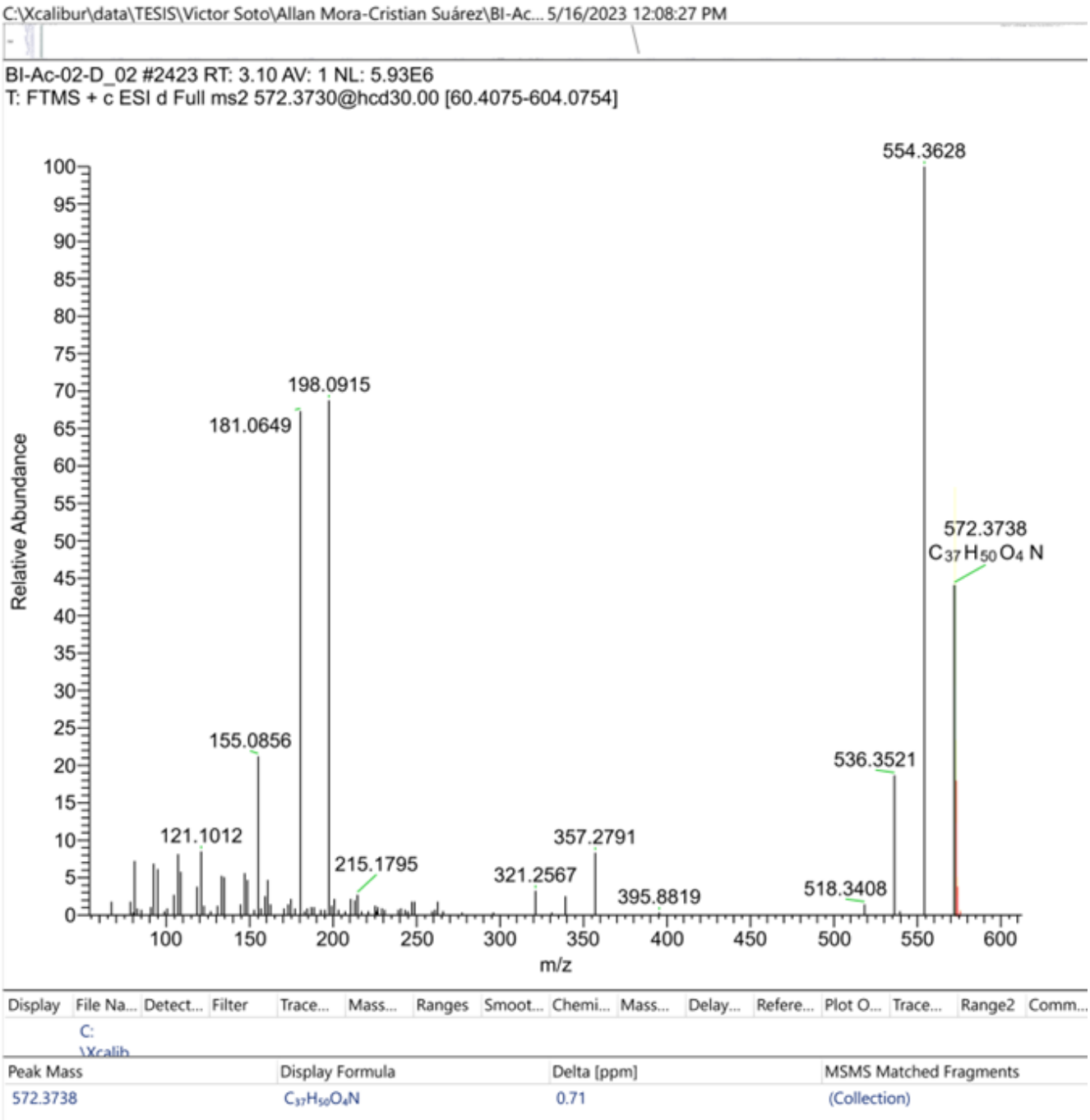


Figure S27. ESI-Orbitrap-MS of the Biphenyl Deoxycholic acid derivative.

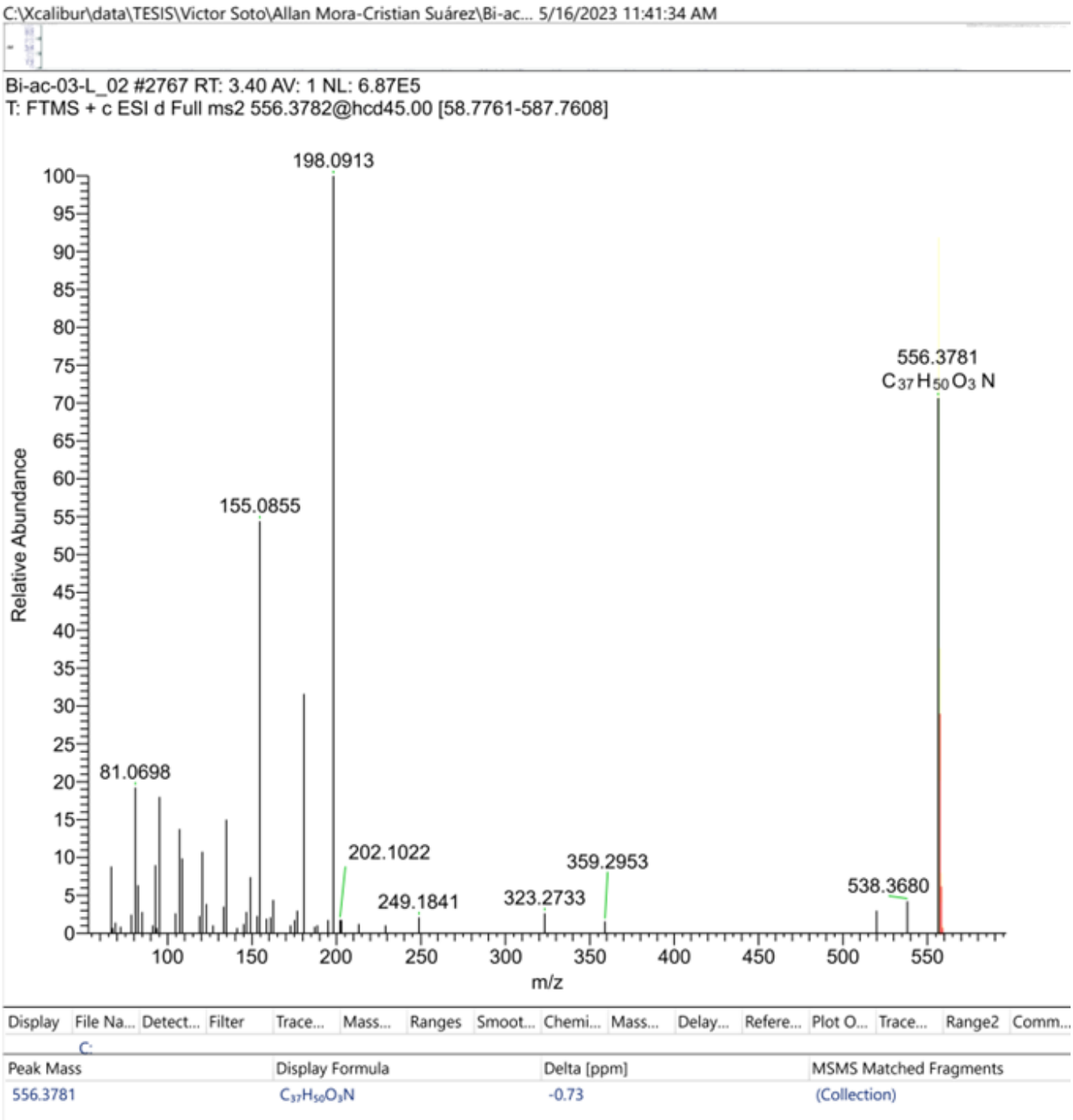


Figure S28. ESI-Orbitrap-MS of the Biphenyl Litocholic acid derivative.

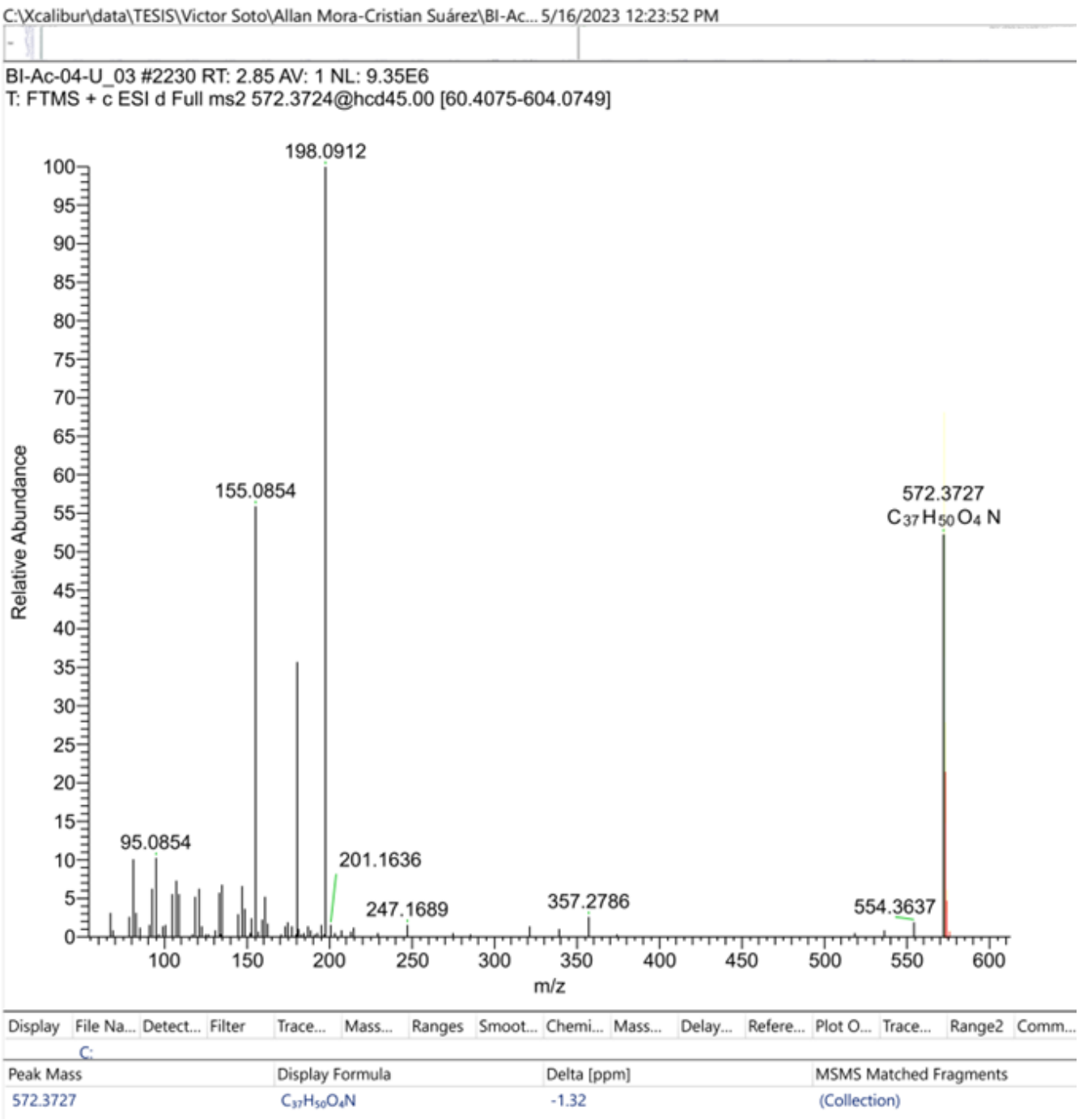


Figure S29. ESI-Orbitrap-MS of the Biphenyl Ursodeoxycholic acid derivative.

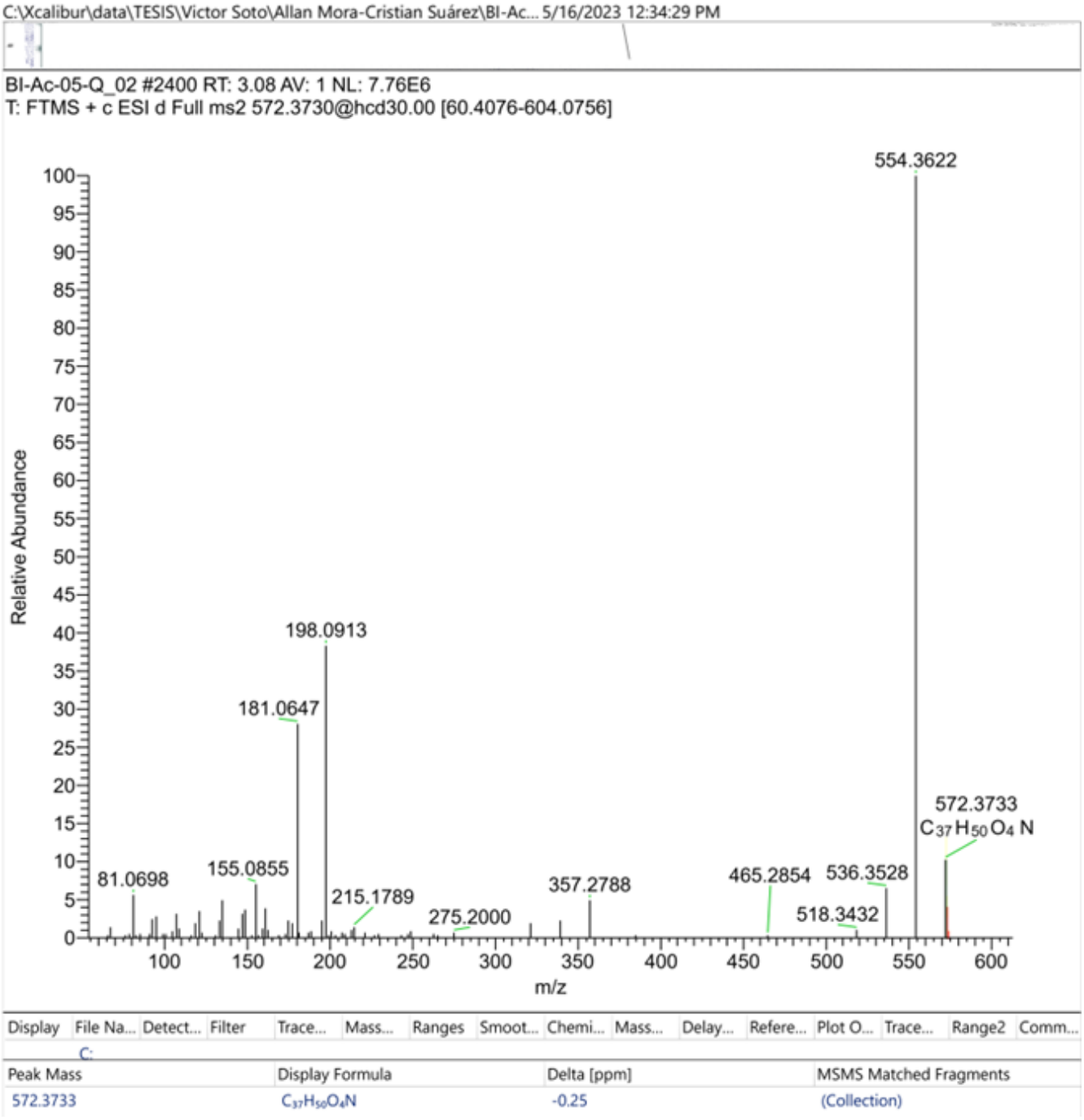


Figure S30. ESI-Orbitrap-MS of the Biphenyl Chenodeoxycholic acid derivative.

3 Optical properties

The 4μm thick mesoporous TiO_2 films sensitized with the various dyenamo blue:coadsrober ratios were washed with a 0.5μL tetrabutylammonium hydroxide. This led to dye getting de-sorbed from the titania. 3mL of dichloromethane was added to the vial and the absorption spectra measured.

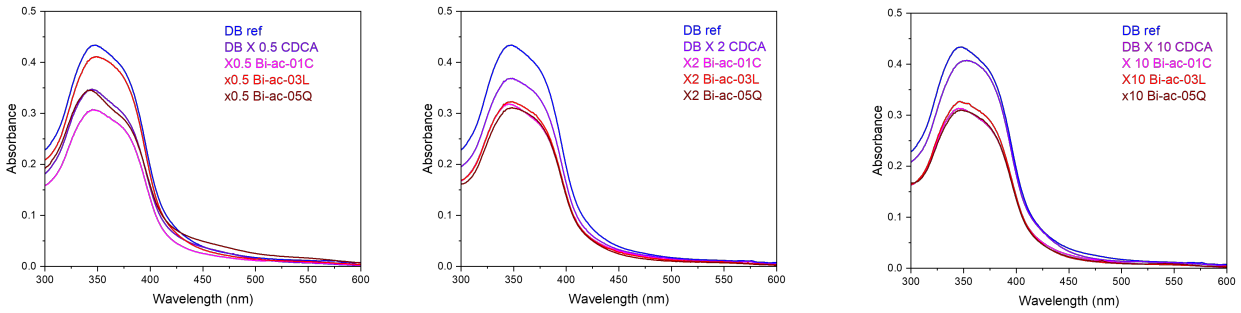


Figure S31. UV-Vis absorption spectra of the dye with different concentrations of the coadsorbers (given in the legends) desorbed from the 4μm thick titania films.

4 Photovoltaic performance

Dye:Co-sensitizer	Jsc (mA/cm2)	Voc (V)	FF	PCE (%)
0.075mM DB	9.14 (7.56 ± 0.92)	0.74 (0.75 ± 0.01)	0.76 (0.74 ± 0.02)	5.17 (4.19 ± 0.64)
1:10 DB:CDCA	12 (11.68 ± 0.35)	0.74 (0.75 ± 0.01)	0.72 (0.72 ± 0.01)	6.4 (6.22 ± 0.16)
1:10 DB:Bi-ac-01C	13.13 (12.53 ± 0.50)	0.76 (0.76 ± 0.01)	0.71 (0.72 ± 0.01)	7.11 (6.9 ± 0.16)
1:10 DB:Bi-ac-03L	13.1 (12.95 ± 0.53)	0.77 (0.75 ± 0.01)	0.75 (0.73 ± 0.01)	7.56 (7.15 ± 0.35)
1:10 DB:Bi-ac-05Q	13.1 (12.87 ± 0.41)	0.76 (0.76 ± 0.02)	0.73 (0.73 ± 0.01)	7.26 (7.09 ± 0.12)

Table S6. Photovoltaic performance with statistical analysis of the Dyenamo blue DSC devices based on the coadsorbers CDCA, BIAC01C, BIAC03L, BIAC05Q under AM1.5G sunlight

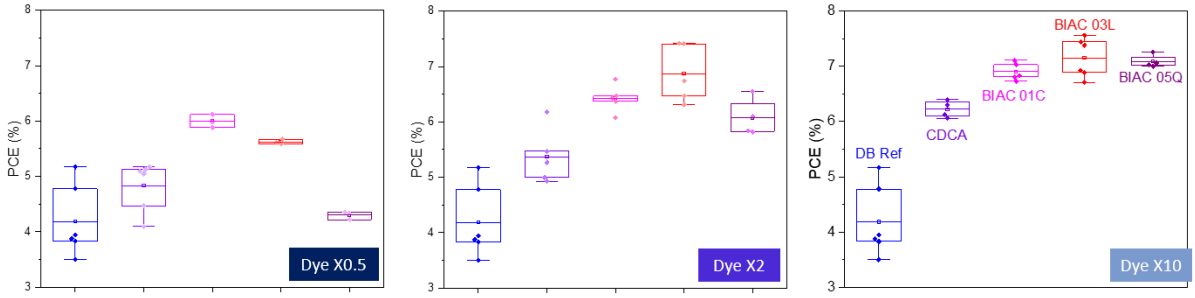


Figure S32. Statistical results showing the change in power conversion efficiencies of the devices upon increasing the concentration of the co-adsorbers from 0.5 times to 10 times the concentration of the dye dyenamo blue.

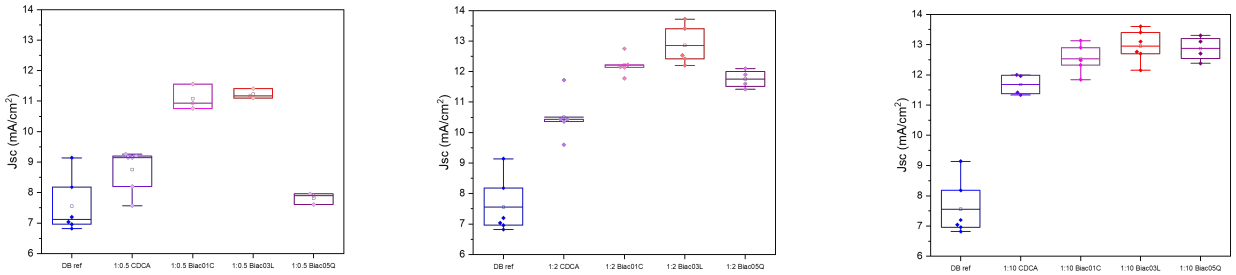


Figure S33. Statistical results showing the chnage in current densities of the devices upon increasing the concentration of the co-adsorbers from 0.5 times to 10 times the concentration of the dye dyenamo blue.

Dye:Co-sensitizer	**Jsc (mA/cm2)**	Voc (V)	FF	PCE (%)
0.075mM DB: D35	10.8 (10.68 ± 0.10)	0.78 (0.77 ± 0.01)	0.7 (0.69 ± 0.02)	5.87 (5.66 ± 0.23)
With CDCA	12.82 (12.63 ± 0.18)	0.79 (0.79 ± 0)	0.72 (0.72 ± 0.01)	7.19 (7.11 ± 0.09)
With Bi-ac-01C	11.57 (11.45 ± 0.12)	0.75 (0.75 ± 0)	0.72 (0.72 ± 0)	6.24 (6.16 ± 0.07)
With Bi-ac-03L	13.73 (13.59 ± 0.13)	0.77 (0.77 ± 0.01)	0.71 (0.71 ± 0.01)	7.37 (7.32 ± 0.06)
With Bi-ac-05Q	12.8 (12.50 ± 0.30)	0.78 (0.77 ± 0.01)	0.73 (0.71 ± 0.03)	7.02 (6.9 ± 0.13)

Table S7. Photovoltaic performance of the Dyenamo blue:D35 co-sensitized DSC devices based on the coadsorbers CDCA, BIAC01C, BIAC03L, BIAC05Q under AM1.5G sunlight.

5 Photoluminescence spectrocopy

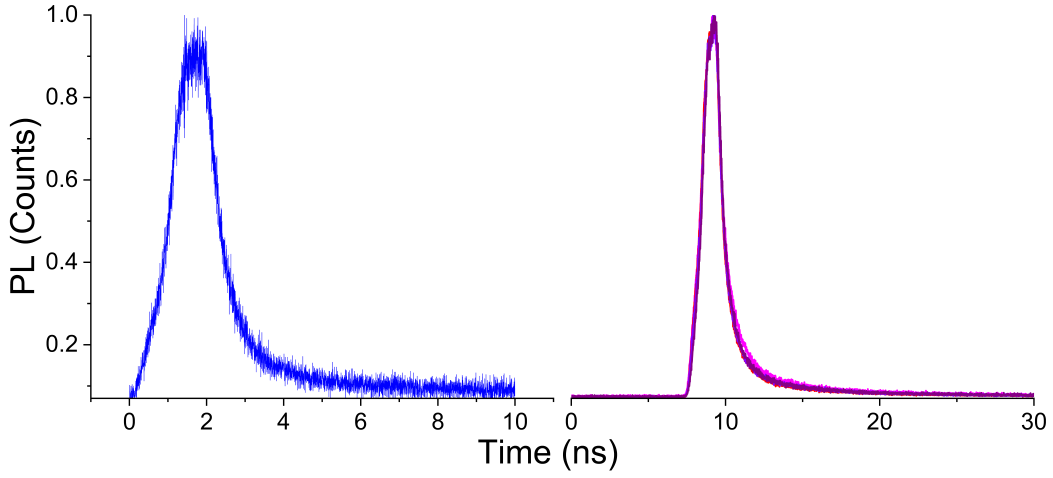


Figure S34. Time-resolved photoluminescence of DB dye and DB with the different coadsorbers on ZrO_2

	B1	tau1 (ns)	Rel 1 (%)	B2	tau2 (ps)	Rel 2 (%)
DB	358.775	0.61	100			
DB+ CDCA	3876.80	0.63	58.29	330.21	5.3	41.71
DB+ BIAC01C	2788.45	0.74	58.88	270.74	5.36	41.12
DB+ BIAC03L	8275.72	0.63	63.27	610	4.93	36.73
DB+ BIAC05Q	3511.72	0.63	61.32	277.48	5.06	38.68

Table S8. Fit parameters for photoluminescence decay lifetimes

6 Transient absorption spectroscopy

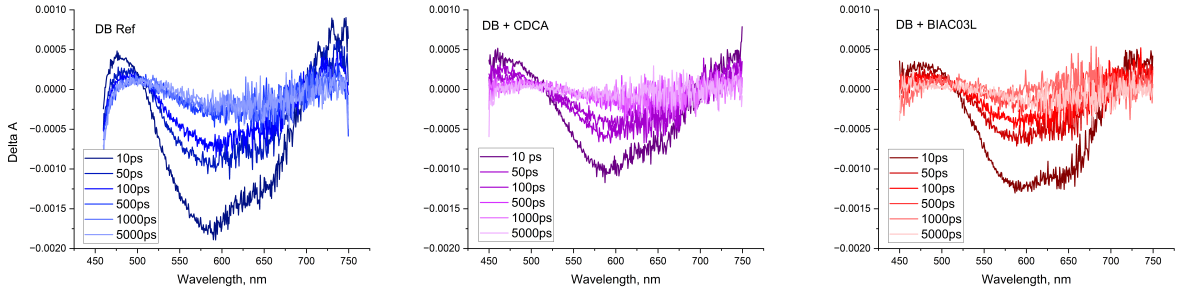


Figure S35. fs-TAS plots of DB dye and DB with the different coadsorbers on ZrO_2

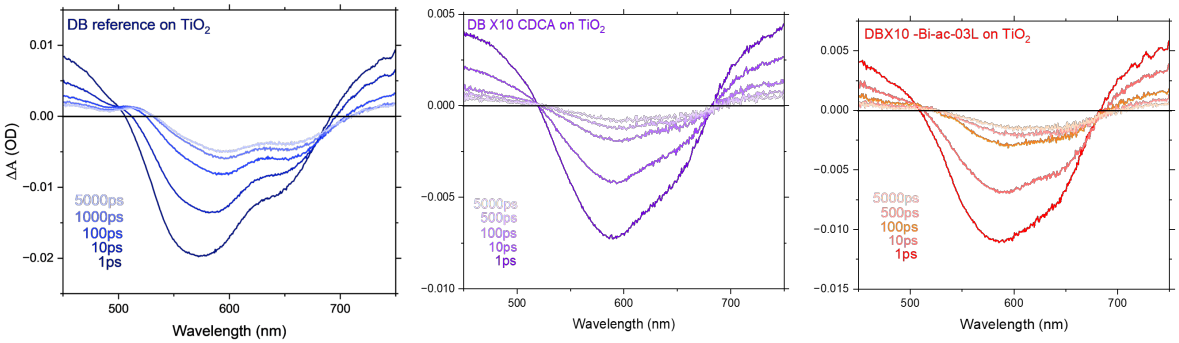


Figure S36. fs-TAS plots of DB dye and DB with the different coadsorbers on TiO_2

	On ZrO_2		On TiO_2	
	rise (ps)	decay (ps)	rise (ps)	decay (ps)
DB	3.4	77.85	6.4	140.5
DB+ CDCA	7.7	245.1	4.6	87.10
DB+ BIAC03L	7.04	188.9	4.6	90.48

Table S9. TA kinetic parameters for DB, DB+CDCA and DB+BIAC03L on ZrO_2 and TiO_2 observed at 710nm