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Supporting information for article:

Chemical characterization, absolute configuration and optical purity of (1*S*)-(+)- and (1*R*)-(-)-10-camphorsulfonic acid

Hong Cheng, Dingce Yan, Liqing Wu, Ping Liang, Yuncheng Cai and Li Li

SUPPORTING INFORMATION

Chemical characterization, absolute configuration and optical purity of (1S)-(+)-and (1R)-(-)-10-camphorsulfonic acid

HONG CHENG[1], DINGCE YAN[1], LIQING WU[2], PING LIANG[1], YUNCHENG CAI[1*] AND LI LI[3**]

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Figure S1: ESI- FT-ICR MS data of (1R)-(-)-CSA

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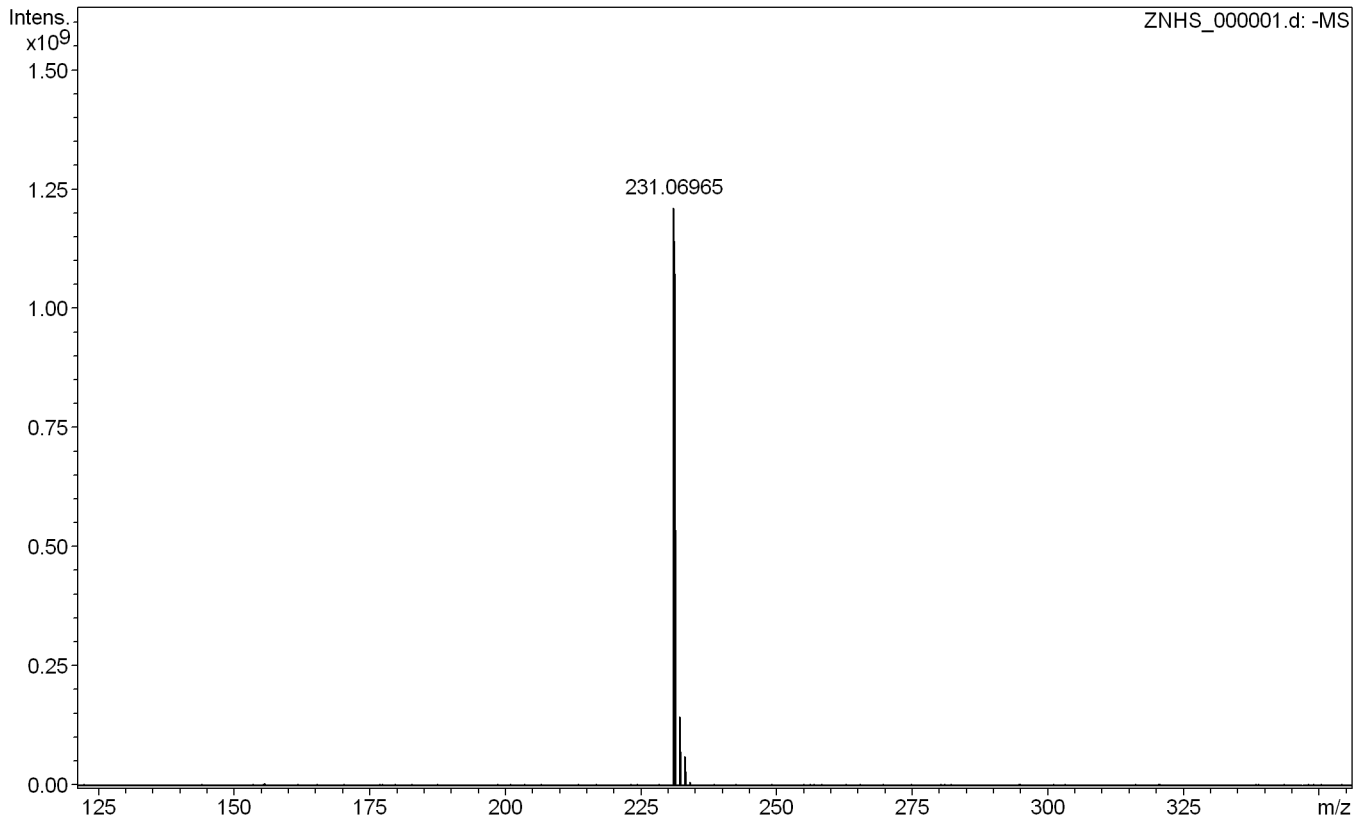

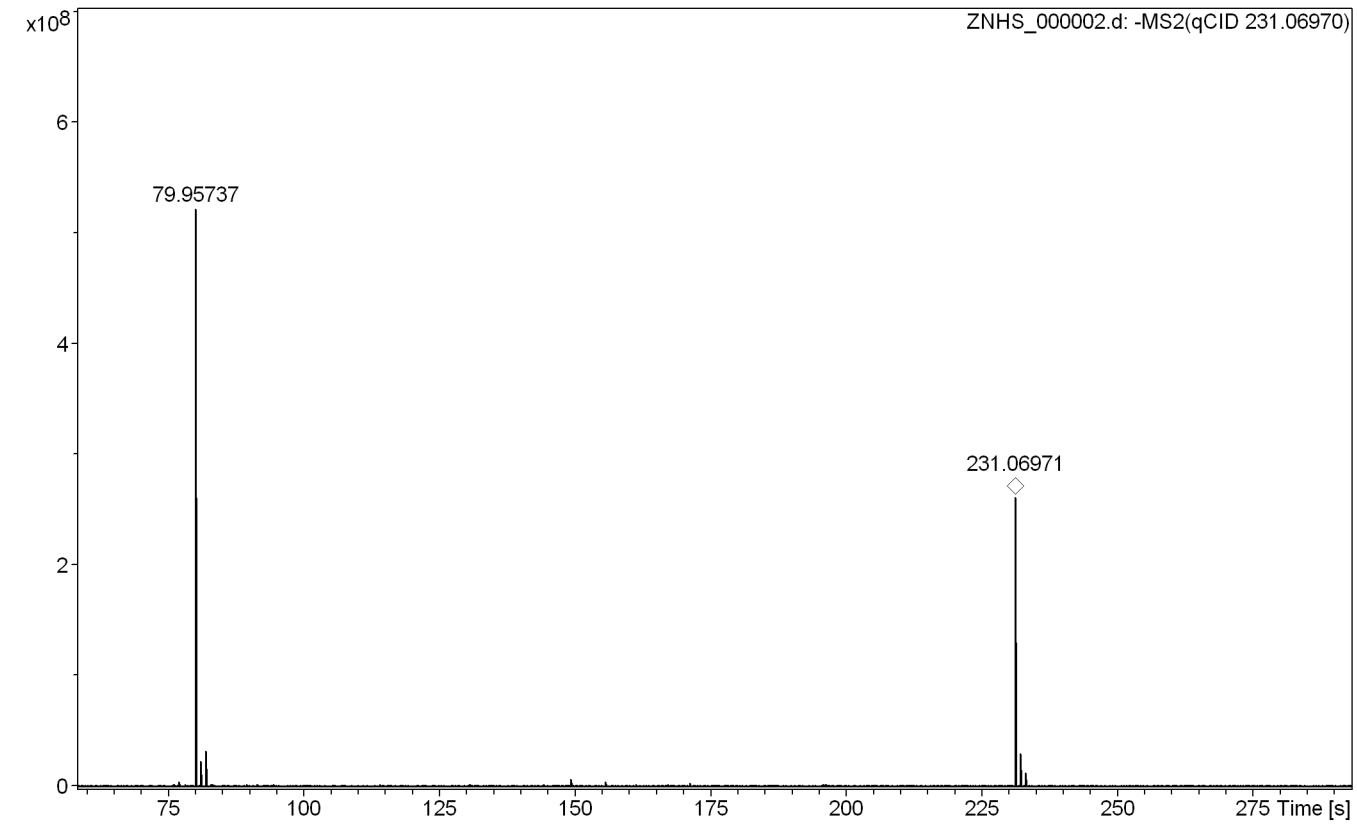

Figure S2: ^{1}H NMR spectra of (1S)-(+)-CSA

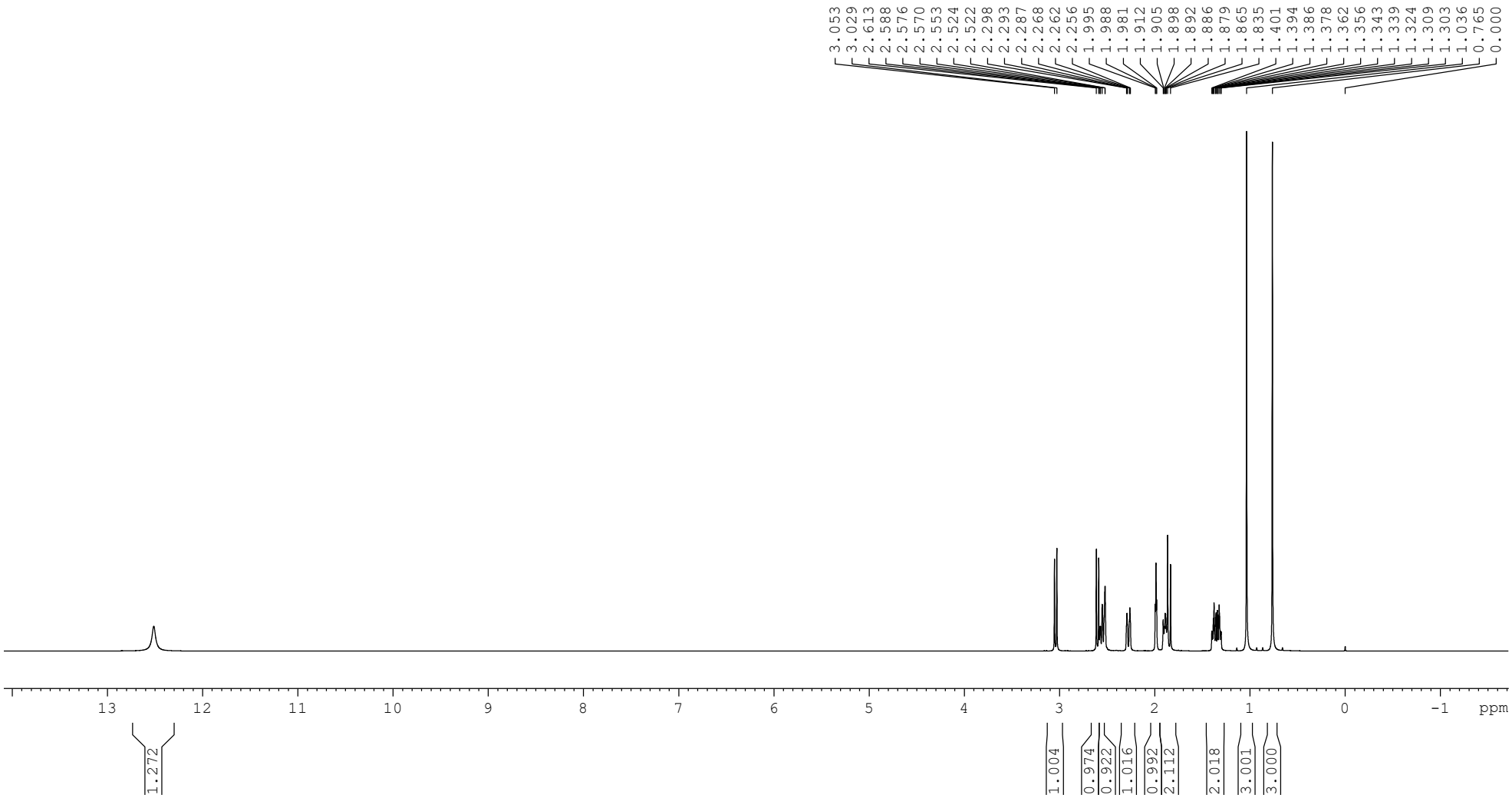

Figure S3: ^{1}H NMR spectra of (1S)-(+)-CSA after deuterium exchange

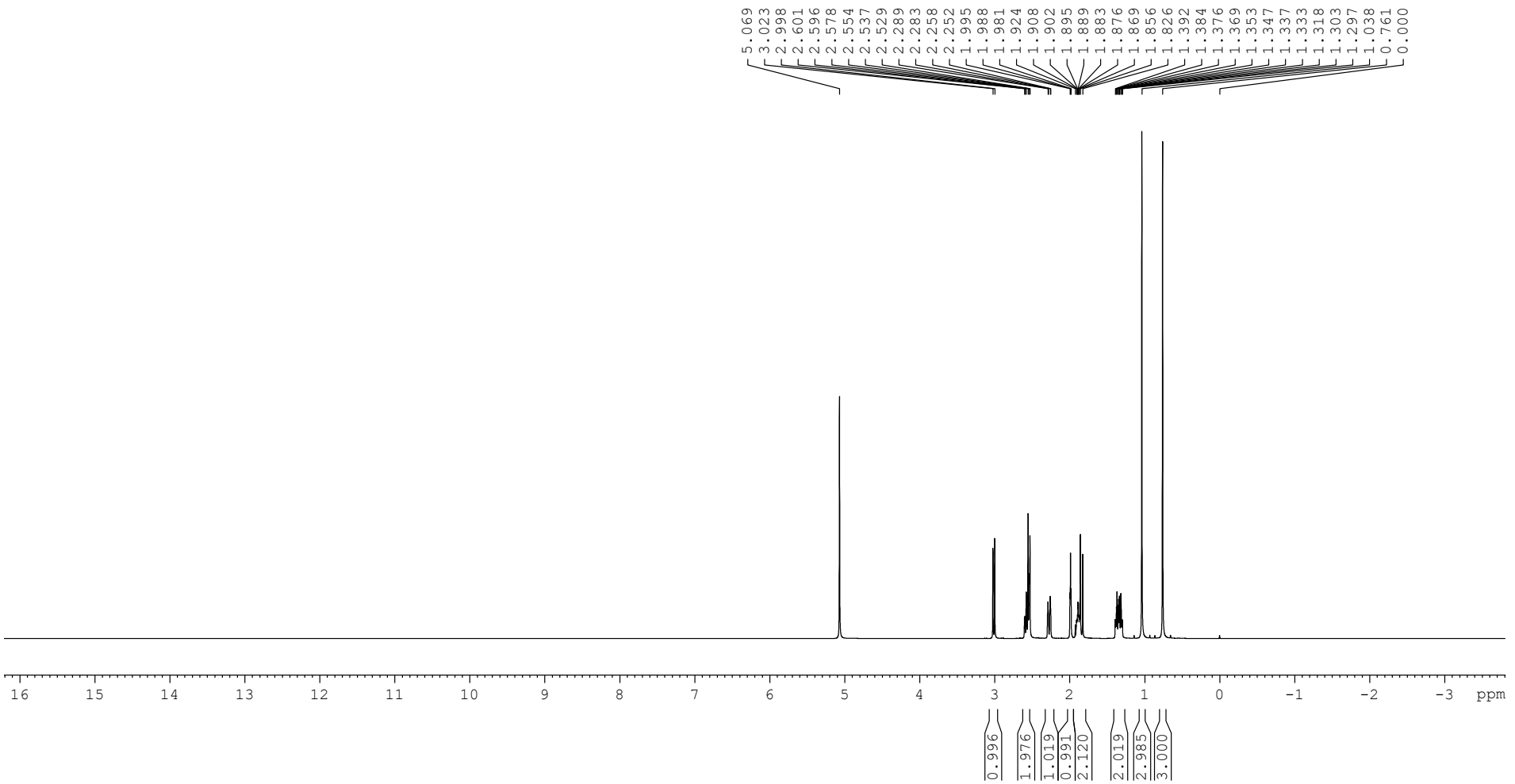

Figure S4: ^{13}C NMR spectra of (1S)-(+)-CSA

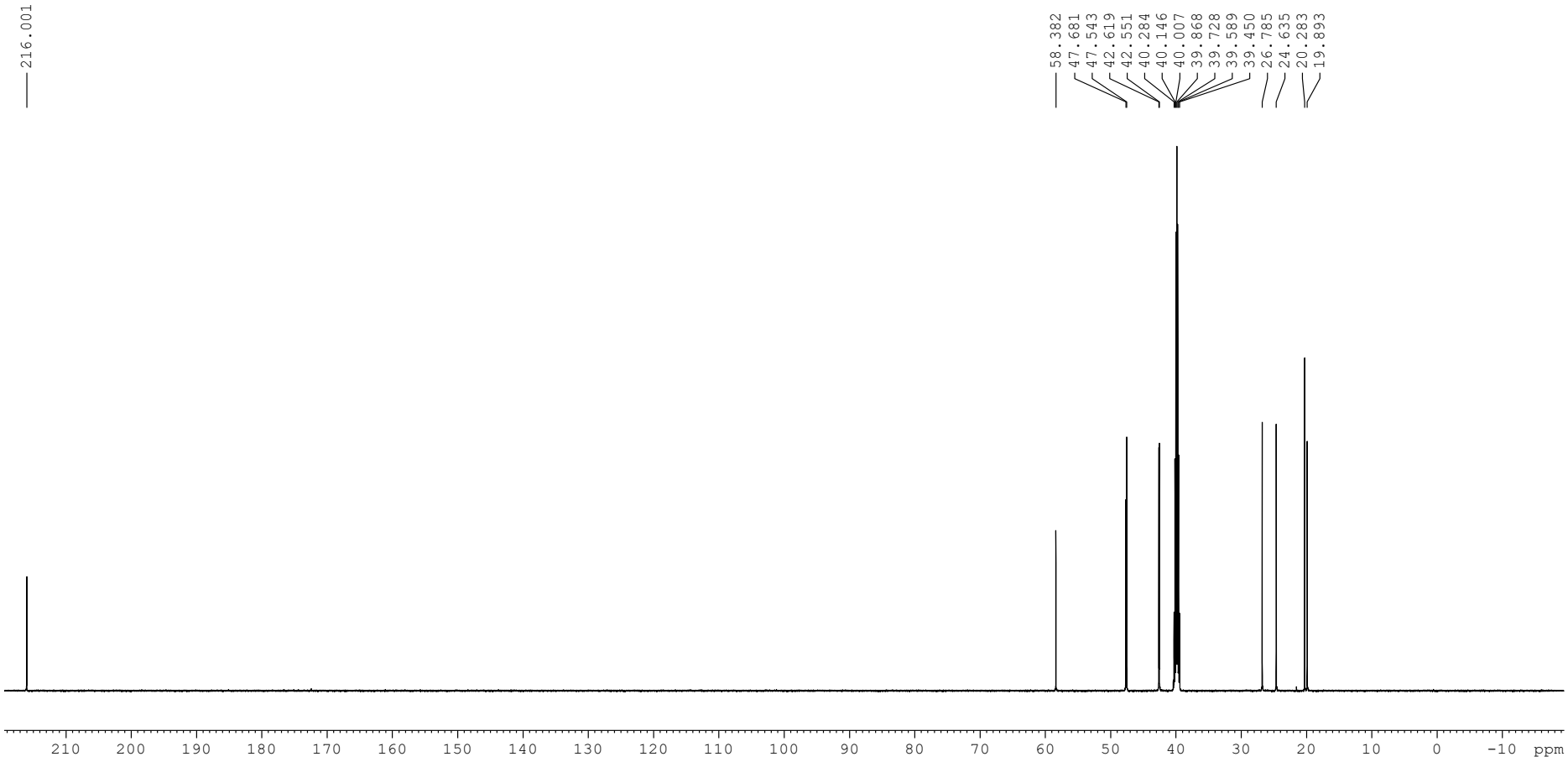

Figure S5: DEPT90 NMR spectra of (1S)-(+)-CSA

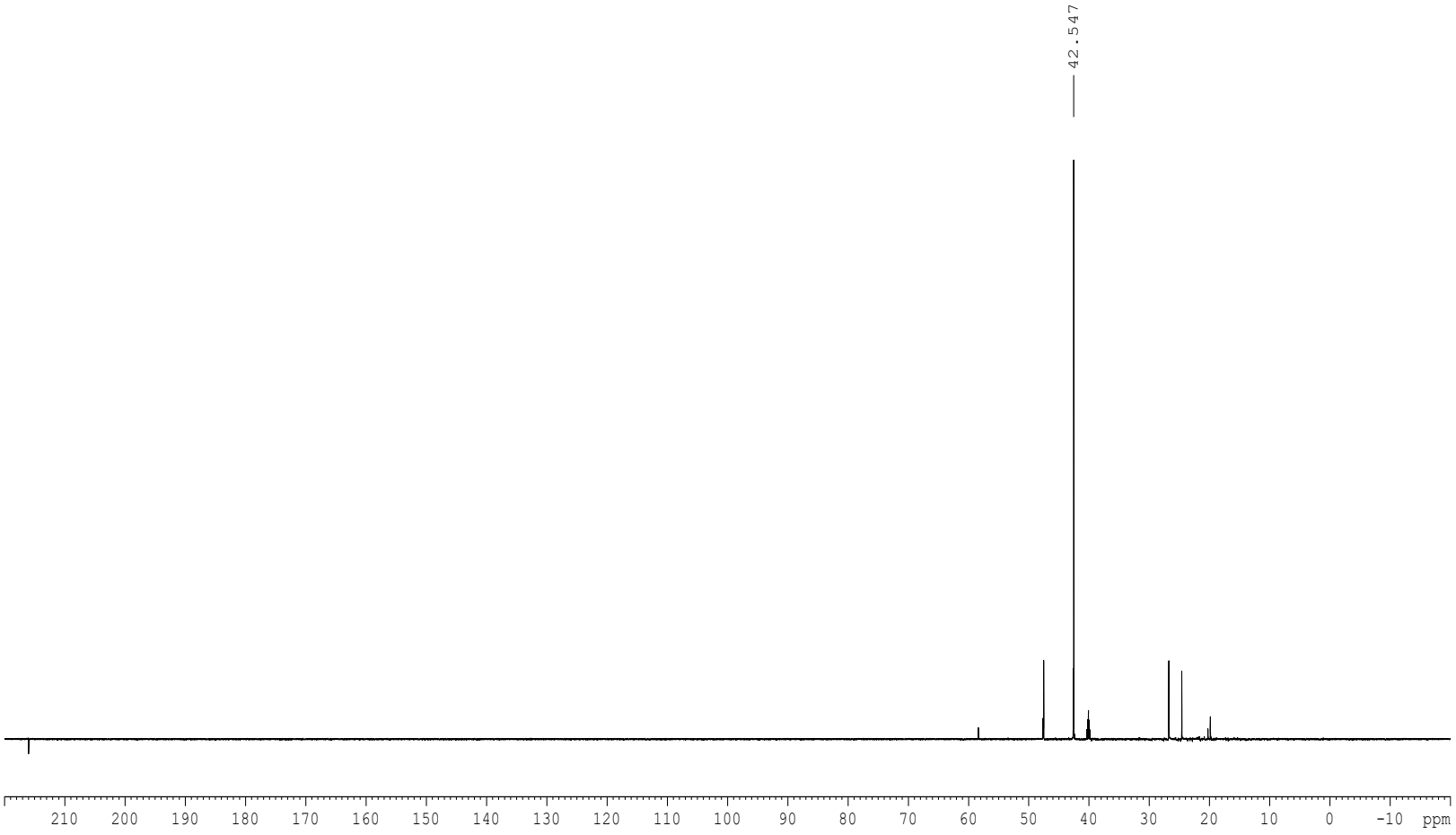

Figure S6: DEPT135 NMR spectra of (1S)-(+)-CSA

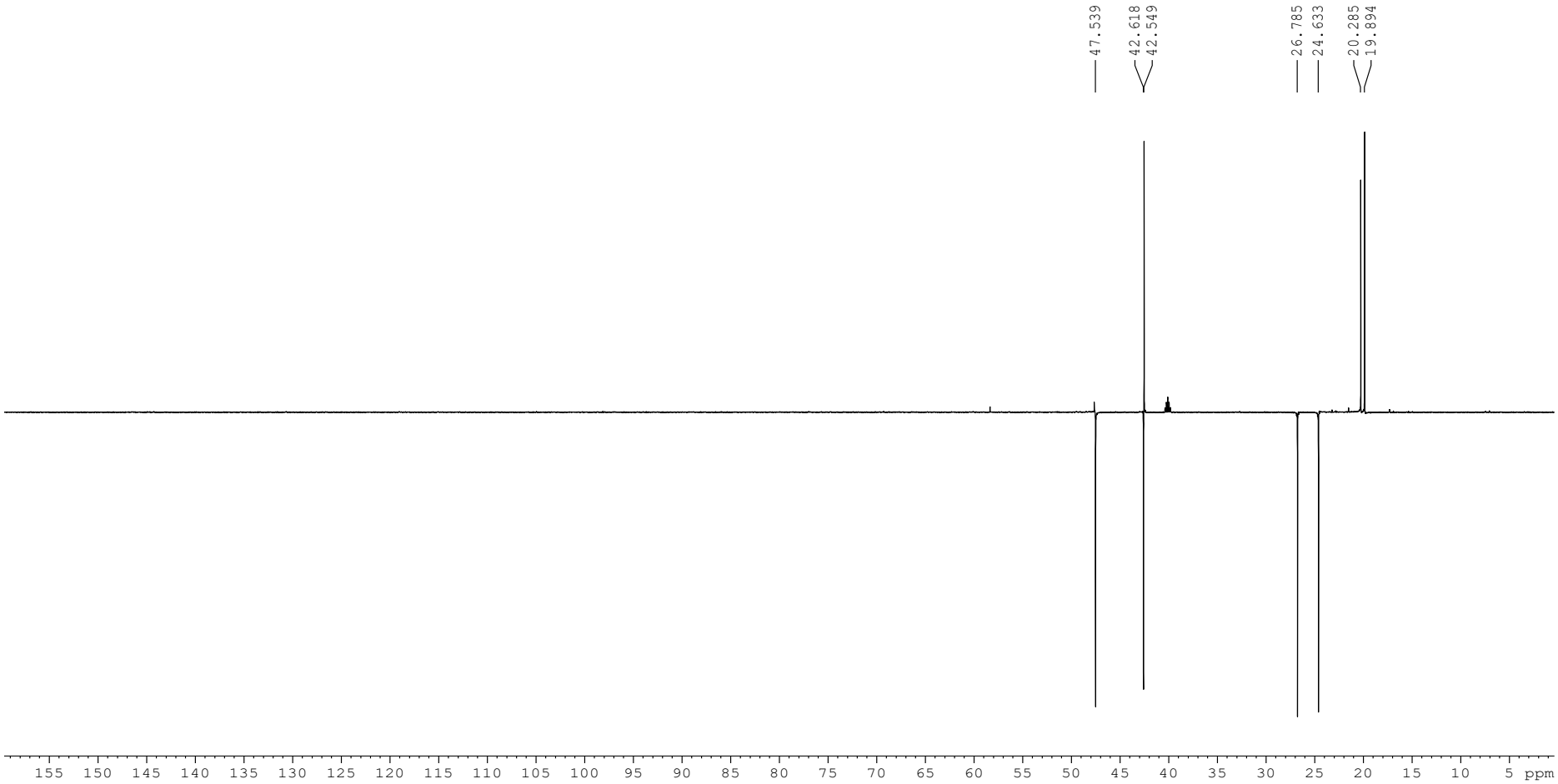

Figure S7: COSY NMR spectra of (1S)-(+)-CSA

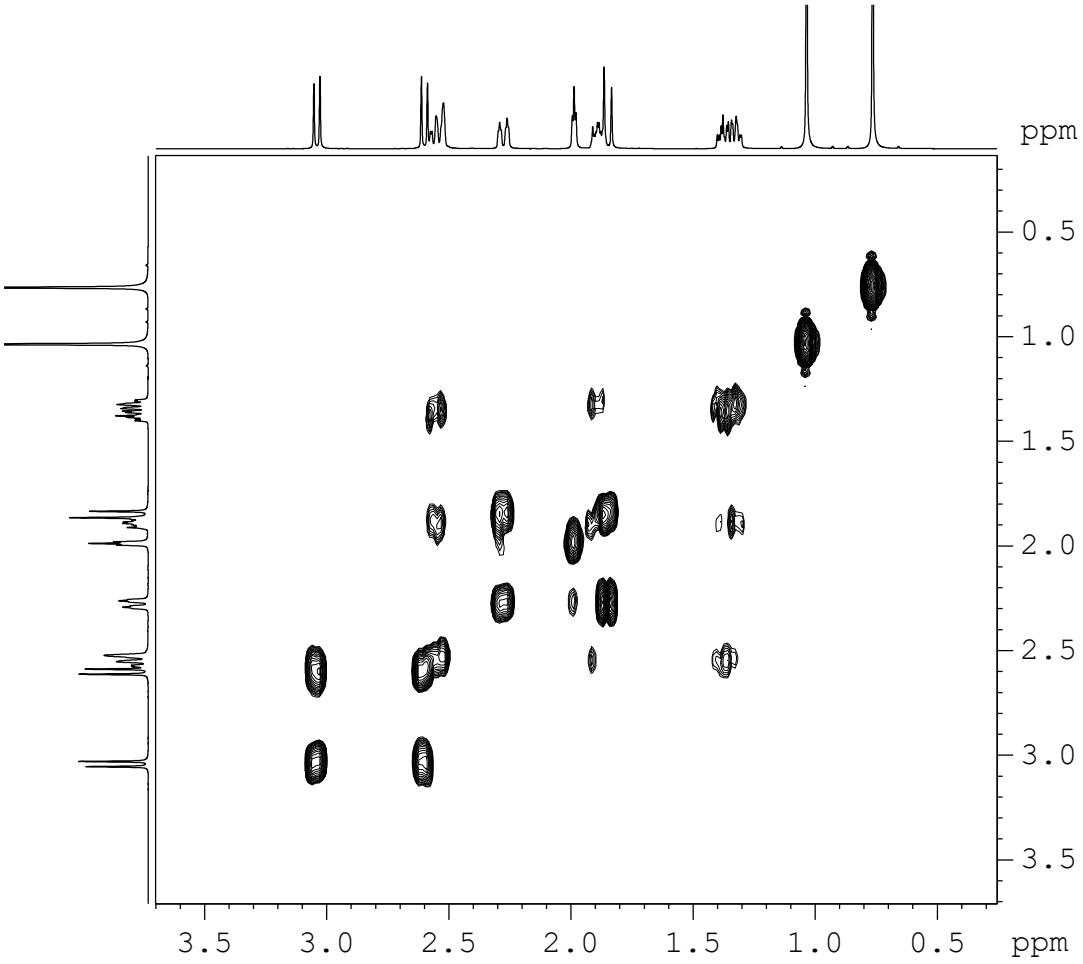

Figure S8: HSQC NMR spectra of (1S)-(+)-CSA

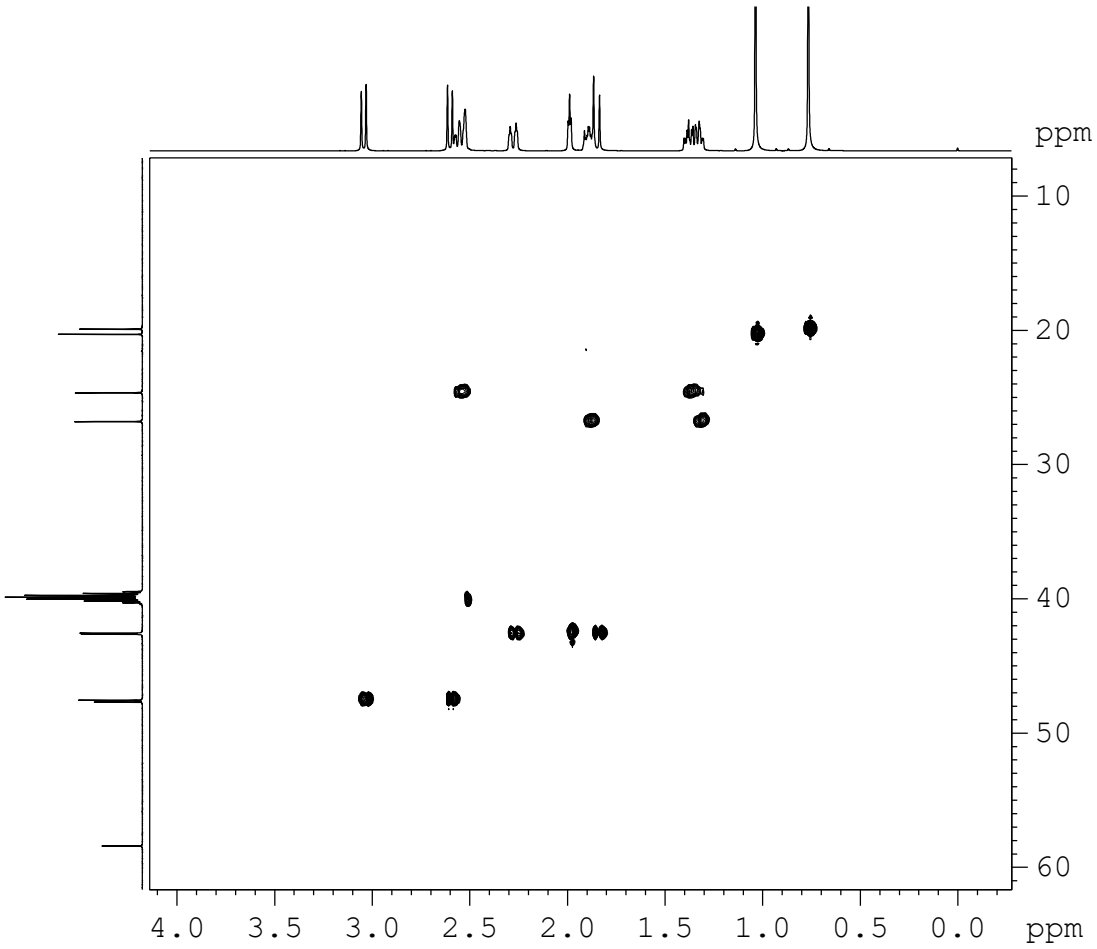

Figure S9: HMBC NMR spectra of (1S)-(+)-CSA

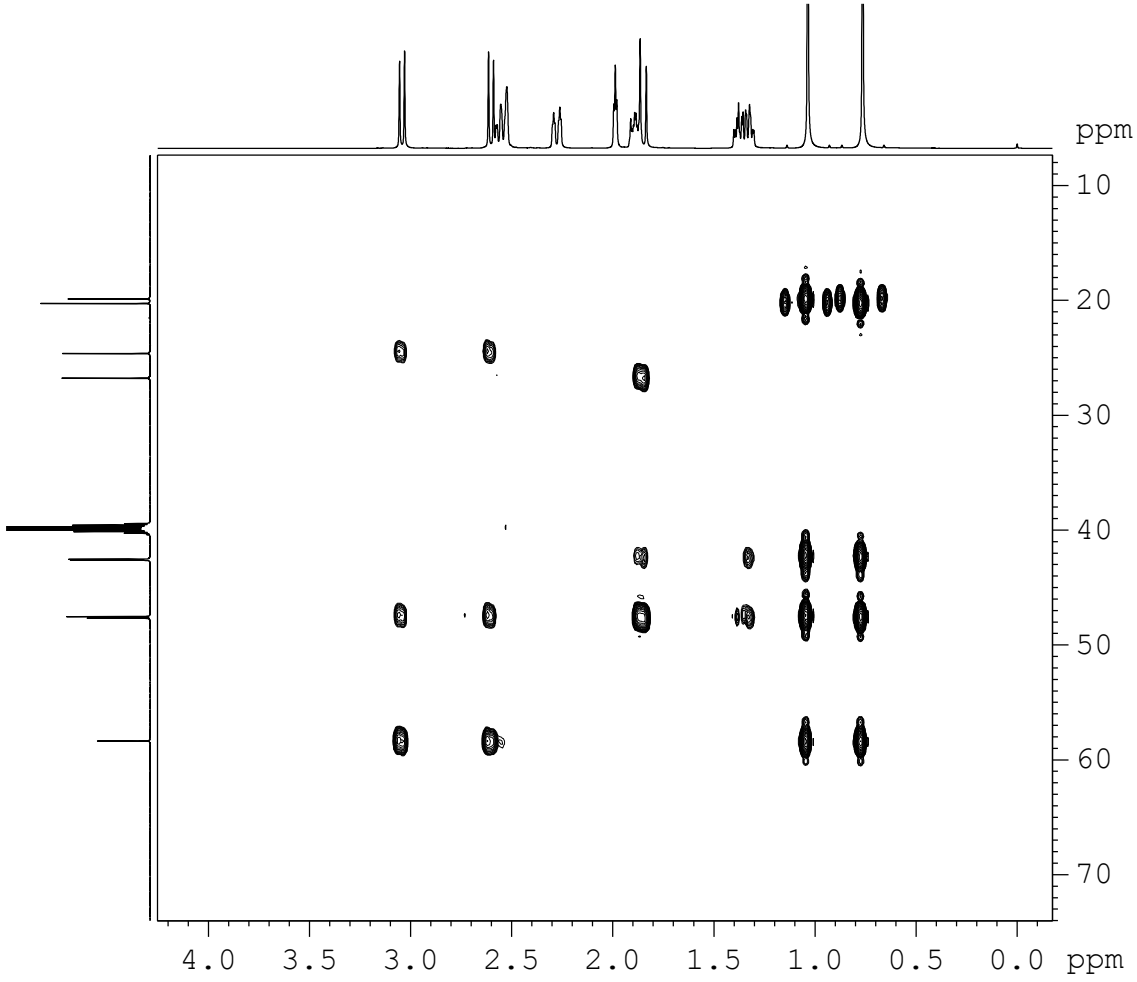

Figure S10: ^{1}H NMR spectra of (1R)-(-)-CSA

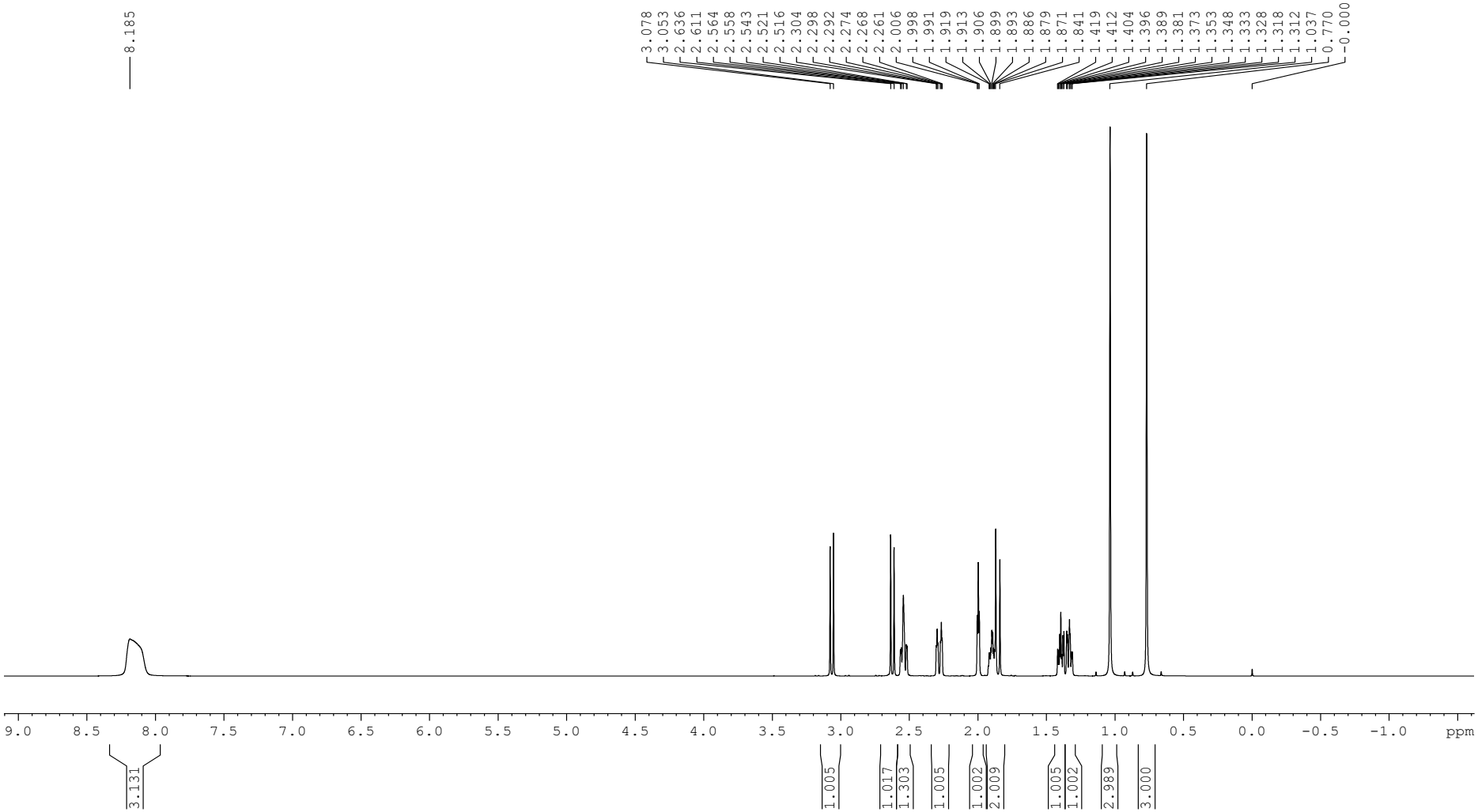

Figure S11: ^{13}C NMR spectra of (1R)-(-)-CSA

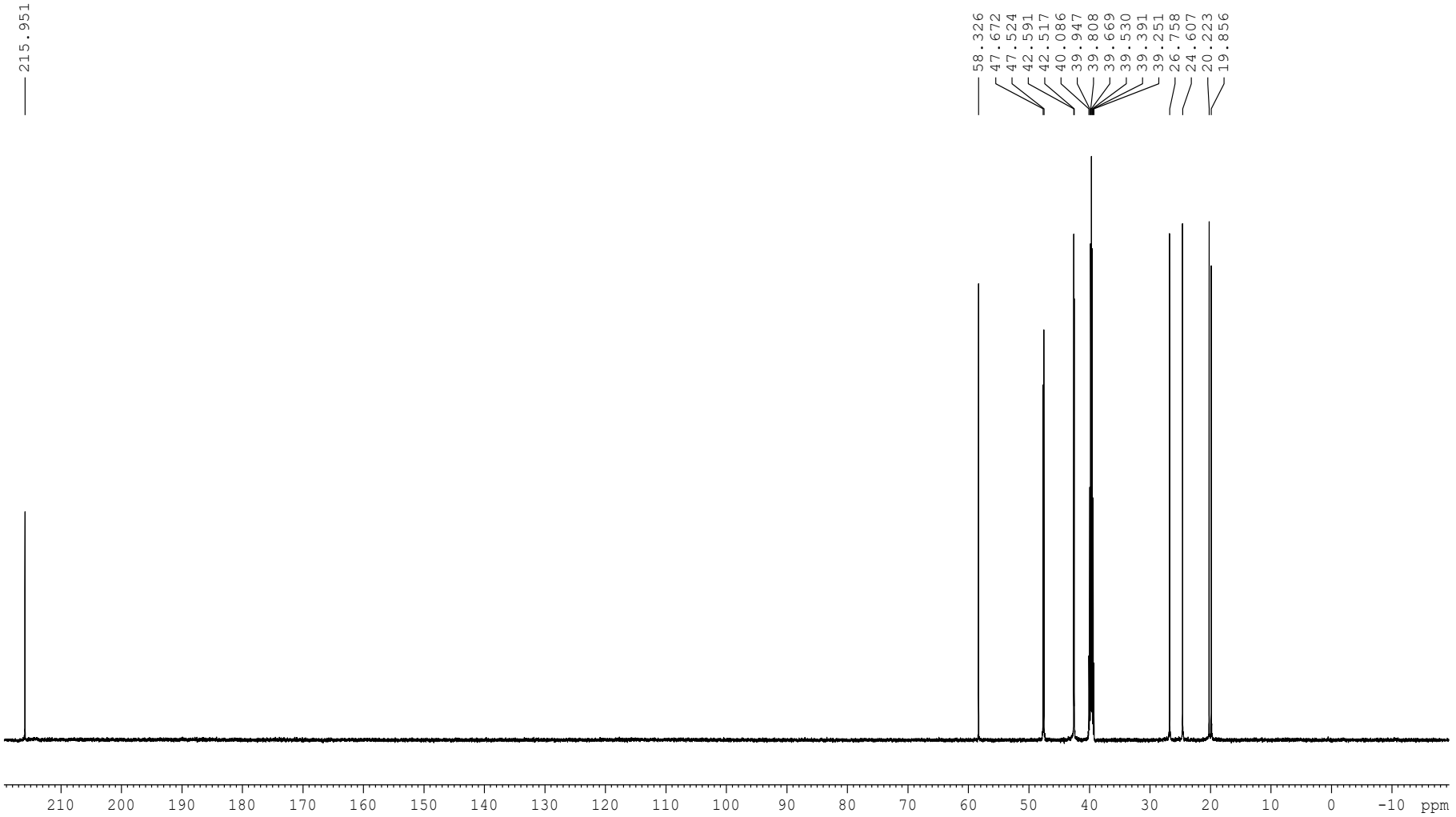

Figure S12: DEPT135 NMR spectra of (1R)-(-)-CSA

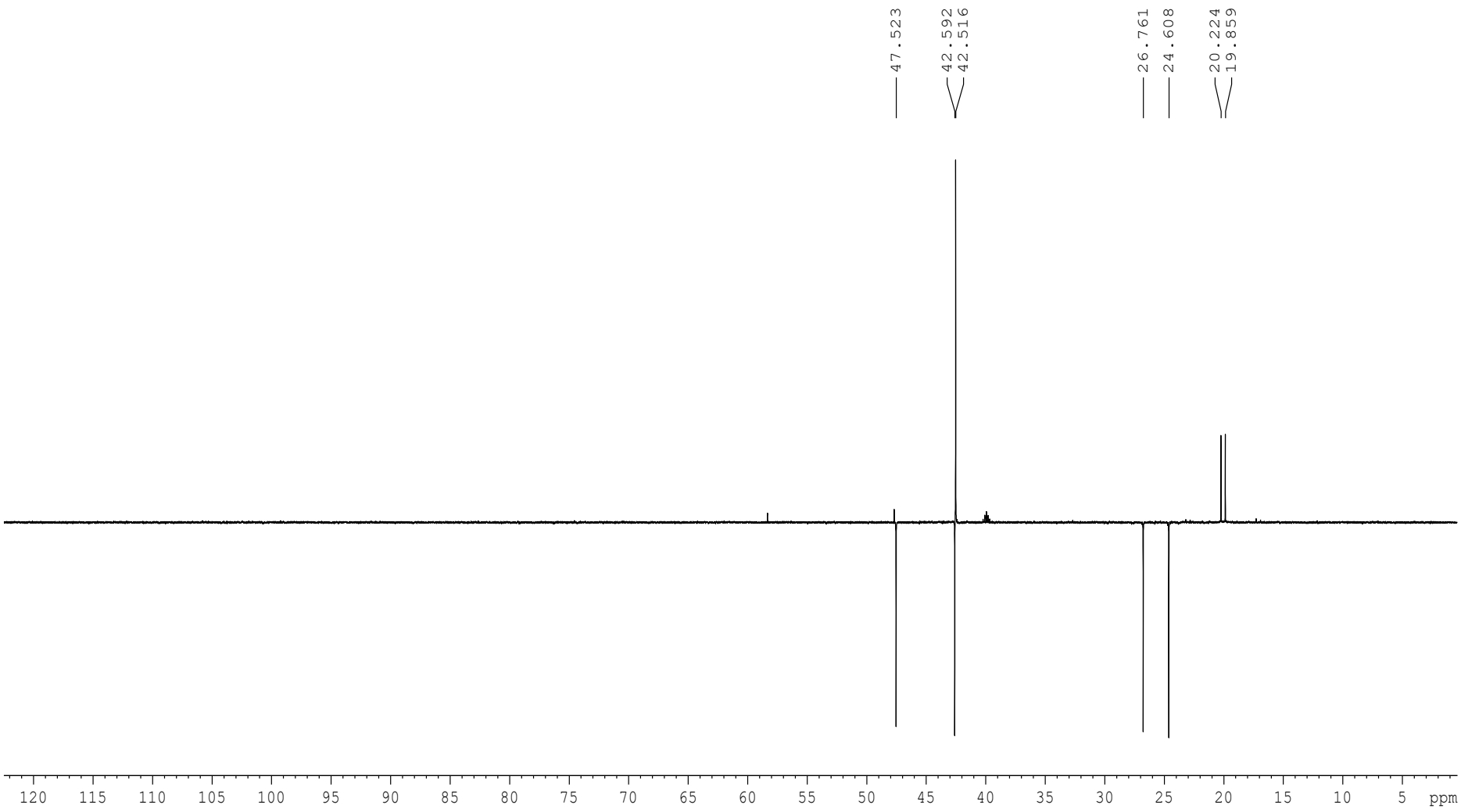

Figure S13: HSQC NMR spectra of (1R)-(-)-CSA

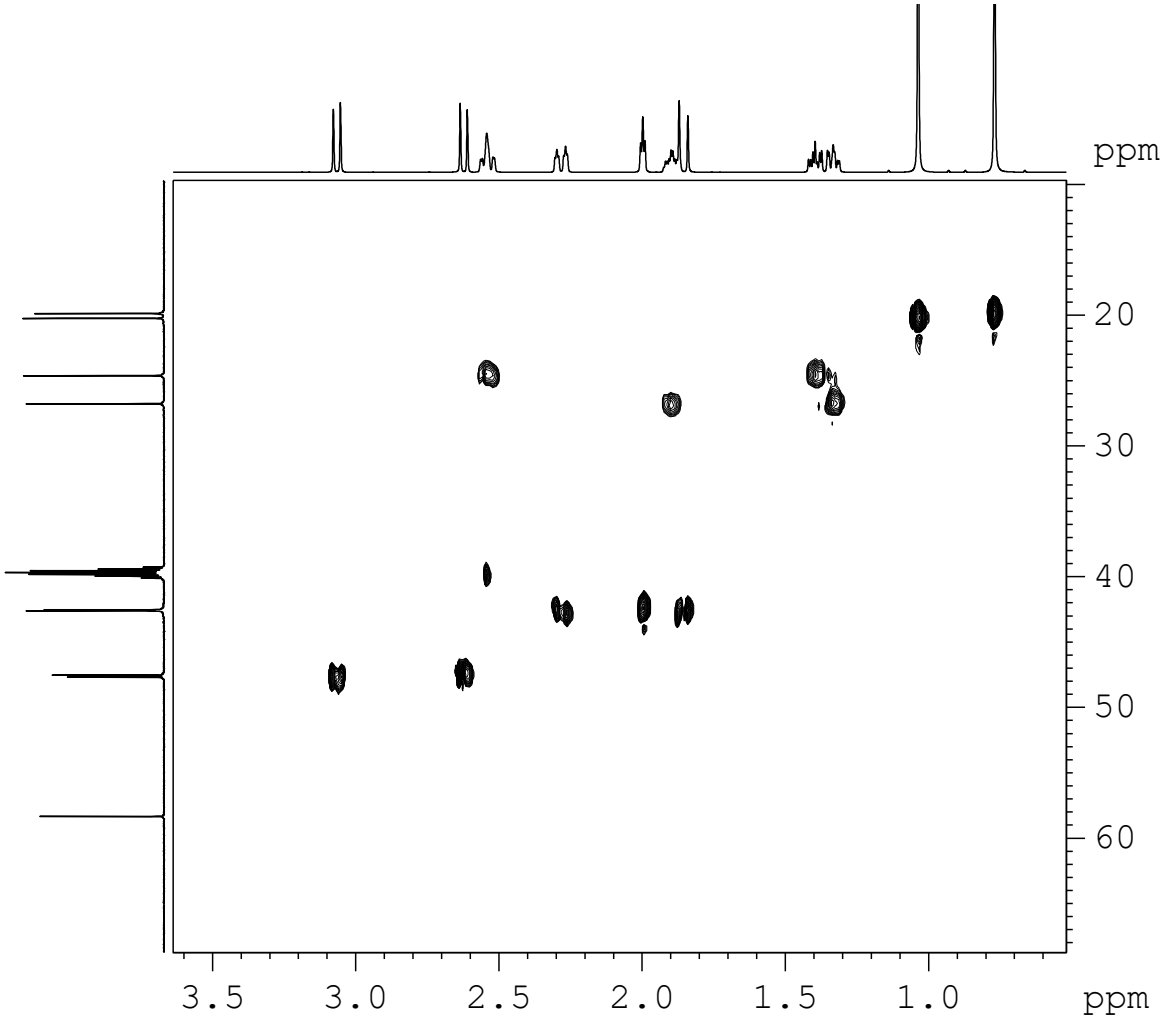

Figure S14: COSY NMR spectra of (1R)-(-)-CSA

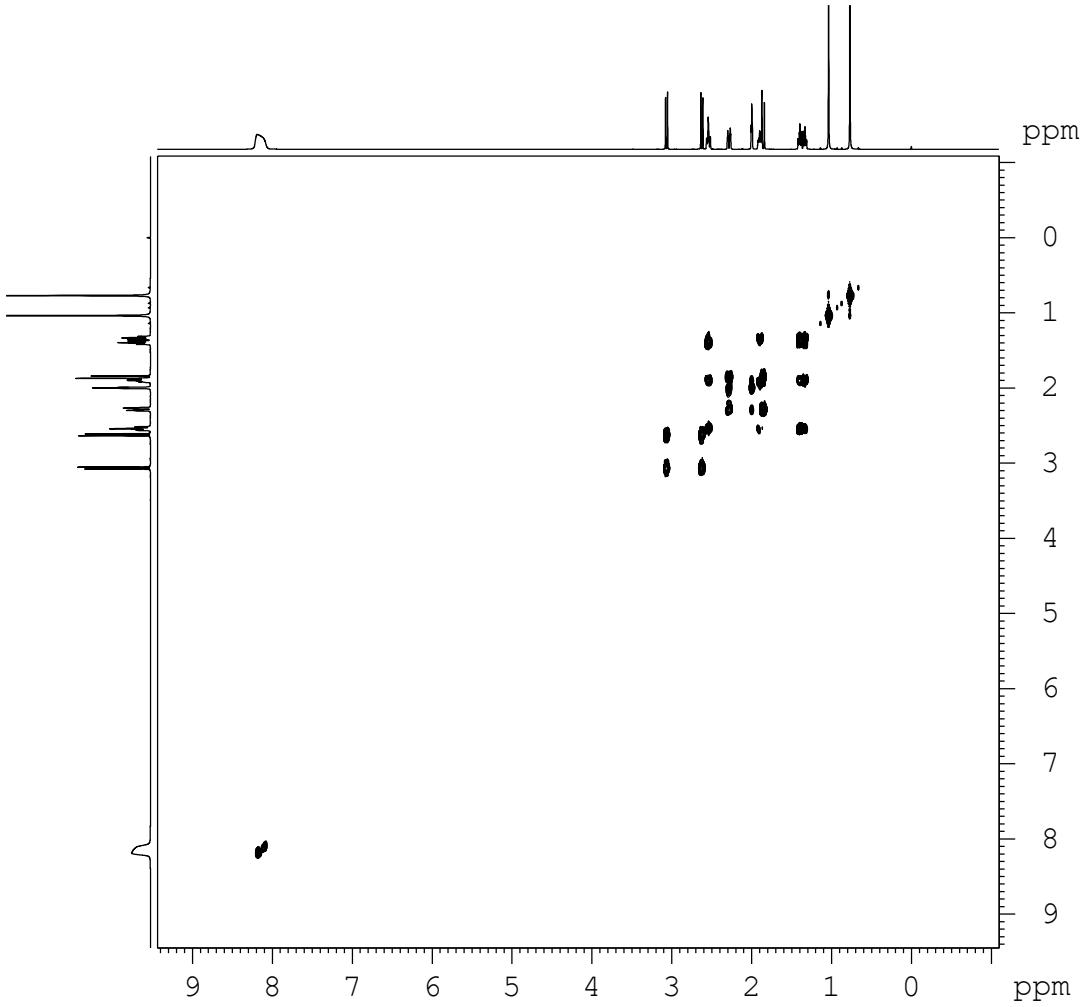

Figure S15: HMBC NMR spectra of (1R)-(-)-CSA

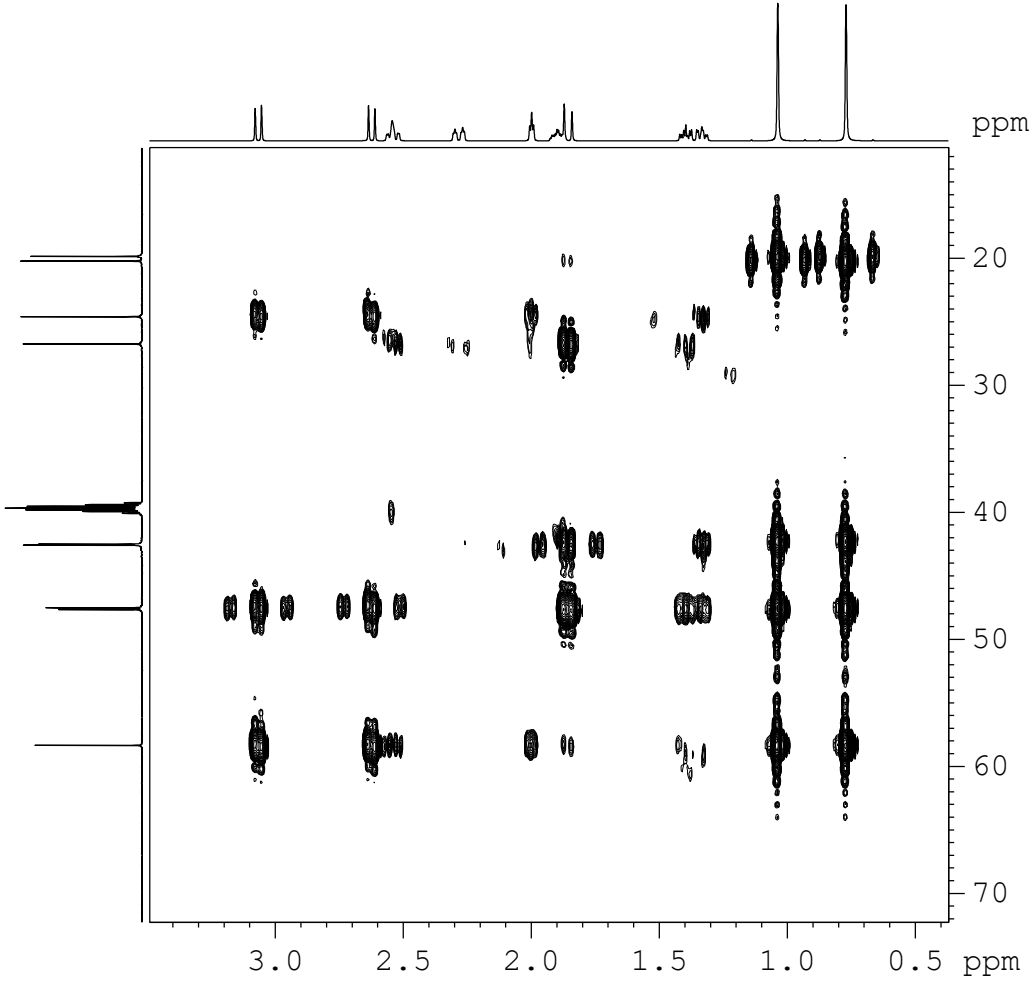

Table S1: Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic

Displacement Parameters ($Å^2 \times 10^3$) for (1S)-(+)-CSA monohydrate. Ueq is defined as 1/3 of the trace of the orthogonalised UIJ tensor.

Atom	*x*	*y*	*z*	U(eq)
S01	7306.8(6)	5568.4(3)	4569.7(3)	9.83(13)
O2	8972.2(19)	5234.6(12)	5123.3(8)	13.8(3)
O3	7233(2)	6841.5(11)	4385.0(8)	16.1(3)
O4	5436.1(19)	5115.0(12)	4918.1(9)	14.2(3)
O1	11574(2)	3854.0(13)	3926.8(9)	18.3(3)
C1	8074(3)	3585.3(15)	3513.7(11)	10.1(3)
C2	10244(3)	3233.9(16)	3658.2(11)	12.4(4)
C3	10443(3)	1957.9(17)	3328.3(13)	16.4(4)
C4	8375(3)	1733.6(16)	2936.9(12)	14.9(4)
C5	6960(3)	1523.0(17)	3696.6(13)	18.1(4)
C6	6838(3)	2772.0(16)	4123.5(12)	14.1(4)
C7	7759(3)	2988.1(15)	2610.1(11)	13.0(4)
C8	9131(3)	3488.0(18)	1908.0(12)	18.6(4)
C9	5615(3)	3054.8(19)	2287.4(14)	20.5(4)
C10	7668(3)	4913.4(14)	3539.0(10)	11.6(3)
O5	12223.2(19)	6244.3(11)	4723.8(9)	14.9(3)

Table S2: Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for (1S)-(+)-CSA monohydrate.
The Anisotropic displacement factor exponent takes the form: $-2\pi 2[h2a*2U11+2hka*b*U12+\cdots]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S01	8.5(2)	9.6(2)	11.3(2)	-1.13(14)	-0.65(15)	0.77(15)
O2	10.9(6)	16.8(6)	13.8(6)	0.1(5)	-2.0(5)	0.9(5)
O3	20.6(7)	9.0(6)	18.5(6)	-1.3(5)	-1.0(5)	1.9(5)
O4	9.5(6)	16.1(6)	17.0(6)	-1.9(5)	1.6(5)	0.8(5)
O1	11.1(6)	19.8(7)	24.0(7)	-6.1(6)	-2.2(5)	-0.5(5)
C1	10.5(8)	9.4(7)	10.4(8)	-0.8(6)	0.8(6)	-0.3(6)
C2	12.4(9)	13.8(8)	11.0(8)	-0.3(7)	0.5(7)	0.8(7)
C3	16.2(10)	12.7(9)	20.5(9)	-3.0(7)	0.7(7)	2.8(8)
C4	17.4(9)	10.2(9)	17.0(8)	-3.5(7)	1.8(7)	-1.3(7)
C5	20.1(9)	11.7(8)	22.4(9)	0.7(7)	4.3(8)	-3.3(7)
C6	14.2(9)	12.0(8)	16.1(8)	0.7(7)	4.4(7)	-1.5(7)
C7	15.2(9)	11.7(8)	11.9(8)	-2.0(6)	-0.5(7)	-1.3(7)
C8	26.1(10)	17.6(9)	12.0(8)	-2.7(7)	3.9(8)	-3.7(8)
C9	20.8(10)	20.4(10)	20.4(9)	-3.5(8)	-6.3(8)	-1.4(8)
C10	14.5(9)	10.7(8)	9.6(7)	0.6(6)	-0.3(7)	1.6(7)
O5	11.7(6)	11.0(6)	21.9(7)	-2.2(5)	-0.6(6)	0.0(5)

Table S3: Bond Lengths for (1S)-(+)-CSA monohydrate

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S01	O2	1.4607(13)	C1	C10	1.519(2)
S01	O3	1.4611(12)	C2	C3	1.529(3)
S01	O4	1.4616(13)	C3	C4	1.539(3)
S01	C10	1.7771(17)	C4	C5	1.533(3)
O1	C2	1.209(2)	C4	C7	1.555(2)
C1	C2	1.529(2)	C5	C6	1.555(2)
C1	C6	1.557(2)	C7	C8	1.534(3)
C1	C7	1.569(2)	C7	C9	1.529(3)

Table S4: Bond Angles for (1S)-(+)-CSA monohydrate

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O2	S01	O3	113.15(8)	C1	C2	C3	106.08(15)
O2	S01	O4	110.71(8)	C2	C3	C4	101.94(15)
O2	S01	C10	108.52(8)	C3	C4	C7	102.76(15)
O3	S01	O4	112.66(8)	C5	C4	C3	106.46(16)
O3	S01	C10	103.56(7)	C5	C4	C7	103.01(15)
O4	S01	C10	107.80(8)	C4	C5	C6	102.74(14)
C2	C1	C6	105.61(14)	C5	C6	C1	104.11(14)
C2	C1	C7	98.58(14)	C4	C7	C1	93.51(13)
C6	C1	C7	102.66(14)	C8	C7	C1	113.33(15)
C10	C1	C2	114.98(15)	C8	C7	C4	113.79(16)
C10	C1	C6	117.78(14)	C9	C7	C1	113.52(15)
C10	C1	C7	114.82(14)	C9	C7	C4	113.75(16)
O1	C2	C1	127.47(17)	C9	C7	C8	108.49(16)
O1	C2	C3	126.31(17)	C1	C10	S01	117.09(12)

Table S5: Hydrogen Bonds for (1S)-(+)-CSA monohydrate

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
O5	H5C	O4[1]	0.85	1.68	2.5253(18)	172.7
O5	H5D	O2	0.85	1.71	2.5412(19)	165.7

[1]1+X,+Y,+Z

Table S6: Torsion Angles for (1S)-(+)-CSA monohydrate

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O2	S01	C10	C1	51.95(16)	C5	C4	C7	C9	-62.10(18)
O3	S01	C10	C1	172.44(14)	C6	C1	C2	O1	-118.21(19)
O4	S01	C10	C1	-67.99(16)	C6	C1	C2	C3	66.03(17)
O1	C2	C3	C4	-170.47(18)	C6	C1	C7	C4	-51.80(16)
C1	C2	C3	C4	5.36(18)	C6	C1	C7	C8	-169.62(16)
C2	C1	C6	C5	-72.10(17)	C6	C1	C7	C9	66.02(18)
C2	C1	C7	C4	56.42(15)	C6	C1	C10	S01	41.7(2)
C2	C1	C7	C8	-61.39(18)	C7	C1	C2	O1	135.99(19)
C2	C1	C7	C9	174.25(16)	C7	C1	C2	C3	-39.77(16)
C2	C1	C10	S01	-83.84(17)	C7	C1	C6	C5	30.70(18)
C2	C3	C4	C5	-76.13(18)	C7	C1	C10	S01	162.77(13)
C2	C3	C4	C7	31.79(16)	C7	C4	C5	C6	-38.46(18)
C3	C4	C5	C6	69.28(18)	C10	C1	C2	O1	13.4(3)
C3	C4	C7	C1	-54.99(16)	C10	C1	C2	C3	-162.37(14)
C3	C4	C7	C8	62.44(18)	C10	C1	C6	C5	157.90(16)
C3	C4	C7	C9	-172.62(15)	C10	C1	C7	C4	179.13(15)
C4	C5	C6	C1	4.33(19)	C10	C1	C7	C8	61.3(2)
C5	C4	C7	C1	55.53(16)	C10	C1	C7	C9	-63.0(2)
C5	C4	C7	C8	172.96(16)					

Table S7: Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for (1S)-(+)-CSA monohydrate

Atom	*x*	*y*	*z*	U(eq)
H3A	10721.09	1408.66	3795.18	20
H3B	11479.17	1893	2896.05	20
H4	8342.56	1111.51	2494.72	18
H5A	7495.28	938.07	4093.26	22
H5B	5664.74	1260.72	3498.84	22
H6A	7405.64	2759.1	4698.37	17
H6B	5471.77	3042.02	4159.49	17
H8A	10466.59	3529.61	2123.79	28
H8B	8691.87	4269.78	1748.51	28
H8C	9093.2	2977.37	1412.31	28
H9A	5345.75	3842.32	2079.07	31
H9B	4723.08	2871.15	2751.84	31
H9C	5428.8	2492.83	1828.57	31
H10A	6492.5	5068.48	3194.67	14
H10B	8771.82	5315.74	3262.21	14
H5C	13245.48	5814.95	4803.66	22
H5D	11253.6	5803.54	4869.54	22
H5E	12220(50)	6890(30)	5010(19)	41(8)

Table S8: Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters (Å2×103) for (1R)-(-)-CSA monohydrate. Ueq is defined as 1/3 of the trace of the orthogonalised UIJ tensor

Atom	*x*	*y*	*z*	U(eq)
S001	7302.6(6)	4432.7(4)	4569.4(3)	12.26(13)
O1	8968(2)	4767.5(13)	5122.3(9)	16.2(3)
O5	12218(2)	3755.2(12)	4722.7(9)	17.2(3)
O4	11571(2)	6147.1(13)	3926.5(10)	20.9(3)
O3	5431.9(19)	4887.0(12)	4917.8(9)	16.6(3)
O2	7229(2)	3157.7(11)	4385.7(8)	18.6(3)
C2	10243(3)	6767.6(17)	3657.9(12)	14.8(4)
C1	8073(3)	6416.3(16)	3513.3(12)	12.5(4)
C9	9131(3)	6511.6(19)	1909.8(13)	21.1(4)
C4	8372(3)	8269.9(17)	2935.0(13)	17.3(4)
C7	7758(3)	7014.1(16)	2609.7(11)	15.3(4)
C10	7665(3)	5087.8(15)	3539.5(11)	14.0(4)
C5	6958(3)	8480.4(17)	3694.3(14)	20.6(4)
C6	6839(3)	7232.0(17)	4121.7(13)	16.4(4)
C8	5615(3)	6946(2)	2287.2(14)	23.1(4)
C3	10442(3)	8043.2(18)	3327.0(13)	18.9(4)

Table S9: Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for (1R)-(-)-CSA monohydrate. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\cdots]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S001	10.1(2)	12.6(2)	14.1(2)	1.11(15)	-0.59(16)	-0.77(15)
O1	11.7(6)	20.1(7)	16.8(6)	-0.4(5)	-2.2(5)	-1.0(5)
O5	13.1(6)	14.1(6)	24.4(7)	2.2(5)	-0.7(6)	0.2(5)
O4	13.1(7)	22.8(7)	26.9(8)	5.7(6)	-1.8(6)	0.4(6)
O3	11.2(6)	19.0(7)	19.7(7)	1.7(6)	2.2(5)	-0.7(5)
O2	22.2(7)	12.4(6)	21.2(6)	1.8(5)	-1.1(6)	-1.6(6)
C2	14.4(9)	16.5(9)	13.4(8)	0.1(8)	0.6(7)	-0.1(7)
C1	11.3(8)	13.0(8)	13.0(8)	0.7(7)	0.7(7)	0.2(7)
C9	28.3(11)	20.6(10)	14.4(9)	2.4(8)	3.5(8)	3.7(9)
C4	18.6(10)	13.4(9)	20.0(9)	3.3(7)	2.0(7)	2.2(7)
C7	16.4(9)	14.3(8)	15.2(8)	1.8(7)	-0.4(7)	1.9(7)
C10	16.0(9)	13.8(8)	12.3(8)	-0.7(6)	-0.3(7)	-1.5(8)
C5	21.7(10)	14.9(9)	25.2(10)	-0.7(8)	4.3(8)	2.9(8)
C6	16.8(10)	14.1(9)	18.3(9)	-0.9(7)	4.5(8)	1.2(7)
C8	22.4(11)	24.0(11)	23.0(10)	3.2(9)	-7.0(8)	1.3(9)
C3	17.3(10)	15.6(9)	23.7(10)	2.9(8)	0.7(8)	-2.7(8)

Table S10: Bond Lengths for (1R)-(-)-CSA monohydrate

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S001	O1	1.4604(14)	C1	C10	1.518(2)
S001	O3	1.4615(14)	C1	C6	1.555(3)
S001	O2	1.4613(13)	C9	C7	1.533(3)
S001	C10	1.7764(18)	C4	C7	1.554(3)
O4	C2	1.207(2)	C4	C5	1.533(3)
C2	C1	1.528(3)	C4	C3	1.540(3)
C2	C3	1.528(3)	C7	C8	1.527(3)
C1	C7	1.569(2)	C5	C6	1.553(3)

Table S11: Bond Angles for (1R)-(-)-CSA monohydrate

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	S001	O3	110.67(8)	C6	C1	C7	102.61(14)
O1	S001	O2	113.15(8)	C5	C4	C7	102.99(15)
O1	S001	C10	108.47(9)	C5	C4	C3	106.42(16)
O3	S001	C10	107.84(9)	C3	C4	C7	102.62(15)
O2	S001	O3	112.65(8)	C9	C7	C1	113.21(15)
O2	S001	C10	103.61(8)	C9	C7	C4	113.83(16)
O4	C2	C1	127.47(18)	C4	C7	C1	93.57(13)
O4	C2	C3	126.33(18)	C8	C7	C1	113.51(16)
C3	C2	C1	106.05(15)	C8	C7	C9	108.53(17)
C2	C1	C7	98.61(15)	C8	C7	C4	113.75(17)
C2	C1	C6	105.55(15)	C1	C10	S001	117.14(12)
C10	C1	C2	115.00(16)	C4	C5	C6	102.76(15)
C10	C1	C7	114.85(15)	C5	C6	C1	104.19(15)
C10	C1	C6	117.80(15)	C2	C3	C4	102.03(15)

Table S12: Hydrogen Bonds for (1R)-(-)-CSA monohydrate

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
O5	H5C	O3[1]	0.85	1.68	2.5261(18)	173.6
O5	H5D	O1	0.85	1.71	2.5408(19)	164.8
O5	H5E	O2[2]	0.87(3)	1.68(3)	2.5559(18)	177(3)

[1]1+X,+Y,+Z; [2]1/2+X,1/2-Y,1-Z

Table S13: Torsion Angles for (1R)-(-)-CSA monohydrate

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O1	S001	C10	C1	-51.90(17)	C10	C1	C7	C4	-179.23(15)
O4	C2	C1	C7	-136.0(2)	C10	C1	C7	C8	62.9(2)
O4	C2	C1	C10	-13.3(3)	C10	C1	C6	C5	-157.79(16)
O4	C2	C1	C6	118.3(2)	C5	C4	C7	C1	-55.47(17)
O4	C2	C3	C4	170.45(19)	C5	C4	C7	C9	-172.80(16)
O3	S001	C10	C1	68.00(16)	C5	C4	C7	C8	62.18(19)
O2	S001	C10	C1	-172.39(14)	C5	C4	C3	C2	76.00(19)
C2	C1	C7	C9	61.39(19)	C6	C1	C7	C9	169.56(16)
C2	C1	C7	C4	-56.46(15)	C6	C1	C7	C4	51.71(16)
C2	C1	C7	C8	-174.31(17)	C6	C1	C7	C8	-66.14(19)
C2	C1	C10	S001	83.80(18)	C6	C1	C10	S001	-41.7(2)
C2	C1	C6	C5	72.21(18)	C3	C2	C1	C7	39.69(17)
C1	C2	C3	C4	-5.29(19)	C3	C2	C1	C10	162.34(15)
C4	C5	C6	C1	-4.4(2)	C3	C2	C1	C6	-66.05(18)
C7	C1	C10	S001	-162.74(13)	C3	C4	C7	C1	54.95(16)
C7	C1	C6	C5	-30.59(19)	C3	C4	C7	C9	-62.38(19)
C7	C4	C5	C6	38.47(19)	C3	C4	C7	C8	172.60(16)
C7	C4	C3	C2	-31.83(17)	C3	C4	C5	C6	-69.10(19)
C10	C1	C7	C9	-61.4(2)					

Table S14: Hydrogen Atom Coordinates (Å×10^4) and Isotropic

Displacement Parameters (Å^2×10^3) for (1R)-(-)-CSA monohydrate

Atom	*x*	*y*	*z*	U(eq)
H5C	13247.4	4181.74	4796.88	26
H5D	11255.31	4205.4	4863.31	26
H9A	10469	6479.39	2123.93	32
H9B	9082.36	7016.07	1410.97	32
H9C	8701.32	5724.74	1756.42	32
H4	8340.01	8892.43	2492.91	21
H10A	8768.49	4684.2	3263.05	17
H10B	6488.88	4932.82	3195.39	17
H5A	5661.45	8741.77	3496.9	25
H5B	7492.89	9066.84	4090.23	25
H6A	5472.43	6961.43	4158.72	20
H6B	7408.19	7246.26	4695.92	20
H8A	5346.97	6157.28	2079.75	35
H8B	5429.24	7507.79	1827.95	35
H8C	4722.8	7130.73	2751.05	35
H3A	11478.48	8106.6	2894.8	23
H3B	10721.63	8593.68	3793.01	23
H5E	12250(50)	3090(30)	5014(18)	37(8)

Figure S16: CIF report of (1S)-(+)-CSA monohydrate

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 20220428_1

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: 20220428_1

```
Bond precision:   C-C = 0.0028 A          Wavelength=1.54184

Cell:             a=6.72815(4)     b=11.24661(6)     c=15.51195(8)
                  alpha=90         beta=90           gamma=90
Temperature:      100 K

                 Calculated                Reported
Volume           1173.772(11)              1173.772(10)
Space group      P 21 21 21                P 21 21 21
Hall group       P 2ac 2ab                 P 2ac 2ab
Moiety formula   C10 H15 O4 S, H3 O        C10 H15 O4 S, H3 O
Sum formula      C10 H18 O5 S              C10 H18 O5 S
Mr               250.30                    250.30
Dx,g cm-3        1.416                     1.416
Z                4                         4
Mu (mm-1)        2.522                     2.522
F000             536.0                     536.0
F000'            539.00
h,k,lmax         8,14,19                   8,13,19
Nref             2379[ 1395]               2349
Tmin,Tmax        0.399,0.469               0.628,1.000
Tmin'            0.246

Correction method= # Reported T Limits: Tmin=0.628 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.68/0.99        Theta(max)= 73.951

R(reflections)= 0.0219( 2349)                wR2(reflections)=
                                             0.0574( 2349)
S = 1.127                Npar= 155
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT313_ALERT_2_C Oxygen with Three Covalent Bonds (rare) ..... O5 Check

Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 2 Report
PLAT142_ALERT_4_G s.u. on b - Axis Small or Missing ..... 0.00006 Ang.
PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing ..... 0.00008 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 1 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 2 Note
H3 O
PLAT791_ALERT_4_G Model has Chirality at C1 (Sohnke SpGr) S Verify
PLAT791_ALERT_4_G Model has Chirality at C4 (Sohnke SpGr) R Verify
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 9 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 1 Note
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities ..... Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 9 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
11 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
7 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 19/02/2022; check.def file version of 19/02/2022

Datablock 20220428_1 - ellipsoid plot

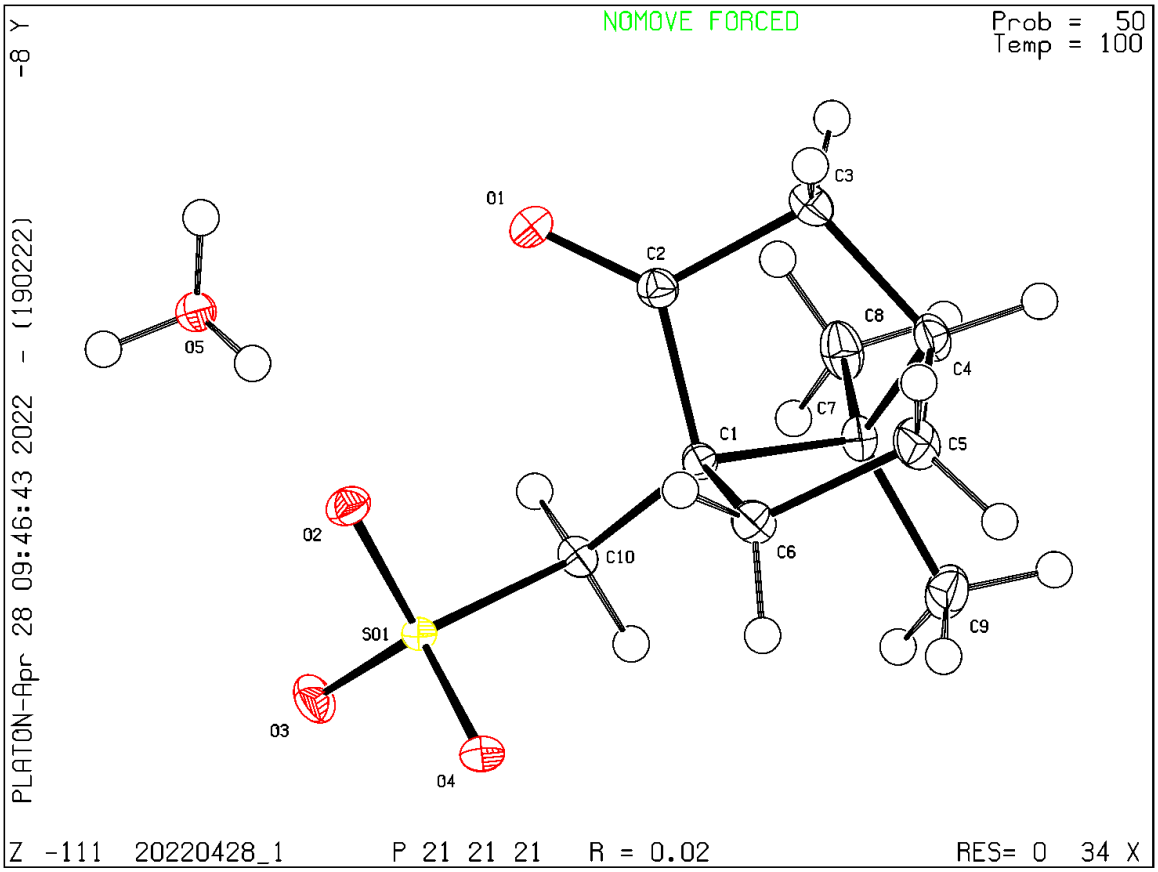

Figure S17: CIF report of (1R)-(-)-CSA monohydrate

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 20220502_2

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: 20220502_2

```
Bond precision:   C-C = 0.0029 A           Wavelength=1.54184

Cell:             a=6.72595(5)     b=11.23408(8)     c=15.51954(11)
                  alpha=90         beta=90           gamma=90
Temperature:      100 K
```

	Calculated	Reported
Volume	1172.654(15)	1172.654(14)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C10 H15 O4 S, H3 O	C10 H15 O4 S, H3 O
Sum formula	C10 H18 O5 S	C10 H18 O5 S
Mr	250.30	250.30
Dx,g cm-3	1.418	1.418
Z	4	4
Mu (mm-1)	2.524	2.524
F000	536.0	536.0
F000'	539.00	
h,k,lmax	8,13,19	8,13,19
Nref	2373[1391]	2348
Tmin,Tmax	0.573,0.881	0.464,1.000
Tmin'	0.394	

```
Correction method= # Reported T Limits: Tmin=0.464 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.69/0.99        Theta(max)= 73.853

R(reflections)= 0.0222( 2338)                    wR2(reflections)=
                                                 0.0587( 2348)
S = 1.140                  Npar= 155
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

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Alert level G

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PLAT142_ALERT_4_G s.u. on b - Axis Small or Missing ..... 0.00008 Ang.
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PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 2 Note
H3 O
PLAT791_ALERT_4_G Model has Chirality at C1 (Sohnke SpGr) R Verify
PLAT791_ALERT_4_G Model has Chirality at C4 (Sohnke SpGr) S Verify
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 11 Note
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities ..... Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 10 Info

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PLATON version of 19/02/2022; check.def file version of 19/02/2022

Datablock 20220502_2 - ellipsoid plot

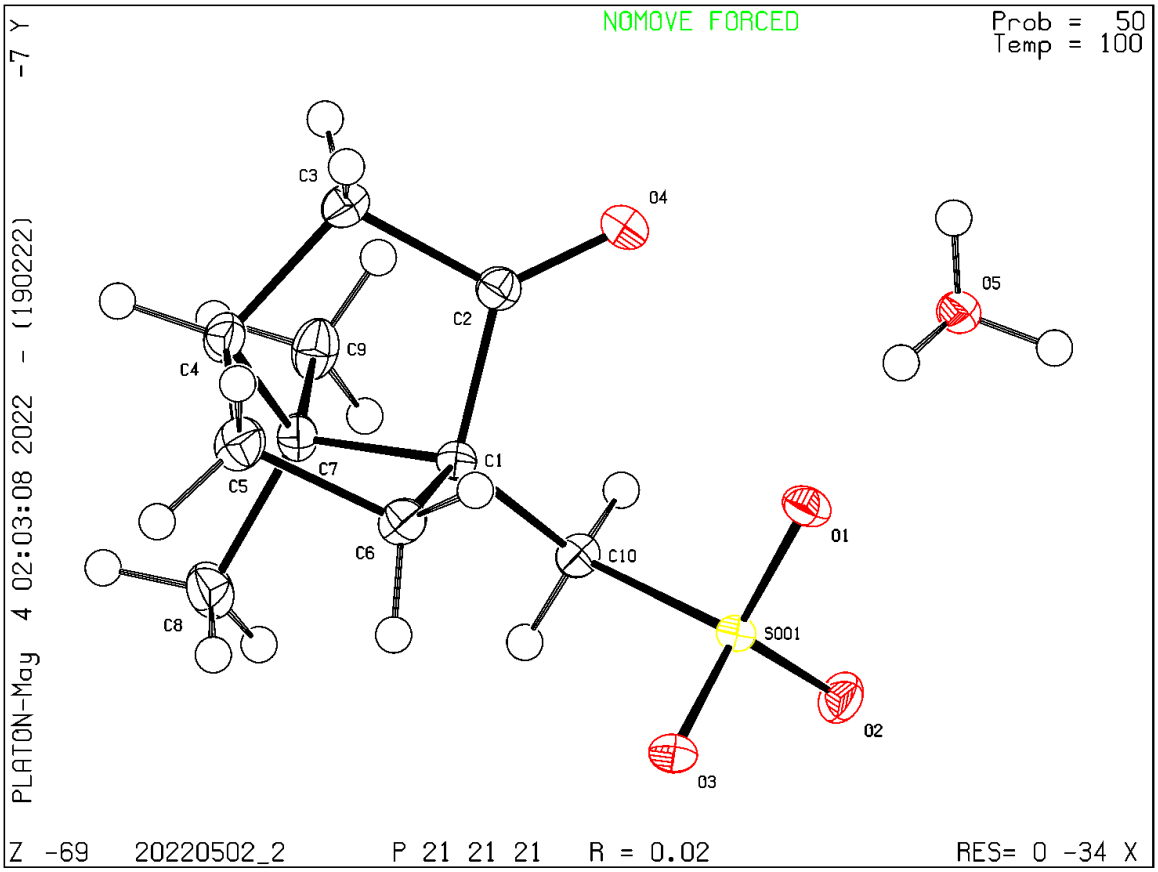
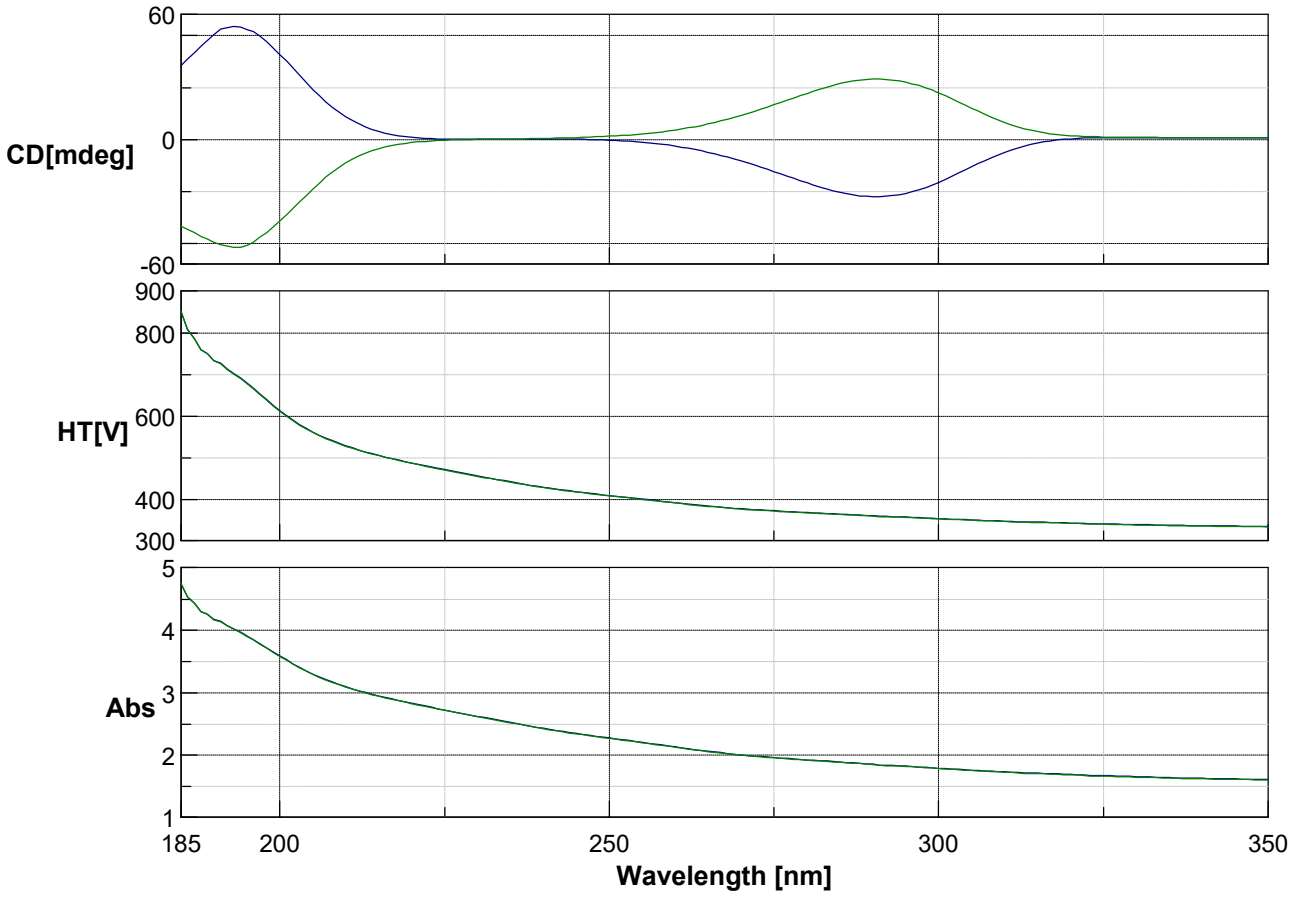


Figure S18: Electronic circular dichroism spectra of (1S)-(+)-CSA and (1R)-(-)-CSA



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Response	1 sec
Sensitivity	Standard
Measurement range	350 - 185 nm
Data pitch	1nm
Scanning speed	50 nm/min
Accumulation	3
Cell Length	0.1 cm
Temperature	Room Temperature
Sample name	
Operator	atc
Comment	