

SUMMARY OF SERVICES REQUESTED

The Client has requested structure elucidation of two 10-OH-HHC cannabinoid samples by NMR, LC-MS, and GC-MS. The samples were labeled as QC-I-57-001 and QC-I-57-002.

MATERIALS AND METHODS

LC-MS Analysis

LC-MS analysis was completed using an Agilent 1200 HPLC coupled to an Agilent 6125A single quadrupole mass spectrometer. Samples were prepared at approximately 1 mg/mL in chloroform (QC-I-57-001) or DMSO (QC-I-57-002) and analyzed using the method parameters listed in Table 1.

Table 1. Instrument parameters for LC-MS Analysis

Column	Agilent Zorbax SB-C8, 2.1 x 50 mm, 5 µm particle	
Flow rate	0.5 mL/min	
Detection (UV)	210 nm	
Detection (MS)	Dual Mode ESI/APCI Full scan (100-1500 m/z) positive and negative mode	
Injection Volume	1 µL	
Mobile Phase A	90:10:0.1 Water:Methanol:Acetic Acid	
Mobile Phase B	10:90:0.1 Water:Methanol:Acetic Acid	
Gradient	Time (minutes)	%B
	0	0
	8	100
	16	100
	16.1	0
	22	0
Method Run Time	22 minutes	

GC-MS Analysis

GC-MS analysis was completed using an Agilent 8890 GC coupled to an Agilent 5977B single quadrupole mass spectrometer. Samples were prepared at approximately 1 mg/mL in chloroform (QC-I-57-001) or dimethyl sulfoxide (QC-I-57-002) and analyzed using the method parameters listed in Table 2.

Table 2. Instrument parameters for GC-MS Analysis

Column	Agilent HP-5ms UI, 30 m x 0.25 mm x 0.25 µm film thickness
Carrier Gas	Helium
Flow Rate	1 mL/min
Detection	Electron Impact ionization Full scan (50-550 m/z) positive mode
MS Transfer Line Temperature	250 °C
Inlet Temperature	250 °C
Injection Mode	Split, 20:1
Injection Volume	1 µL
Temperature Program	60 °C for 3 min; 20 °C/min to 300 °C; 300 °C for 3 min
Method Run Time	18 minutes
Solvent Delay	6.2 minutes

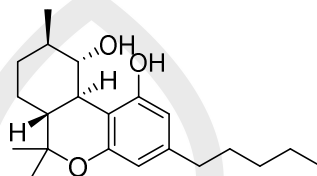
NMR Analysis

NMR analysis was completed using a JEOL ECZ400S spectrometer equipped with a JEOL ROYALPROBE HFX probe. ^1H -NMR spectra were acquired at 399.5822 MHz and ^{13}C -NMR spectra were obtained at 100.4750 MHz. Samples were prepared at approximately 28 mg/mL in chloroform- d (QC-I-57-001) or DMSO- d_6 (QC-I-57-002). Additional experimental parameters are included in the attached NMR reports.

RESULTS

QC-I-57-001

The LC-MS, GC-MS and NMR data for QC-I-57-001 are consistent with 10(S)-hydroxy-9(R)-hexahydrocannabinol. Analytical reports for each method are attached in Appendix A.



10(S)-hydroxy-9(R)-hexahydrocannabinol

Chemical Formula: $\text{C}_{21}\text{H}_{32}\text{O}_3$

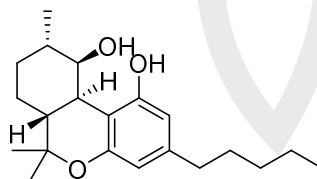
Exact Mass: 332.2351

Molecular Weight: 332.4840

- A single major product is observed at 10.01 minutes by LC-MS with a 333 m/z $[\text{M}+\text{H}]^+$ ion in positive mode and a 331 m/z $[\text{M}-\text{H}]^-$ ion in negative mode confirming a mass of 332 amu.
- A single major product is observed at 16.35 minutes by GC-MS with a 332 m/z $[\text{M}]^+$ ion. A NIST library search using this spectrum matched for 10-hydroxyhexahydrocannabinol with a match score of 72.82.
- Critical correlations were observed in HMBC, COSY, and NOESY experiments to confirm the proposed structure.

QC-I-57-002

The LC-MS, GC-MS and NMR data for QC-I-57-002 are consistent with 10(R)-hydroxy-9(S)-hexahydrocannabinol. Analytical reports for each method are attached in Appendix B.



10(R)-hydroxy-9(S)-hexahydrocannabinol

Chemical Formula: $\text{C}_{21}\text{H}_{32}\text{O}_3$

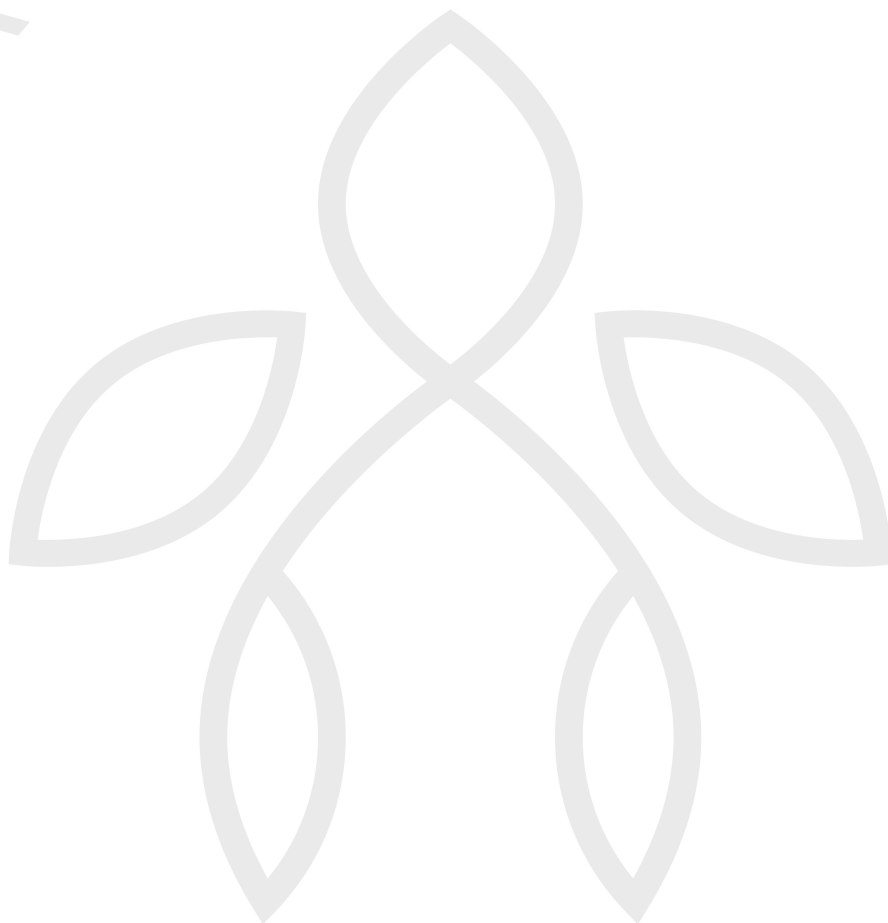
Exact Mass: 332.2351

Molecular Weight: 332.4840

- A single major product is observed at 9.57 minutes by LC-MS with a 333 m/z $[\text{M}+\text{H}]^+$ ion in positive mode and a 331 m/z $[\text{M}-\text{H}]^-$ ion in negative mode confirming a mass of 332 amu.
- A single major product is observed at 15.88 minutes by GC-MS with a 332 m/z $[\text{M}]^+$ ion. A NIST library search using this spectrum matched for 10-hydroxyhexahydrocannabinol with a match score of 79.98.
- Critical correlations were observed in HMBC, COSY, and NOESY experiments to confirm the proposed structure.

APPENDIX A – ANALYTICAL REPORTS FOR QC-I-57-001

A P R I C I T Y



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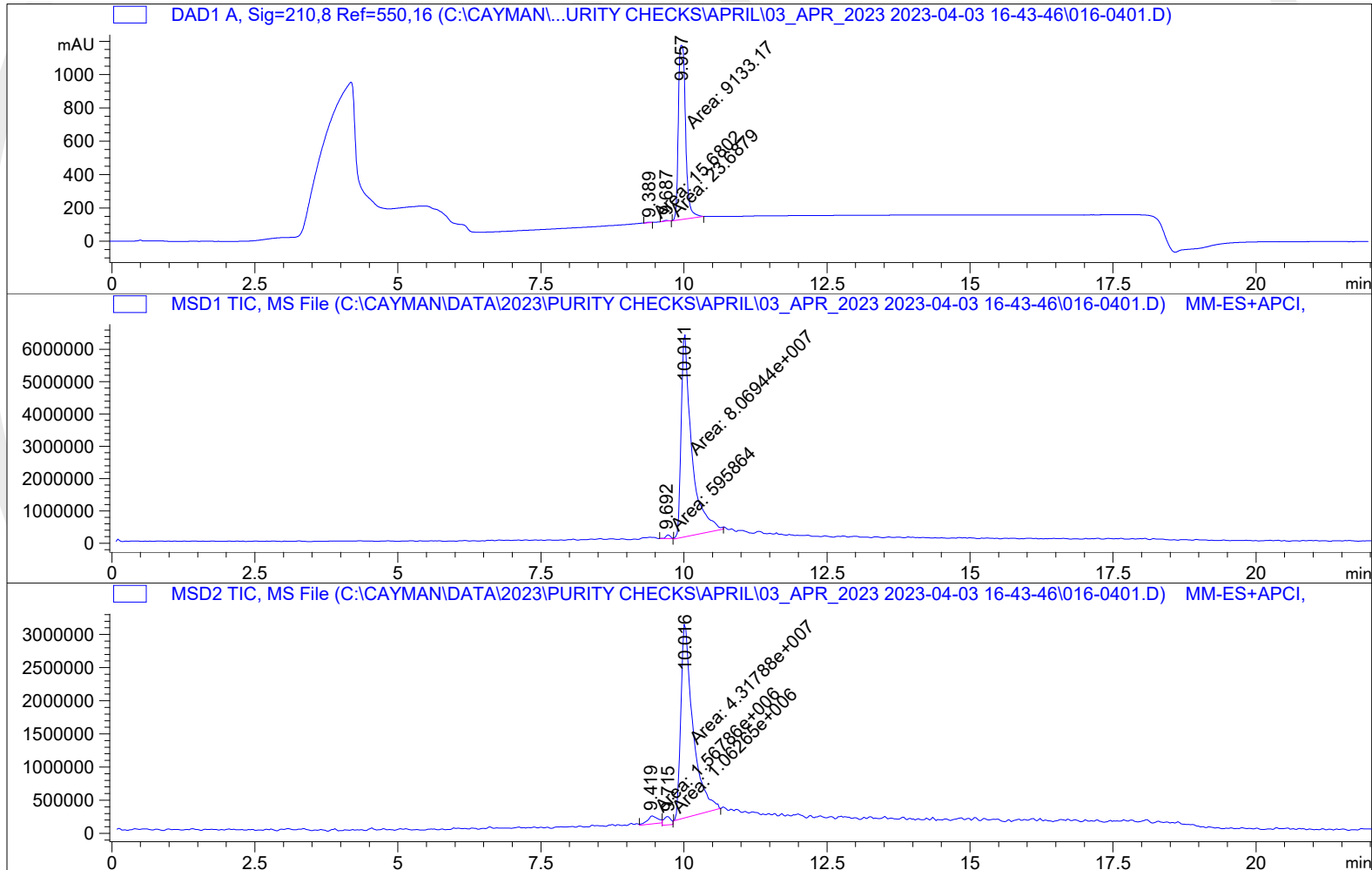
Acq. Operator : Seq. Line : 4
Acq. Instrument : LCMS01 Location : Vial 16
Injection Date : 4/3/2023 5:57:47 PM Inj : 1
Inj Volume : 1.0 µl

Method : C:\CAYMAN\DATA\2023\PURITY CHECKS\APRIL\03_APR_2023 2023-04-03 16-43-46\C8_ACOH.M (Sequence Method)
Last changed : 4/3/2023 4:43:01 PM
Method Info : A: 90:10:0.1 H2O:MeOH:AcOH
B: 10:90:0.1 H2O:MeOH:AcOH

0-8 min: 0%B to 100%B
8-16 min: Hold 100% B
16-16.1 min: 100% to 0% B
16.1-22 mins re-equilibrate to 0% B

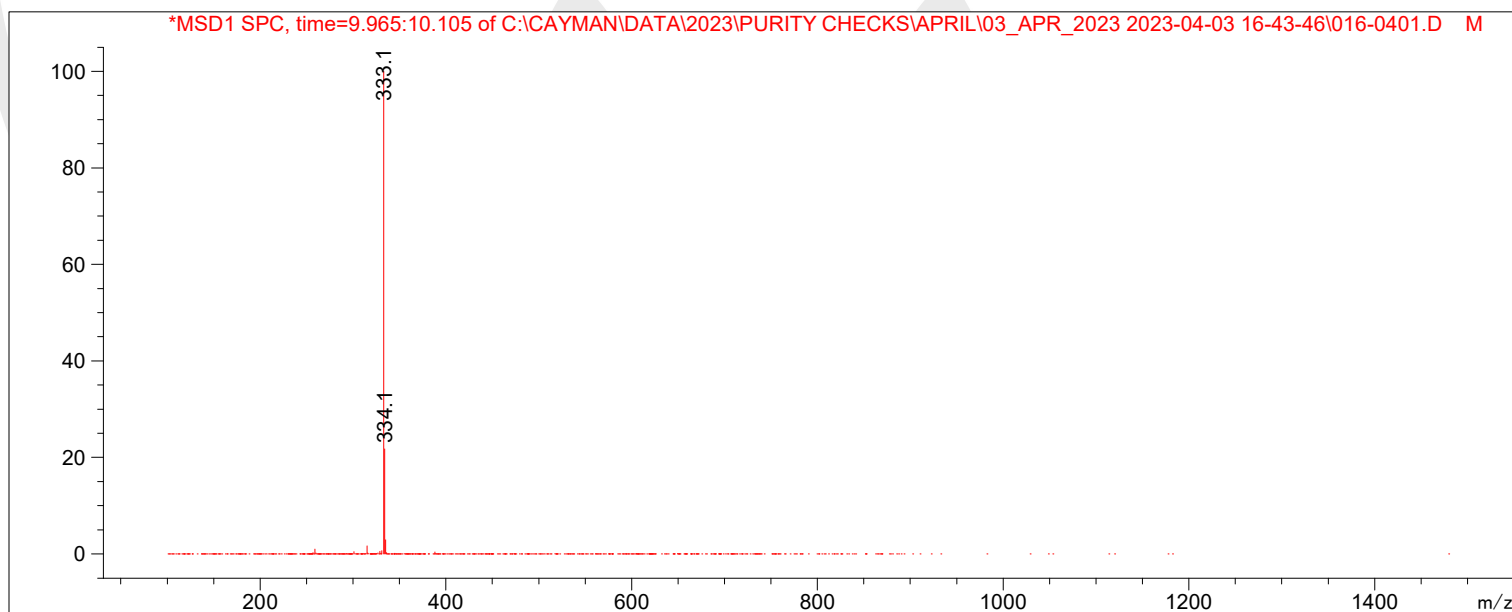
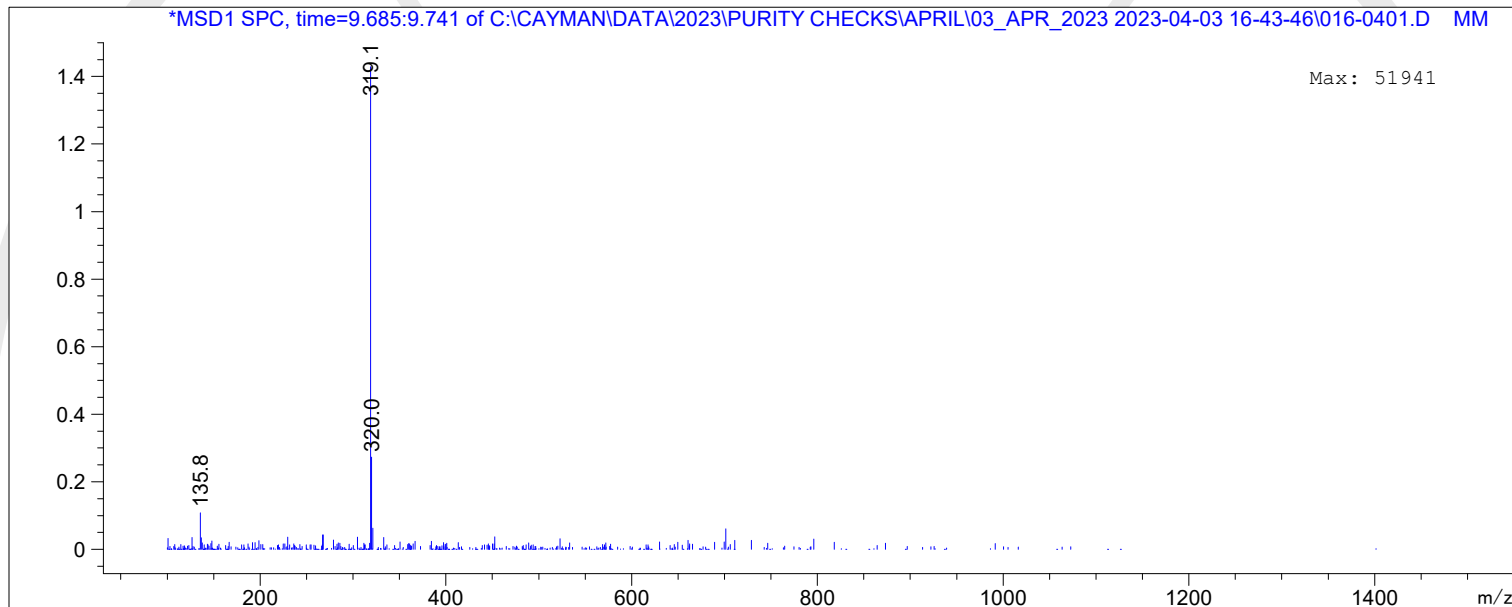
Agilent Zorbax 5µ C8 50x2.1 mm
0.5 ml/min 210 nm

Additional Info : Peak(s) manually integrated



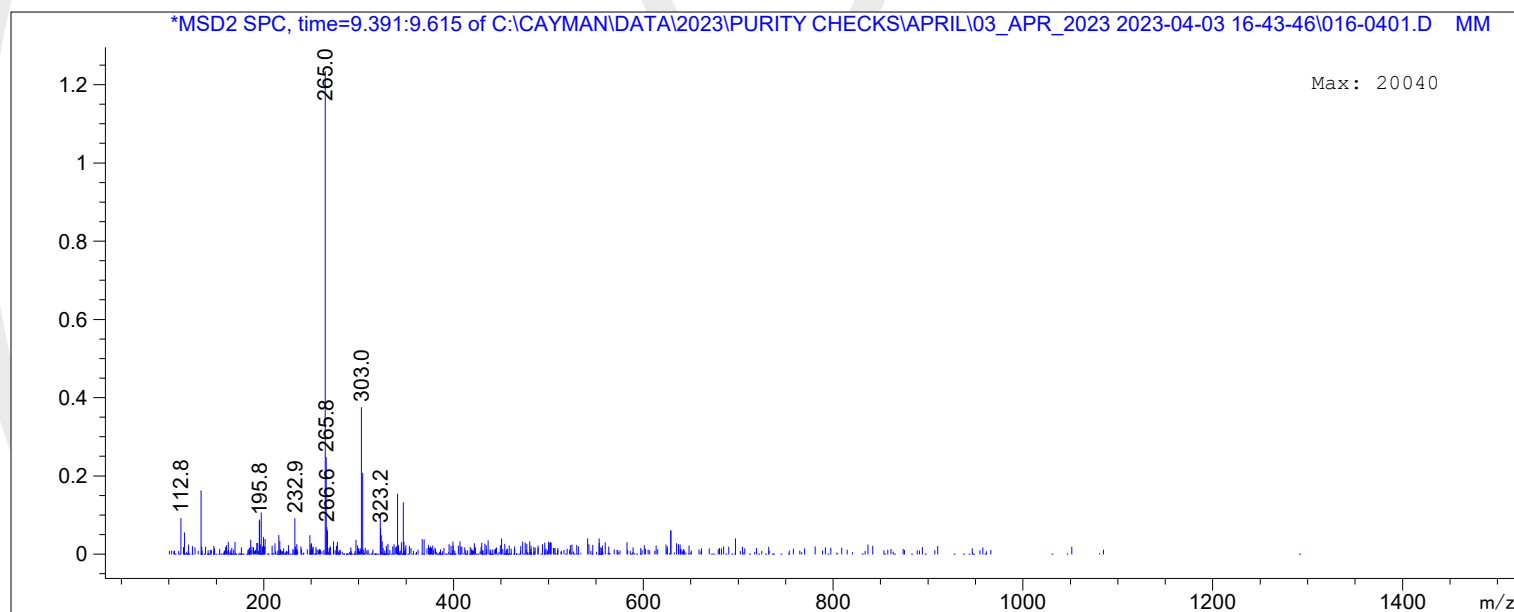
MS Signal: MSD1 TIC, MS File, MM-ES+APCI, Pos, Fast Scan, Frag: 70, "+DUAL"
Spectra averaged over upper half of peaks.
Noise Cutoff: 1000 counts.
Reportable Ion Abundance: > 10%.

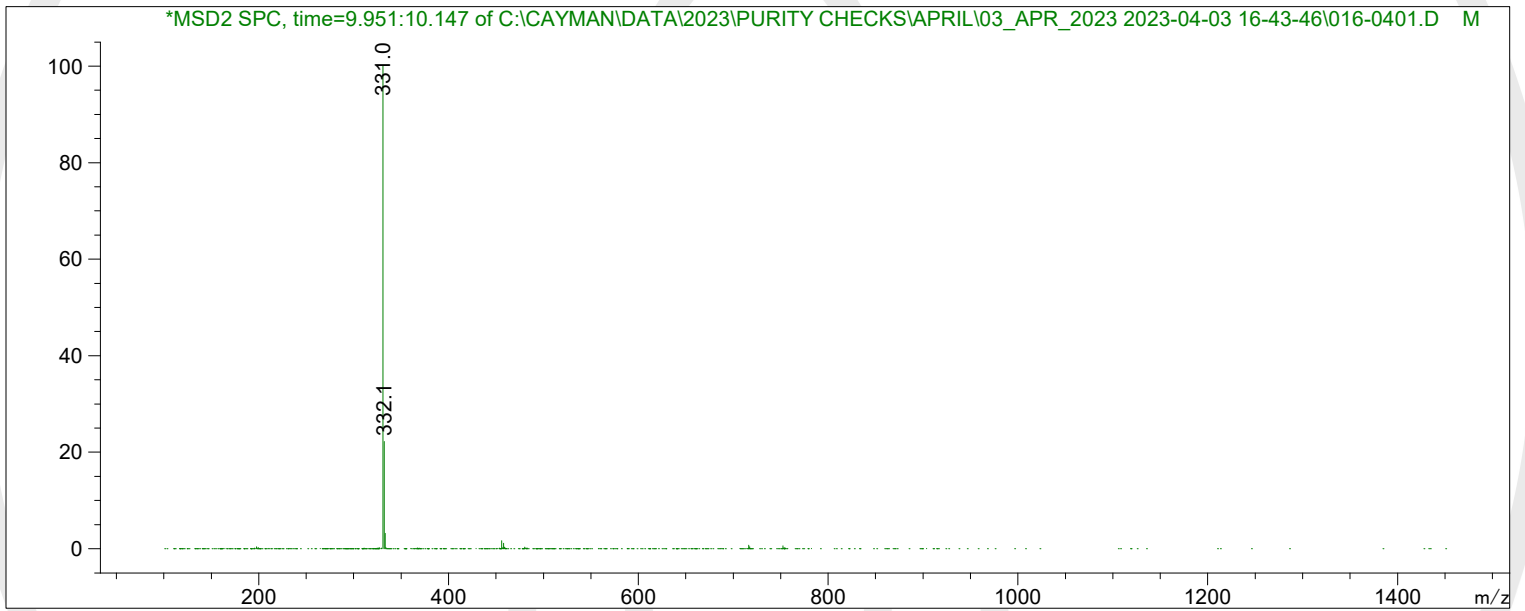
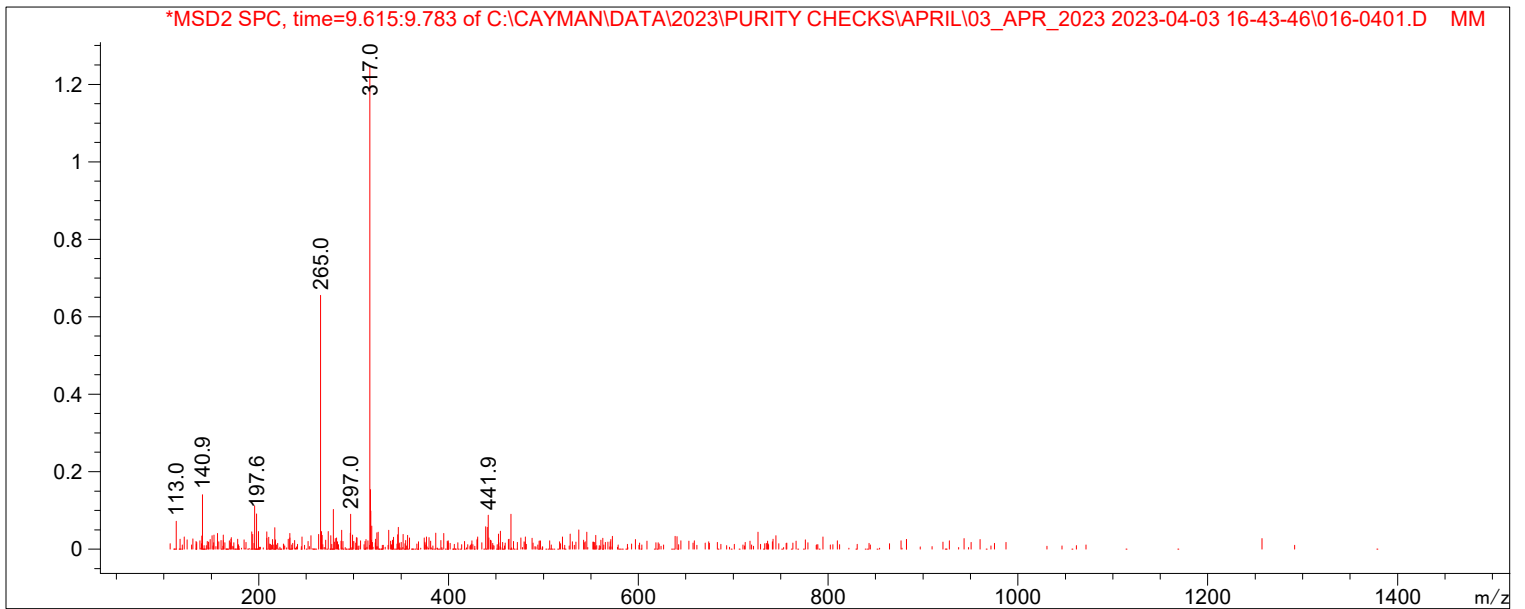
Retention Time (MS)	MS Area	Mol. Weight or Ion
9.692	595864	320.00 I 319.10 I
10.011	80694448	334.10 I 333.10 I



MS Signal: MSD2 TIC, MS File, MM-ES+APCI, Neg, Fast Scan, Frag: 70, "--DUAL"
Spectra averaged over upper half of peaks.
Noise Cutoff: 1000 counts.
Reportable Ion Abundance: > 10%.

Retention Time (MS)	MS Area	Mol. Weight or Ion
9.419	1567861	347.20 I
		341.00 I
		304.10 I
		303.05 I
		265.80 I
		264.95 I
		133.95 I
9.715	1062647	317.90 I
		317.00 I
		265.05 I
		140.85 I
10.016	43178832	332.10 I
		331.05 I





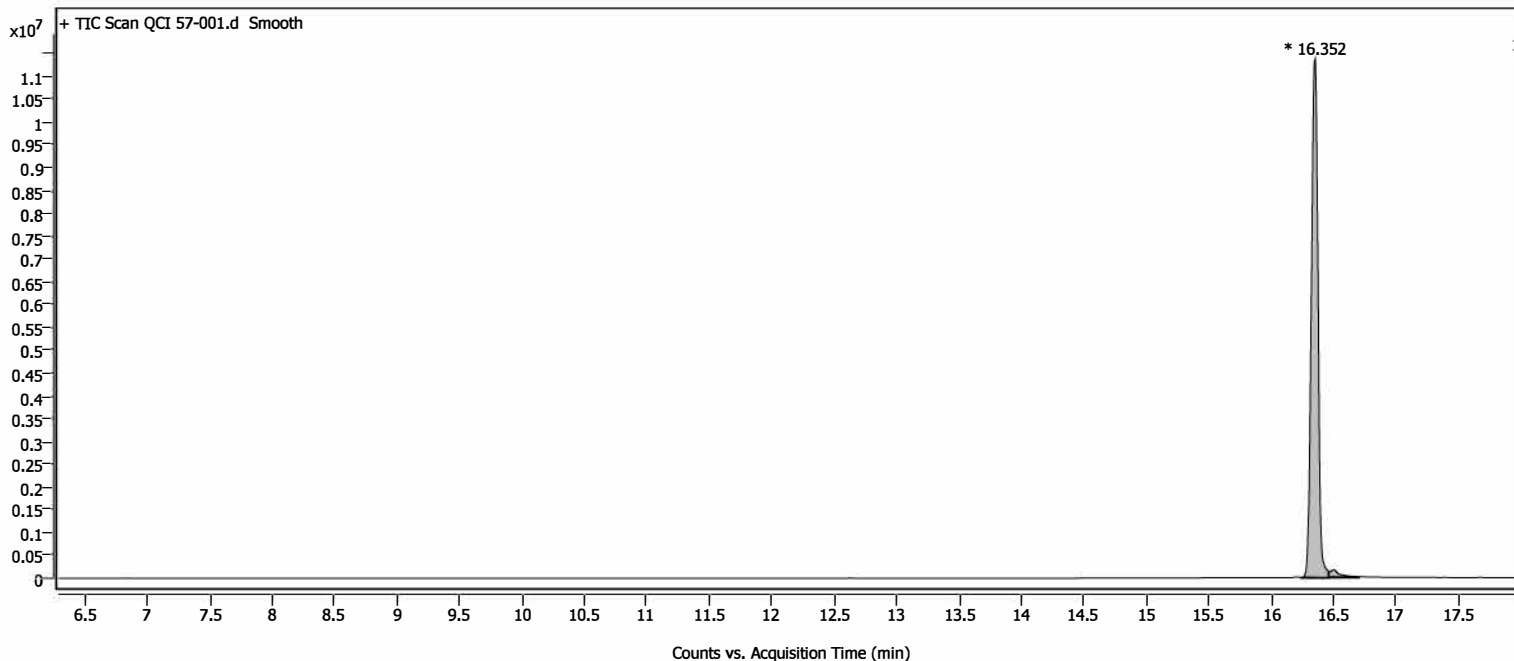
*** End of Report ***

Analysis Report

Sample Information

Name	QC-I-57-001	Data File Path	C:\MassHunter\GCMS\1\data\2023\April\03Apr23\QCI 57-001.D
Instrument	GCMS	Acq. Time (Local)	4/3/2023 11:41:14 AM (UTC-04:00)
MS Type	Q	Method Path (Acq)	C:\MassHunter\GCMS\1\methods\DMSO delay_60-300_20C_EI_GCMS Analysis.M
Inj. Vol. (ul)	1	Method Path (DA)	DMSO delay_60-300_20C_EI_GCMS Analysis.M
Position	2	Version (Acq SW)	MassHunter GC/MS Acquisition 10.0.368 14-Feb-2019 Copyright © 1989-2018 Agilent Technologies, Inc.
		Operator	KRH

Sample Chromatograms



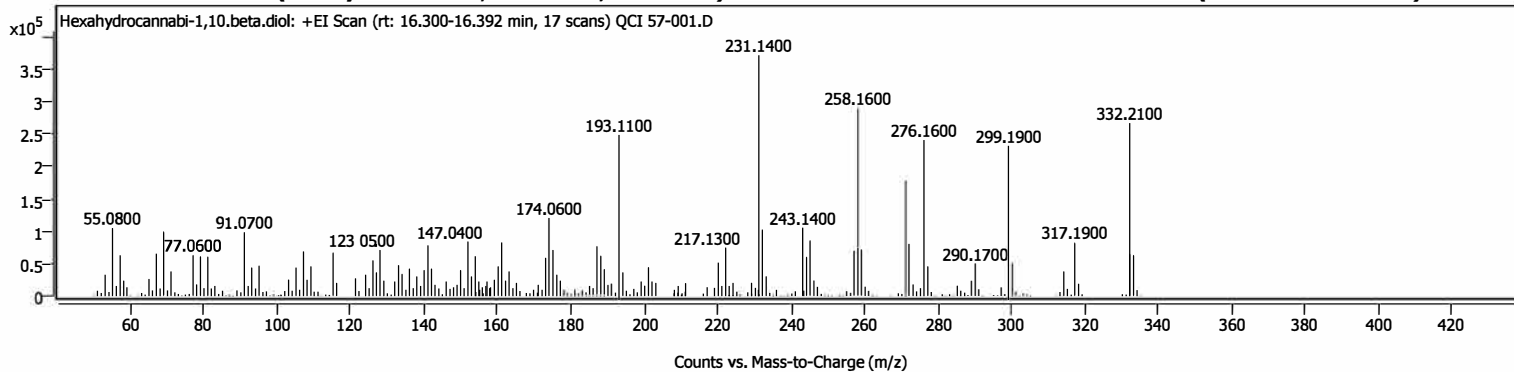
Chromatogram Peaks

Peak	RT	Height	Area	Area Sum %
1	16.352	11377479	42381151	97.88
2	16.501	162361	916263	2.12

Sample Spectra

Peak 1 from + TIC Scan Smo (Hexahydrocannabinol-1,10.beta.diol; C₂₁H₃₂O₃)

+ Scan (rt: 16.300-16.392 min)



Analysis Report

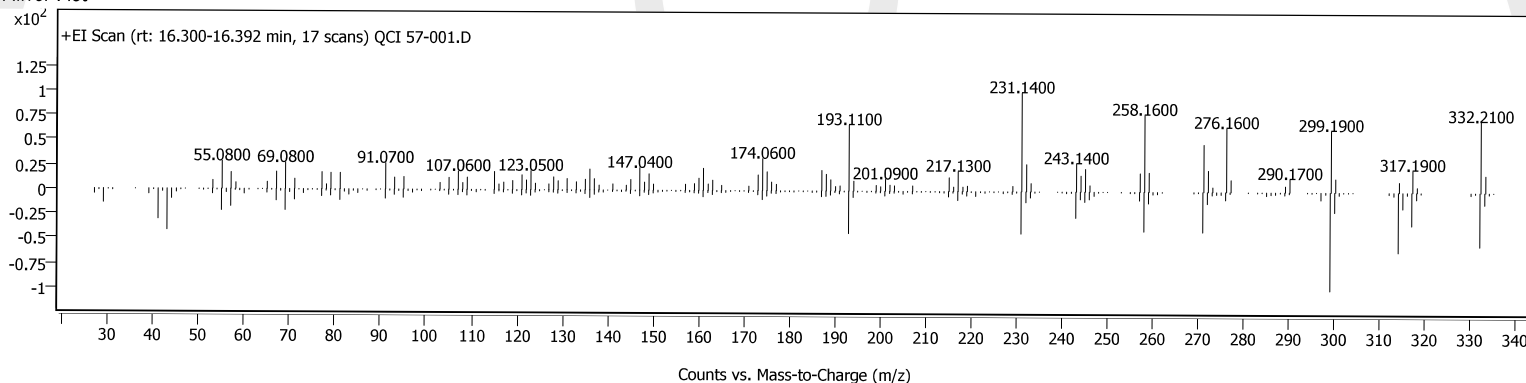
Spectrum Peaks (Max. 20)

m/z	Z	Abund	Abund %
55.0800		104701	28.21
69.0800		99725	26.87
91.0700		98188	26.46
136.0500		77997	21.01
147.0400		83841	22.59
161.0600		82358	22.19
174.0600		120238	32.40
187.0700		76879	20.71
193.1100	1	248359	66.92
231.1400	1	371149	100.00
232.1400	1	102134	27.52
243.1400		104972	28.28
245.1500	1	85777	23.11
258.1600	1	288992	77.86
271.1600		178000	47.96
272.1700	1	79992	21.55
276.1600	1	240531	64.81
299.1900	1	231238	62.30
317.1900	1	82705	22.28
332.2100	1	266606	71.83

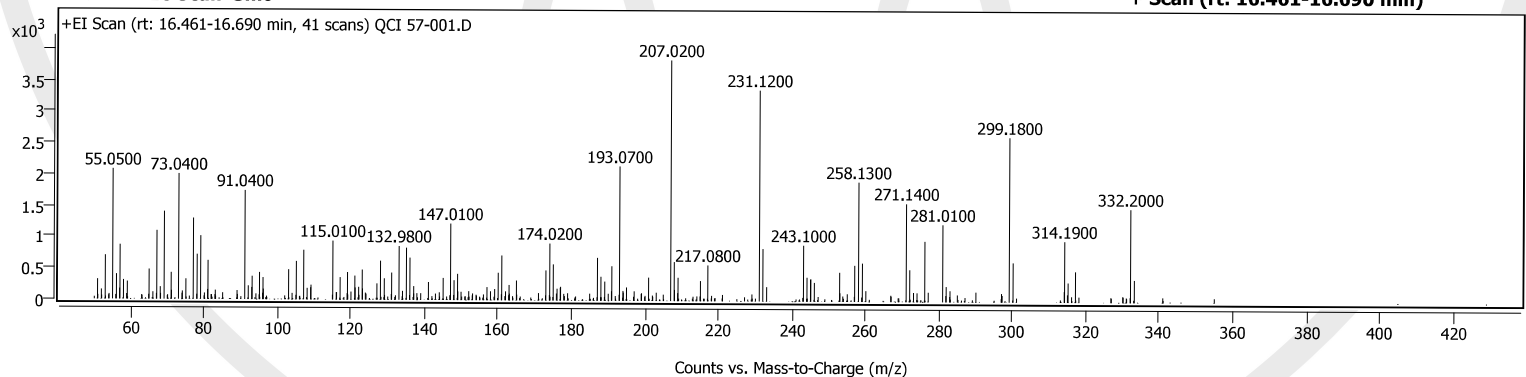
Spectrum Identification Table (Max. 1)

Best	Name	Formula	CAS	Score	Score (Lib)	Lib/DB
Yes	Hexahydrocannabinol-1,10.beta.diol	C21H32O3	1010196-54-2	72.82	72.82	NIST20.L

Mirror Plot



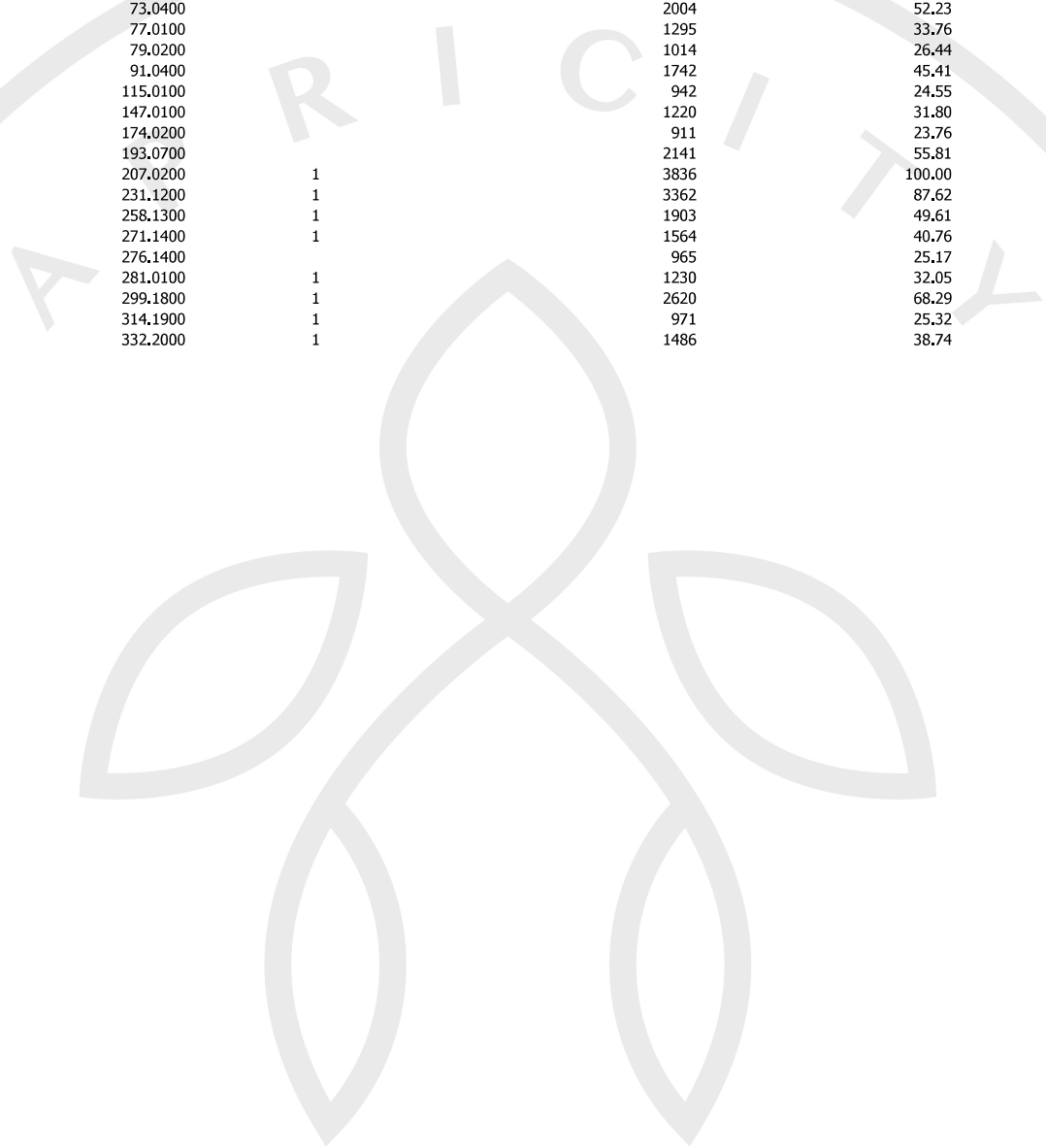
Peak 2 from + TIC Scan Smo

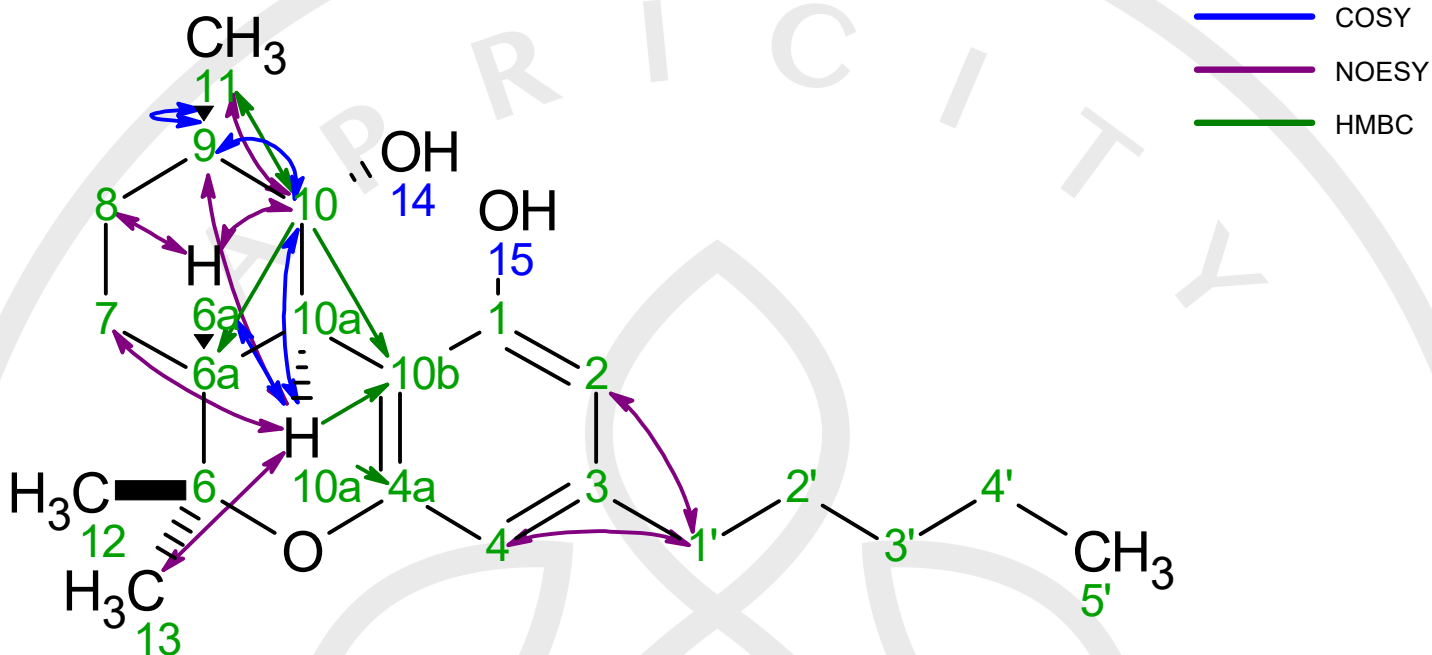


Analysis Report

Spectrum Peaks (Max. 20)

m/z	Z	Abund	Abund %
55.0500		2080	54.21
67.0400		1099	28.64
69.0500		1405	36.62
73.0400		2004	52.23
77.0100		1295	33.76
79.0200		1014	26.44
91.0400		1742	45.41
115.0100		942	24.55
147.0100		1220	31.80
174.0200		911	23.76
193.0700		2141	55.81
207.0200	1	3836	100.00
231.1200	1	3362	87.62
258.1300	1	1903	49.61
271.1400	1	1564	40.76
276.1400		965	25.17
281.0100	1	1230	32.05
299.1800	1	2620	68.29
314.1900	1	971	25.32
332.2000	1	1486	38.74





Critical Correlations

HMBC

- Proton 10: ${}^3J_{CH}$ to carbons 6a, 10b, and 11
- Proton 10a: ${}^2J_{CH}$ to carbon 10b; ${}^3J_{CH}$ to carbon 4a

COSY

- Proton 6a: ${}^3J_{HH}$ (~10.3 Hz) to proton 10a, indicating axial-axial coupling
- Proton 10a: ${}^3J_{HH}$ (~9.6 Hz) to proton 10, indicating axial-axial coupling
- Proton 10: ${}^3J_{HH}$ (~2.4 Hz) to proton 9, indicating axial-equatorial coupling
- Proton 9: ${}^3J_{HH}$ to protons 11

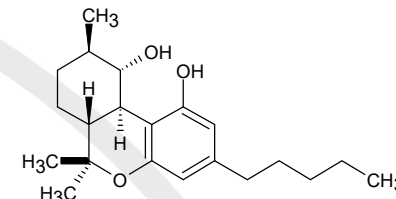
NOESY

- Proton 1' to protons 2, 4: confirms normal attachment of pentyl chain (abnormal at position 1)
- Proton 6a to protons 10 and 8: 1,3 diaxial interactions confirming axial positions for 6a, 10 and 8
- Proton 10a to protons 7, 9, and 13: 1,3 diaxial interactions confirming axial positions for 7, 9, 10a and 13
- Proton 10 to protons 11: with 10 in the axial position, nOe to 11 suggests 11 is equatorial

QC-I-57-001

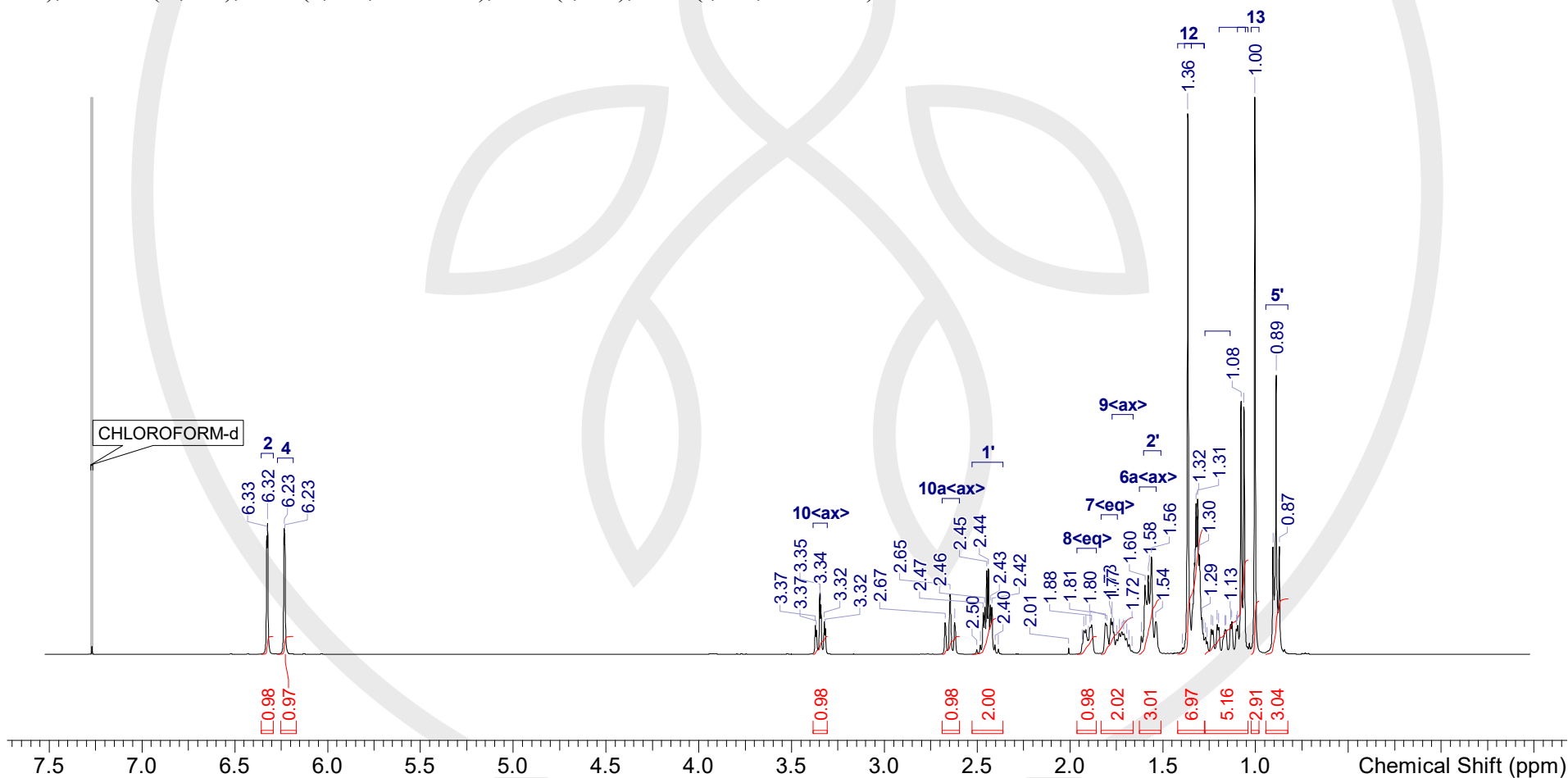
Proposed Structure

10(S)-hydroxy-9(R)-Hexahydrocannabinol



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Date	28 Mar 2023 14:51:53	Nucleus	1H
Solvent	CHLOROFORM-d	Number of Transients	16
Temperature (degree C)	21.900	Origin	JEOL ECZ400S Sc v601

¹H NMR (CHLOROFORM-d, 400 MHz) δ 6.33 (d, 1H, *J*=1.7 Hz), 6.23 (d, 1H, *J*=1.7 Hz), 3.34 (dt, 1H, *J*=2.4, 9.6 Hz), 2.65 (t, 1H, *J*=10.3 Hz), 2.4-2.5 (m, 2H), 1.9-2.0 (m, 1H), 1.7-1.8 (m, 1H), 1.7-1.8 (m, 1H), 1.5-1.6 (m, 1H), 1.5-1.6 (m, 2H), 1.36 (s, 3H), 1.3-1.4 (m, 2H), 1.3-1.3 (m, 2H), 1.1-1.3 (m, 1H), 1.1-1.2 (m, 1H), 1.07 (d, 3H, *J*=6.5 Hz), 1.00 (s, 3H), 0.89 (t, 3H, *J*=6.9 Hz)

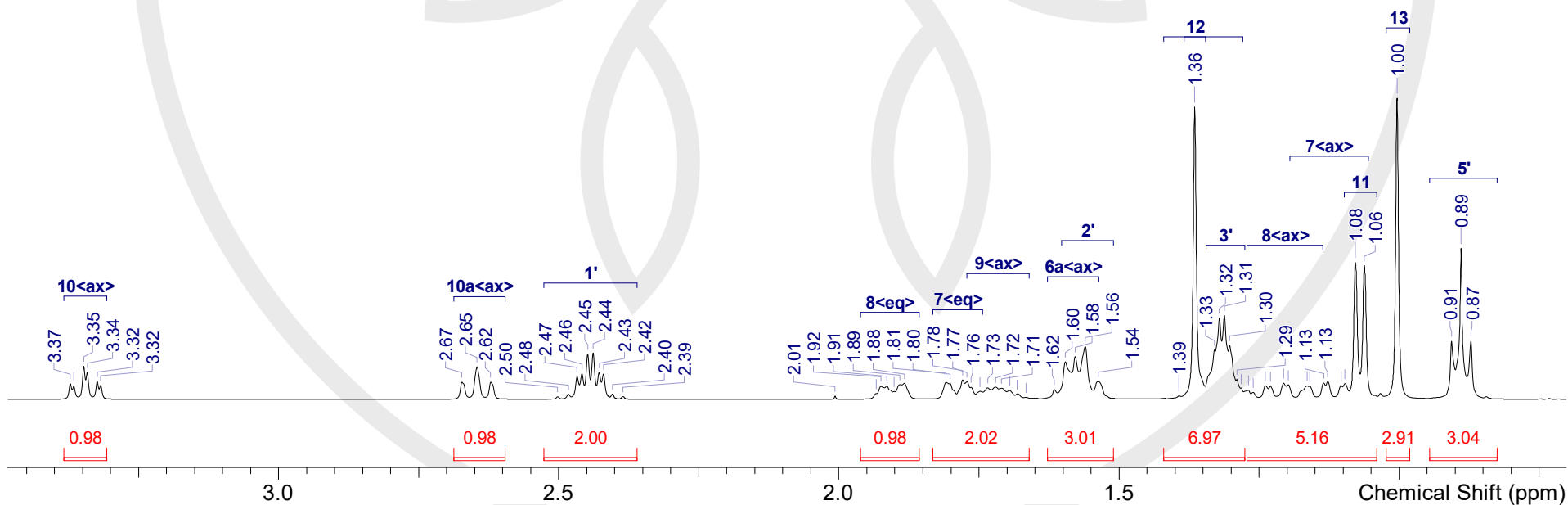
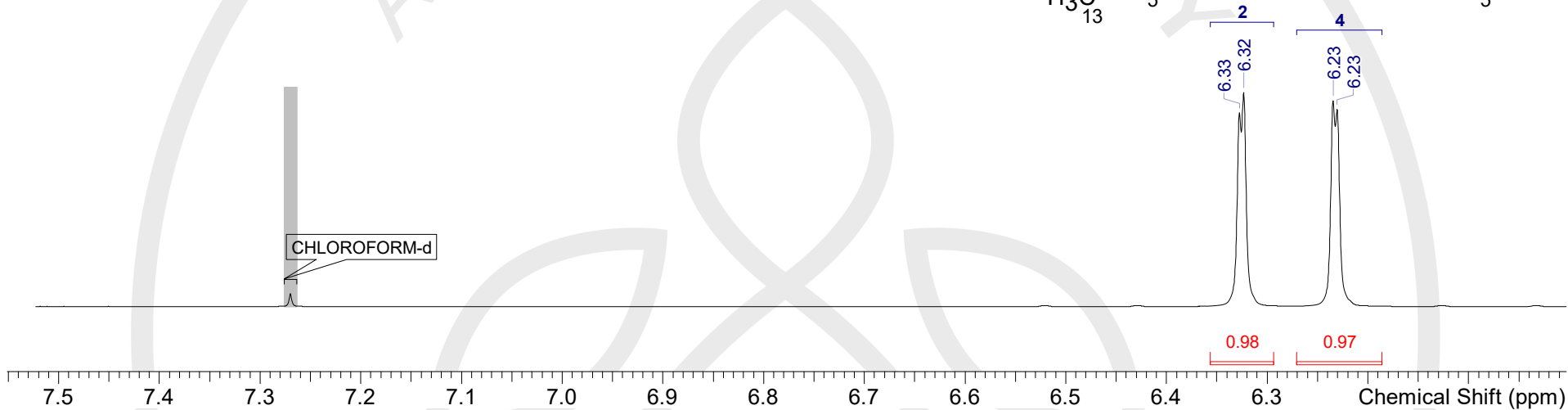
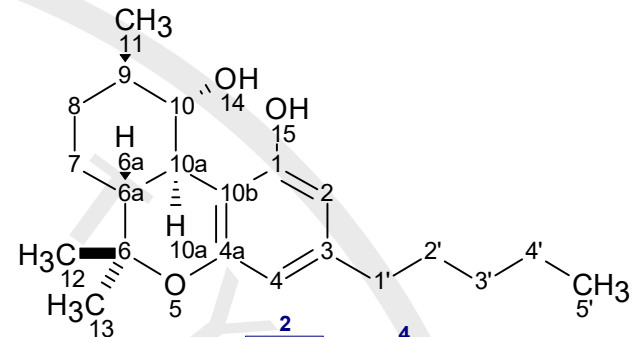




QC-I-57-001

Proposed Structure

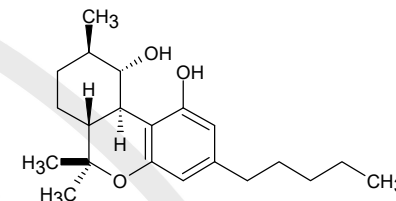
10(S)-hydroxy-9(R)-Hexahydrocannabinol



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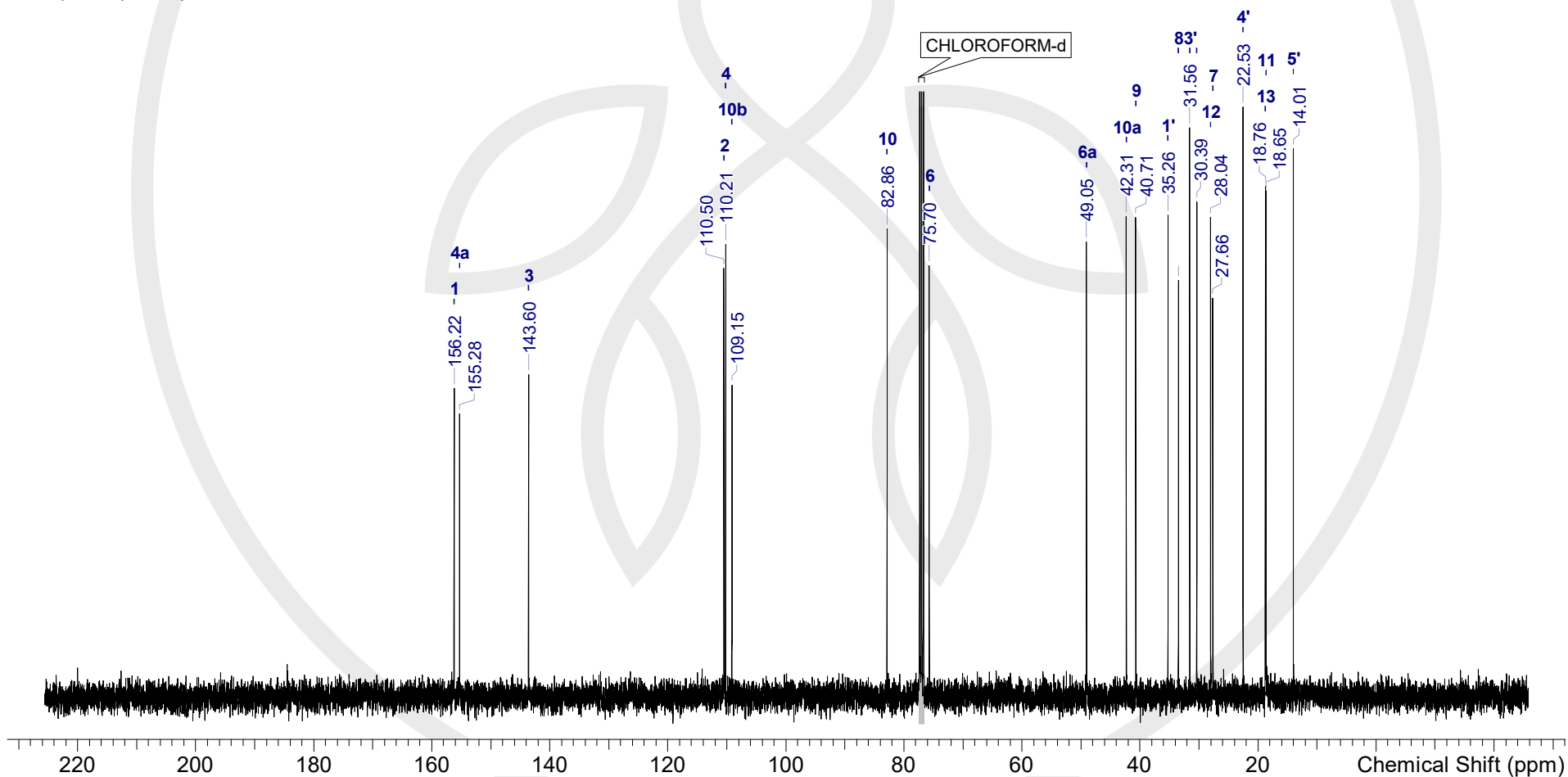
Proposed Structure

10(S)-hydroxy-9(R)-Hexahydrocannabinol



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Solvent	CHLOROFORM-d	Number of Transients	256
Temperature (degree C)	22.100	Frequency (MHz)	100.4750
		Origin	JEOL ECZ400S Sc v601

^{13}C NMR (CHLOROFORM-d, 100 MHz) δ 156.2, 155.3, 143.6, 110.5, 110.2, 109.1, 82.9, 75.7, 49.1, 42.3, 40.7, 35.3, 33.5, 31.6, 30.4, 28.0, 27.7, 22.5, 18.8, 18.6, 14.0

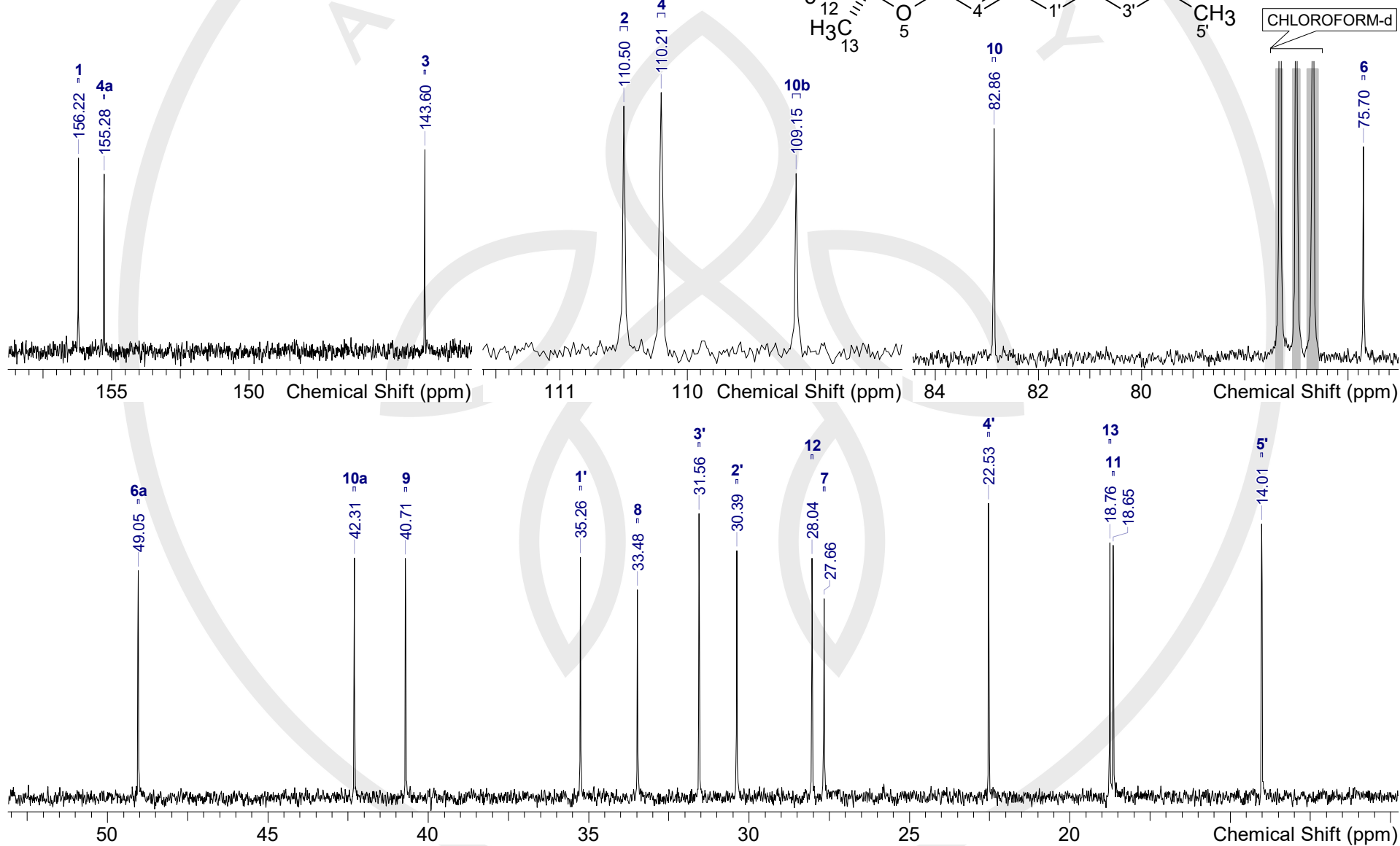
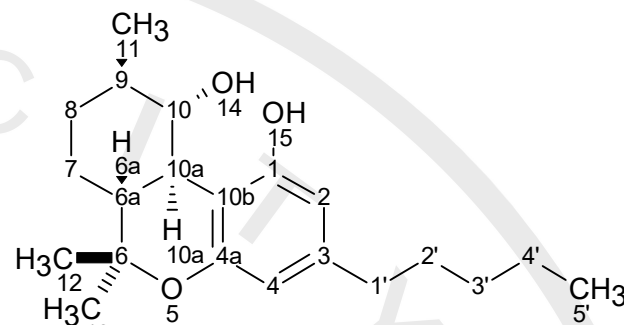




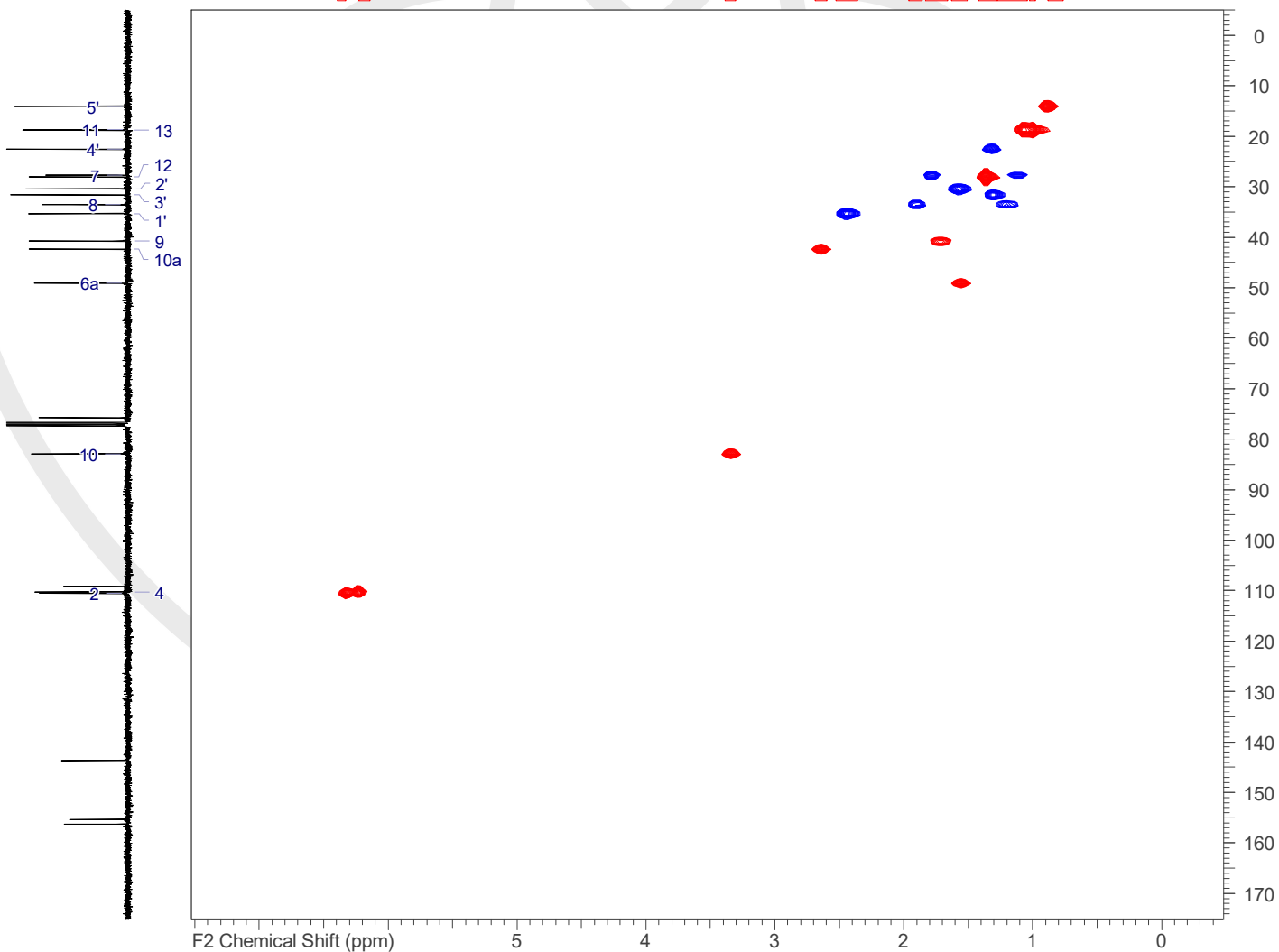
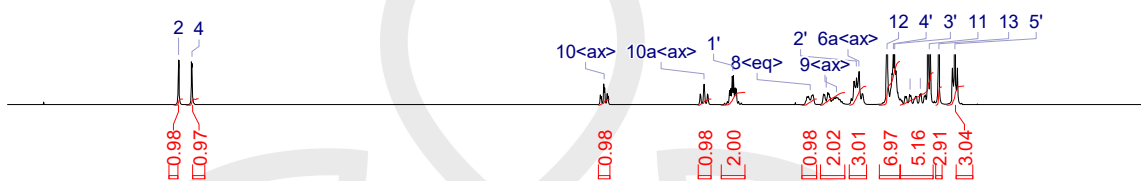
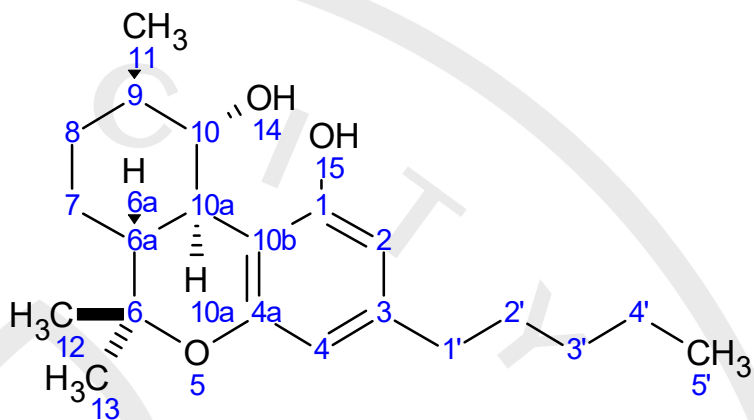
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Proposed Structure

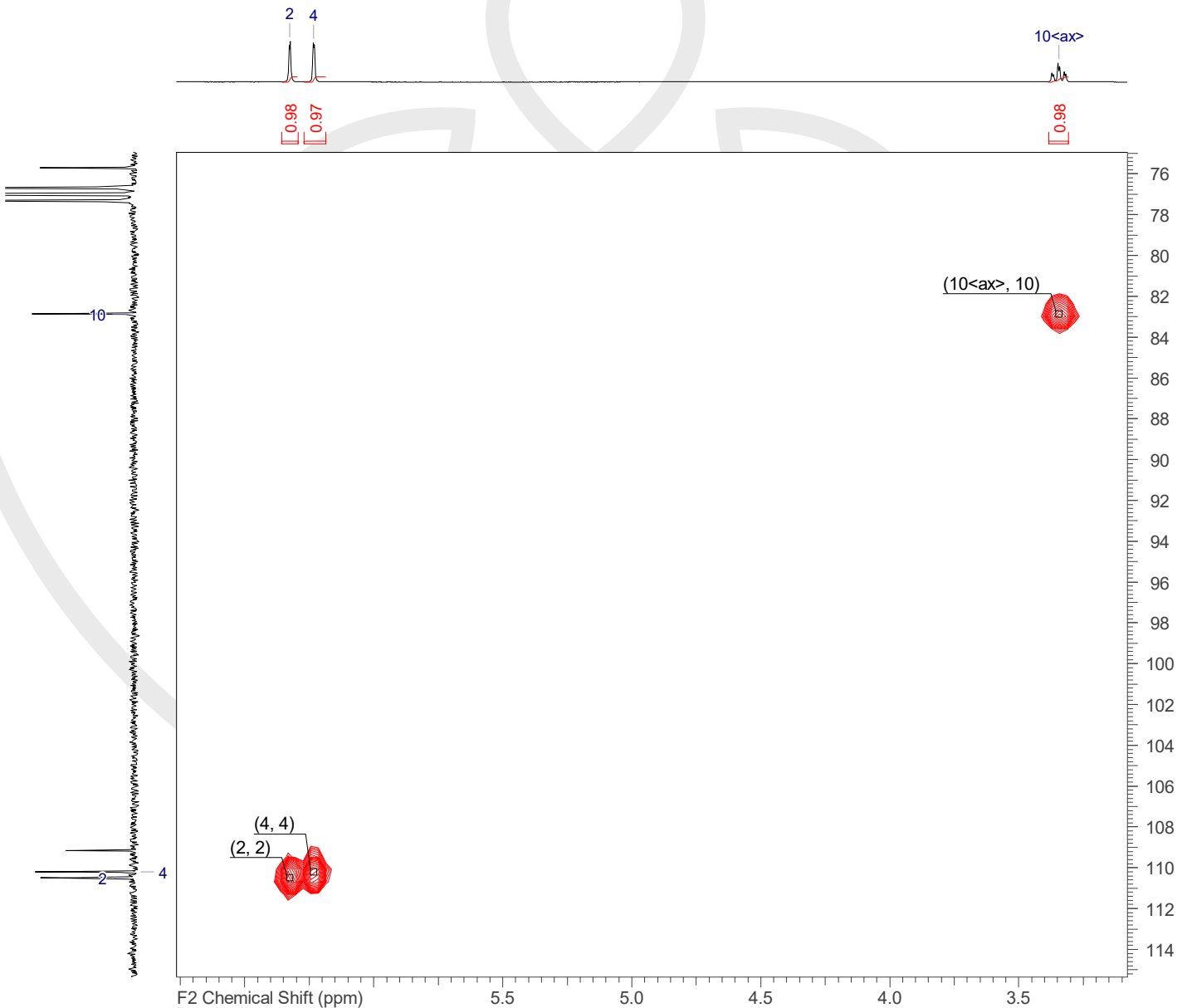
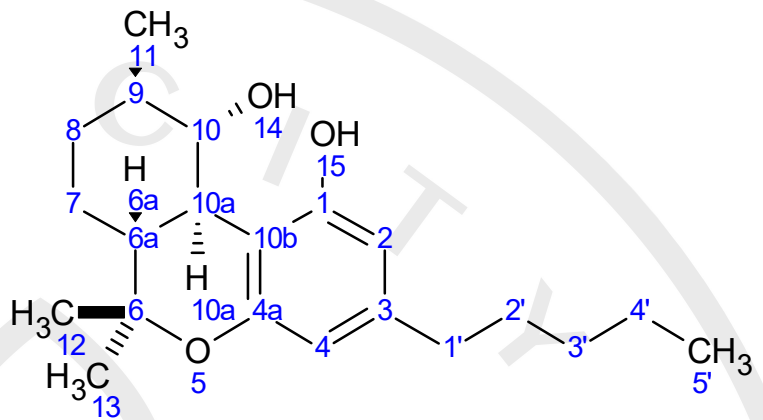
10(S)-hydroxy-9(R)-Hexahydrocannabinol



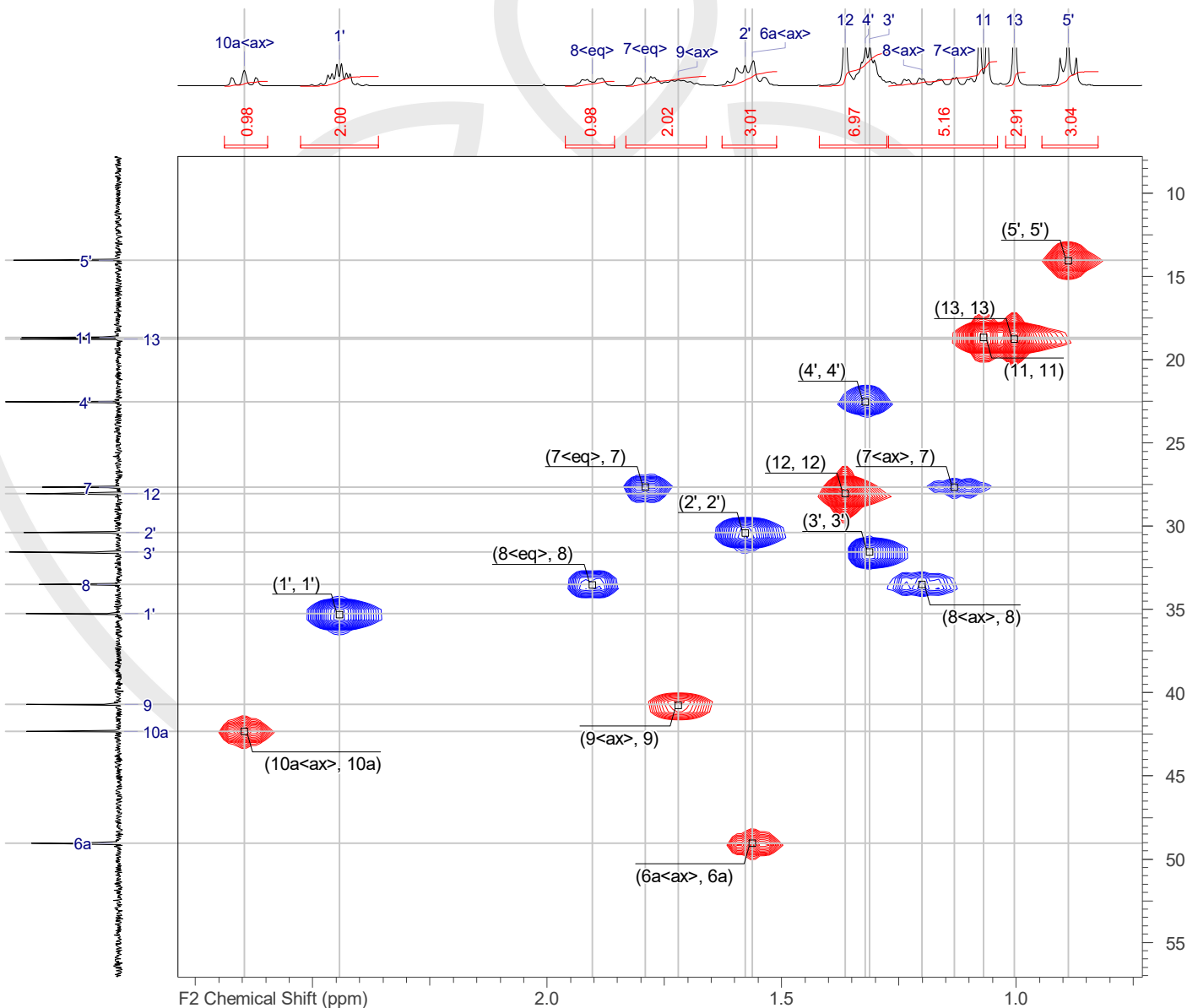
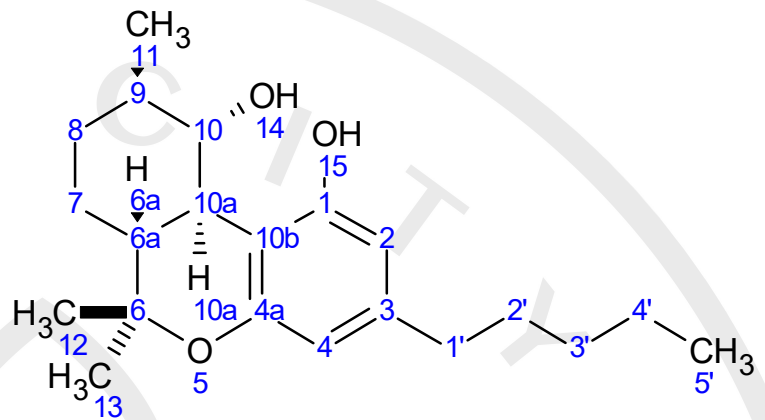
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Nucleus	(1H, 13C)
Number of Transients	2
Origin	JEOL ECZ400S Sc v601
Original Points Count	(1000, 512)
Pulse Sequence	ghsqcad.jxp
Spectrum Type	HSQC-DEPT
Sweep Width (Hz)	(3198.10, 18080.89)
Temperature (degree C)	22.400
Title	QC-I-57-001



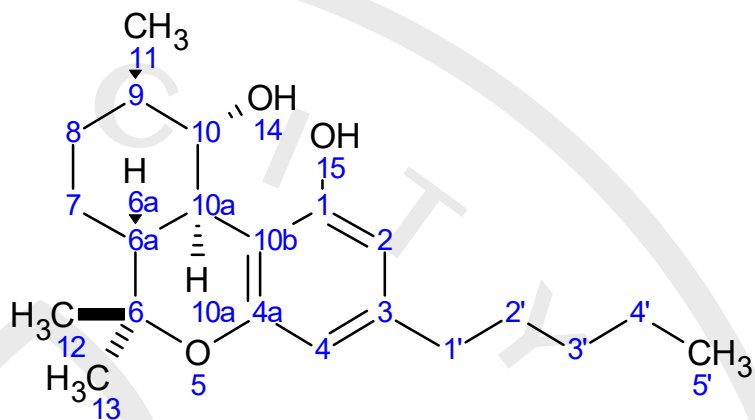
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Nucleus	(1H, 13C)
Number of Transients	2
Origin	JEOL ECZ400S Sc v601
Original Points Count	(1000, 512)
Pulse Sequence	ghsqcad.jxp
Spectrum Type	HSQC-DEPT
Sweep Width (Hz)	(3198.10, 18080.89)
Temperature (degree C)	22.400
Title	QC-I-57-001



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Nucleus	(1H, 13C)
Number of Transients	2
Origin	JEOL ECZ400S Sc v601
Original Points Count	(1000, 512)
Pulse Sequence	ghsqcad.jxp
Spectrum Type	HSQC-DEPT
Sweep Width (Hz)	(3198.10, 18080.89)
Temperature (degree C)	22.400
Title	QC-I-57-001

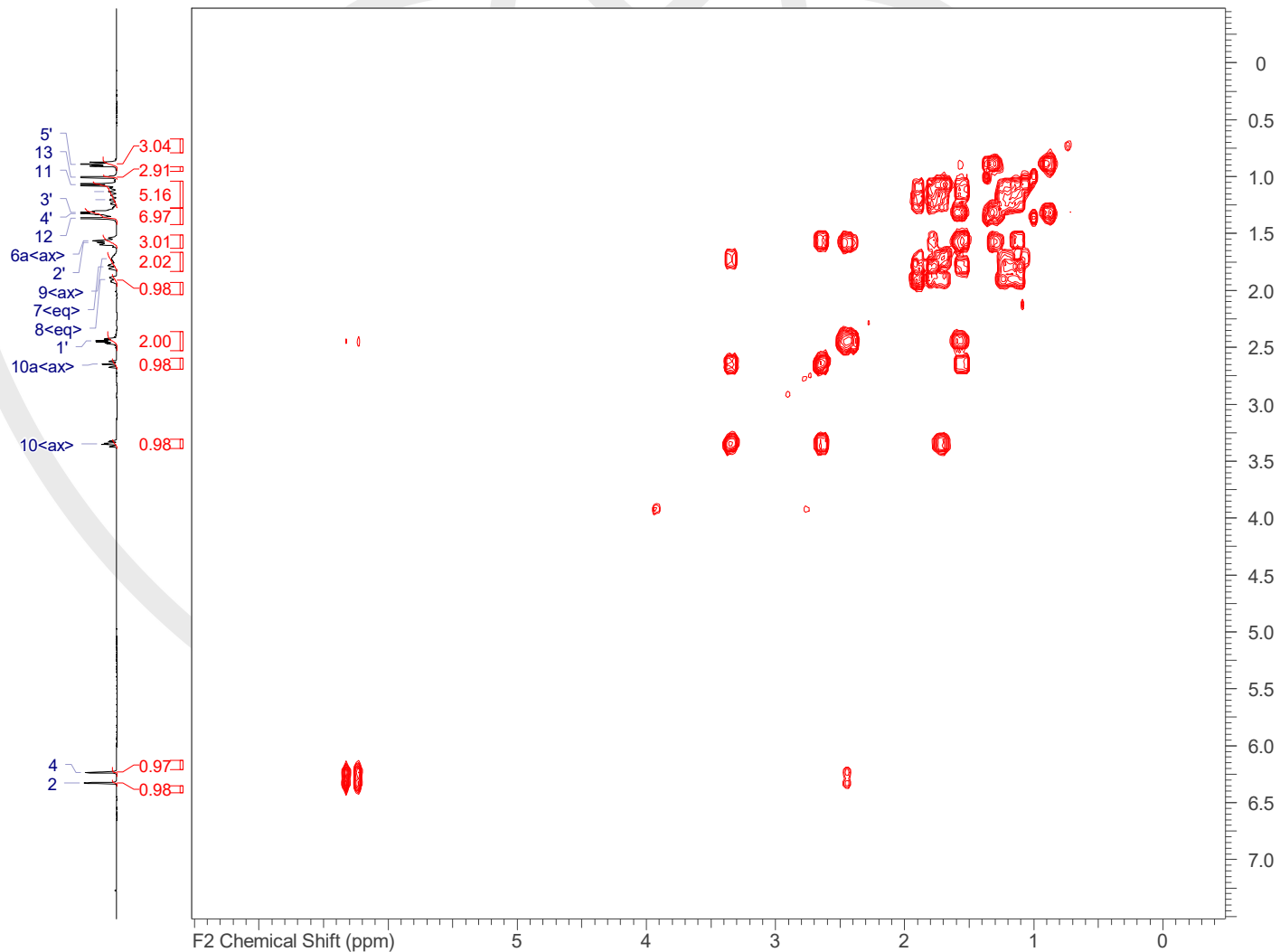
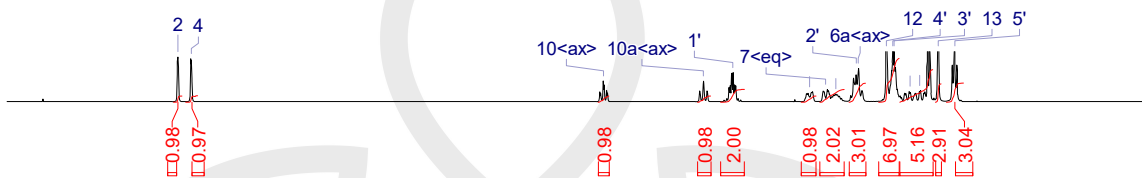
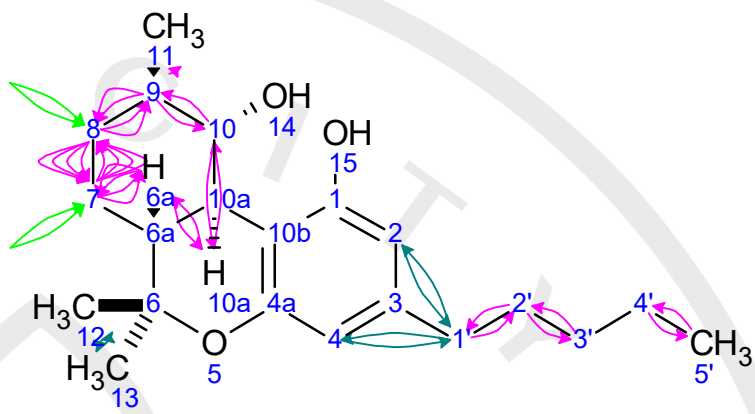


Acquisition Time (sec)	(0.2502, 0.0283)
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Nucleus	(1H, 13C)
Number of Transients	2
Origin	JEOL ECZ400S Sc v601
Original Points Count	(1000, 512)
Pulse Sequence	ghsqcad.jxp
Spectrum Type	HSQC-DEPT
Sweep Width (Hz)	(3198.10, 18080.89)
Temperature (degree C)	22.400
Title	QC-I-57-001

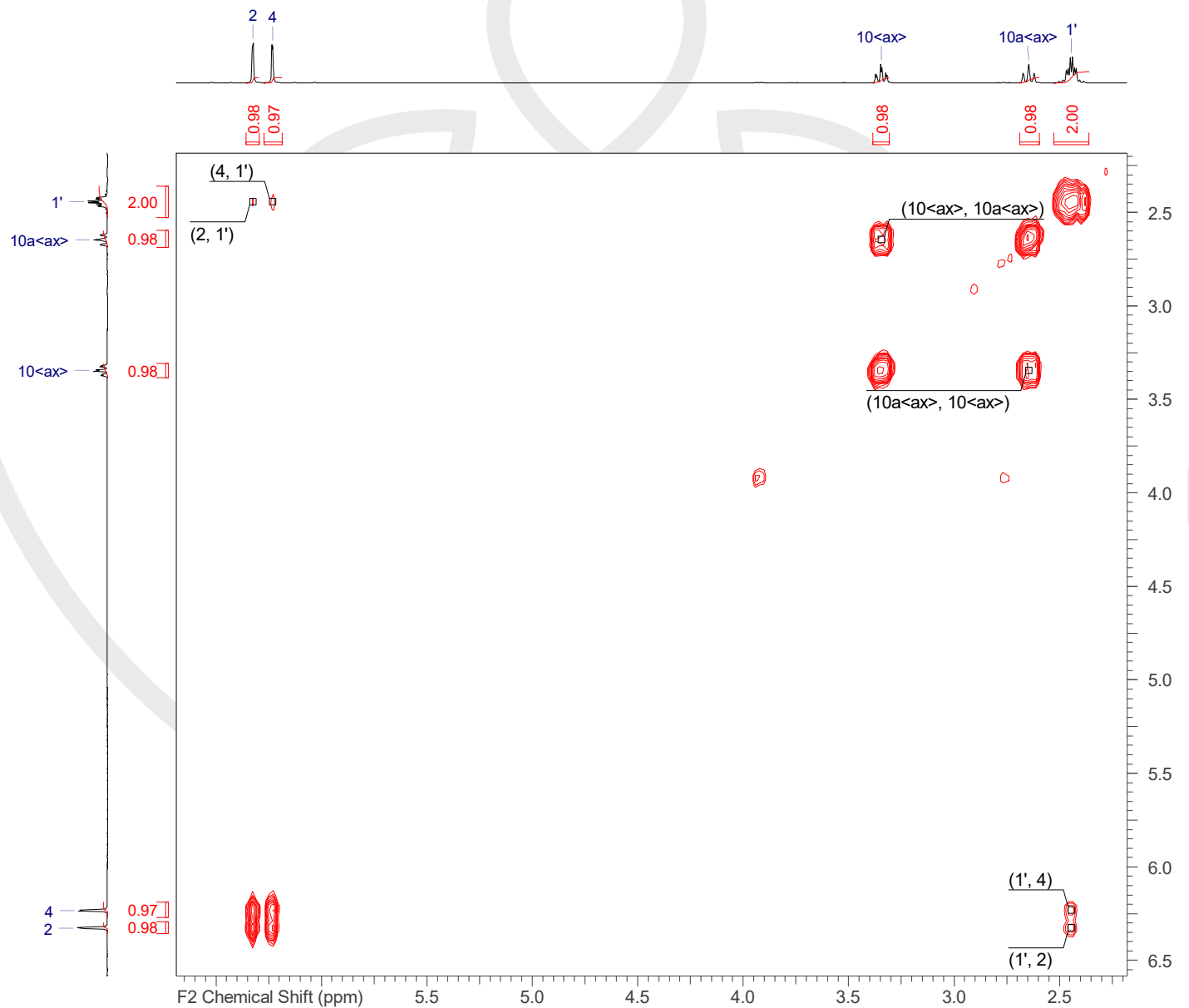
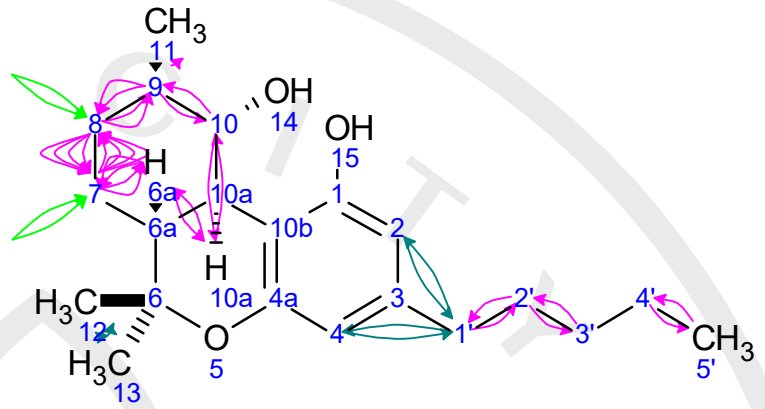


No	F2 Atom	F1 Atom	F2 (ppm)	F1 (ppm)
1	1'	1'	2.44	35.31
2	2	2	6.33	110.50
3	2'	2'	1.58	30.42
4	3'	3'	1.31	31.56
5	4	4	6.23	110.21
6	4'	4'	1.32	22.52
7	5'	5'	0.89	14.05
8	6a<ax>	6a	1.56	49.05
9	7<ax>	7	1.13	27.66
10	7<eq>	7	1.79	27.66
11	8<ax>	8	1.20	33.51
12	8<eq>	8	1.90	33.52
13	9<ax>	9	1.72	40.76
14	10<ax>	10	3.34	82.86
15	10a<ax>	10a	2.65	42.31
16	11	11	1.07	18.65
17	12	12	1.36	28.05
18	13	13	1.00	18.76

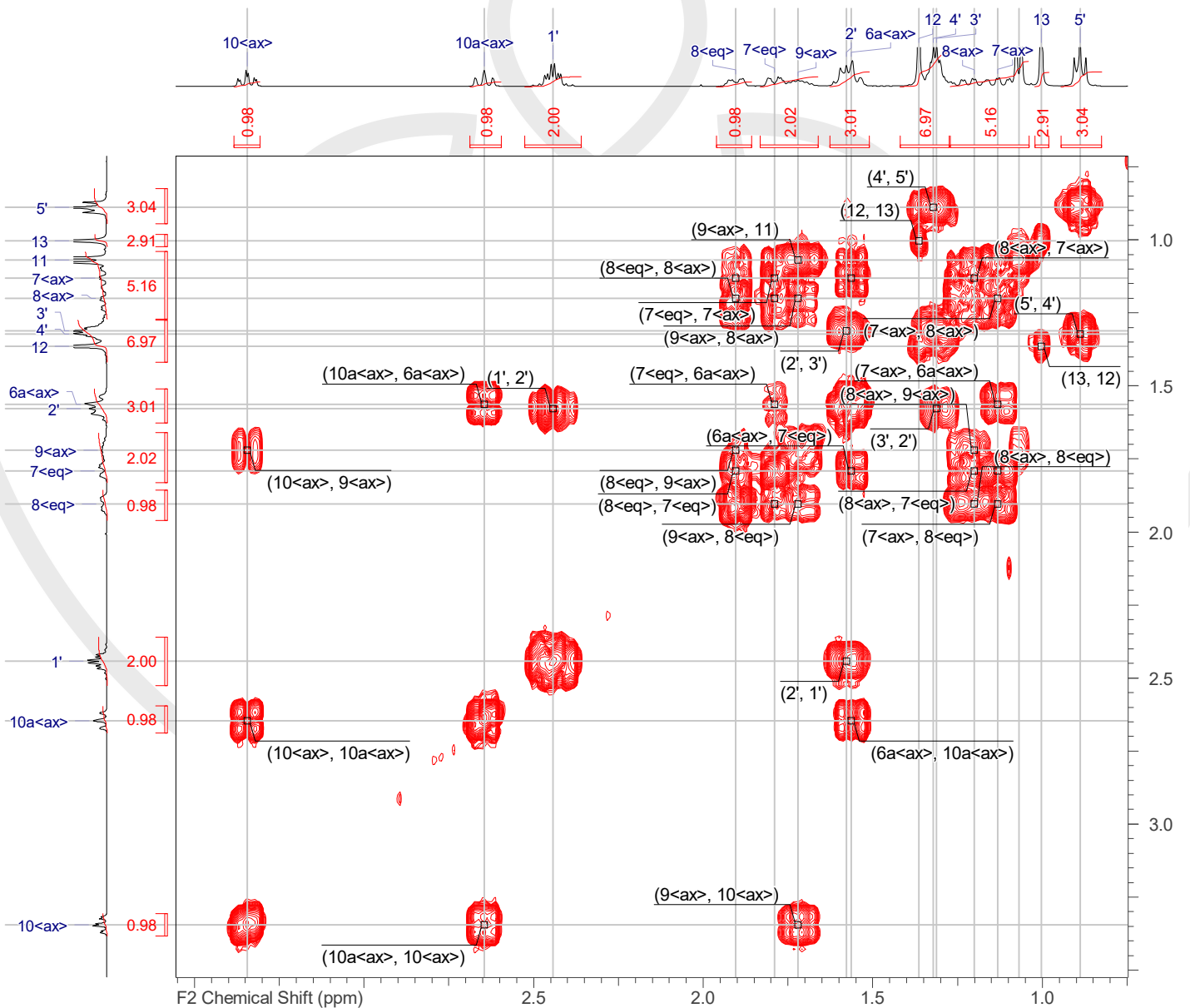
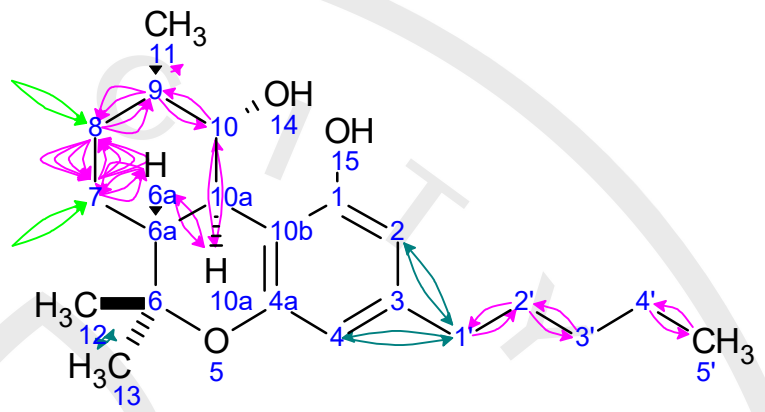
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Date Stamp	28 Mar 2023 15:47:36
File Name	\\sulfur\private\nmrdata\JEOL_2023\QC-I-57-001\QC-I-57-001_DQF_COSY_28-Mar-2023-1-1.jdf
Frequency (MHz)	(399.5822, 399.5822)
Nucleus	(1H, 1H)
Number of Transients	2
Origin	JEOL ECZ400S Sc v601
Original Points Count	(2560, 256)
Pulse Sequence	dqf cosy pfg.jxp
Spectrum Type	COSY
Sweep Width (Hz)	(3197.13, 3195.17)
Temperature (degree C)	22.200
Title	QC-I-57-001



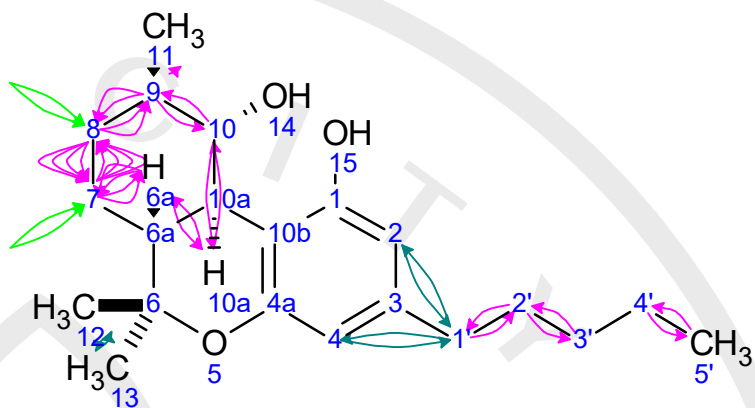
Acquisition Time (sec)	(0.6406, 0.0801)
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File Name	\\sulfur\private\nmrdata\JEOL_2023\QC-I-57-001\QC-I-57-001_DQF_COSY_28-Mar-2023-1-1.jdf
Frequency (MHz)	(399.5822, 399.5822)
Nucleus	(1H, 1H)
Number of Transients	2
Origin	JEOL ECZ400S Sc v601
Original Points Count	(2560, 256)
Pulse Sequence	dqf cosy pfg.jxp
Spectrum Type	COSY
Sweep Width (Hz)	(3197.13, 3195.17)
Temperature (degree C)	22.200
Title	QC-I-57-001



Acquisition Time (sec)	(0.6406, 0.0801)
Date Stamp	28 Mar 2023 15:47:36
File Name	\\sulfur\private\nmrdata\JEOL_2023\QC-I-57-001\QC-I-57-001_DQF_COSY_28-Mar-2023-1-1.jdf
Frequency (MHz)	(399.5822, 399.5822)
Nucleus	(1H, 1H)
Number of Transients	2
Origin	JEOL ECZ400S Sc v601
Original Points Count	(2560, 256)
Pulse Sequence	dqf cosy pfg.jxp
Spectrum Type	COSY
Sweep Width (Hz)	(3197.13, 3195.17)
Temperature (degree C)	22.200
Title	QC-I-57-001



Acquisition Time (sec)	(0.6406, 0.0801)
Date Stamp	28 Mar 2023 15:47:36
File Name	\\sulfur\private\nmrdata\JEOL_2023\QC-I-57-001\QC-I-57-001_DQF_COSY_28-Mar-2023-1-1.jdf
Frequency (MHz)	(399.5822, 399.5822)
Nucleus	(1H, 1H)
Number of Transients	2
Origin	JEOL ECZ400S Sc v601
Original Points Count	(2560, 256)
Pulse Sequence	dqf cosy pfg.jxp
Spectrum Type	COSY
Sweep Width (Hz)	(3197.13, 3195.17)
Temperature (degree C)	22.200
Title	QC-I-57-001



No	F2 Atom	F1 Atom	F2 (ppm)	F1 (ppm)
1	2	1'	6.33	2.44
2	2'	1'	1.58	2.44
3	4	1'	6.23	2.44
4	1'	2	2.44	6.33
5	1'	2'	2.44	1.58
6	3'	2'	1.31	1.58
7	2'	3'	1.58	1.31
8	1'	4	2.44	6.23
9	5'	4'	0.89	1.32
10	4'	5'	1.32	0.89
11	7<ax>	6a<ax>	1.13	1.56
12	7<eq>	6a<ax>	1.79	1.56
13	10a<ax>	6a<ax>	2.65	1.56
14	6a<ax>	7<ax>	1.56	1.13
15	7<eq>	7<ax>	1.79	1.13
16	8<ax>	7<ax>	1.20	1.13
17	8<eq>	7<ax>	1.90	1.13
18	6a<ax>	7<eq>	1.56	1.79
19	7<ax>	7<eq>	1.13	1.79
20	8<ax>	7<eq>	1.20	1.79
21	8<eq>	7<eq>	1.90	1.79
22	7<ax>	8<ax>	1.13	1.20
23	7<eq>	8<ax>	1.79	1.20
24	8<eq>	8<ax>	1.90	1.20
25	9<ax>	8<ax>	1.72	1.20
26	7<ax>	8<eq>	1.13	1.90
27	7<eq>	8<eq>	1.79	1.90
28	8<ax>	8<eq>	1.20	1.90
29	9<ax>	8<eq>	1.72	1.90
30	8<ax>	9<ax>	1.20	1.72
31	8<eq>	9<ax>	1.90	1.72
32	10<ax>	9<ax>	3.34	1.72
33	9<ax>	10<ax>	1.72	3.34

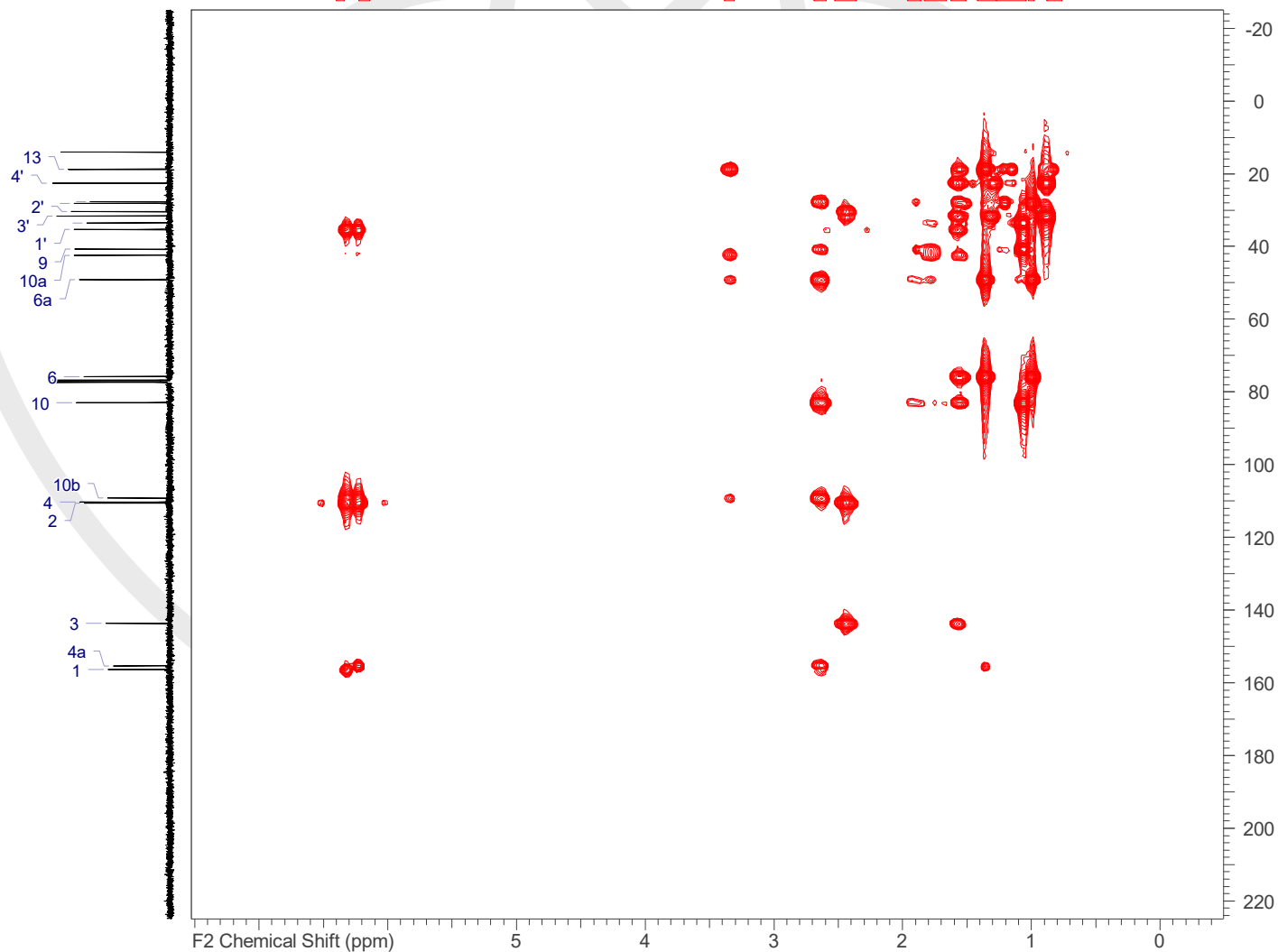
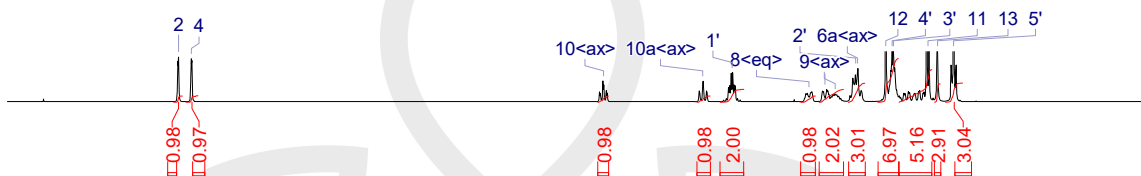
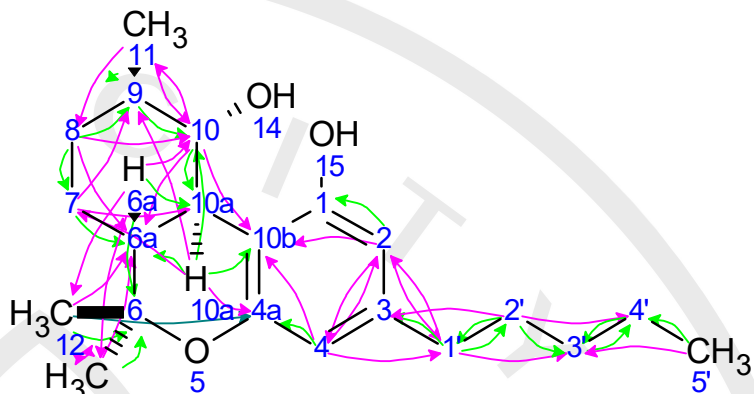
No	F2 Atom	F1 Atom	F2 (ppm)	F1 (ppm)
34	10a<ax>	10<ax>	2.65	3.34
35	6a<ax>	10a<ax>	1.56	2.65
36	10<ax>	10a<ax>	3.34	2.65
37	9<ax>	11	1.72	1.07
38	13	12	1.00	1.36
39	12	13	1.36	1.00

QC-I-57-001

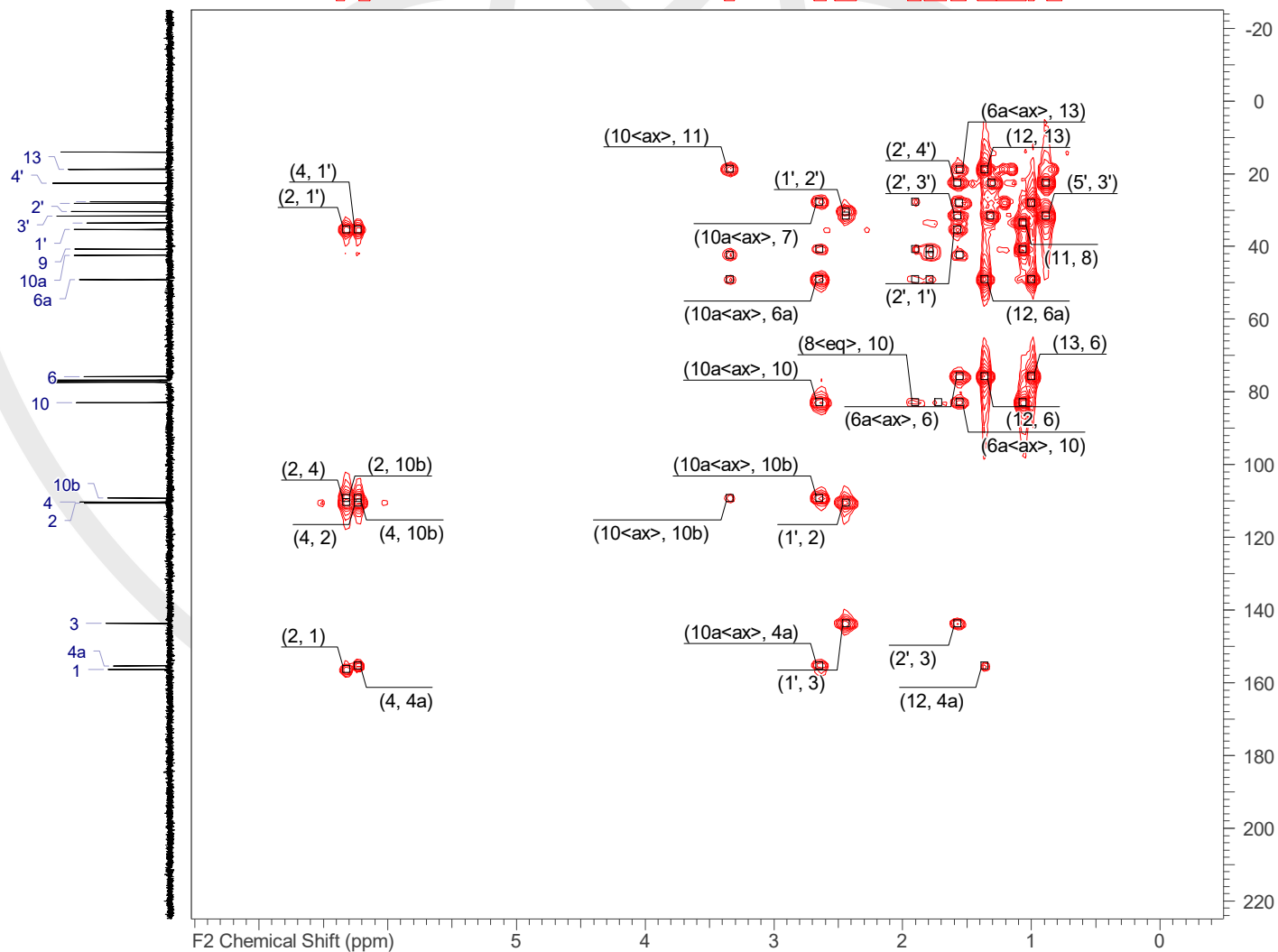
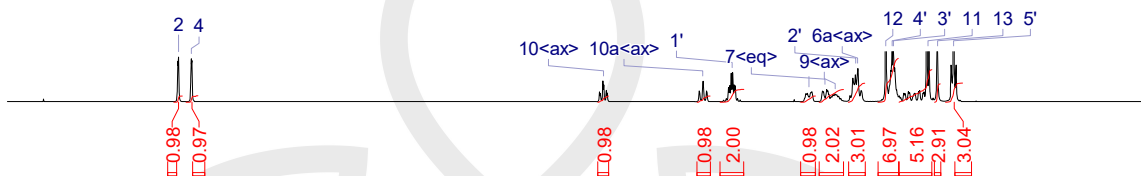
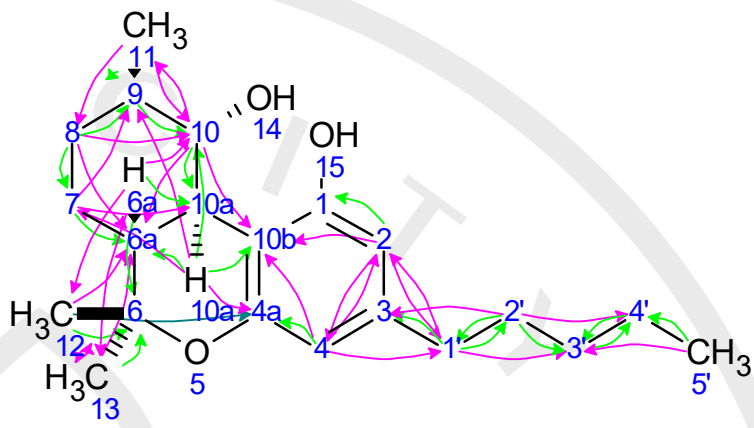
Proposed Structure

10(S)-hydroxy-9(R)-Hexahydrocannabinol

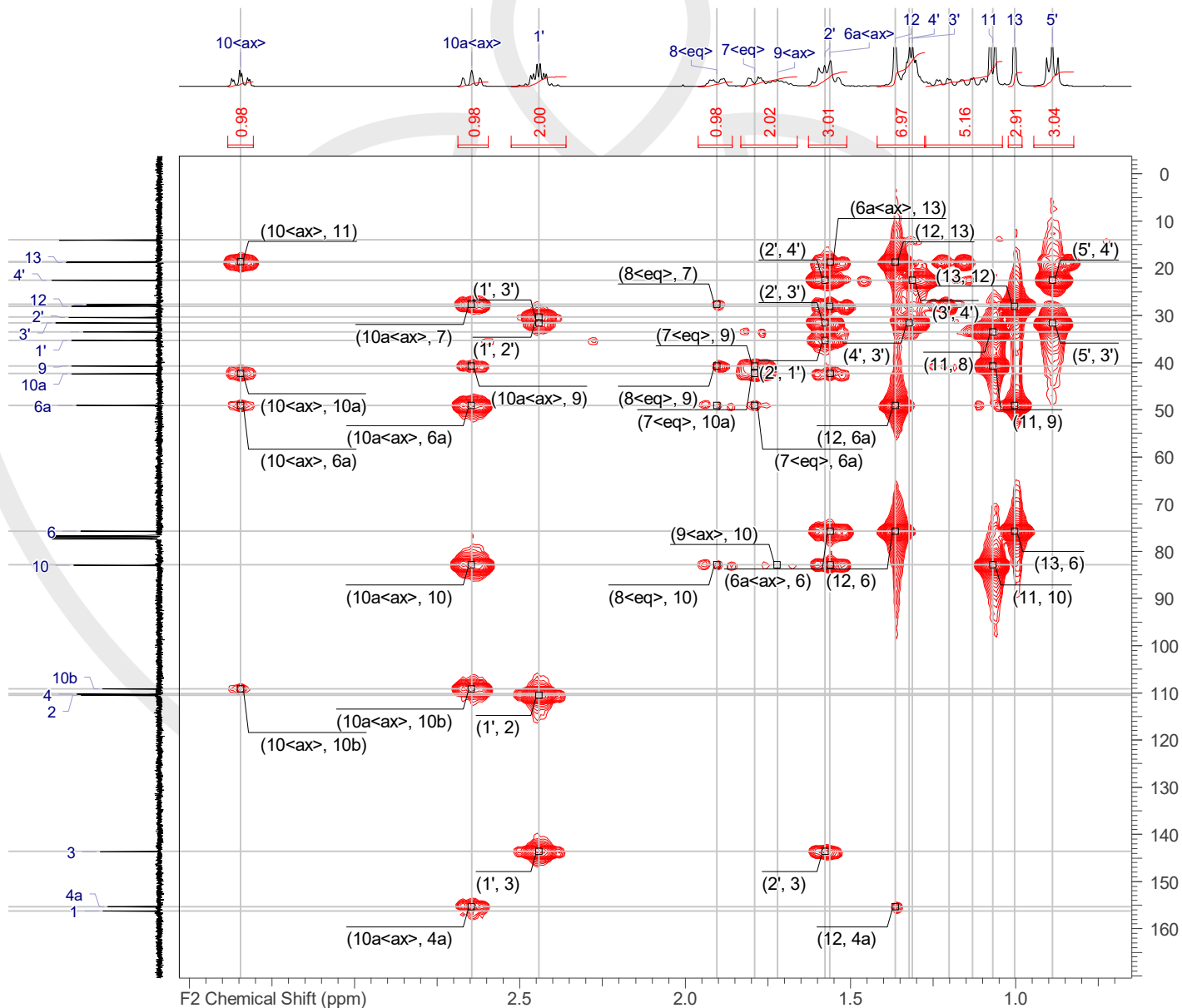
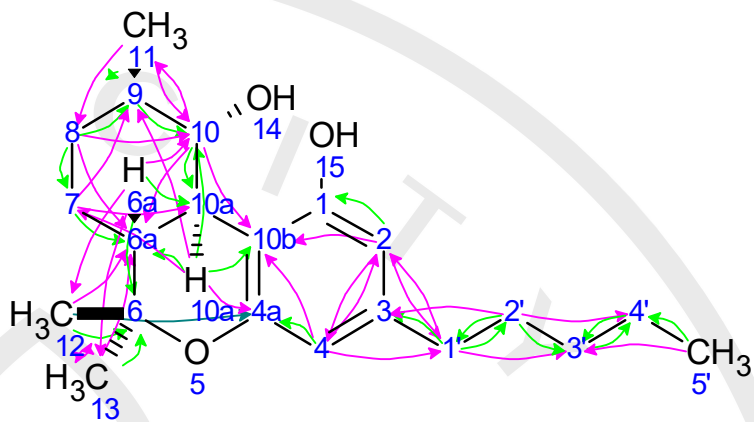
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Date Stamp	28 Mar 2023 15:13:30
File Name	\\sulfur\private\nmrdata\JEOL_2023\QC-I-57-001\QC-I-57-001_HMBC_28-Mar-2023-1-1.jdf
Frequency (MHz)	(399.5822, 100.4750)
Nucleus	(1H, 13C)
Number of Transients	4
Origin	JEOL ECZ400S Sc v601
Original Points Count	(1599, 256)
Pulse Sequence	hmbc_pfg.jxp
Spectrum Type	HMBC
Sweep Width (Hz)	(3202.20, 25101.09)
Temperature (degree C)	22.200
Title	QC-I-57-001



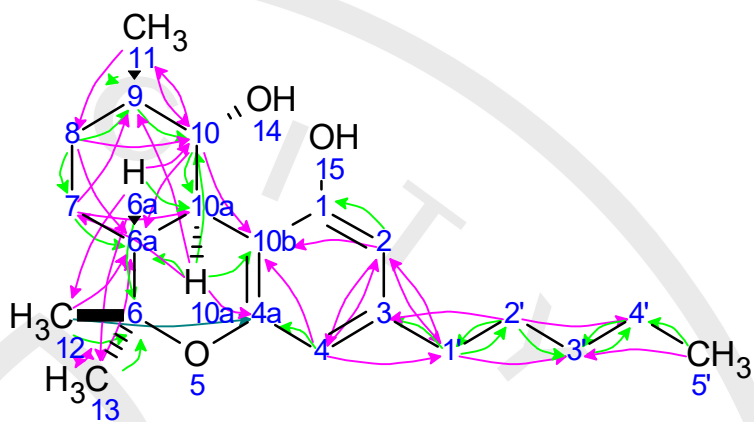
Acquisition Time (sec)	(0.3996, 0.0102)
Date Stamp	28 Mar 2023 15:13:30
File Name	\\sulfur\private\nmrdata\JEOL_2023\QC-I-57-001\QC-I-57-001_HMBC_28-Mar-2023-1-1.jdf
Frequency (MHz)	(399.5822, 100.4750)
Nucleus	(1H, 13C)
Number of Transients	4
Origin	JEOL ECZ400S Sc v601
Original Points Count	(1599, 256)
Pulse Sequence	hmbc_pfg.jxp
Spectrum Type	HMBC
Sweep Width (Hz)	(3202.20, 25101.09)
Temperature (degree C)	22.200
Title	QC-I-57-001



Acquisition Time (sec)	(0.3996, 0.0102)
Date Stamp	28 Mar 2023 15:13:30
File Name	\\sulfur\private\nmrdata\JEOL_2023\QC-I-57-001\QC-I-57-001_HMBC_28-Mar-2023-1-1.jdf
Frequency (MHz)	(399.5822, 100.4750)
Nucleus	(1H, 13C)
Number of Transients	4
Origin	JEOL ECZ400S Sc v601
Original Points Count	(1599, 256)
Pulse Sequence	hmbc_pfg.jxp
Spectrum Type	HMBC
Sweep Width (Hz)	(3202.20, 25101.09)
Temperature (degree C)	22.200
Title	QC-I-57-001



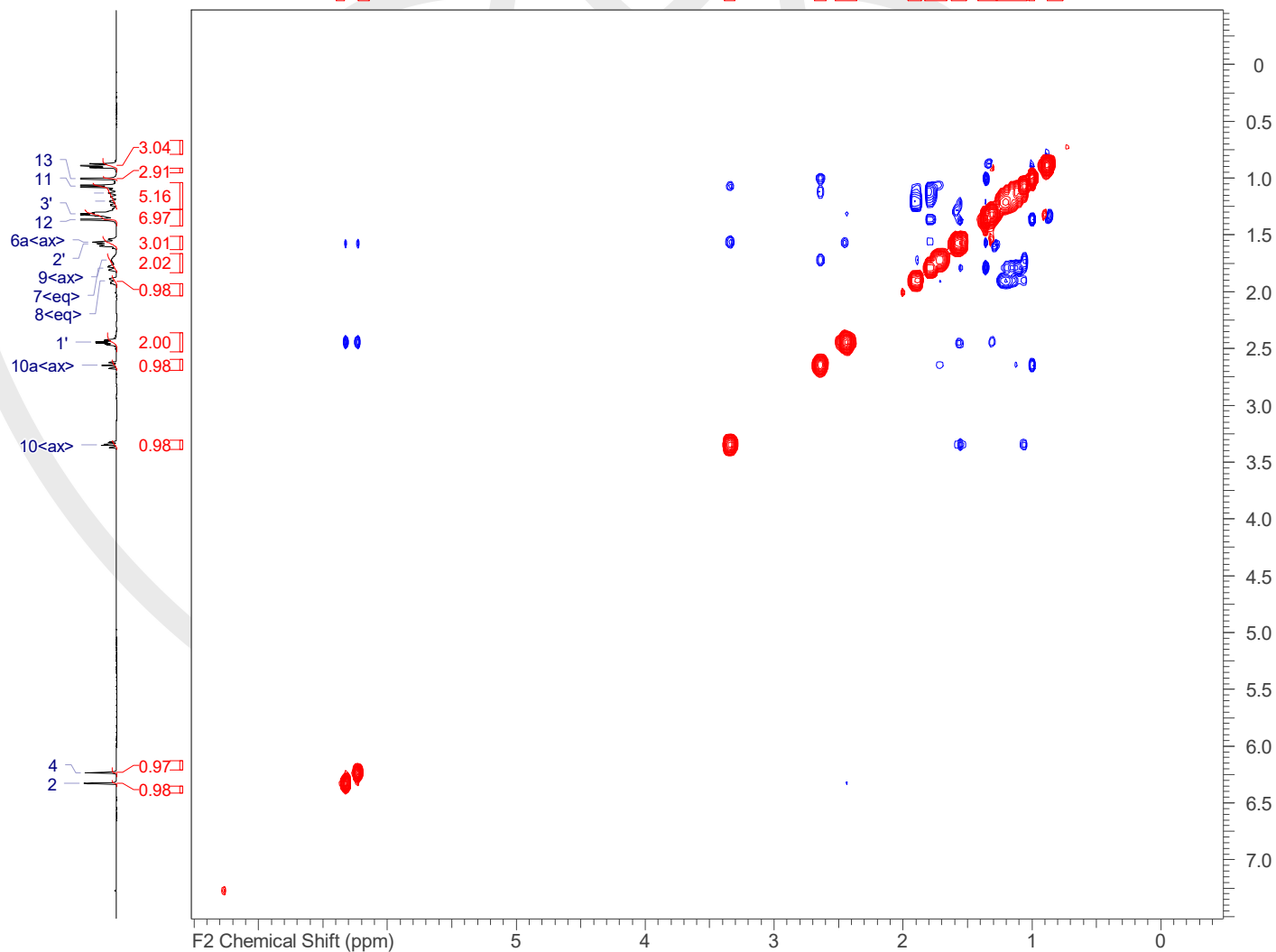
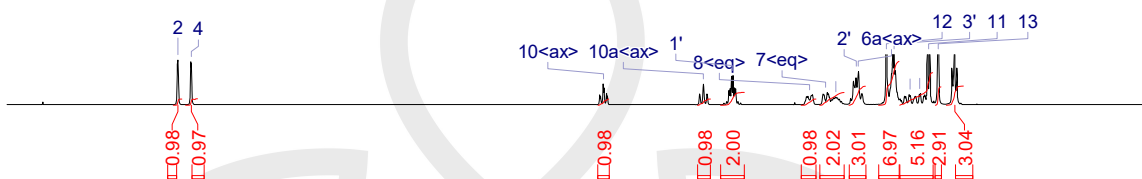
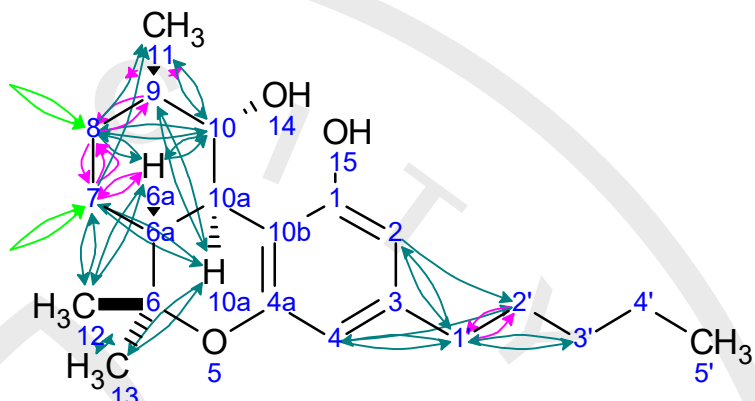
Acquisition Time (sec)	(0.3996, 0.0102)
Date Stamp	28 Mar 2023 15:13:30
File Name	\\sulfur\private\nmrdata\JEOL_2023\QC-I-57-001\QC-I-57-001_HMBC_28-Mar-2023-1-1.jdf
Frequency (MHz)	(399.5822, 100.4750)
Nucleus	(1H, 13C)
Number of Transients	4
Origin	JEOL ECZ400S Sc v601
Original Points Count	(1599, 256)
Pulse Sequence	hmbc_pfg.jxp
Spectrum Type	HMBC
Sweep Width (Hz)	(3202.20, 25101.09)
Temperature (degree C)	22.200
Title	QC-I-57-001



No	F2 Atom	F1 Atom	F2 (ppm)	F1 (ppm)
1	2	1	6.33	156.22
2	2	1'	6.33	35.26
3	2'	1'	1.58	35.26
4	4	1'	6.23	35.26
5	1'	2	2.44	110.50
6	4	2	6.23	110.50
7	1'	2'	2.44	30.39
8	1'	3	2.44	143.60
9	2'	3	1.58	143.60
10	1'	3'	2.44	31.56
11	2'	3'	1.58	31.56
12	4'	3'	1.32	31.56
13	5'	3'	0.89	31.56
14	2	4	6.33	110.21
15	2'	4'	1.58	22.53
16	3'	4'	1.31	22.53
17	5'	4'	0.89	22.53
18	4	4a	6.23	155.28
19	10a<ax>	4a	2.65	155.28
20	12	4a	1.36	155.28
21	6a<ax>	6	1.56	75.70
22	12	6	1.36	75.70
23	13	6	1.00	75.70
24	7<eq>	6a	1.79	49.05
25	8<eq>	6a	1.90	49.05
26	10<ax>	6a	3.34	49.05
27	10a<ax>	6a	2.65	49.05
28	12	6a	1.36	49.05
29	13	6a	1.00	49.05
30	8<eq>	7	1.90	27.66
31	10a<ax>	7	2.65	27.66
32	11	8	1.07	33.48
33	7<eq>	9	1.79	40.71

No	F2 Atom	F1 Atom	F2 (ppm)	F1 (ppm)
34	8<eq>	9	1.90	40.71
35	10a<ax>	9	2.65	40.71
36	11	9	1.07	40.71
37	6a<ax>	10	1.56	82.86
38	8<eq>	10	1.90	82.86
39	9<ax>	10	1.72	82.86
40	10a<ax>	10	2.65	82.86
41	11	10	1.07	82.86
42	6a<ax>	10a	1.56	42.31
43	7<eq>	10a	1.79	42.31
44	10<ax>	10a	3.34	42.31
45	2	10b	6.33	109.15
46	4	10b	6.23	109.15
47	10<ax>	10b	3.34	109.15
48	10a<ax>	10b	2.65	109.15
49	10<ax>	11	3.34	18.65
50	6a<ax>	12	1.56	28.04
51	13	12	1.00	28.04
52	6a<ax>	13	1.56	18.76
53	12	13	1.36	18.76

Acquisition Time (sec)	(0.6406, 0.0801)
Date Stamp	28 Mar 2023 16:06:46
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Frequency (MHz)	(399.5822, 399.5822)
Nucleus	(1H, 1H)
Number of Transients	4
Origin	JEOL ECZ400S Sc v601
Original Points Count	(2560, 256)
Pulse Sequence	noesy phase pfgz
Spectrum Type	NOESY
Sweep Width (Hz)	(3197.13, 3195.17)
Temperature (degree C)	22.200
Title	QC-I-57-001

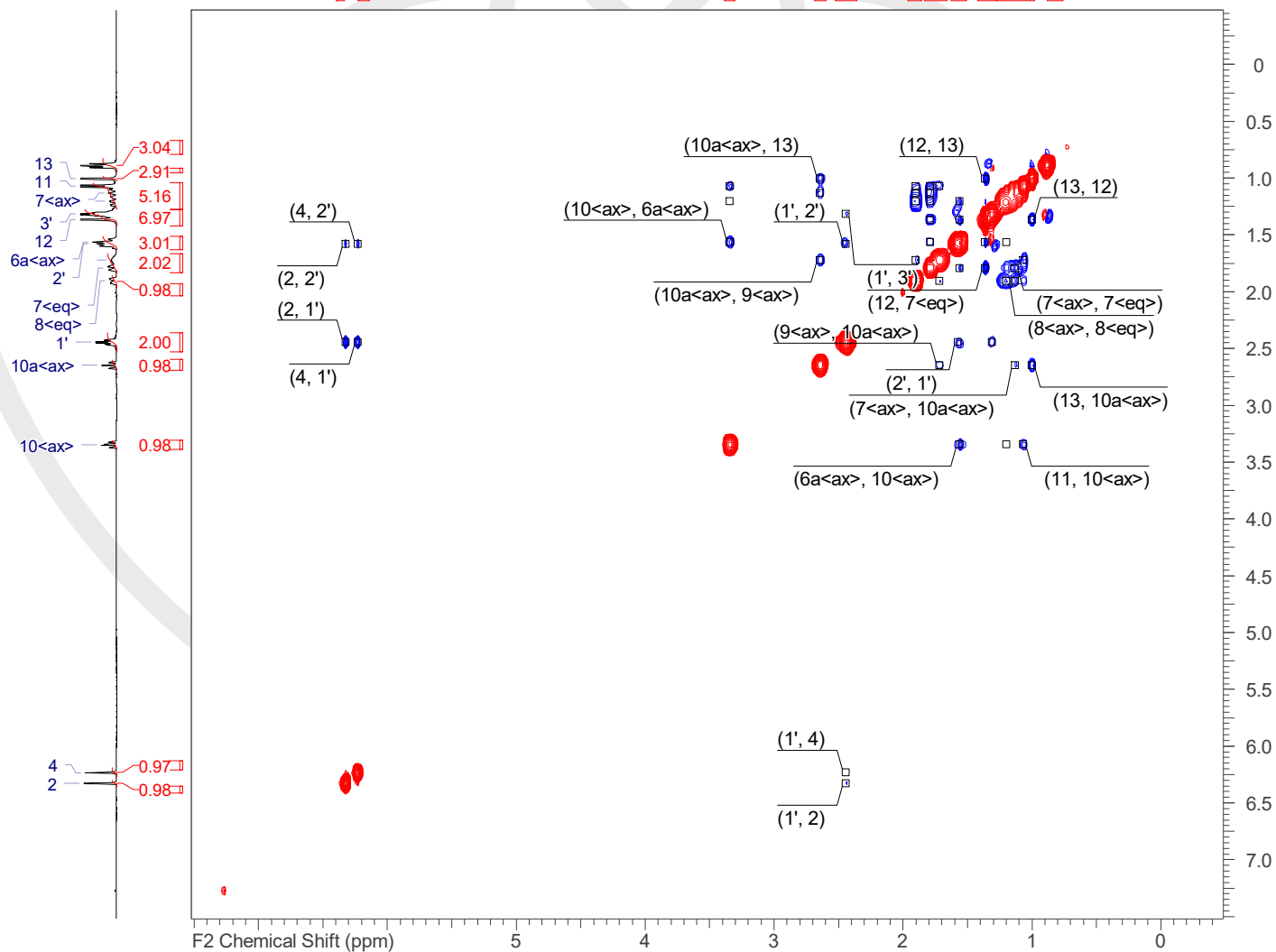
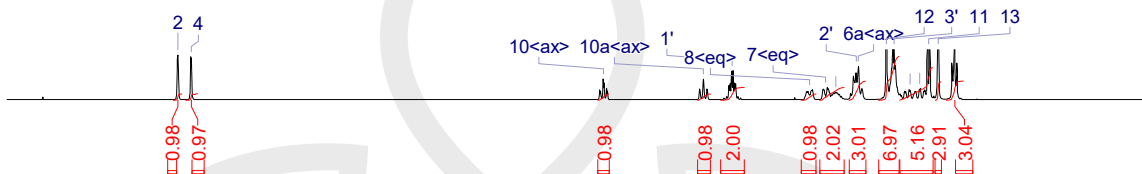
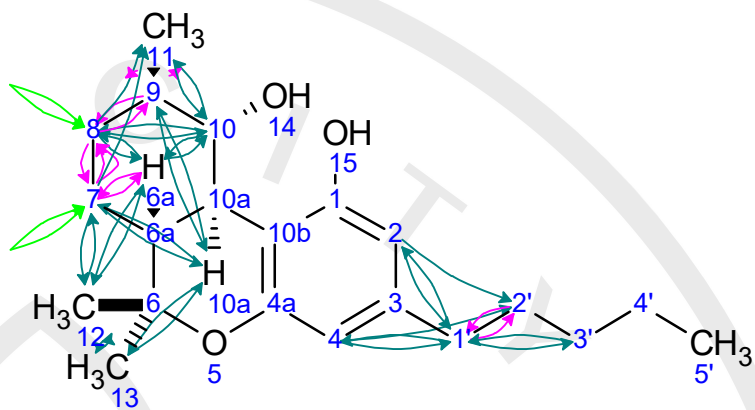


QC-I-57-001

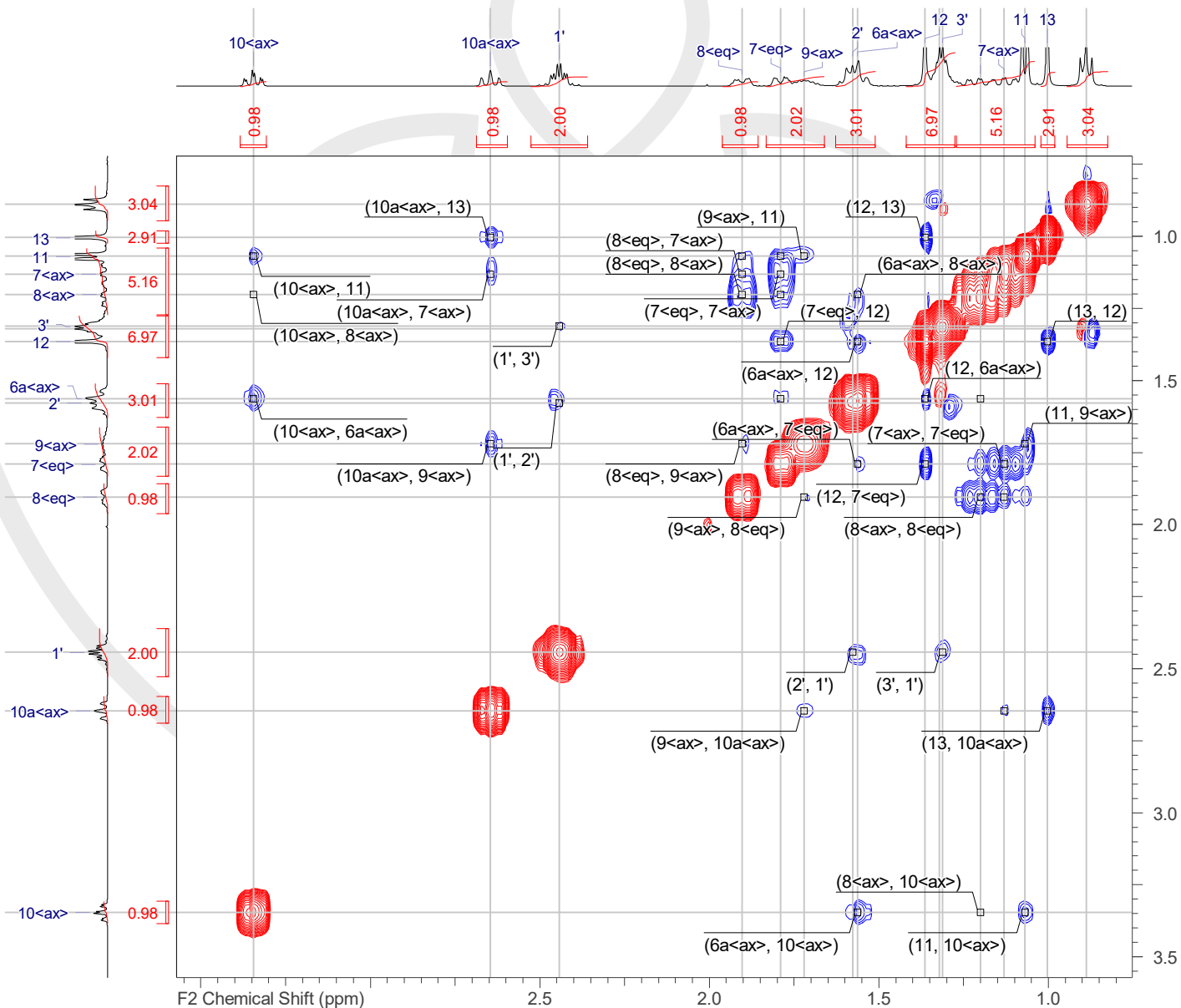
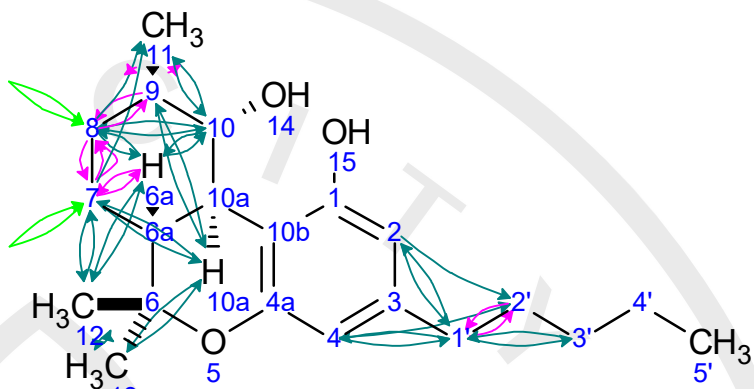
Proposed Structure

10(S)-hydroxy-9(R)-Hexahydrocannabinol

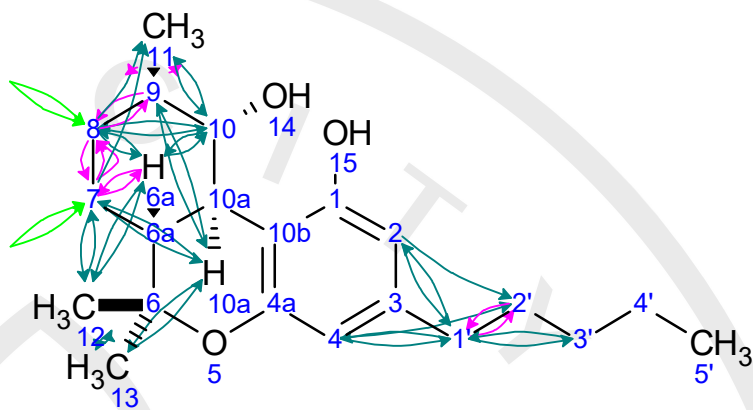
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Date Stamp	28 Mar 2023 16:06:46
File Name	\\sulfur\private\nmrdata\JEOL_2023\QC-I-57-001\QC-I-57-001_NOESY_28-Mar-2023-1-1.jdf
Frequency (MHz)	(399.5822, 399.5822)
Nucleus	(1H, 1H)
Number of Transients	4
Origin	JEOL ECZ400S Sc v601
Original Points Count	(2560, 256)
Pulse Sequence	noesy phase pfgz
Spectrum Type	NOESY
Sweep Width (Hz)	(3197.13, 3195.17)
Temperature (degree C)	22.200
Title	QC-I-57-001



Acquisition Time (sec)	(0.6406, 0.0801)
Date Stamp	28 Mar 2023 16:06:46
File Name	\\sulfur\private\nmrdata\JEOL_2023\QC-I-57-001\QC-I-57-001_NOESY_28-Mar-2023-1-1.jdf
Frequency (MHz)	(399.5822, 399.5822)
Nucleus	(1H, 1H)
Number of Transients	4
Origin	JEOL ECZ400S Sc v601
Original Points Count	(2560, 256)
Pulse Sequence	noesy phase pfgz
Spectrum Type	NOESY
Sweep Width (Hz)	(3197.13, 3195.17)
Temperature (degree C)	22.200
Title	QC-I-57-001



Acquisition Time (sec)	(0.6406, 0.0801)
Date Stamp	28 Mar 2023 16:06:46
File Name	\\sulfur\private\nmrdata\JEOL_2023\QC-I-57-001\QC-I-57-001_NOESY_28-Mar-2023-1-1.jdf
Frequency (MHz)	(399.5822, 399.5822)
Nucleus	(1H, 1H)
Number of Transients	4
Origin	JEOL ECZ400S Sc v601
Original Points Count	(2560, 256)
Pulse Sequence	noesy phase pfgz
Spectrum Type	NOESY
Sweep Width (Hz)	(3197.13, 3195.17)
Temperature (degree C)	22.200
Title	QC-I-57-001

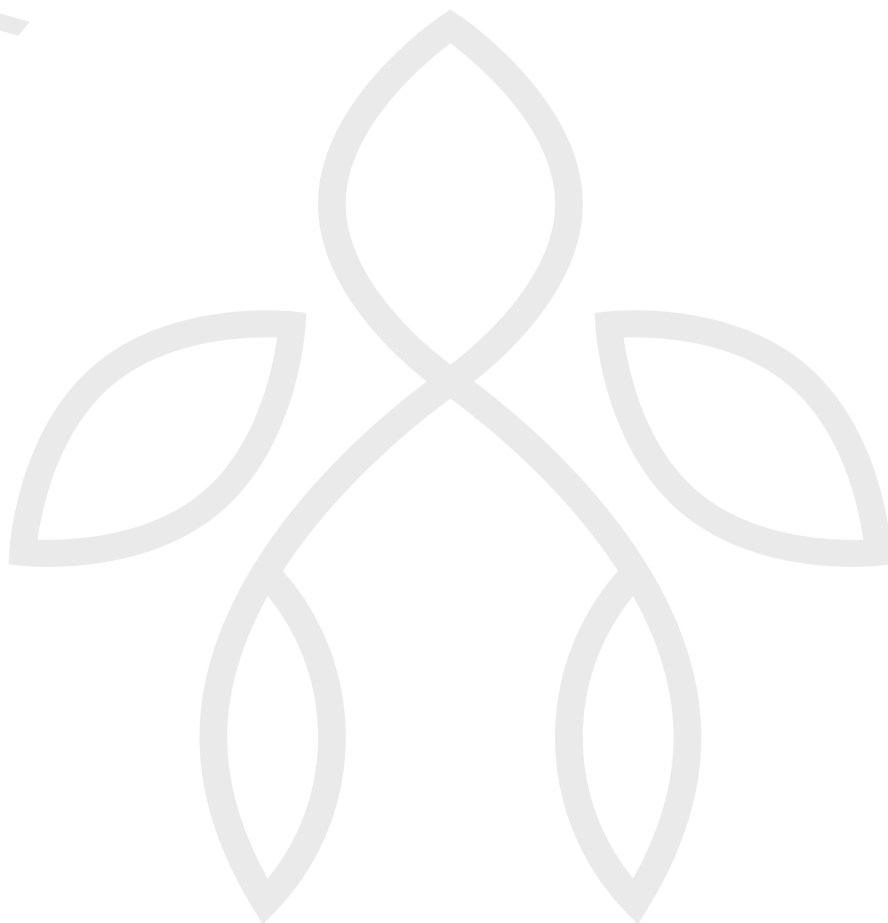


No	F2 Atom	F1 Atom	F2 (ppm)	F1 (ppm)
1	2	1'	6.33	2.44
2	2'	1'	1.58	2.44
3	3'	1'	1.31	2.44
4	4	1'	6.23	2.44
5	1'	2	2.44	6.33
6	1'	2'	2.44	1.58
7	2	2'	6.33	1.58
8	4	2'	6.23	1.58
9	1'	3'	2.44	1.31
10	1'	4	2.44	6.23
11	7<eq>	6a<ax>	1.79	1.56
12	8<ax>	6a<ax>	1.20	1.56
13	10<ax>	6a<ax>	3.34	1.56
14	12	6a<ax>	1.36	1.56
15	7<eq>	7<ax>	1.79	1.13
16	8<eq>	7<ax>	1.90	1.13
17	10a<ax>	7<ax>	2.65	1.13
18	6a<ax>	7<eq>	1.56	1.79
19	7<ax>	7<eq>	1.13	1.79
20	12	7<eq>	1.36	1.79
21	6a<ax>	8<ax>	1.56	1.20
22	7<eq>	8<ax>	1.79	1.20
23	8<eq>	8<ax>	1.90	1.20
24	10<ax>	8<ax>	3.34	1.20
25	7<ax>	8<eq>	1.13	1.90
26	8<ax>	8<eq>	1.20	1.90
27	9<ax>	8<eq>	1.72	1.90
28	8<eq>	9<ax>	1.90	1.72
29	10a<ax>	9<ax>	2.65	1.72
30	11	9<ax>	1.07	1.72
31	6a<ax>	10<ax>	1.56	3.34
32	8<ax>	10<ax>	1.20	3.34
33	11	10<ax>	1.07	3.34

No	F2 Atom	F1 Atom	F2 (ppm)	F1 (ppm)
34	7<ax>	10a<ax>	1.13	2.65
35	9<ax>	10a<ax>	1.72	2.65
36	13	10a<ax>	1.00	2.65
37	7<eq>	11	1.79	1.07
38	8<eq>	11	1.90	1.07
39	9<ax>	11	1.72	1.07
40	10<ax>	11	3.34	1.07
41	6a<ax>	12	1.56	1.36
42	7<eq>	12	1.79	1.36
43	13	12	1.00	1.36
44	10a<ax>	13	2.65	1.00
45	12	13	1.36	1.00

APPENDIX A – ANALYTICAL REPORTS FOR QC-I-57-002

A P R I C I T Y



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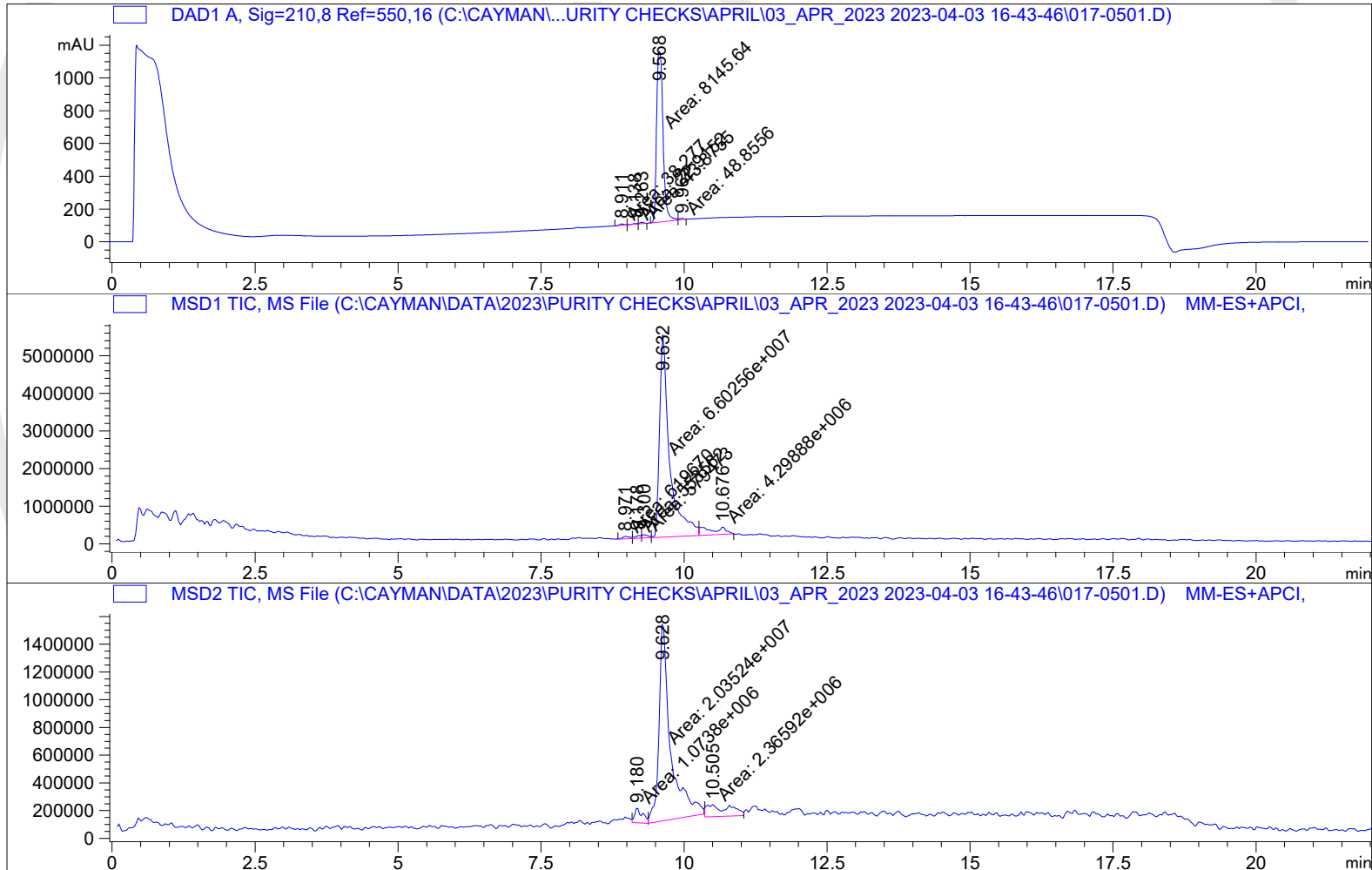
Acq. Operator : Seq. Line : 5
Acq. Instrument : LCMS01 Location : Vial 17
Injection Date : 4/3/2023 6:21:44 PM Inj : 1
Inj Volume : 1.0 µl

Method : C:\CAYMAN\DATA\2023\PURITY CHECKS\APRIL\03_APR_2023 2023-04-03 16-43-46\C8_ACOH.M (Sequence Method)
Last changed : 4/3/2023 4:43:01 PM
Method Info : A: 90:10:0.1 H2O:MeOH:AcOH
B: 10:90:0.1 H2O:MeOH:AcOH

0-8 min: 0%B to 100%B
8-16 min: Hold 100% B
16-16.1 min: 100% to 0% B
16.1-22 mins re-equilibrate to 0% B

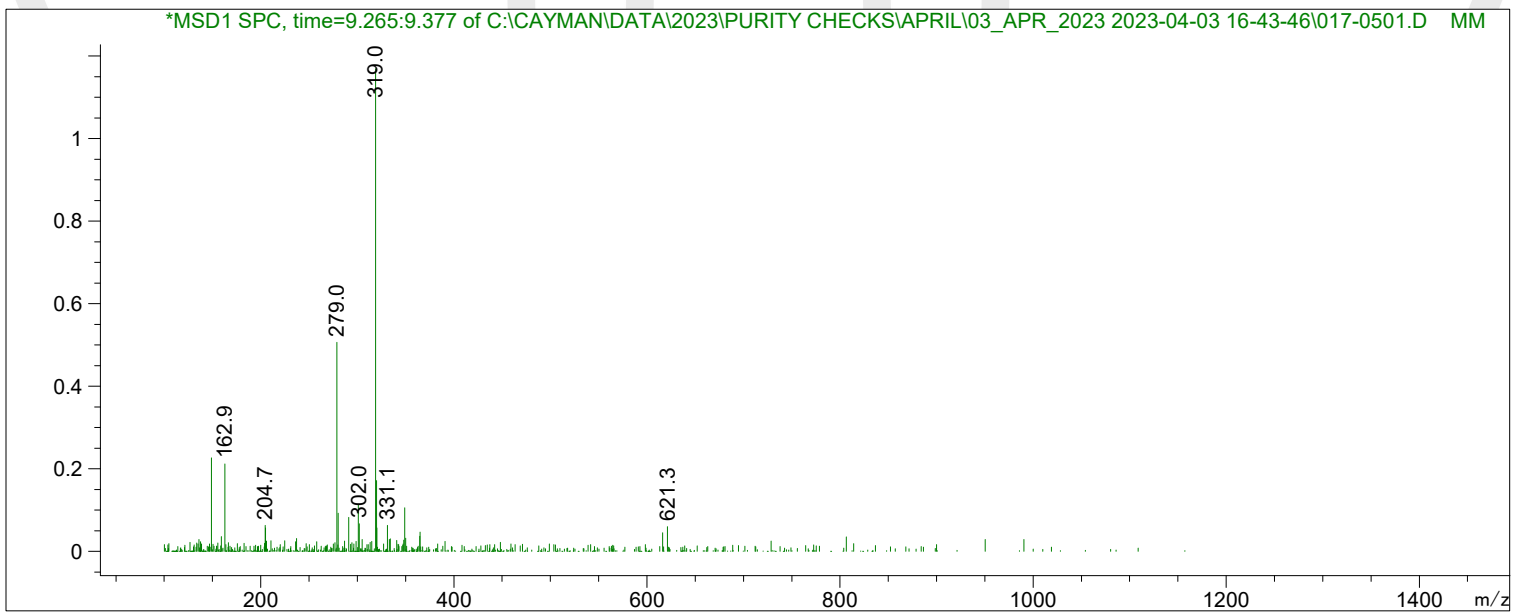
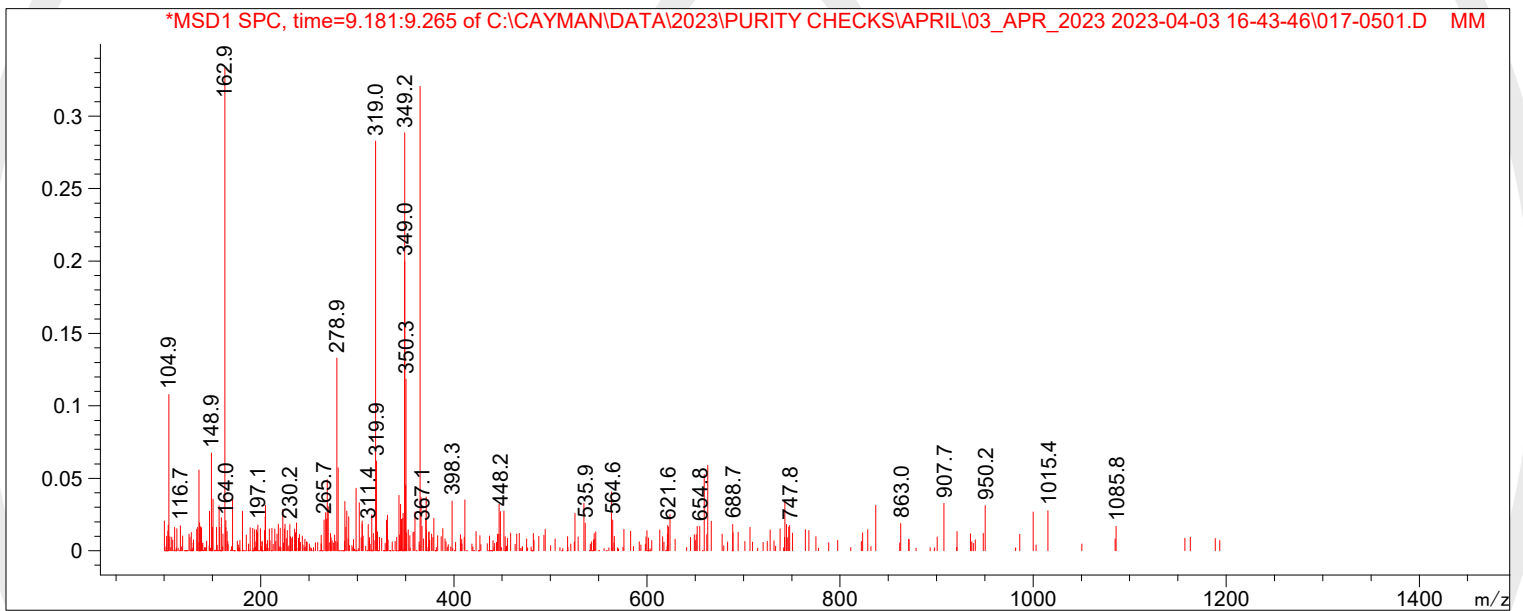
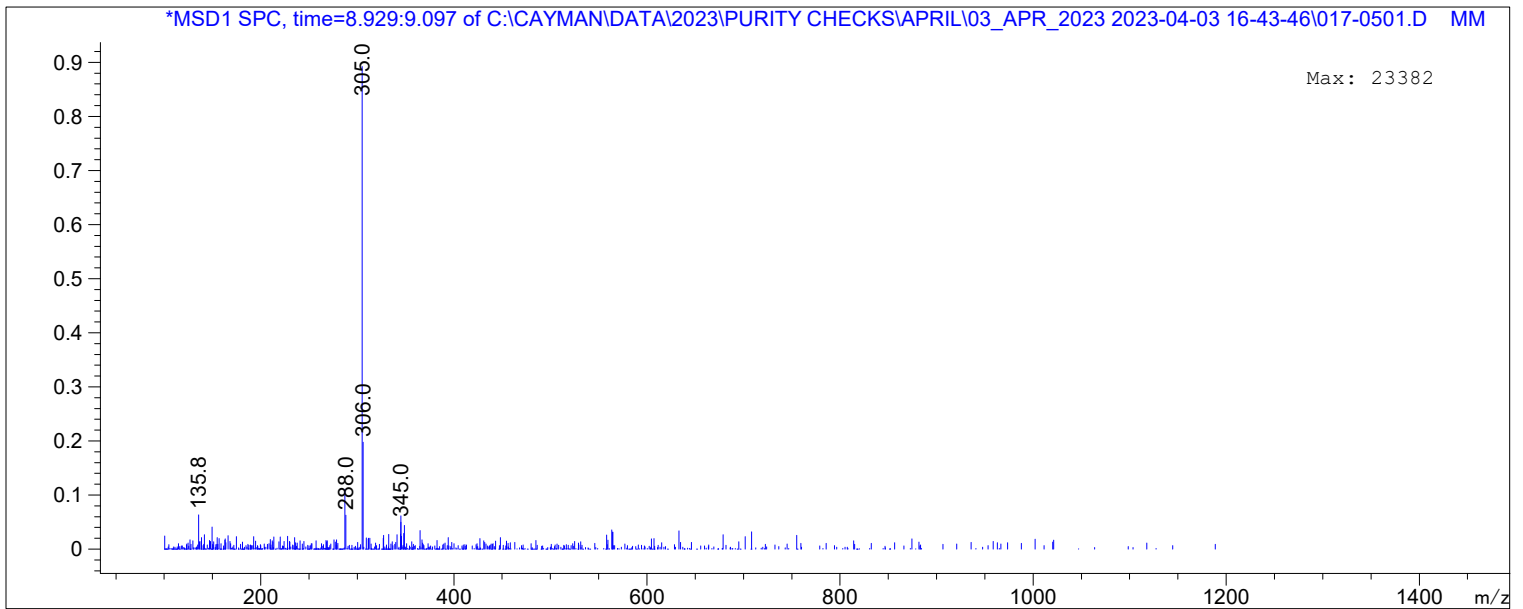
Agilent Zorbax 5µ C8 50x2.1 mm
0.5 ml/min 210 nm

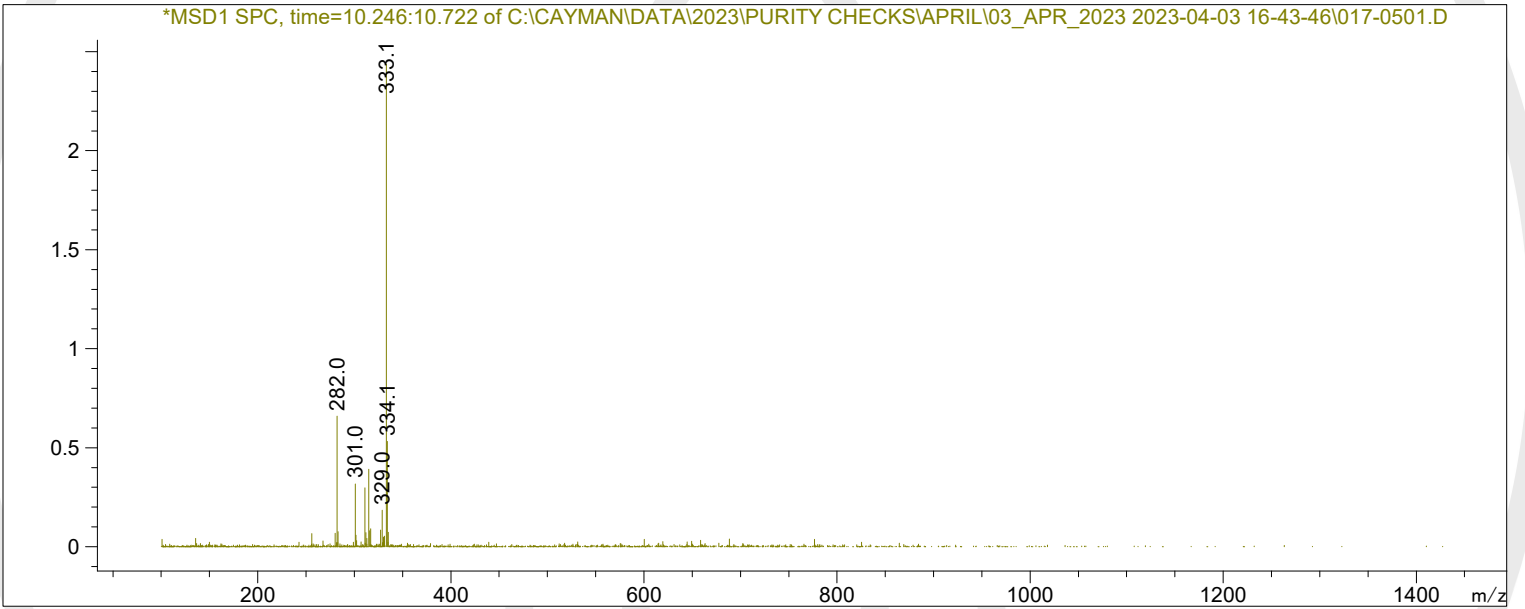
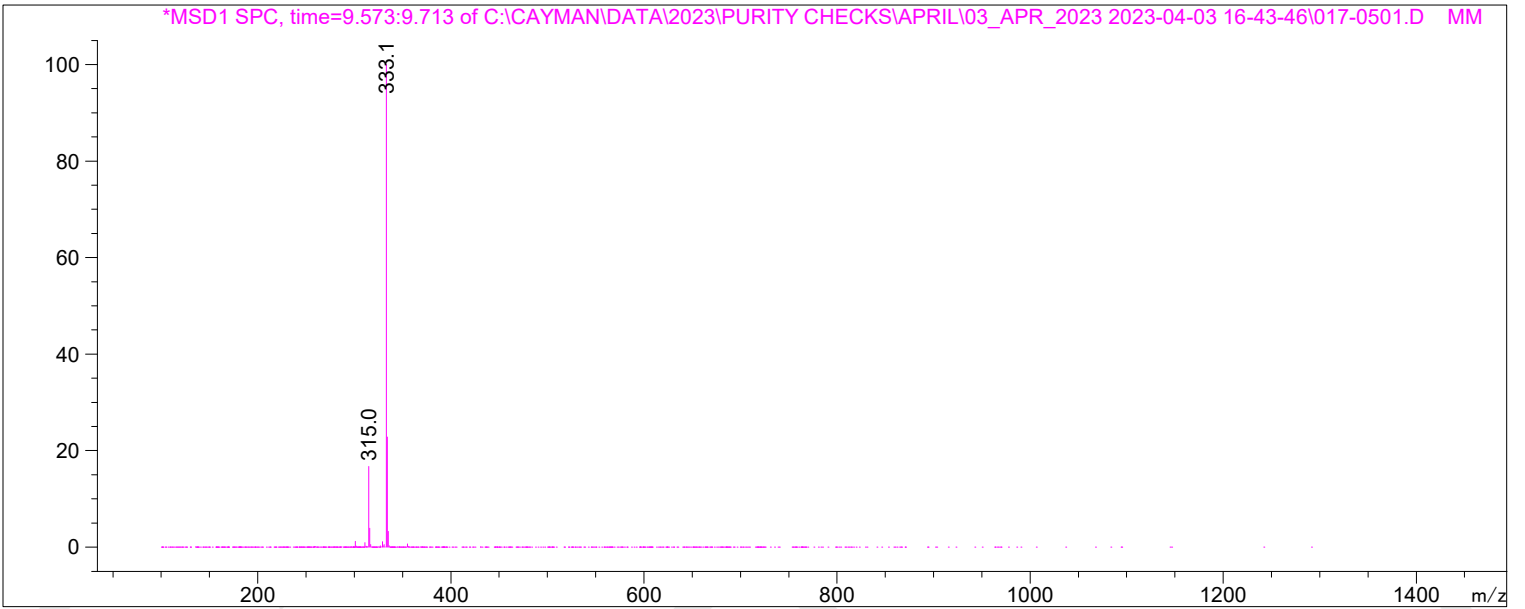
Additional Info : Peak(s) manually integrated



MS Signal: MSD1 TIC, MS File, MM-ES+APCI, Pos, Fast Scan, Frag: 70, "+DUAL"
Spectra averaged over upper half of peaks.
Noise Cutoff: 1000 counts.
Reportable Ion Abundance: > 10%.

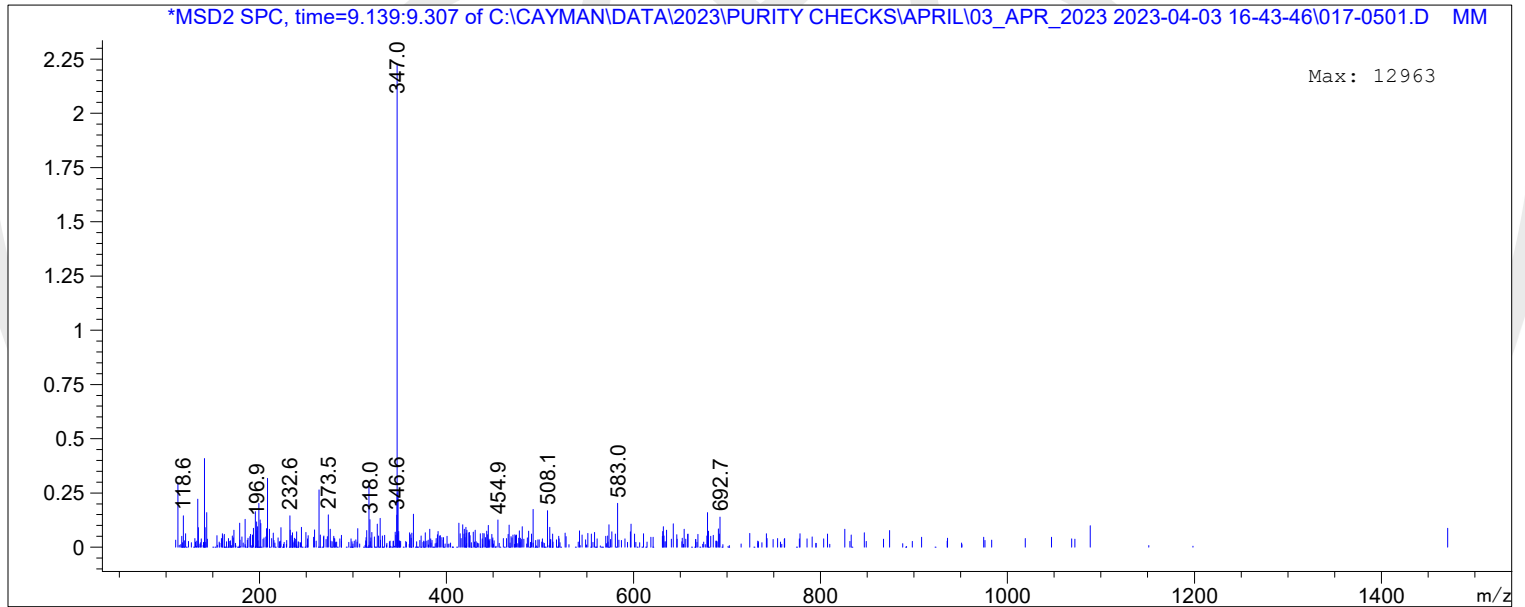
Retention Time (MS)	MS Area	Mol. Weight or Ion
8.971	619670	306.05 I
		305.05 I
		287.05 I
9.178	553562	663.10 I
		659.40 I
		563.15 I
		365.00 I
		350.30 I
		349.95 I
		349.20 I
		349.00 I
		343.05 I
		319.90 I
		319.00 I
		298.80 I
		280.20 I
		278.85 I
268.85 I		
9.300	579473	162.85 I
		148.85 I
		136.00 I
		104.90 I
		320.00 I
		319.00 I
9.632	66025612	278.95 I
		162.90 I
		148.80 I
		334.10 I
10.676	4298884	333.10 I
		315.05 I
		315.10 I
		311.00 I
		301.05 I
282.05 I		

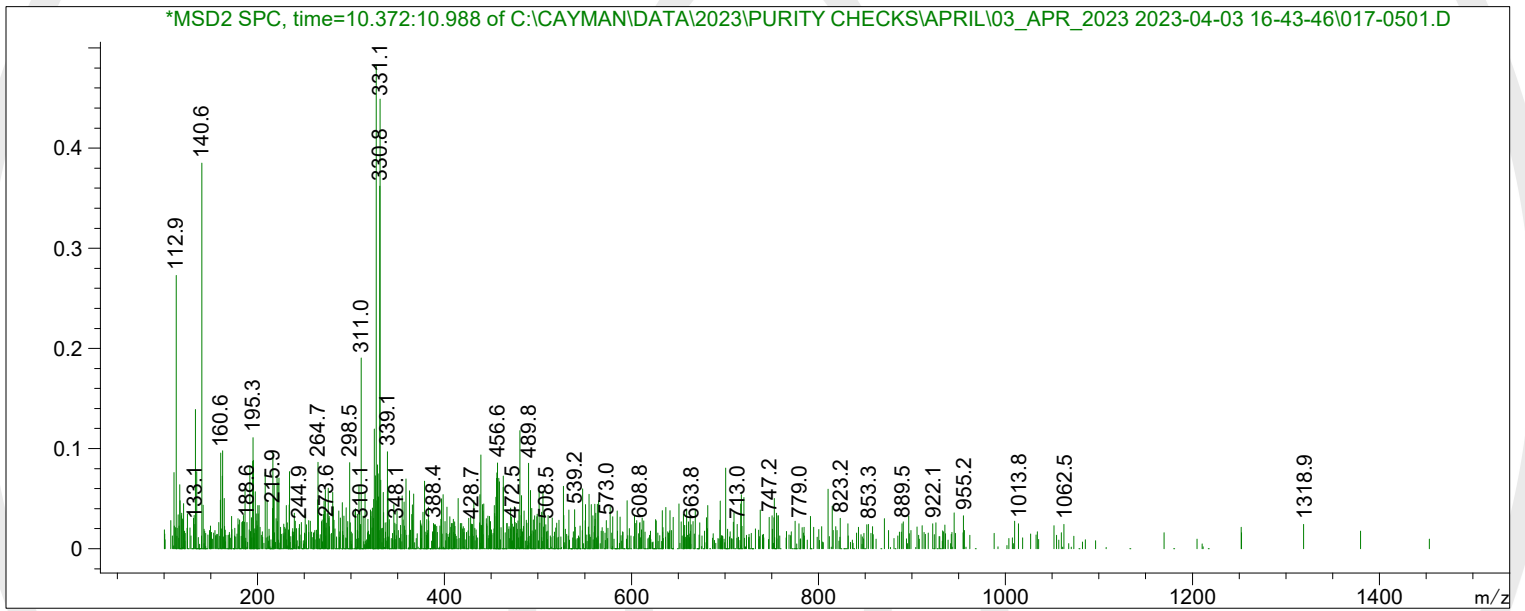
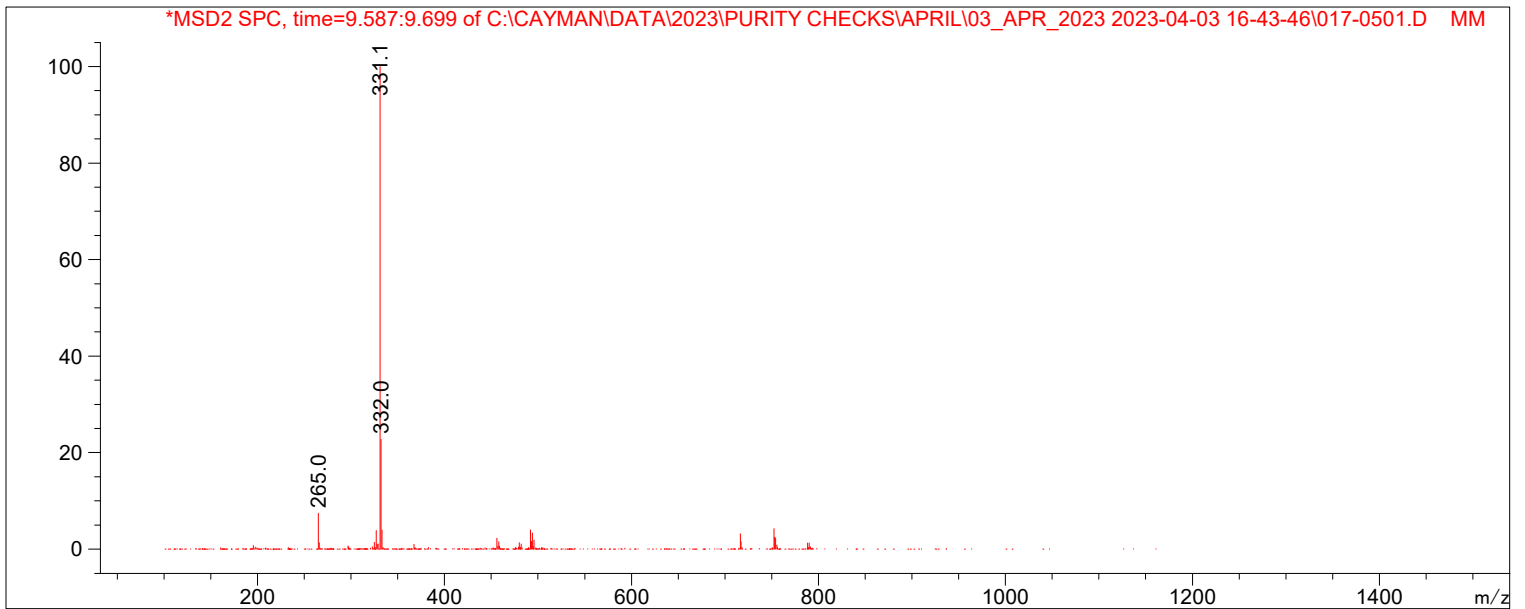




MS Signal: MSD2 TIC, MS File, MM-ES+APCI, Neg, Fast Scan, Frag: 70, "--DUAL"
Spectra averaged over upper half of peaks.
Noise Cutoff: 1000 counts.
Reportable Ion Abundance: > 10%.

Retention Time (MS)	MS Area	Mol. Weight or Ion
9.180	1073801	348.25 I
		347.30 I
		347.05 I
		316.95 I
		263.80 I
		208.50 I
		140.95 I
		112.90 I
9.628	20352394	332.05 I
		331.10 I
10.505	2365915	331.10 I
		330.80 I
		327.00 I
		310.95 I
		140.55 I
		112.95 I





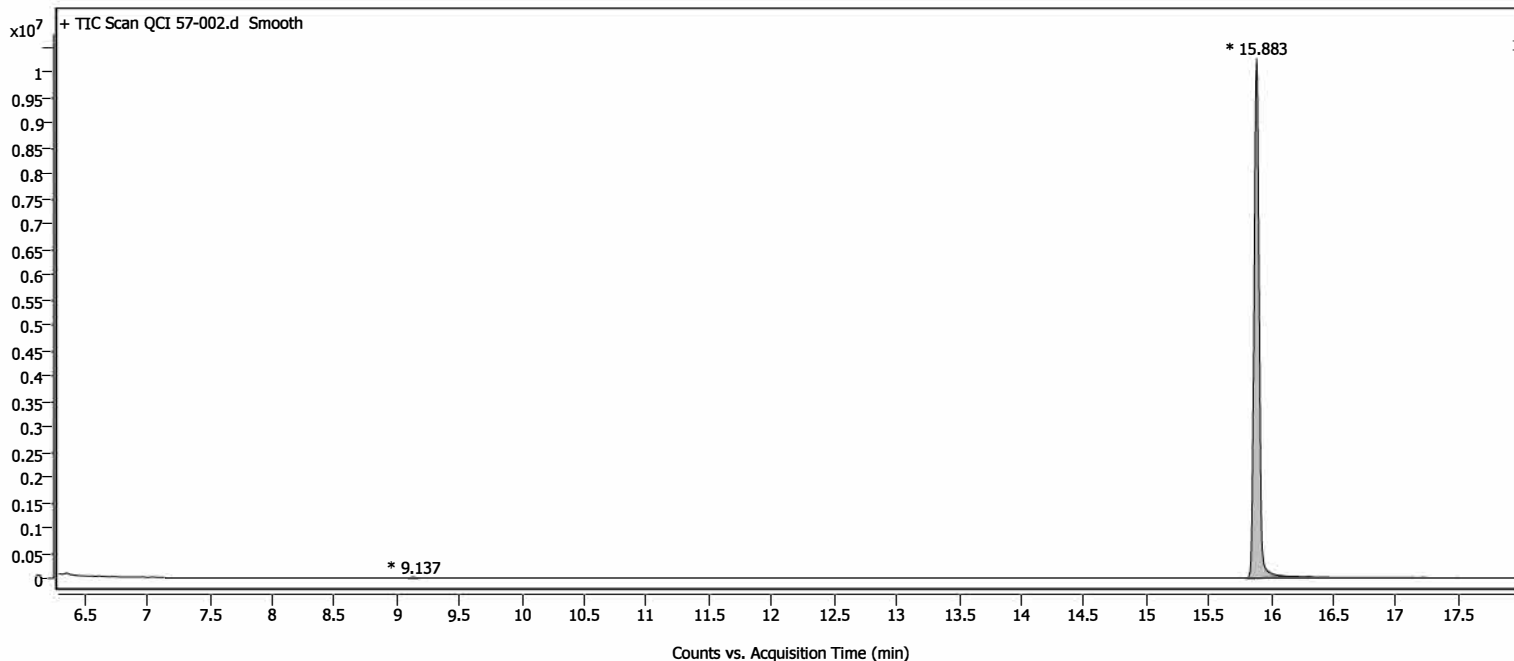
*** End of Report ***

Analysis Report

Sample Information

Name	QC-157-002	Data File Path	C:\MassHunter\GCMS\1\data\2023\April\03Apr23\QCI 57-002.D
Instrument	GCMS	Acq. Time (Local)	4/3/2023 12:03:40 PM (UTC-04:00)
MS Type	Q	Method Path (Acq)	C:\MassHunter\GCMS\1\methods\DMSO delay_60-300_20C_EI_GCMS Analysis.M
Inj. Vol. (ul)	1	Method Path (DA)	DMSO delay_60-300_20C_EI_GCMS Analysis.M
Position	3	Version (Acq SW)	MassHunter GC/MS Acquisition 10.0.368 14-Feb-2019 Copyright © 1989-2018 Agilent Technologies, Inc.
		Operator	KRH

Sample Chromatograms



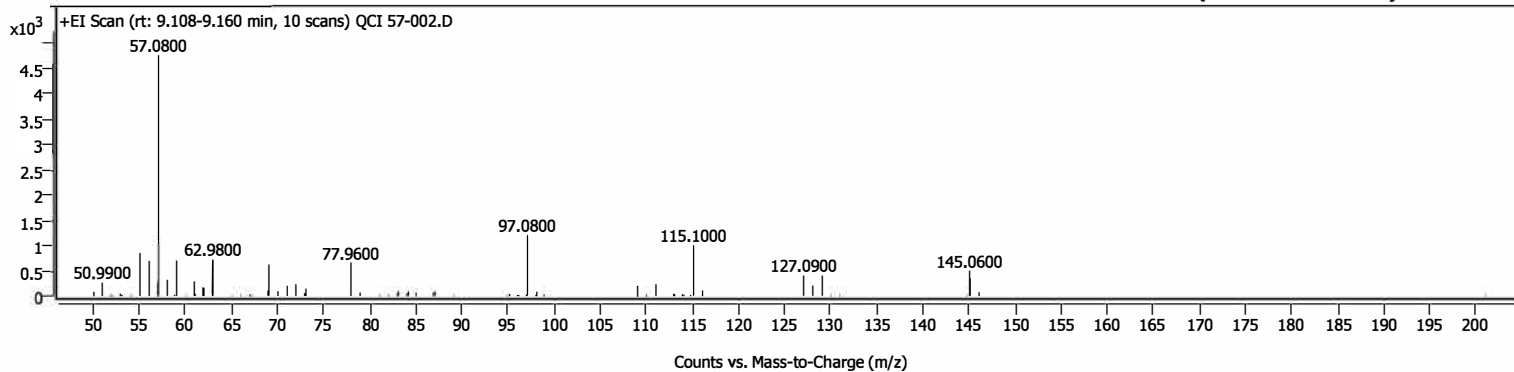
Chromatogram Peaks

Peak	RT	Height	Area	Area Sum %
1	9.137	24928	50584	0.17
2	15.883	10269174	29414210	99.83

Sample Spectra

Peak 1 from + TIC Scan Smo

+ Scan (rt: 9.108-9.160 min)



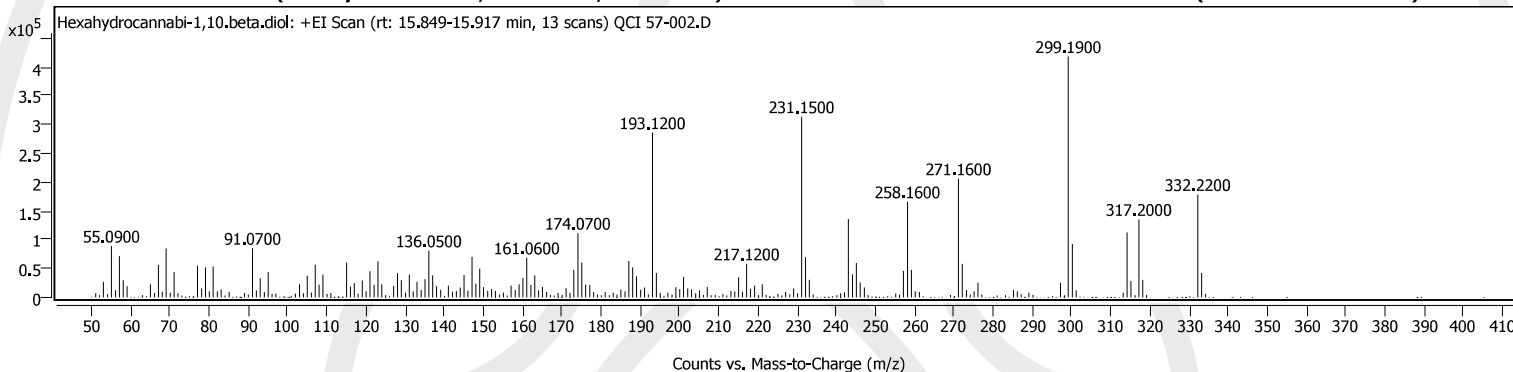
Analysis Report

Spectrum Peaks (Max. 20)

m/z	Z	Abund	Abund %
50.9900		271	5.68
55.0500		850	17.80
56.0700		694	14.54
56.9900		279	5.85
57.0800	1	4774	100.00
58.0400	1	316	6.62
59.0600		697	14.60
60.9700		289	6.05
62.9800		727	15.22
69.0500		624	13.07
71.9900		231	4.85
77.9600		662	13.87
97.0800	1	1214	25.43
111.0400		228	4.77
115.1000	1	1008	21.12
127.0900		406	8.50
128.0600		203	4.25
129.1000		399	8.36
145.0600	1	504	10.55
145.1300		342	7.17

Peak 2 from + TIC Scan Smo (Hexahydrocannabinol-1,10.beta.diol; C21H32O3)

+ Scan (rt: 15.849-15.917 min)



Spectrum Peaks (Max. 20)

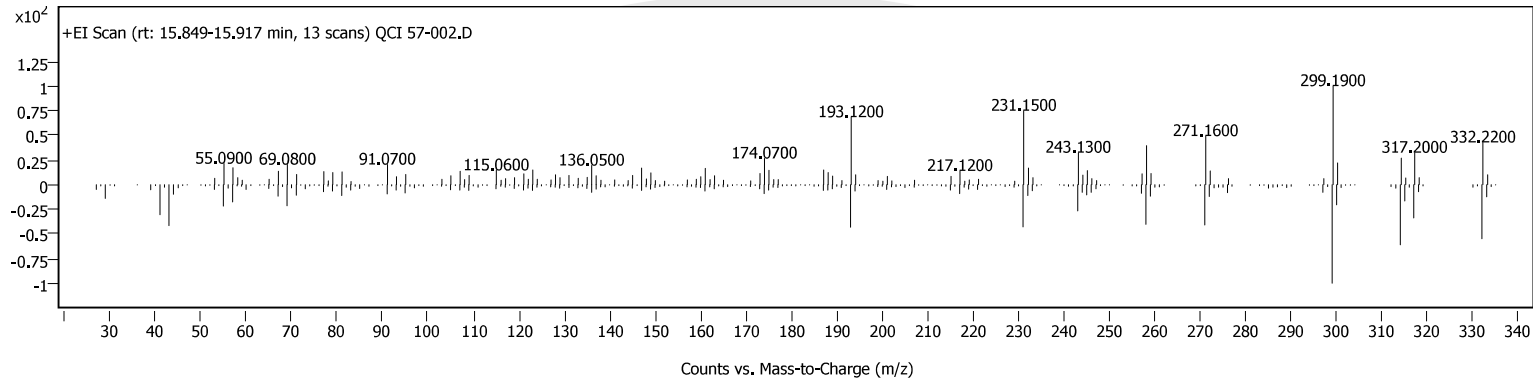
m/z	Z	Abund	Abund %
55.0900		89072	21.29
57.0900		71426	17.07
69.0800		85119	20.35
91.0700		85270	20.38
136.0500		81131	19.39
147.0500		70633	16.88
161.0600		68702	16.42
174.0700		111537	26.66
187.0800		62910	15.04
193.1200	1	285853	68.33
231.1500	1	313652	74.97
232.1500	1	69701	16.66
243.1300	1	135899	32.48
258.1600	1	166042	39.69
271.1600	1	206047	49.25
299.1900	1	418366	100.00
300.2000	1	92469	22.10
314.2000	1	112762	26.95
317.2000	1	135489	32.39
332.2200	1	178494	42.66

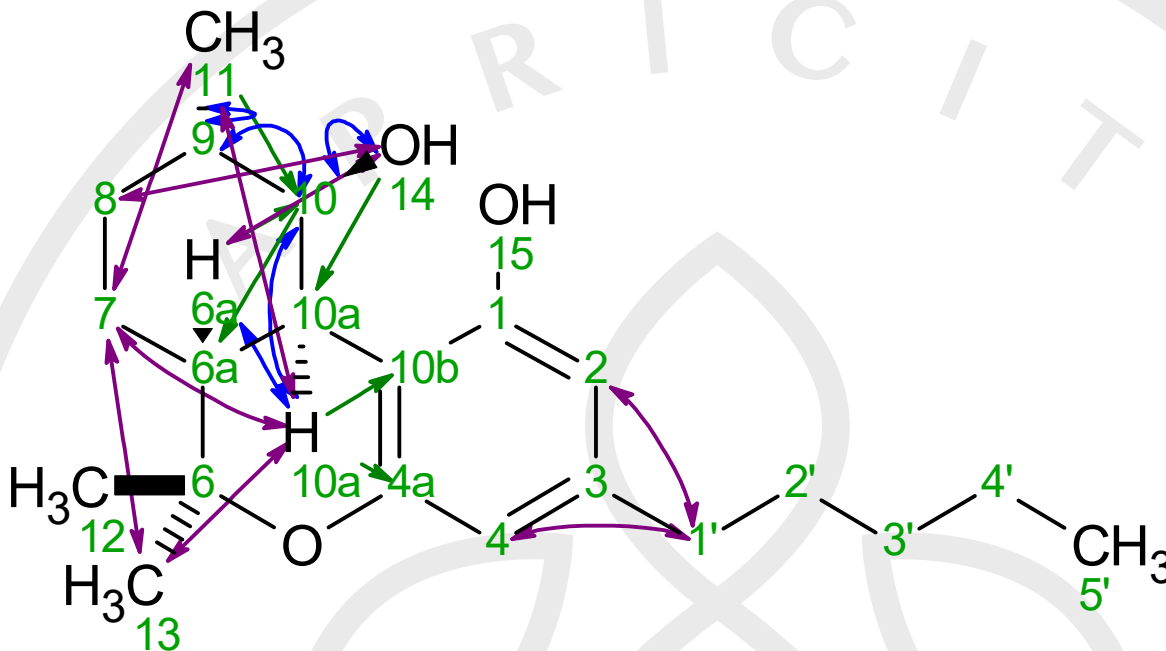
Spectrum Identification Table (Max. 1)




Best	Name	Formula	CAS	Score	Score (Lib)	Lib/DB
Yes	Hexahydrocannabinol-1,10.beta.diol	C21H32O3	1010196-54-2	79.98	79.98	NIST20.L

Analysis Report

Mirror Plot





 COSY
 NOESY
 HMBC

Critical Correlations

HMBC

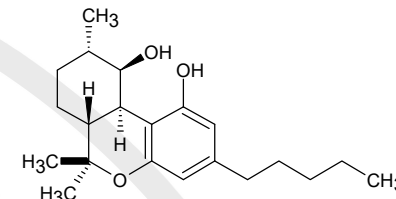
- Proton 10: $^3J_{CH}$ to carbon 6a
- Proton 10a: $^2J_{CH}$ to carbon 10b; $^3J_{CH}$ to carbon 4a
- Proton 11: $^3J_{CH}$ to carbon 10
- Proton 14: $^3J_{CH}$ to carbon 10a

COSY

- Proton 6a: $^3J_{HH}$ (~11.7 Hz) to proton 10a, indicating axial-axial coupling
- Proton 10a: $^3J_{HH}$ (~1.1 Hz) to proton 10, indicating equatorial coupling
- Proton 10: $^3J_{HH}$ to proton 9; $^3J_{HH}$ to proton 14 indicating hydroxyl attachment at 10
- Proton 9: $^3J_{HH}$ to protons 11

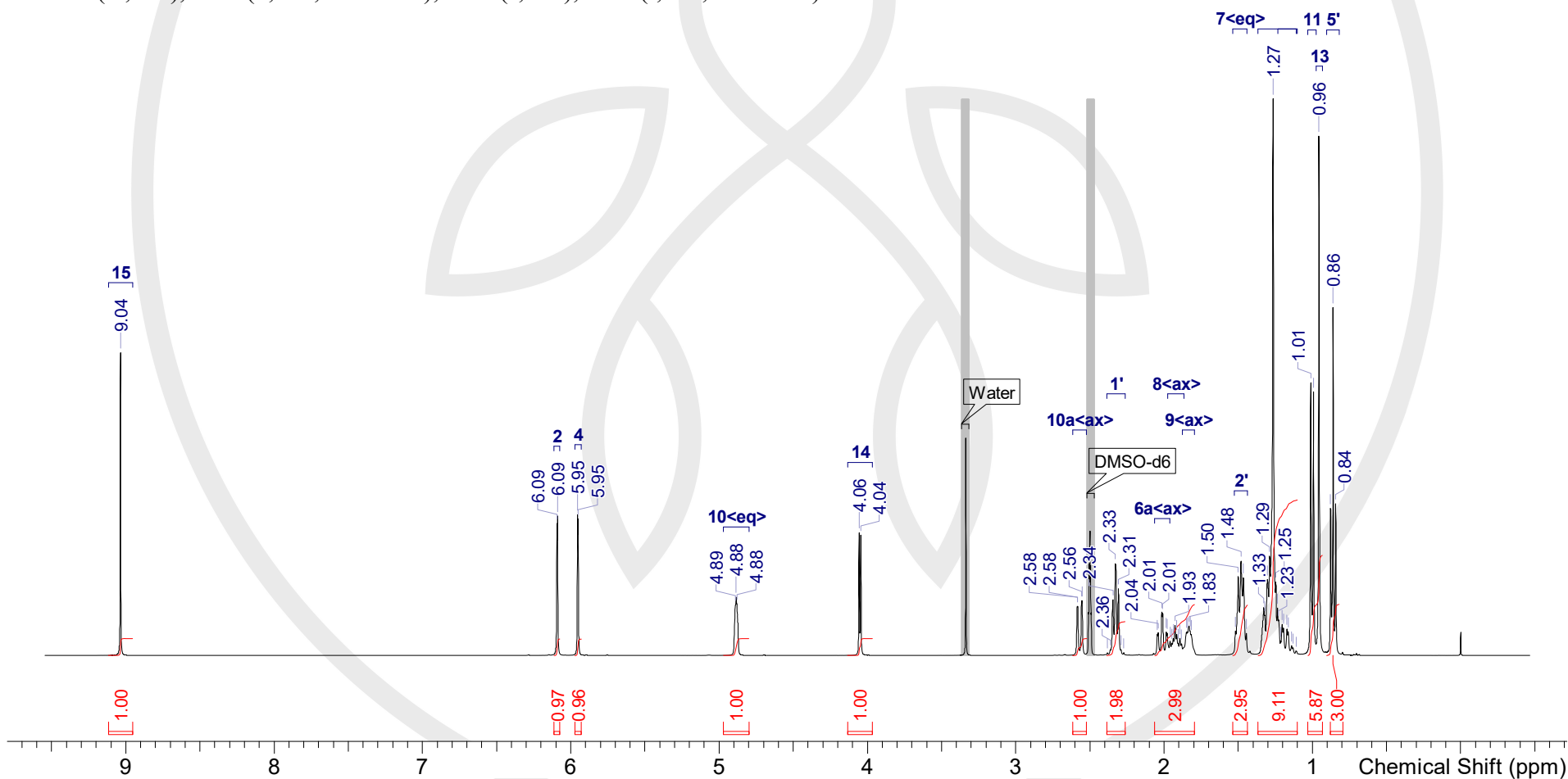
NOESY

- Proton 1' to protons 2, 4: confirms normal attachment of pentyl chain (abnormal at position 1)
- Proton 14 to protons 6a and 8: 1,3 diaxial interactions confirming axial positions of 6a, 8, and hydroxyl -OH 14
- Proton 10a to protons 7, 11, and 13: 1,3 diaxial interactions confirming axial positions of 7, 11, 10a and 13



File Name	\\sulfur\private\nmrdata\JEOL_2023\QC-I-57-002\QC-I-57-002 PROTON 29-Mar-2023-1-1.jdf		
Date	29 Mar 2023 12:58:29	Nucleus	1H
Solvent	DMSO-d6	Number of Transients	16
Temperature (degree C)	21.000	Frequency (MHz)	399.5822
		Origin	JEOL ECZ400S Sc v601

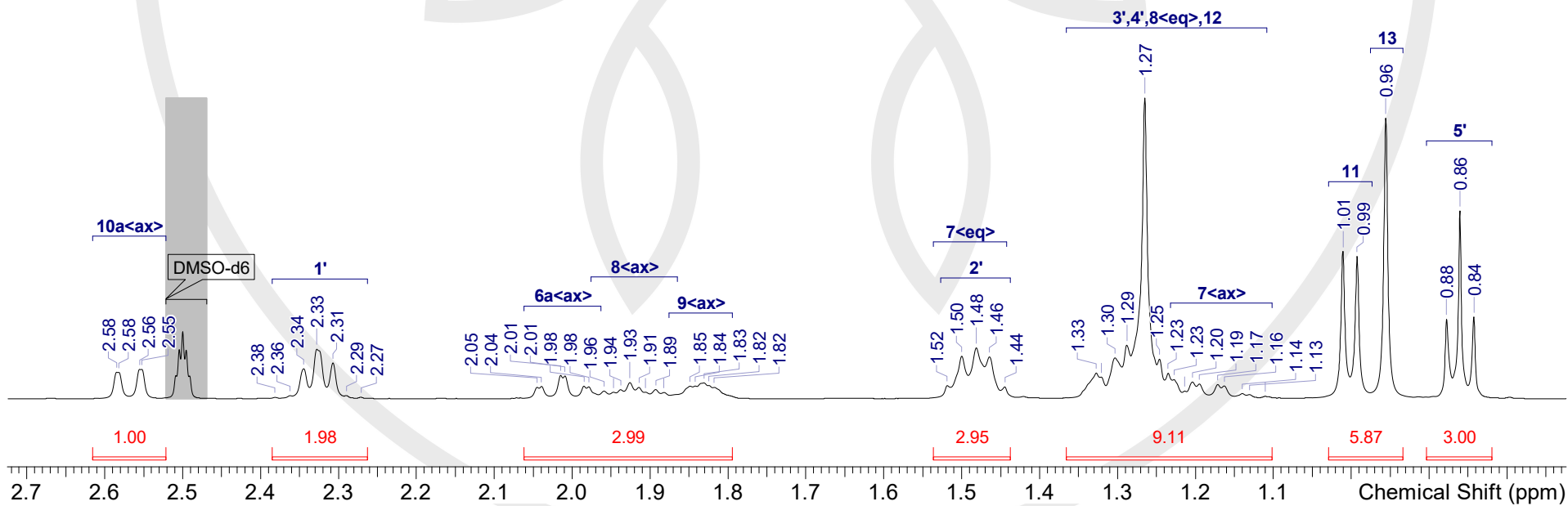
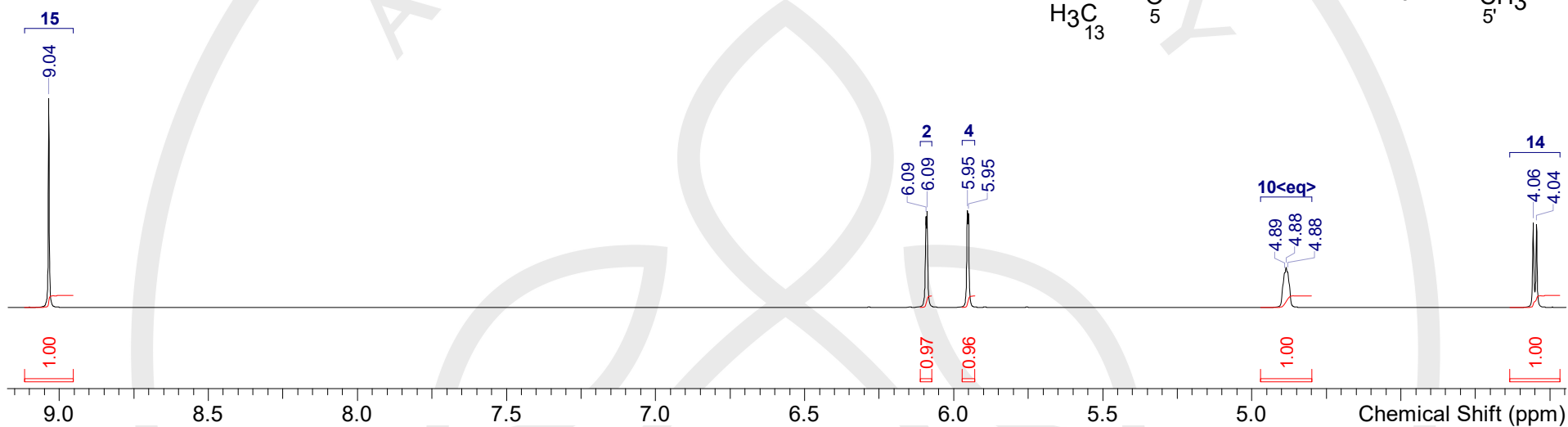
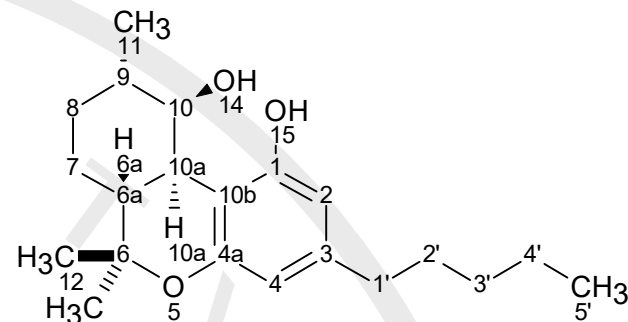
¹H NMR (DMSO-d₆, 400 MHz) δ 9.04 (s, 1H), 6.09 (d, 1H, *J*=1.5 Hz), 5.95 (d, 1H, *J*=1.5 Hz), 4.8-5.0 (m, 1H), 4.05 (d, 1H, *J*=4.6 Hz), 2.57 (dd, 1H, *J*=1.1, 11.7 Hz), 2.3-2.4 (m, 2H), 2.01 (dt, 1H, *J*=2.3, 12.2 Hz), 1.9-2.0 (m, 1H), 1.8-1.9 (m, 1H), 1.4-1.5 (m, 1H), 1.4-1.5 (m, 2H), 1.1-1.4 (m, 8H), 1.1-1.2 (m, 1H), 1.00 (d, 3H, *J*=7.2 Hz), 0.96 (s, 3H), 0.86 (t, 3H, *J*=7.0 Hz)



QC-I-57-002

Proposed Structure

10(R)-hydroxy-9(S)-Hexahydrocannabinol

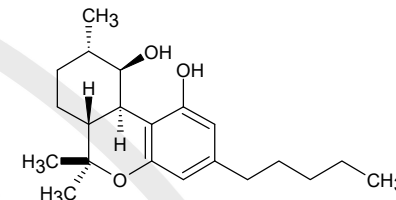




QC-I-57-002

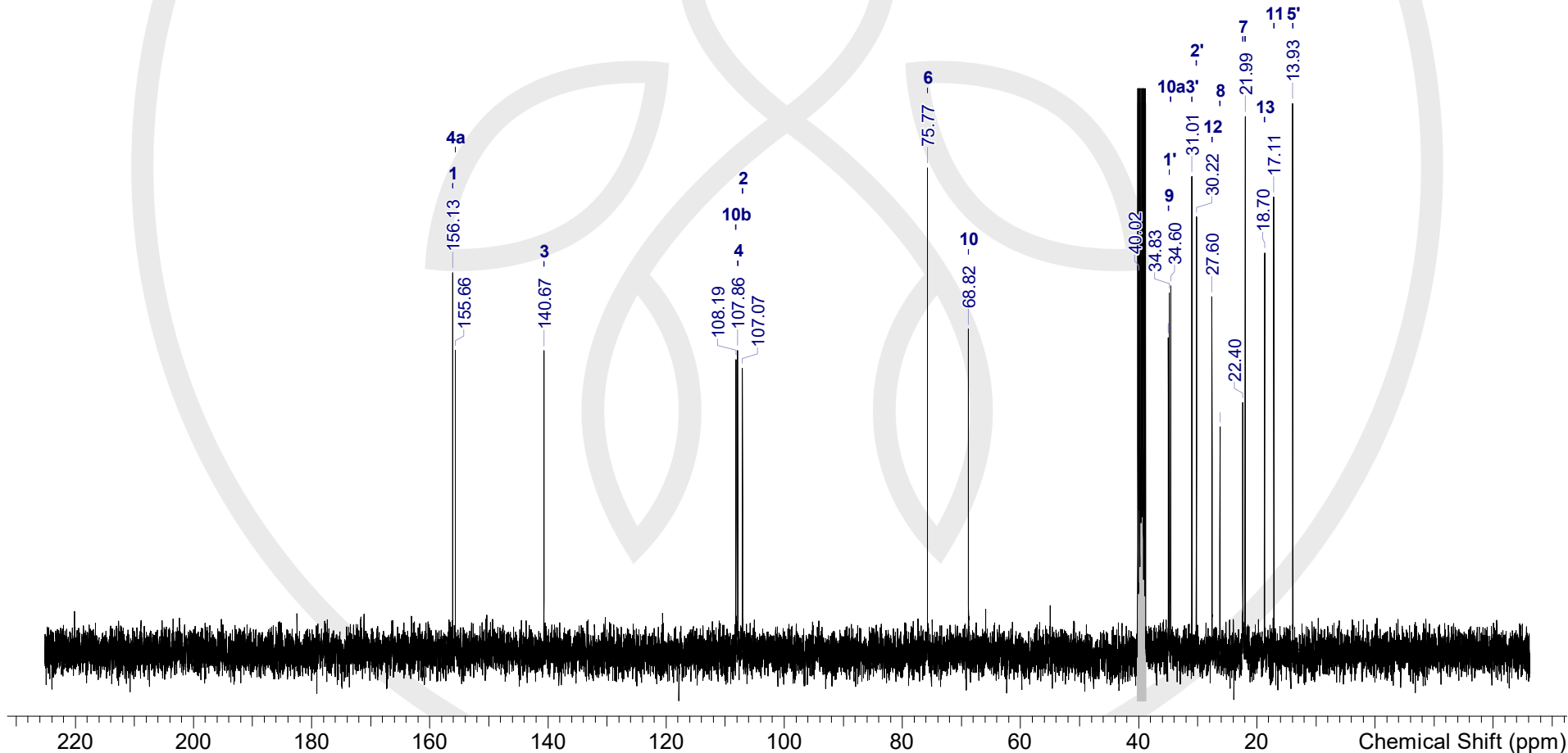
Proposed Structure

10(R)-hydroxy-9(S)-Hexahydrocannabinol



File Name	\\sulfur\private\nmrdata\JEOL_2023\QC-I-57-002\QC-I-57-002 CARBON 29-Mar-2023-1-1.jdf				
Date	29 Mar 2023 13:12:04	Nucleus	13C	Frequency (MHz)	100.4750
Solvent	DMSO-d6	Number of Transients	256	Origin	JEOL ECZ400S Sc v601
Temperature (degree C)	21.100				

^{13}C NMR (DMSO- d_6 , 100 MHz) δ 156.1, 155.7, 140.7, 108.2, 107.9, 107.1, 75.8, 68.8, 40.0, 35.0, 34.8, 34.6, 31.0, 30.2, 27.6, 26.3, 22.4, 22.0, 18.7, 17.1, 13.9

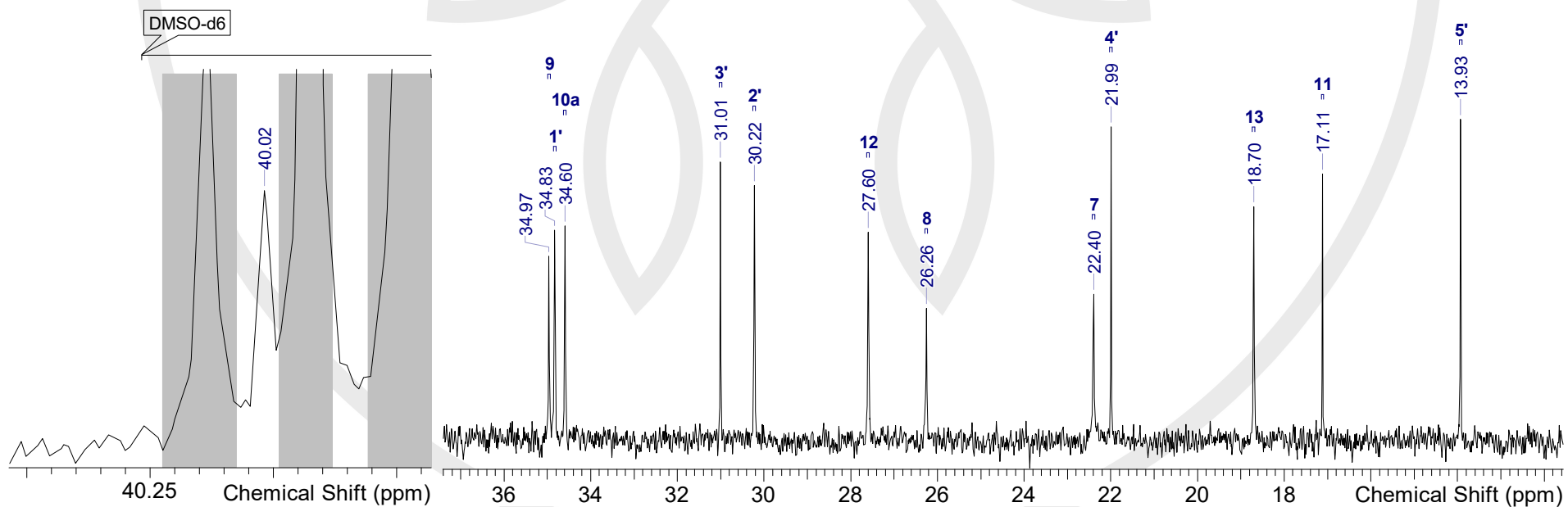
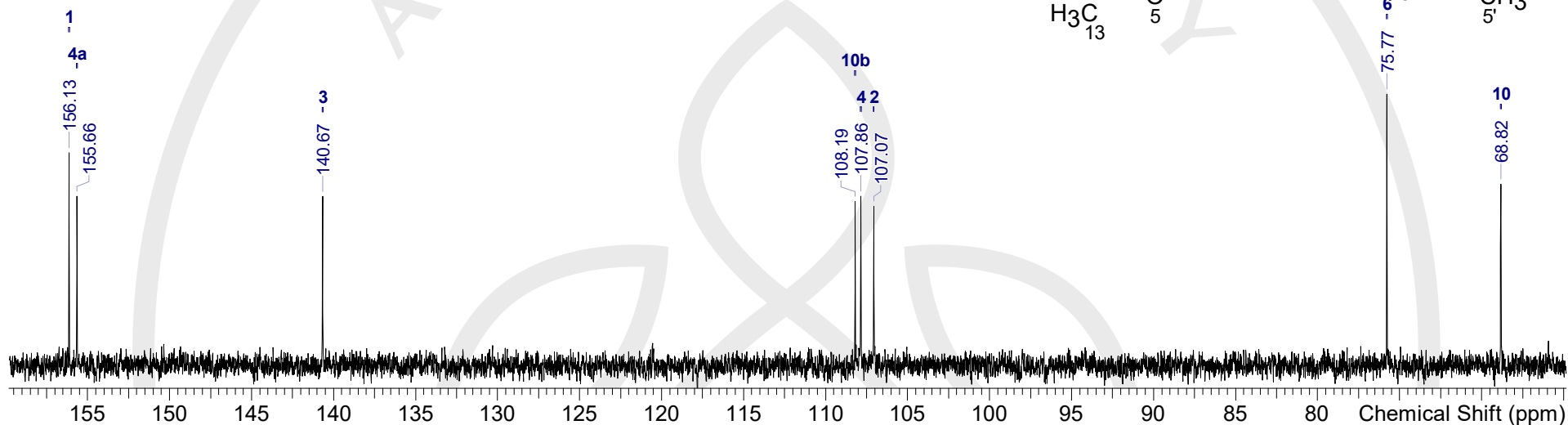
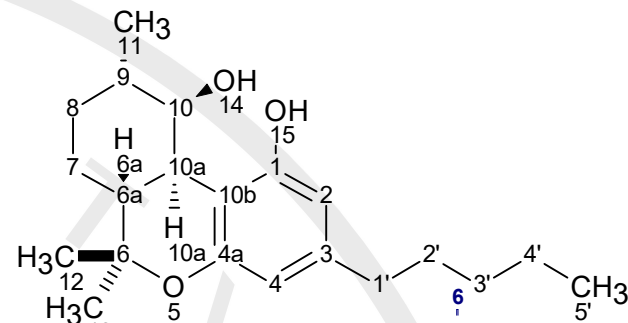




QC-I-57-002

Proposed Structure

10(R)-hydroxy-9(S)-Hexahydrocannabinol

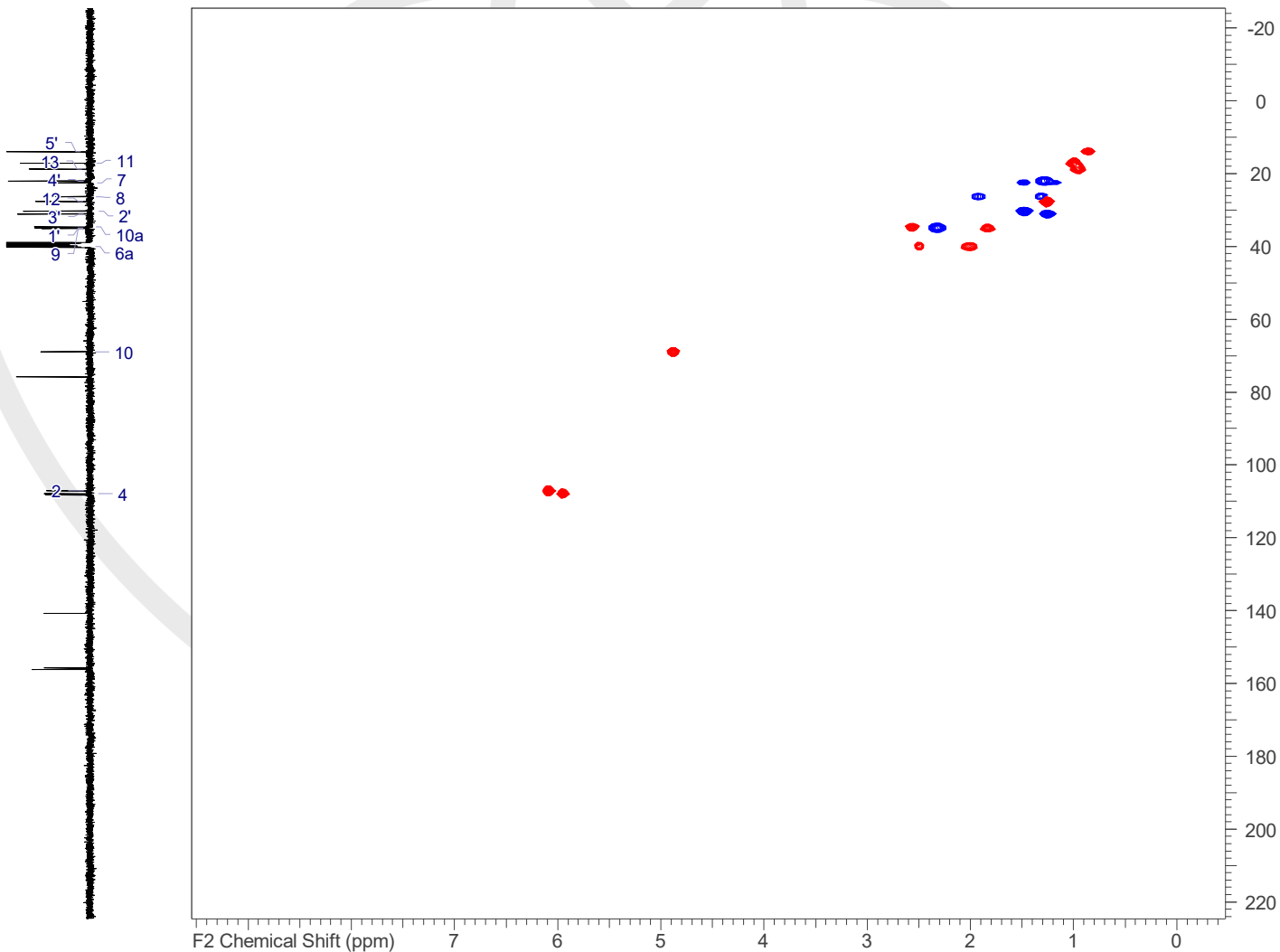
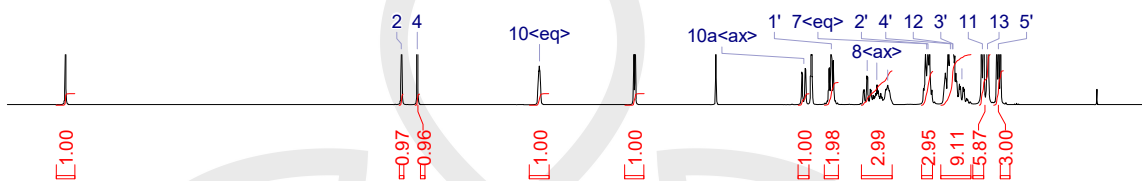
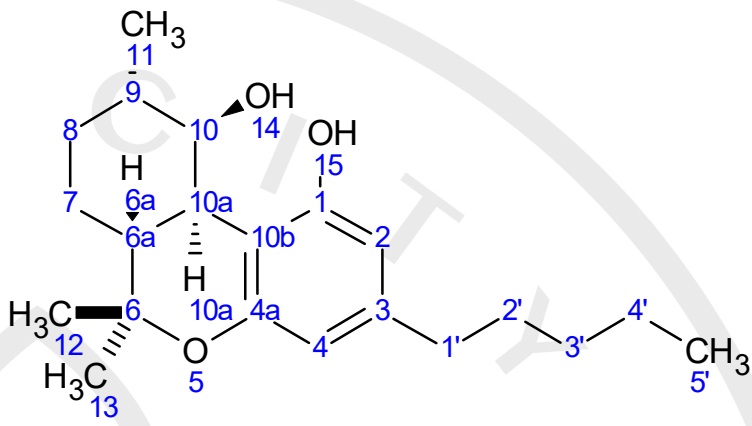


QC-I-57-002

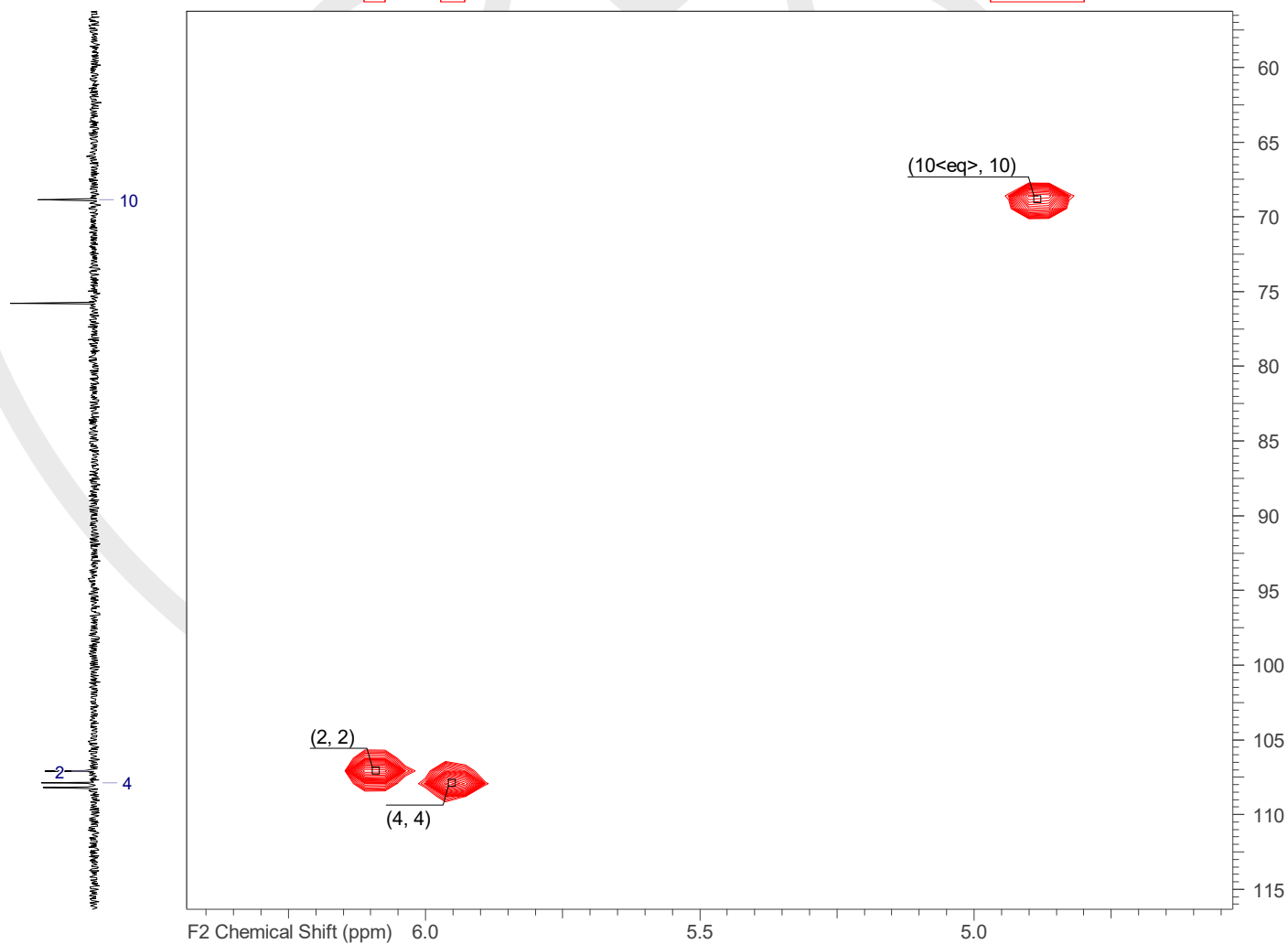
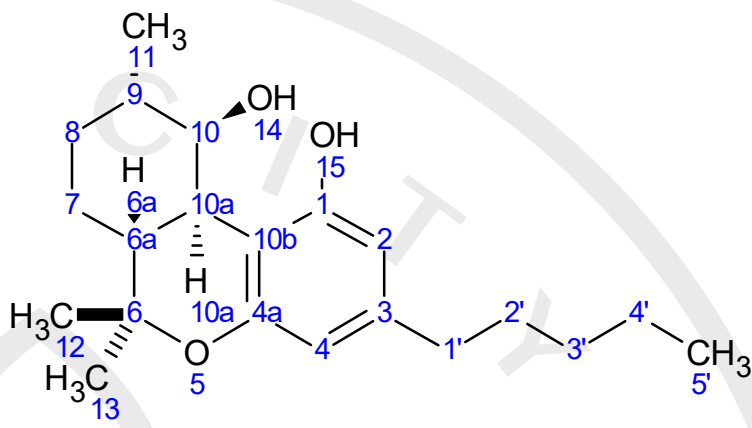
Proposed Structure

10(R)-hydroxy-9(S)-Hexahydrocannabinol

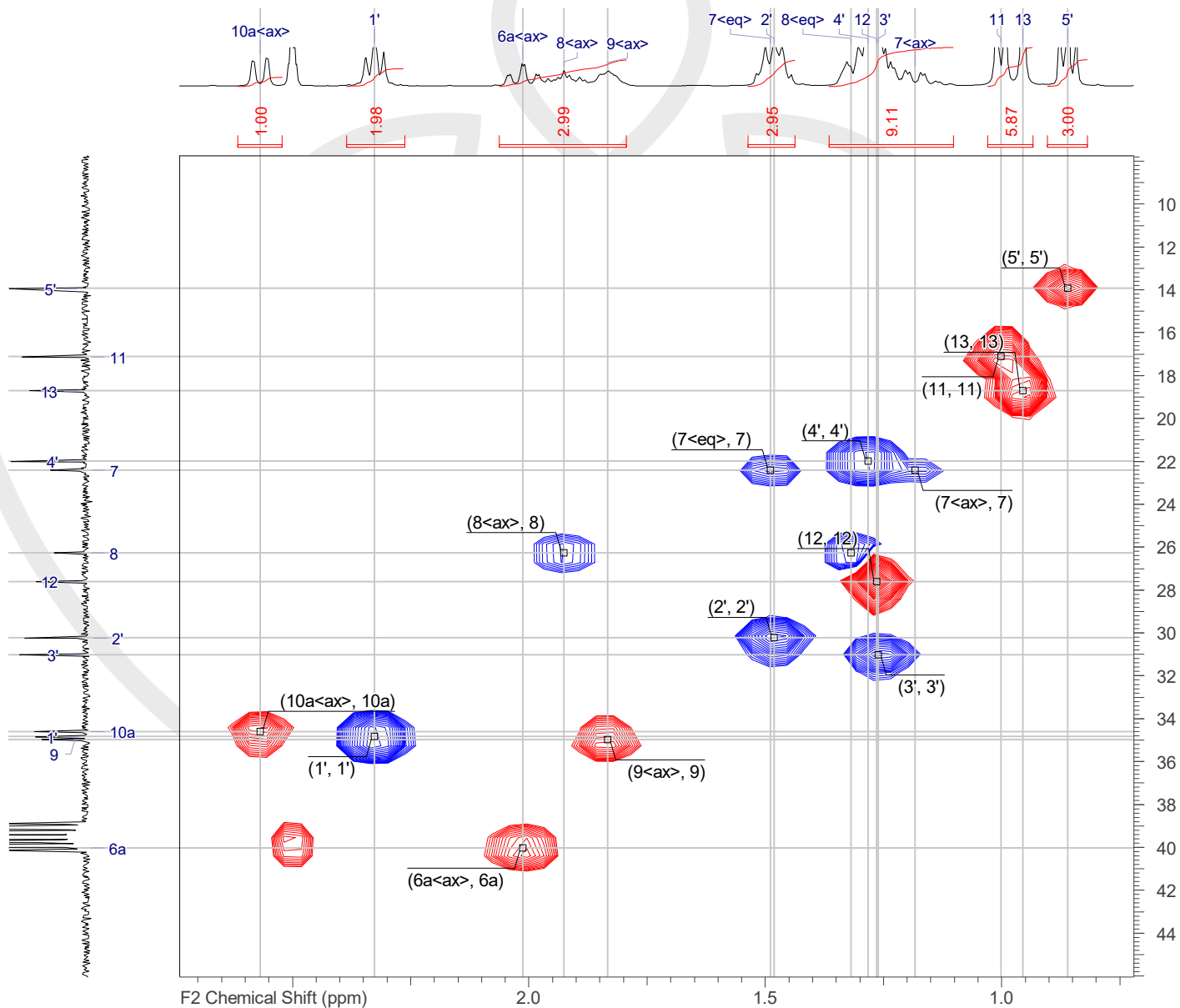
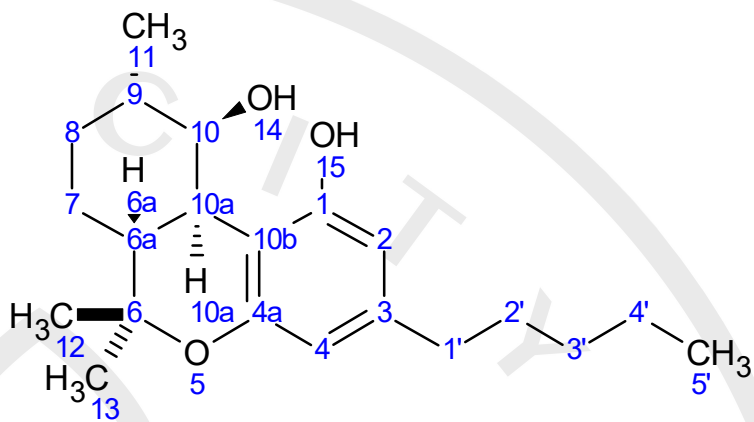
Acquisition Time (sec)	(0.2000, 0.0204)
Date Stamp	29 Mar 2023 13:12:14
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Frequency (MHz)	(399.5822, 100.4750)
Nucleus	(1H, 13C)
Number of Transients	2
Origin	JEOL ECZ400S Sc v601
Original Points Count	(1000, 512)
Pulse Sequence	ghsqcad.jxp
Spectrum Type	HSQC-DEPT
Sweep Width (Hz)	(4001.46, 25113.36)
Temperature (degree C)	21.400
Title	QC-I-57-002



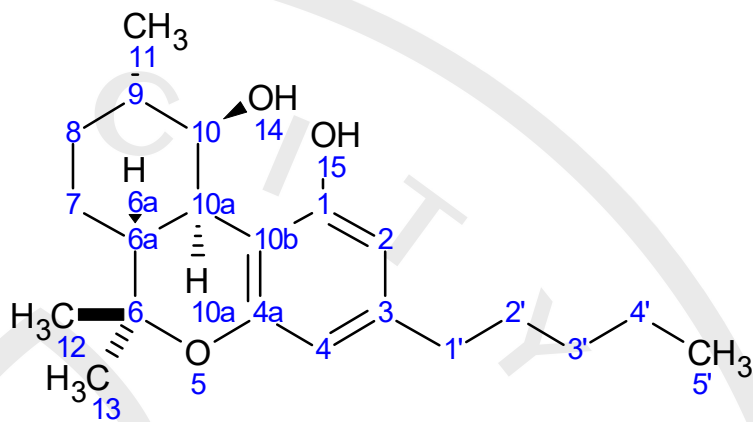
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Frequency (MHz)	(399.5822, 100.4750)
Nucleus	(1H, 13C)
Number of Transients	2
Origin	JEOL ECZ400S Sc v601
Original Points Count	(1000, 512)
Pulse Sequence	ghsqcad.jxp
Spectrum Type	HSQC-DEPT
Sweep Width (Hz)	(4001.46, 25113.36)
Temperature (degree C)	21.400
Title	QC-I-57-002



Acquisition Time (sec)	(0.2000, 0.0204)
Date Stamp	29 Mar 2023 13:12:14
File Name	\\sulfur\private\nmrdata\JEOL_2023\QC-I-57-002\QC-I-57-002_HSQC_29-Mar-2023-1-1.jdf
Frequency (MHz)	(399.5822, 100.4750)
Nucleus	(1H, 13C)
Number of Transients	2
Origin	JEOL ECZ400S Sc v601
Original Points Count	(1000, 512)
Pulse Sequence	ghsqcad.jxp
Spectrum Type	HSQC-DEPT
Sweep Width (Hz)	(4001.46, 25113.36)
Temperature (degree C)	21.400
Title	QC-I-57-002

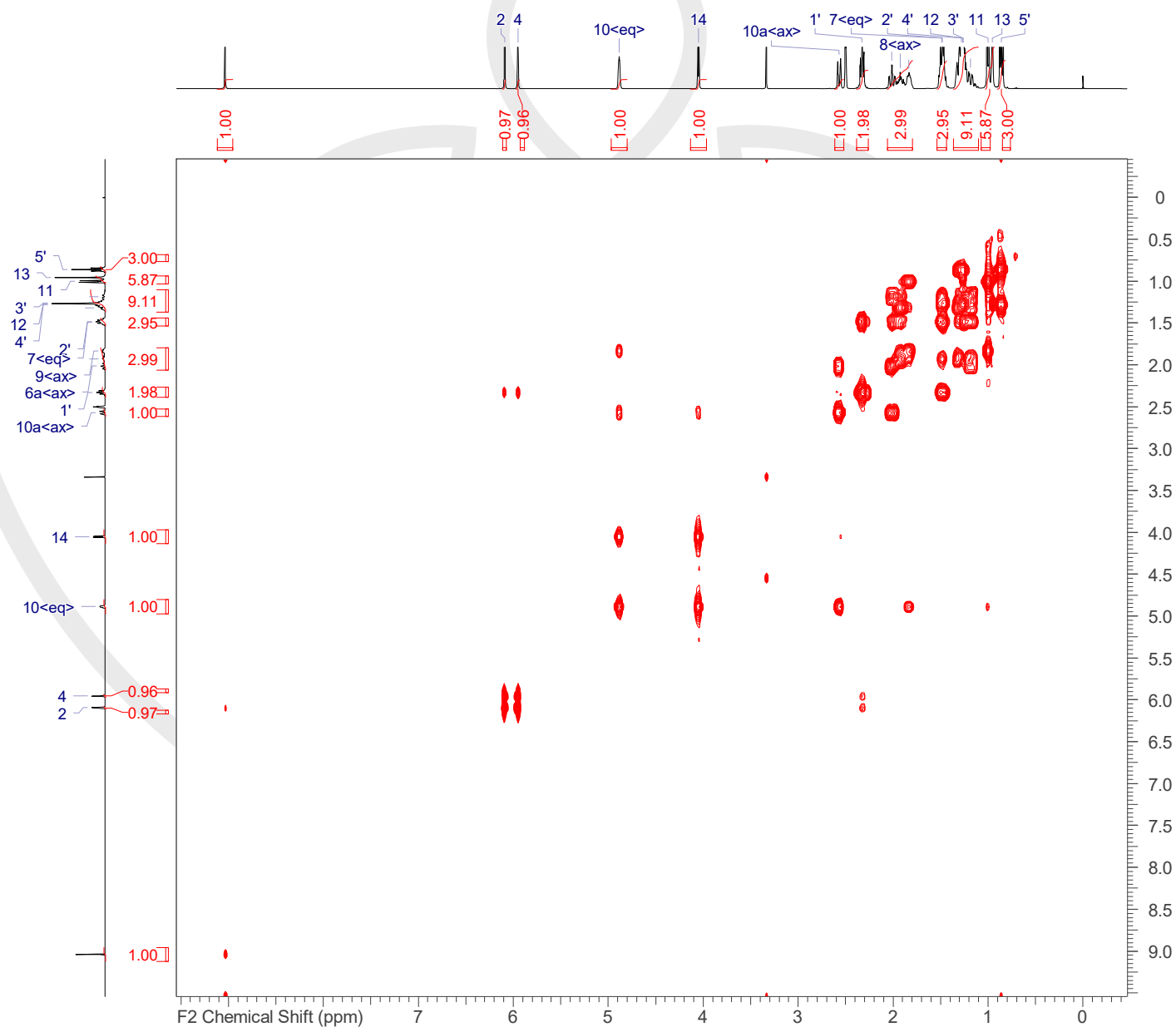
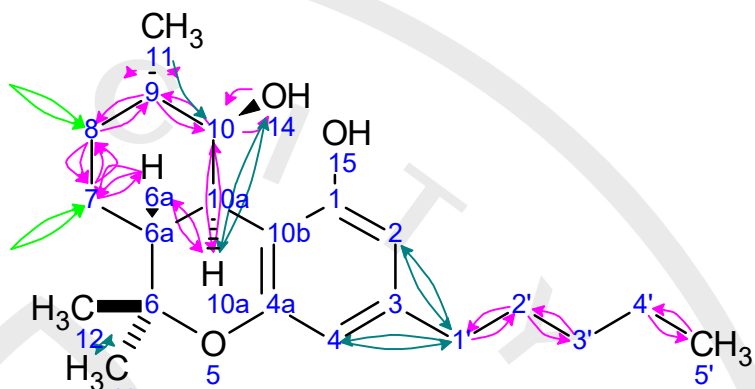


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Frequency (MHz)	(399.5822, 100.4750)
Nucleus	(1H, 13C)
Number of Transients	2
Origin	JEOL ECZ400S Sc v601
Original Points Count	(1000, 512)
Pulse Sequence	ghsqcad.jxp
Spectrum Type	HSQC-DEPT
Sweep Width (Hz)	(4001.46, 25113.36)
Temperature (degree C)	21.400
Title	QC-I-57-002

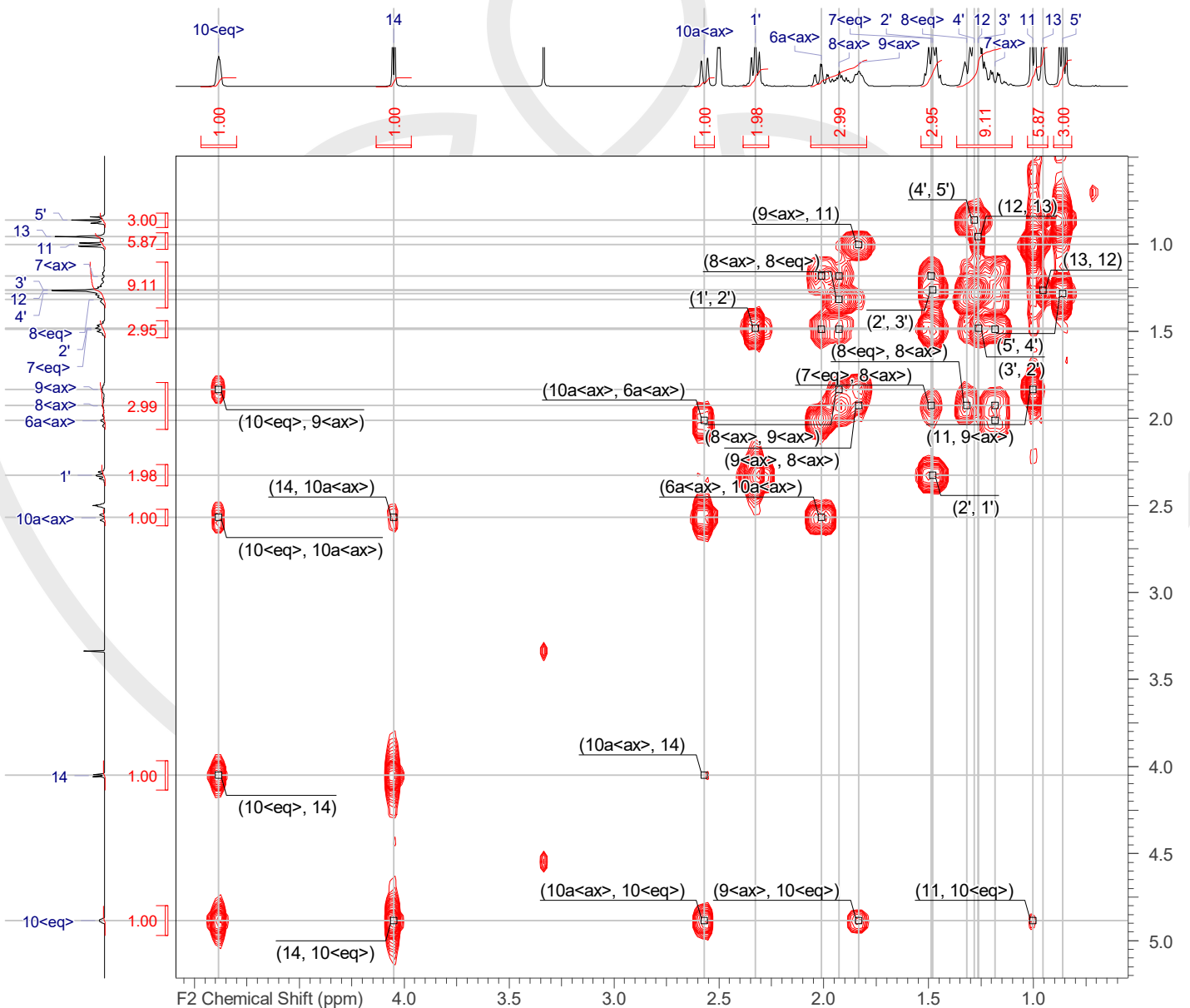
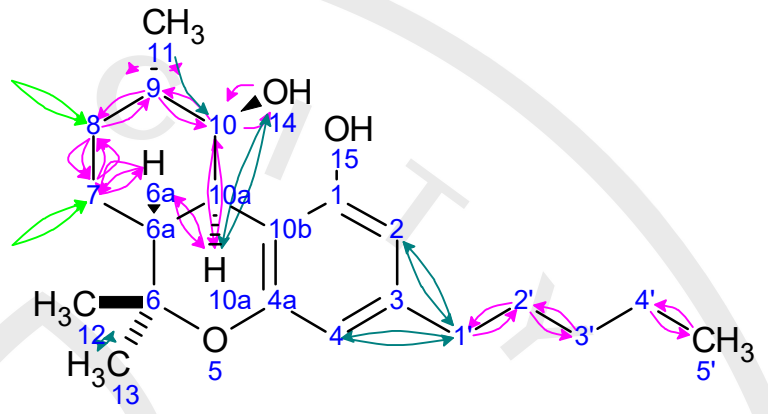


No	F2 Atom	F1 Atom	F2 (ppm)	F1 (ppm)
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2	2	2	6.09	107.07
3	2'	2'	1.48	30.23
4	3'	3'	1.26	31.01
5	4	4	5.95	107.86
6	4'	4'	1.28	21.99
7	5'	5'	0.86	13.93
8	6a<ax>	6a	2.01	40.02
9	7<ax>	7	1.18	22.40
10	7<eq>	7	1.49	22.40
11	8<ax>	8	1.93	26.26
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14	10<eq>	10	4.88	68.82
15	10a<ax>	10a	2.57	34.60
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18	13	13	0.96	18.70

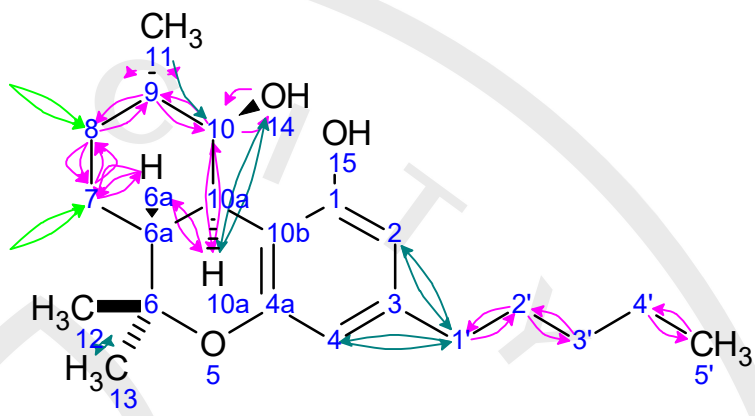
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Frequency (MHz)	(399.5822, 399.5822)
Nucleus	(1H, 1H)
Number of Transients	2
Origin	JEOL ECZ400S Sc v601
Original Points Count	(2560, 256)
Pulse Sequence	dqf cosy pfg.jxp
Spectrum Type	COSY
Sweep Width (Hz)	(4000.24, 3993.89)
Temperature (degree C)	21.300
Title	QC-I-57-002



Acquisition Time (sec)	(0.5120, 0.0641)
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Frequency (MHz)	(399.5822, 399.5822)
Nucleus	(1H, 1H)
Number of Transients	2
Origin	JEOL ECZ400S Sc v601
Original Points Count	(2560, 256)
Pulse Sequence	dqf cosy pfg.jxp
Spectrum Type	COSY
Sweep Width (Hz)	(4000.24, 3993.89)
Temperature (degree C)	21.300
Title	QC-I-57-002



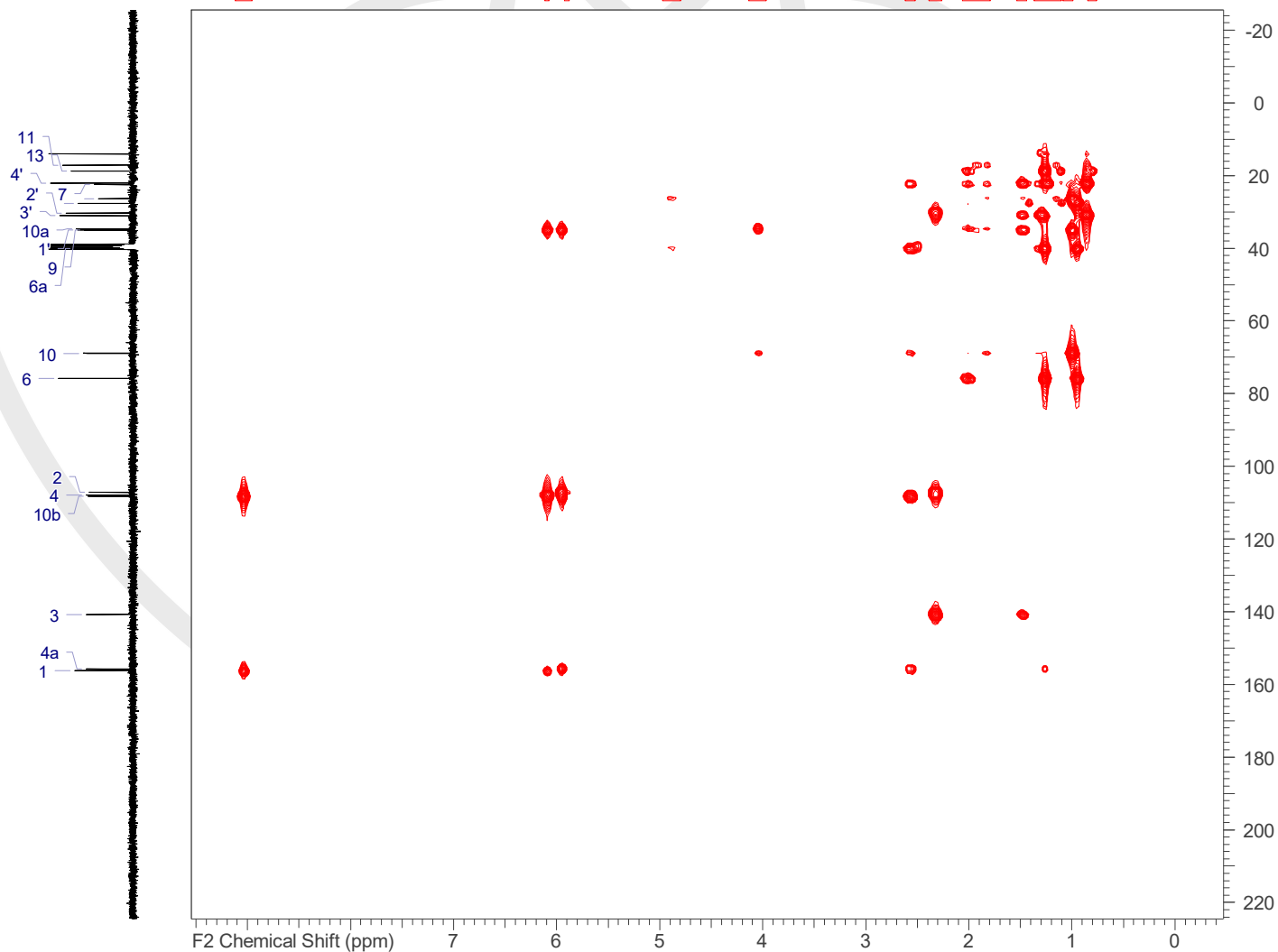
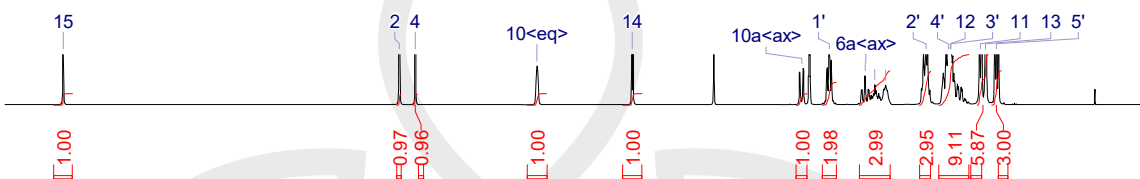
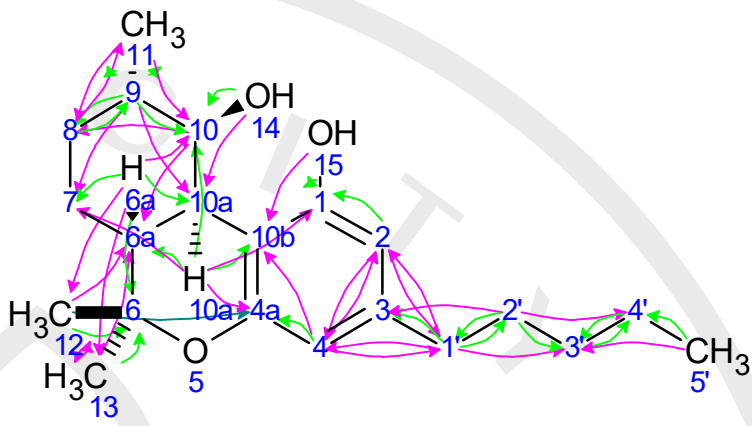
Acquisition Time (sec)	(0.5120, 0.0641)
Date Stamp	29 Mar 2023 14:12:05
File Name	\\sulfur\private\nmrdata\JEOL_2023\QC-I-57-002\QC-I-57-002_DQF_COSY_29-Mar-2023-1-1.jdf
Frequency (MHz)	(399.5822, 399.5822)
Nucleus	(1H, 1H)
Number of Transients	2
Origin	JEOL ECZ400S Sc v601
Original Points Count	(2560, 256)
Pulse Sequence	dqf cosy pfg.jp
Spectrum Type	COSY
Sweep Width (Hz)	(4000.24, 3993.89)
Temperature (degree C)	21.300
Title	QC-I-57-002



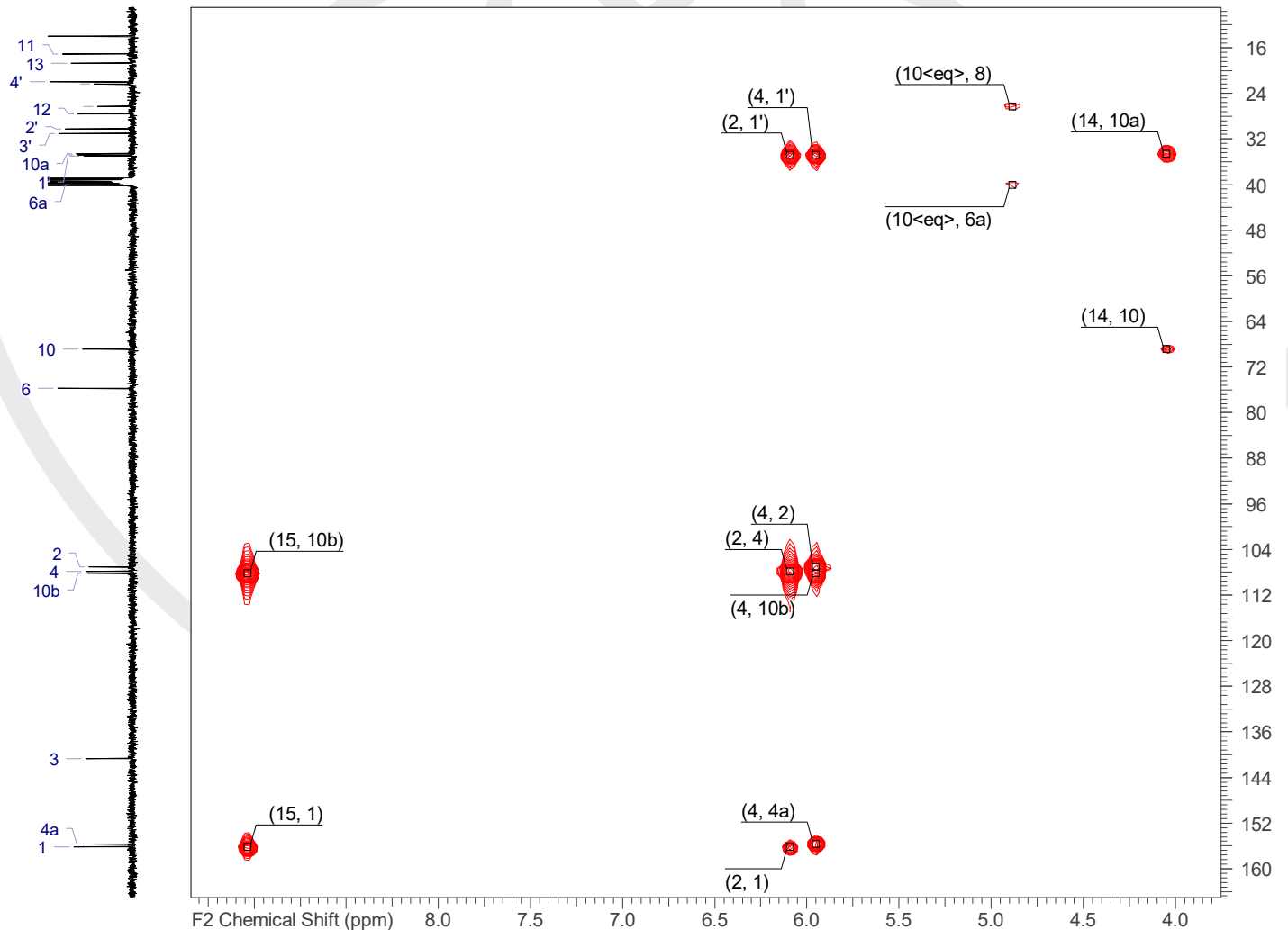
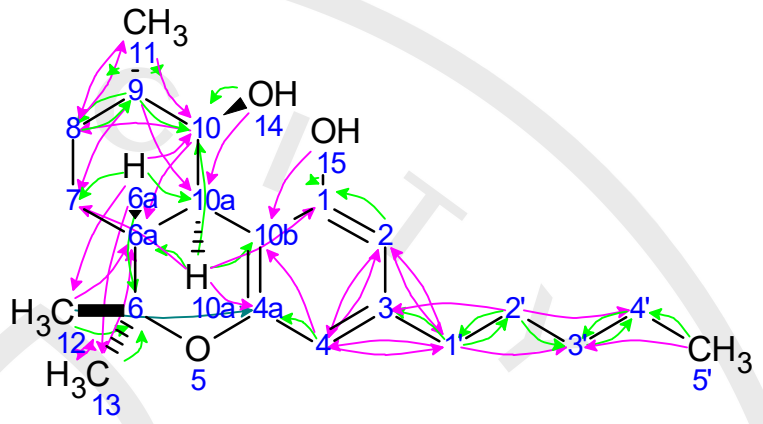
No	F2 Atom	F1 Atom	F2 (ppm)	F1 (ppm)
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2	2'	1'	1.48	2.33
3	4	1'	5.95	2.33
4	1'	2	2.33	6.09
5	1'	2'	2.33	1.48
6	3'	2'	1.26	1.48
7	2'	3'	1.48	1.26
8	1'	4	2.33	5.95
9	5'	4'	0.86	1.28
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12	10a<ax>	6a<ax>	2.57	2.01
13	6a<ax>	7<ax>	2.01	1.18
14	7<eq>	7<ax>	1.49	1.18
15	8<ax>	7<ax>	1.93	1.18
16	6a<ax>	7<eq>	2.01	1.49
17	7<ax>	7<eq>	1.18	1.49
18	8<ax>	7<eq>	1.93	1.49
19	7<ax>	8<ax>	1.18	1.93
20	7<eq>	8<ax>	1.49	1.93
21	8<eq>	8<ax>	1.32	1.93
22	9<ax>	8<ax>	1.83	1.93
23	8<ax>	8<eq>	1.93	1.32
24	8<ax>	9<ax>	1.93	1.83
25	10<eq>	9<ax>	4.88	1.83
26	11	9<ax>	1.00	1.83
27	9<ax>	10<eq>	1.83	4.88
28	10a<ax>	10<eq>	2.57	4.88
29	11	10<eq>	1.00	4.88
30	14	10<eq>	4.05	4.88
31	6a<ax>	10a<ax>	2.01	2.57
32	10<eq>	10a<ax>	4.88	2.57
33	14	10a<ax>	4.05	2.57

No	F2 Atom	F1 Atom	F2 (ppm)	F1 (ppm)
34	9<ax>	11	1.83	1.00
35	13	12	0.96	1.27
36	12	13	1.27	0.96
37	10<eq>	14	4.88	4.05
38	10a<ax>	14	2.57	4.05

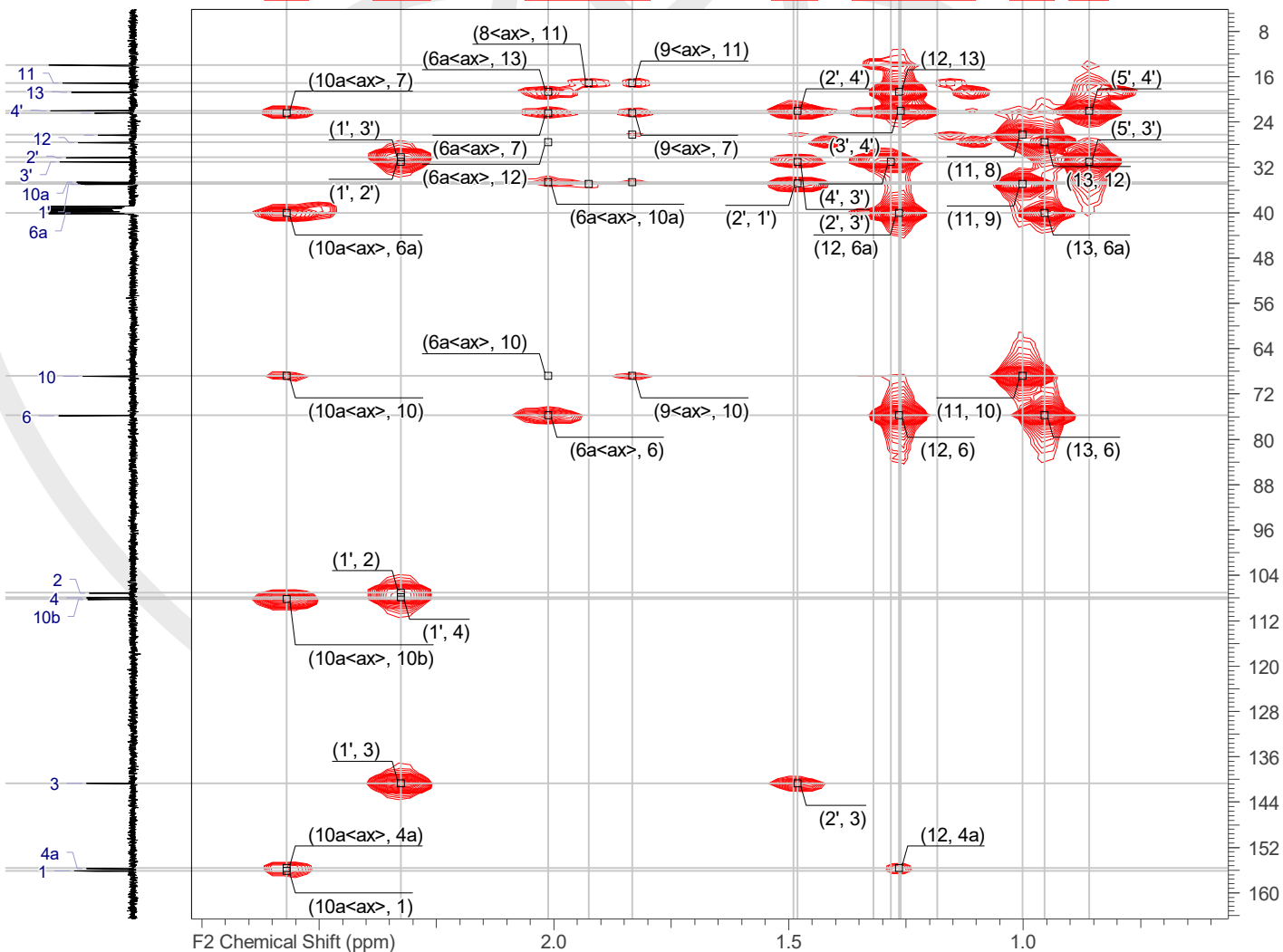
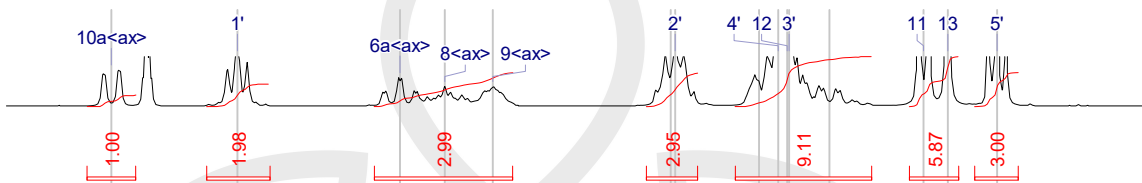
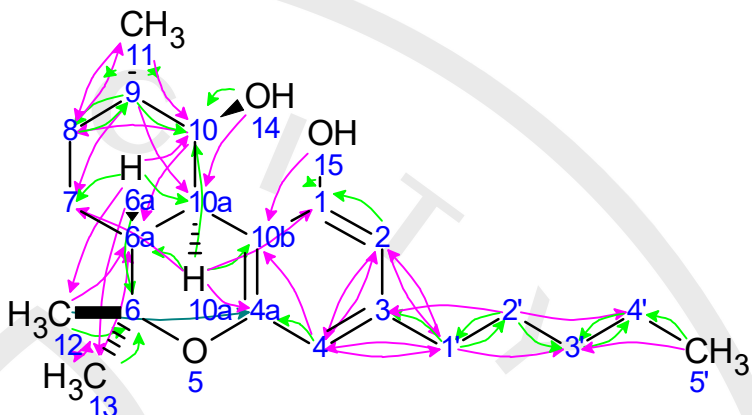
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Frequency (MHz)	(399.5822, 100.4750)
Nucleus	(1H, 13C)
Number of Transients	4
Origin	JEOL ECZ400S Sc v601
Original Points Count	(1999, 512)
Pulse Sequence	hmbc_pfg.jxp
Spectrum Type	HMBC
Sweep Width (Hz)	(4000.24, 25113.36)
Temperature (degree C)	21.400
Title	QC-I-57-002



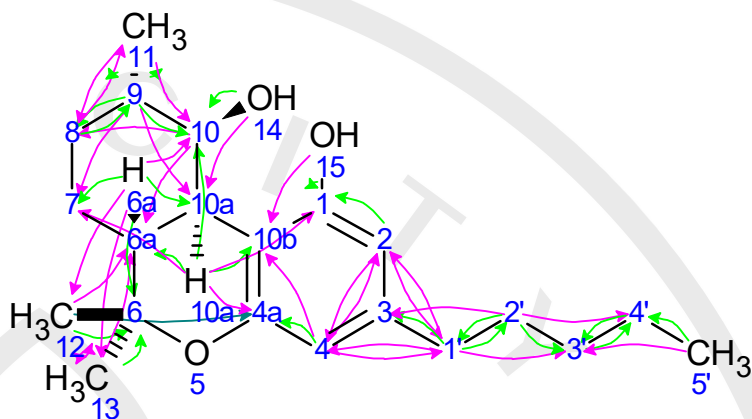
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Frequency (MHz)	(399.5822, 100.4750)
Nucleus	(1H, 13C)
Number of Transients	4
Origin	JEOL ECZ400S Sc v601
Original Points Count	(1999, 512)
Pulse Sequence	hmbc_pfg.jxp
Spectrum Type	HMBC
Sweep Width (Hz)	(4000.24, 25113.36)
Temperature (degree C)	21.400
Title	QC-I-57-002



Acquisition Time (sec)	(0.3998, 0.0204)
Date Stamp	29 Mar 2023 14:30:08
File Name	\\sulfur\private\nmrdata\JEOL_2023\QC-I-57-002\QC-I-57-002_HMBC_29-Mar-2023-1-1.jdf
Frequency (MHz)	(399.5822, 100.4750)
Nucleus	(1H, 13C)
Number of Transients	4
Origin	JEOL ECZ400S Sc v601
Original Points Count	(1999, 512)
Pulse Sequence	hmbc_pfg.jxp
Spectrum Type	HMBC
Sweep Width (Hz)	(4000.24, 25113.36)
Temperature (degree C)	21.400
Title	QC-I-57-002



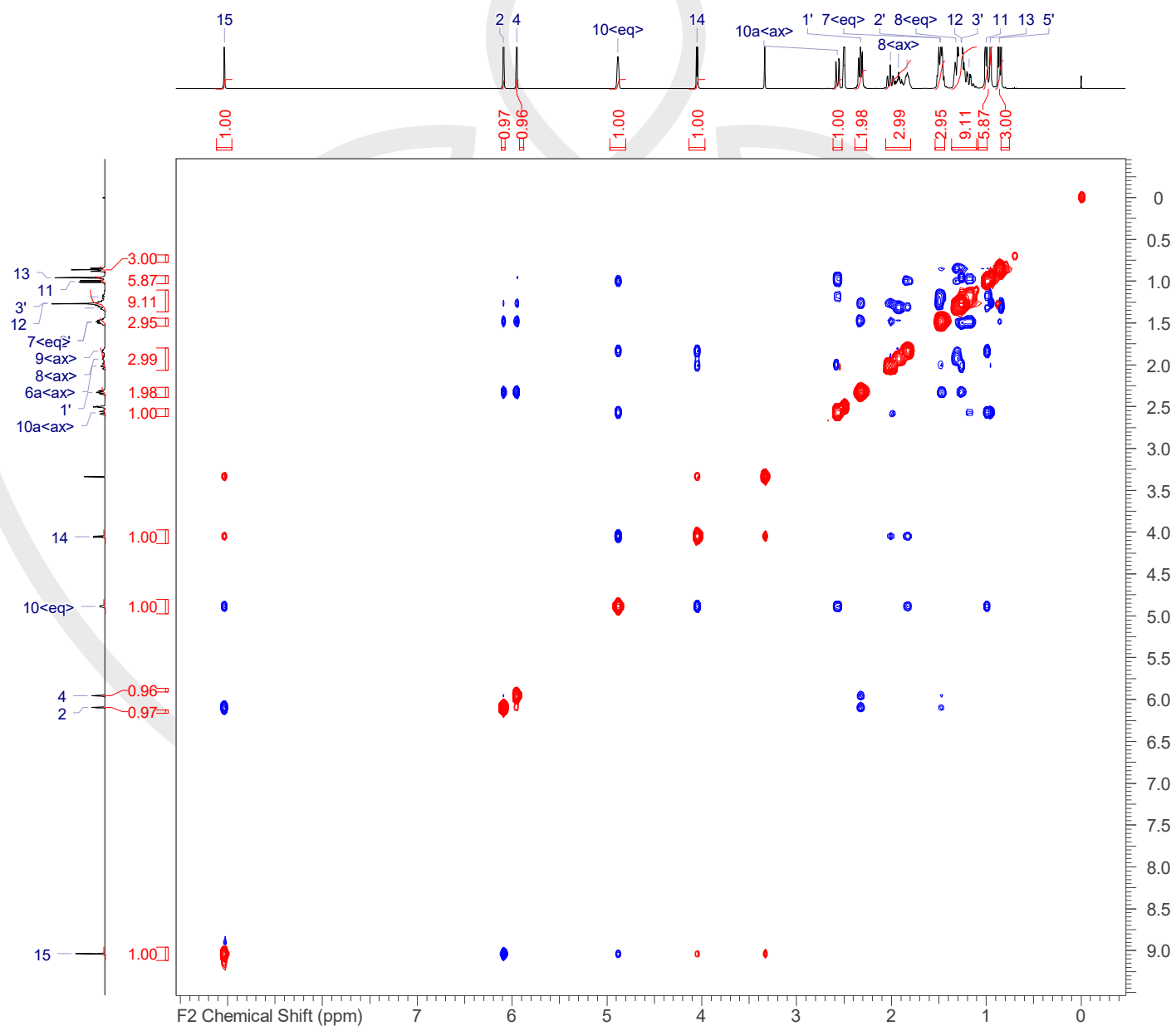
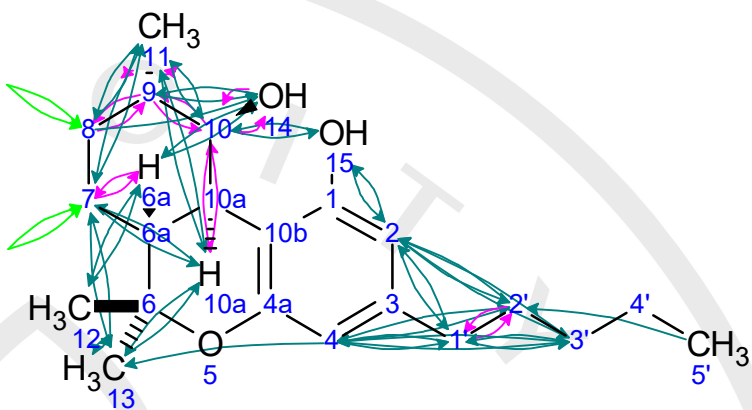
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Frequency (MHz)	(399.5822, 100.4750)
Nucleus	(1H, 13C)
Number of Transients	4
Origin	JEOL ECZ400S Sc v601
Original Points Count	(1999, 512)
Pulse Sequence	hmbc_pfg.jxp
Spectrum Type	HMBC
Sweep Width (Hz)	(4000.24, 25113.36)
Temperature (degree C)	21.400
Title	QC-I-57-002



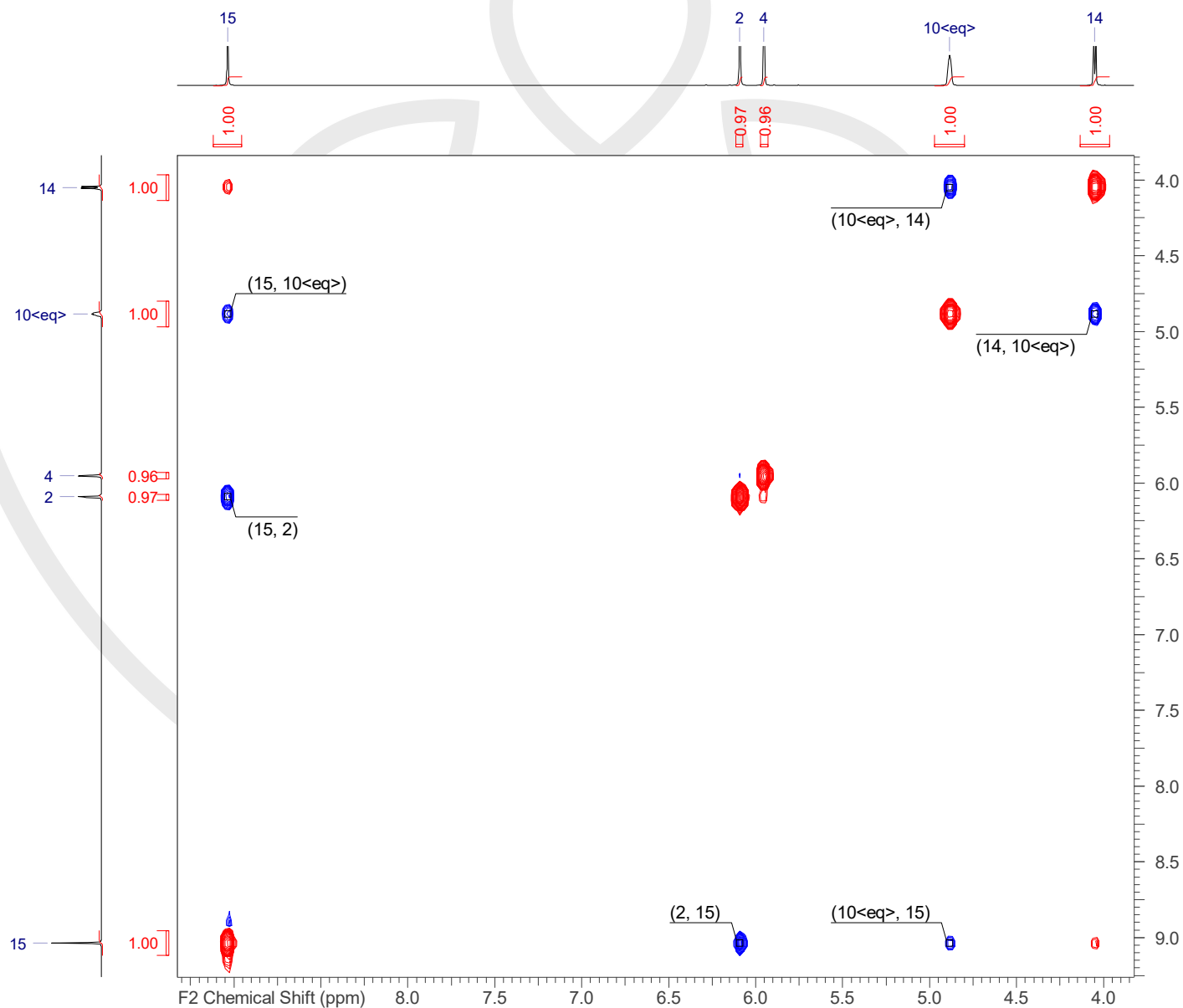
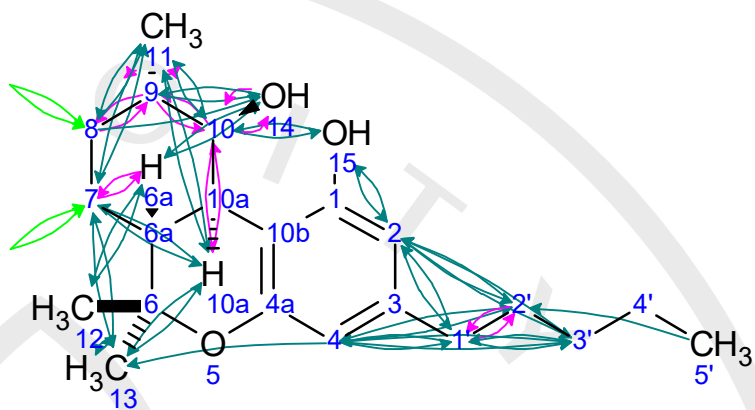
No	F2 Atom	F1 Atom	F2 (ppm)	F1 (ppm)
1	2	1	6.09	156.13
2	10a<ax>	1	2.57	156.13
3	15	1	9.04	156.13
4	2	1'	6.09	34.83
5	2'	1'	1.48	34.83
6	4	1'	5.95	34.83
7	1'	2	2.33	107.07
8	4	2	5.95	107.07
9	1'	2'	2.33	30.23
10	1'	3	2.33	140.67
11	2'	3	1.48	140.67
12	1'	3'	2.33	31.01
13	2'	3'	1.48	31.01
14	4'	3'	1.28	31.01
15	5'	3'	0.86	31.01
16	1'	4	2.33	107.86
17	2	4	6.09	107.86
18	2'	4'	1.48	21.99
19	3'	4'	1.26	21.99
20	5'	4'	0.86	21.99
21	4	4a	5.95	155.66
22	10a<ax>	4a	2.57	155.66
23	12	4a	1.27	155.66
24	6a<ax>	6	2.01	75.77
25	12	6	1.27	75.77
26	13	6	0.96	75.77
27	10<eq>	6a	4.88	40.02
28	10a<ax>	6a	2.57	40.02
29	12	6a	1.27	40.02
30	13	6a	0.96	40.02
31	6a<ax>	7	2.01	22.40
32	9<ax>	7	1.83	22.40
33	10a<ax>	7	2.57	22.40

No	F2 Atom	F1 Atom	F2 (ppm)	F1 (ppm)
34	9<ax>	8	1.83	26.26
35	10<eq>	8	4.88	26.26
36	11	8	1.00	26.26
37	8<ax>	9	1.93	34.97
38	11	9	1.00	34.97
39	6a<ax>	10	2.01	68.82
40	9<ax>	10	1.83	68.82
41	10a<ax>	10	2.57	68.82
42	11	10	1.00	68.82
43	14	10	4.05	68.82
44	6a<ax>	10a	2.01	34.60
45	9<ax>	10a	1.83	34.60
46	14	10a	4.05	34.60
47	4	10b	5.95	108.19
48	10a<ax>	10b	2.57	108.19
49	15	10b	9.04	108.19
50	8<ax>	11	1.93	17.11
51	9<ax>	11	1.83	17.11
52	6a<ax>	12	2.01	27.60
53	13	12	0.96	27.60
54	6a<ax>	13	2.01	18.70
55	12	13	1.27	18.70

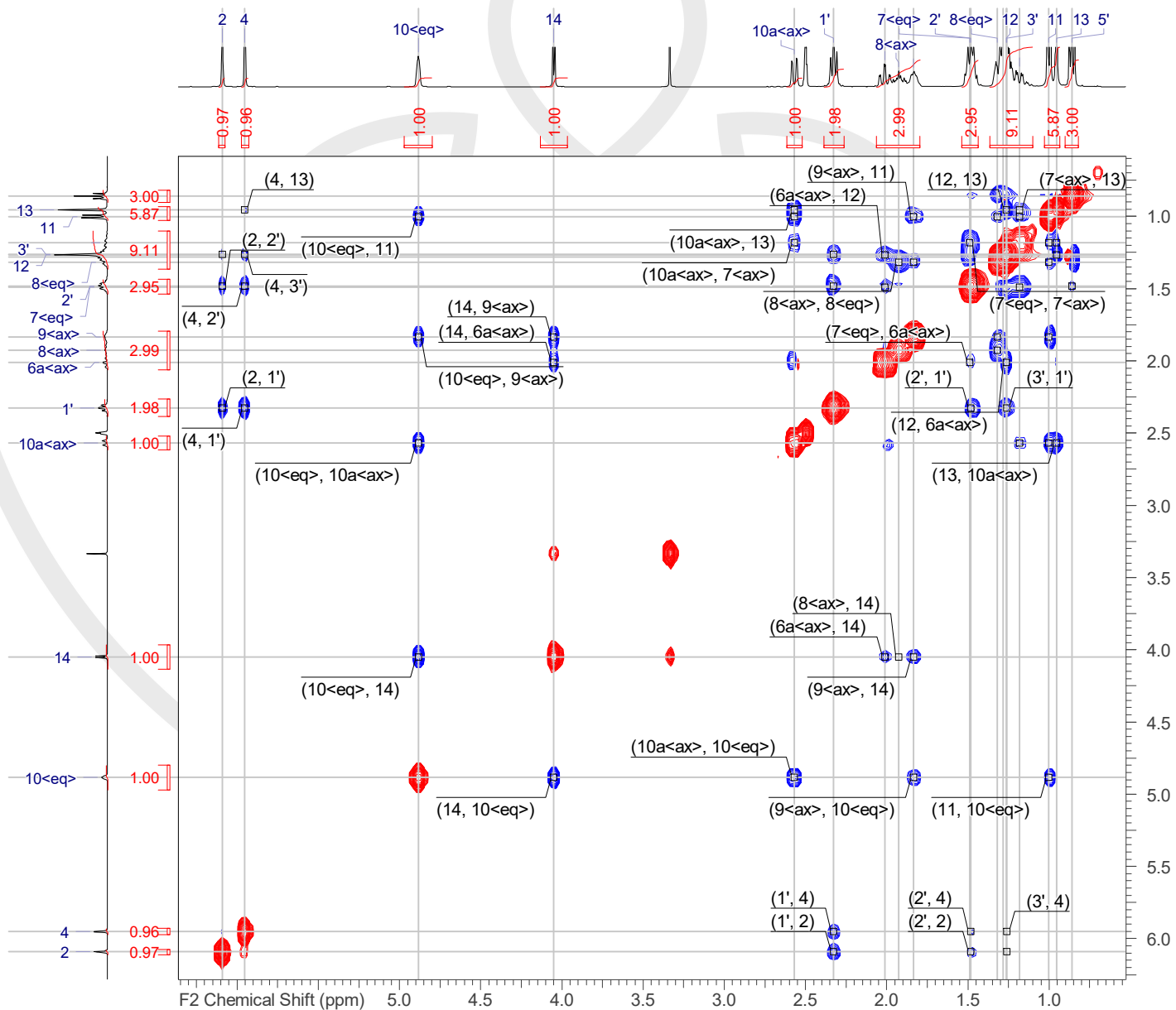
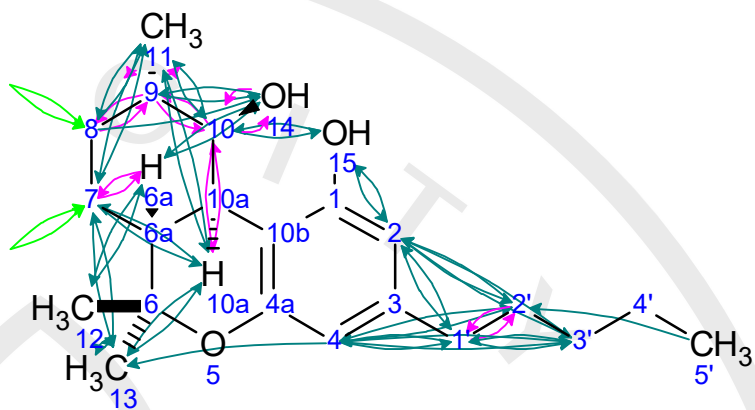
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File Name	\\sulfur\private\nmrdata\JEOL_2023\QC-I-57-002\QC-I-57-002_NOESY_29-Mar-2023-1-1.jdf
Frequency (MHz)	(399.5822, 399.5822)
Nucleus	(1H, 1H)
Number of Transients	4
Origin	JEOL ECZ400S Sc v601
Original Points Count	(2560, 512)
Pulse Sequence	noesy phase pfgz
Spectrum Type	NOESY
Sweep Width (Hz)	(4000.24, 3993.89)
Temperature (degree C)	21.200
Title	QC-I-57-002



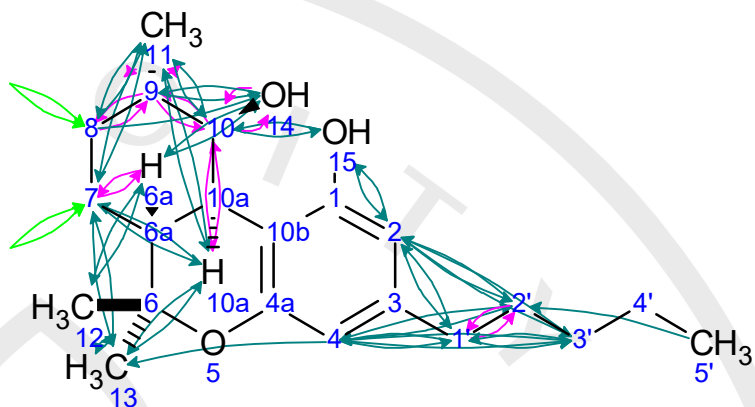
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Frequency (MHz)	(399.5822, 399.5822)
Nucleus	(1H, 1H)
Number of Transients	4
Origin	JEOL ECZ400S Sc v601
Original Points Count	(2560, 512)
Pulse Sequence	noesy phase pfgz
Spectrum Type	NOESY
Sweep Width (Hz)	(4000.24, 3993.89)
Temperature (degree C)	21.200
Title	QC-I-57-002



Acquisition Time (sec)	(0.5120, 0.1281)
Date Stamp	29 Mar 2023 15:38:06
File Name	\\sulfur\private\nmrdata\JEOL_2023\QC-I-57-002\QC-I-57-002_NOESY_29-Mar-2023-1-1.jdf
Frequency (MHz)	(399.5822, 399.5822)
Nucleus	(1H, 1H)
Number of Transients	4
Origin	JEOL ECZ400S Sc v601
Original Points Count	(2560, 512)
Pulse Sequence	noesy phase pfgz
Spectrum Type	NOESY
Sweep Width (Hz)	(4000.24, 3993.89)
Temperature (degree C)	21.200
Title	QC-I-57-002



Acquisition Time (sec)	(0.5120, 0.1281)
Date Stamp	29 Mar 2023 15:38:06
File Name	\\sulfur\private\nmrdata\JEOL_2023\QC-I-57-002\QC-I-57-002_NOESY_29-Mar-2023-1-1.jdf
Frequency (MHz)	(399.5822, 399.5822)
Nucleus	(1H, 1H)
Number of Transients	4
Origin	JEOL ECZ400S Sc v601
Original Points Count	(2560, 512)
Pulse Sequence	noesy phase pfgz
Spectrum Type	NOESY
Sweep Width (Hz)	(4000.24, 3993.89)
Temperature (degree C)	21.200
Title	QC-I-57-002



No	F2 Atom	F1 Atom	F2 (ppm)	F1 (ppm)
1	2	1'	6.09	2.33
2	2'	1'	1.48	2.33
3	3'	1'	1.26	2.33
4	4	1'	5.95	2.33
5	1'	2	2.33	6.09
6	2'	2	1.48	6.09
7	3'	2	1.26	6.09
8	15	2	9.04	6.09
9	1'	2'	2.33	1.48
10	2	2'	6.09	1.48
11	4	2'	5.95	1.48
12	5'	2'	0.86	1.48
13	1'	3'	2.33	1.26
14	2	3'	6.09	1.26
15	4	3'	5.95	1.26
16	1'	4	2.33	5.95
17	2'	4	1.48	5.95
18	3'	4	1.26	5.95
19	7<eq>	6a<ax>	1.49	2.01
20	12	6a<ax>	1.27	2.01
21	14	6a<ax>	4.05	2.01
22	7<eq>	7<ax>	1.49	1.18
23	10a<ax>	7<ax>	2.57	1.18
24	11	7<ax>	1.00	1.18
25	13	7<ax>	0.96	1.18
26	6a<ax>	7<eq>	2.01	1.49
27	7<ax>	7<eq>	1.18	1.49
28	8<eq>	8<ax>	1.32	1.93
29	8<ax>	8<eq>	1.93	1.32
30	9<ax>	8<eq>	1.83	1.32
31	11	8<eq>	1.00	1.32
32	8<eq>	9<ax>	1.32	1.83
33	10<eq>	9<ax>	4.88	1.83

No	F2 Atom	F1 Atom	F2 (ppm)	F1 (ppm)
34	11	9<ax>	1.00	1.83
35	14	9<ax>	4.05	1.83
36	9<ax>	10<eq>	1.83	4.88
37	10a<ax>	10<eq>	2.57	4.88
38	11	10<eq>	1.00	4.88
39	14	10<eq>	4.05	4.88
40	15	10<eq>	9.04	4.88
41	7<ax>	10a<ax>	1.18	2.57
42	10<eq>	10a<ax>	4.88	2.57
43	11	10a<ax>	1.00	2.57
44	13	10a<ax>	0.96	2.57
45	7<ax>	11	1.18	1.00
46	8<eq>	11	1.32	1.00
47	9<ax>	11	1.83	1.00
48	10<eq>	11	4.88	1.00
49	10a<ax>	11	2.57	1.00
50	6a<ax>	12	2.01	1.27
51	13	12	0.96	1.27
52	4	13	5.95	0.96
53	7<ax>	13	1.18	0.96
54	10a<ax>	13	2.57	0.96
55	12	13	1.27	0.96
56	6a<ax>	14	2.01	4.05
57	8<ax>	14	1.93	4.05
58	9<ax>	14	1.83	4.05
59	10<eq>	14	4.88	4.05
60	2	15	6.09	9.04
61	10<eq>	15	4.88	9.04