Electronic Supplementary Material (ESI) for MedChemComm.

T- and B-cell immunosuppressive activity of novel α-santonin analogs with humoral and cellular immune response in Balb/c mice

Nisar A. Dangroo[a], Jasvinder Singh[b,c], Nidhi Gupta[a], Shashank Singh[b,c], Anapurna Kaul[b,c], Mohmmed A. Khuroo[d], and Payare L. Sangwan[a,c,*]

[a]*Bioorganic Chemistry Division,* [b]*Cancer Pharmacology Division, CSIR-Indian Institute of Integrative Medicine, Canal Road Jammu-180001, India*

[c]*Academy of Scientific and Innovative Research (AcSIR), CSIR-IIIM Campus, Jammu, India*

[d]*University of Kashmir, Hazratbal Road, Srinagar, India*

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*Corresponding authors. Tel.: +91 191 2585006-13 Extn. 371; fax +91 191 2586333.

E-mails; plsangwan@iiim.ac.in (P.L. Sangwan)

CONTENTS:

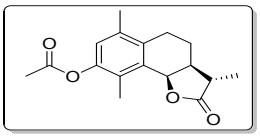
Section A

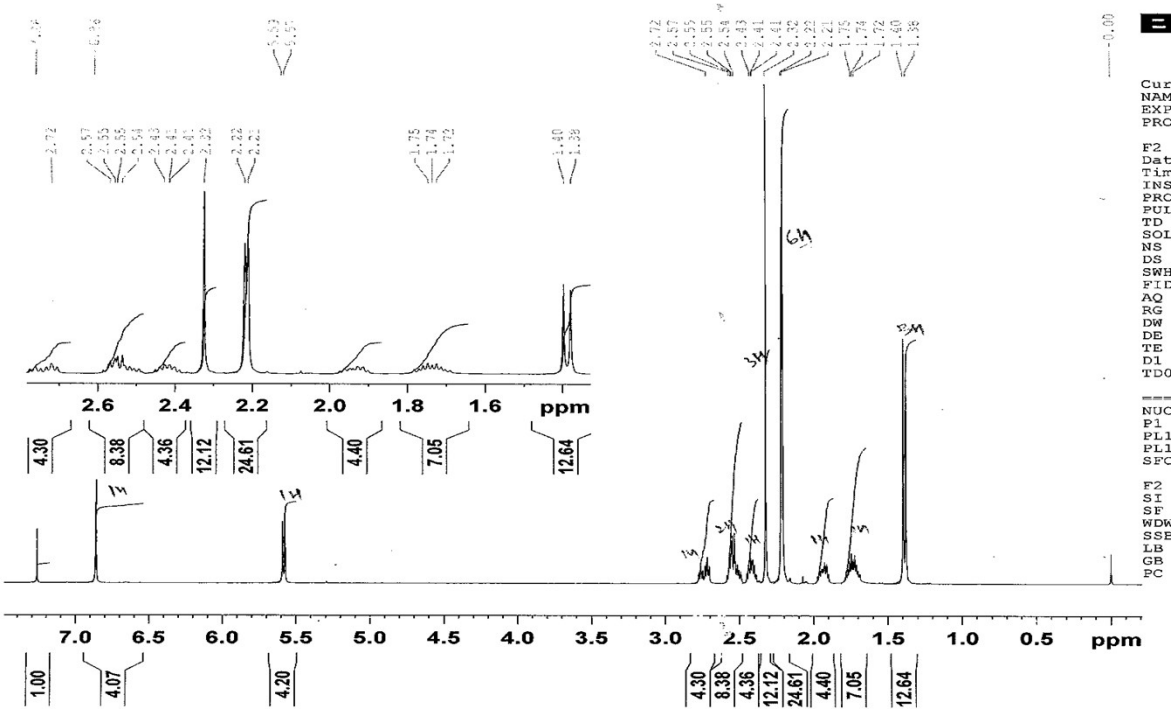
General Methods

All the reagents and solvents for executing the present work were obtained from Sigma Aldrich. Dry DCM was prepared first by distilling it and then refluxing it over CaH_2 (5% w/v) for few hours and again distilled it and finally stored it over 4A° molecular sieves for future use. Pyridine was dried over KOH for one week, then distilled and stored over 4A° molecular sieves and used throughout the synthesis. All the chemical reactions were monitored by TLC on 0.25 mm silica gel 60 F254 plates (E. Merck) using 2% ceric ammonium sulphate solution as a spraying reagent for detection of the spots on the TLC. Purification of all the compounds was carried out by column chromatography using Silica gel 60-120 mesh stationary phase or by recrystillation. ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker DPX 400 and DPX 500 instruments using $CDCl_3$ or CD_3OD as the solvents with TMS as internal standard. The chemical shifts were expressed in ǒ ppm and coupling constants in Hertz. High resolution mass spectra (HREIMS) were recorded on Agilent Technologies 6540 instrument.

Section B: ^{1}H NMR, ^{13}C NMR, DEPT135 and HRMS spectra of compounds

2- ^{1}H NMR





2- HRMS

Data File	SN-AC.d	**Sample Name**	SN-AC
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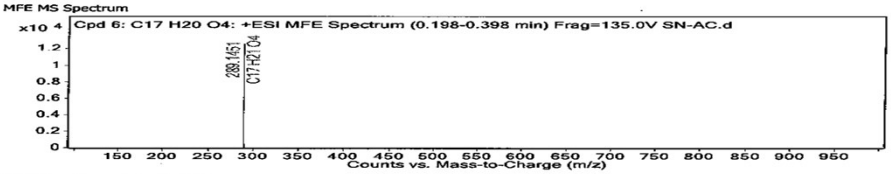
Instrument Name	Instrument 1	**User Name**	
Acq Method	vishal_12-01-13.m	**Acquired Time**	04-06-2015 PM 2:28:06
IRM Calibration Status	[redacted]	**DA Method**	daily_report.m
Comment			
Sample Group	**Info.**		
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)		

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 6: C17 H20 O4	0.26	288.1382	C17 H20 O4	C17 H20 O4	-7.19	C17 H20 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 6: C17 H20 O4	289.1451	0.26	Find by Molecular Feature	288.1382

MFE MS Spectrum



MS Spectrum Peak List

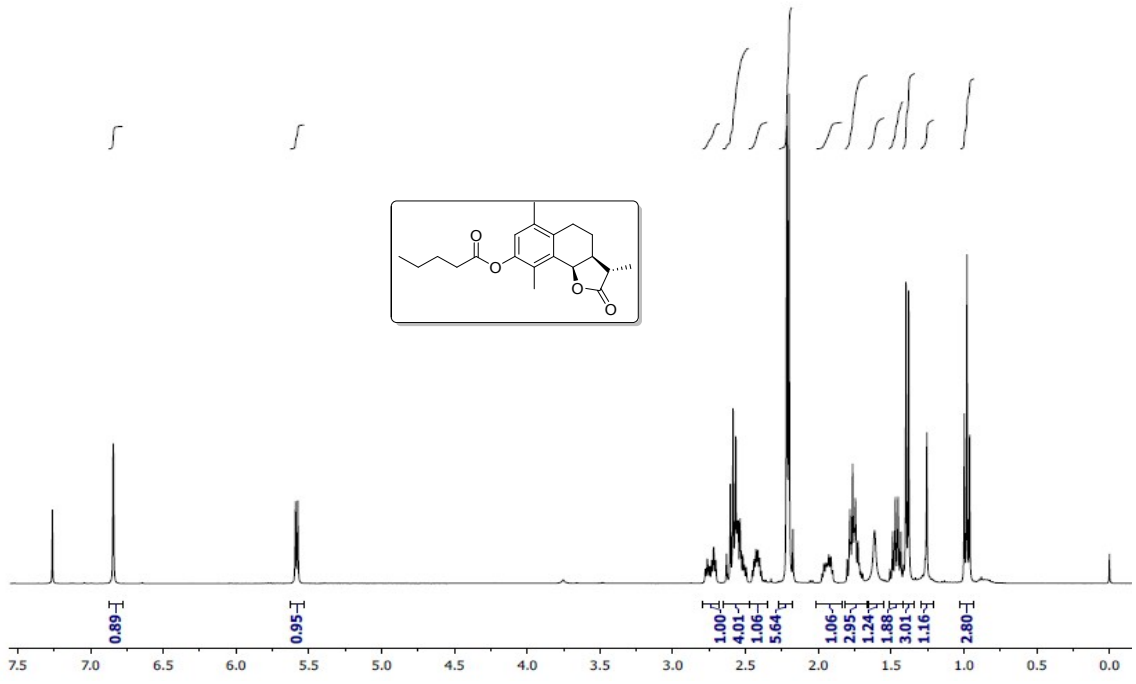
m/z	z	Abund	Formula	Ion
289.1451	1	12623.54	C17 H21 O4	(M+H)+
290.1499	1	2400.3	C17 H21 O4	(M+H)+
291.1572	1	428.05	C17 H21 O4	(M+H)+

Predicted Isotope Match Table

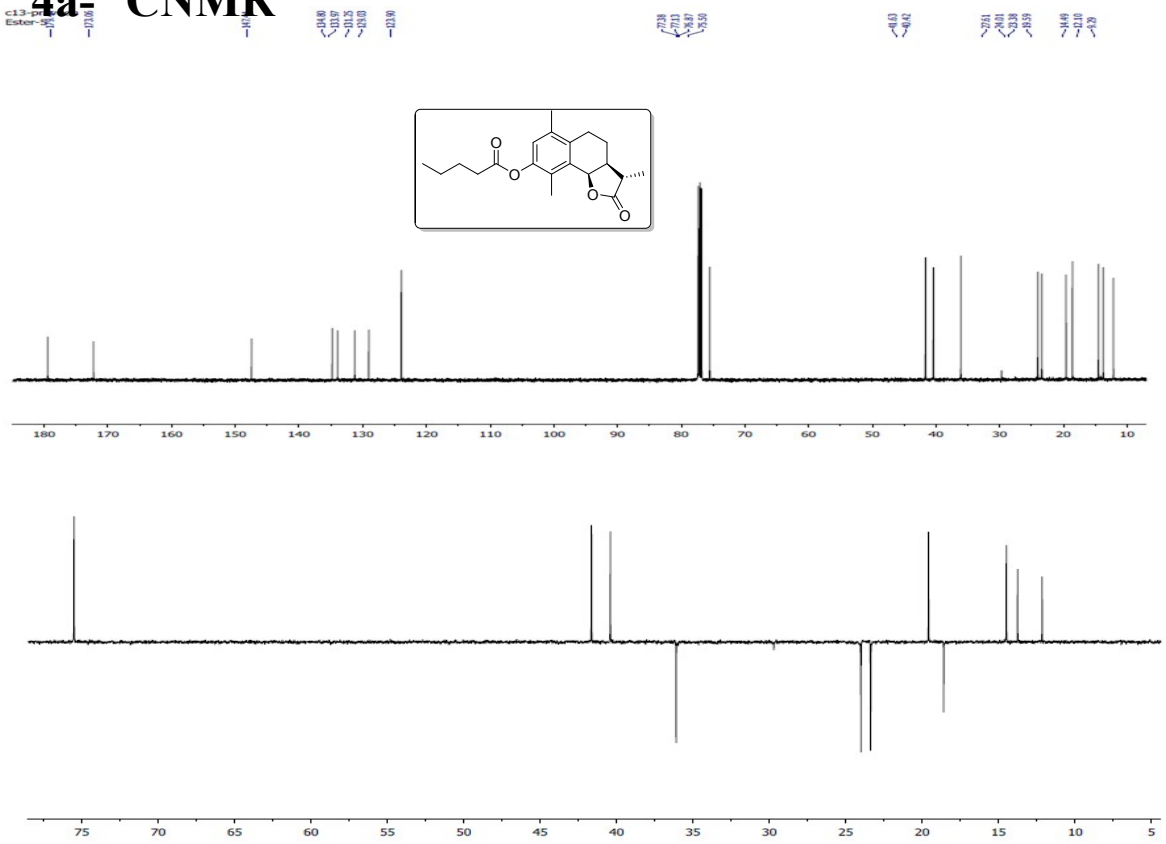
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	289.1451	289.1434	-5.85	100	100	81.7	82.46
2	290.1499	290.1468	-10.47	19.01	18.78	15.53	15.49
3	291.1572	291.1494	-26.96	3.39	2.49	2.77	2.05

--- End Of Report ---

4a-^{1}H NMR



4a-^{13}CNMR



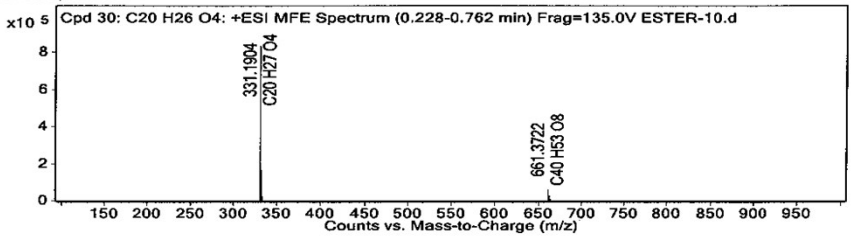
4a-HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 30: C20 H26 O4	0.343	330.1832	C20 H26 O4	C20 H26 O4	-0.22	C20 H26 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 30: C20 H26 O4	331.1904	0.343	Find by Molecular Feature	330.1832

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
331.1904	1	833862.25	C20 H27 O4	(M+H)+
332.194	1	166759.95	C20 H27 O4	(M+H)+
333.1971	1	23436.2	C20 H27 O4	(M+H)+
661.3722	1	62812.54	C40 H53 O8	(2M+H)+
662.3752	1	27424.81	C40 H53 O8	(2M+H)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	331.1904	331.1904	-0.06	100	100	80.98	79.61
2	332.194	332.1938	-0.63	20	22.09	16.2	17.59
3	333.1971	333.1965	-1.7	2.81	3.15	2.28	2.5
4	334.2004	334.1992	-3.53	0.56	0.34	0.46	0.27
5	335.2051	335.2019	-9.51	0.11	0.03	0.09	0.02

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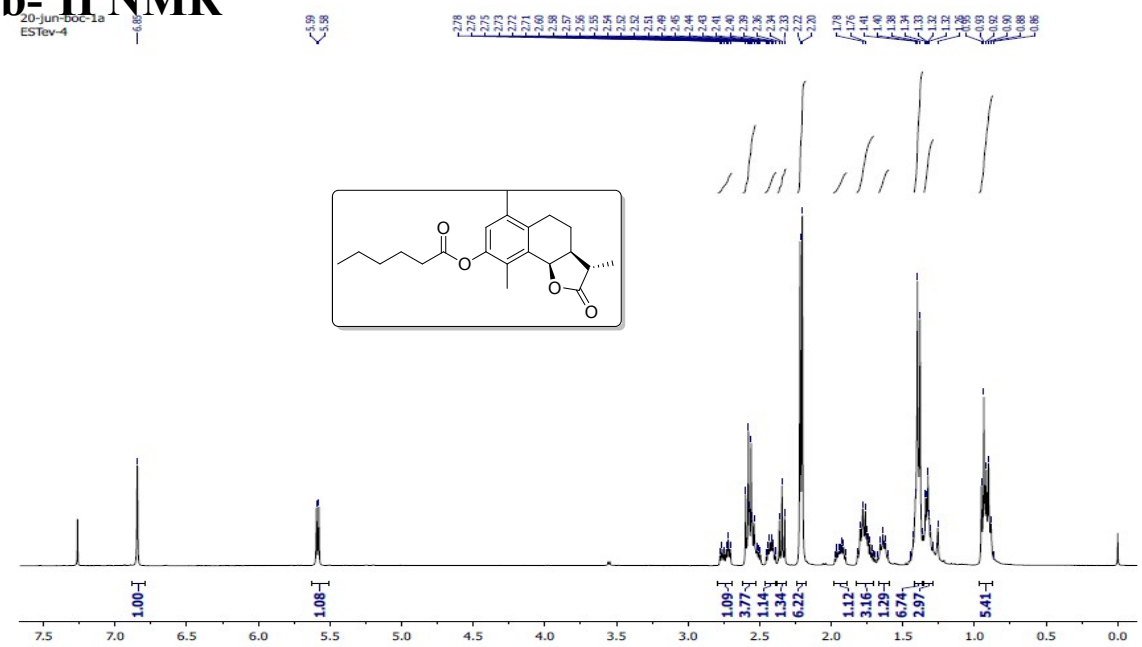
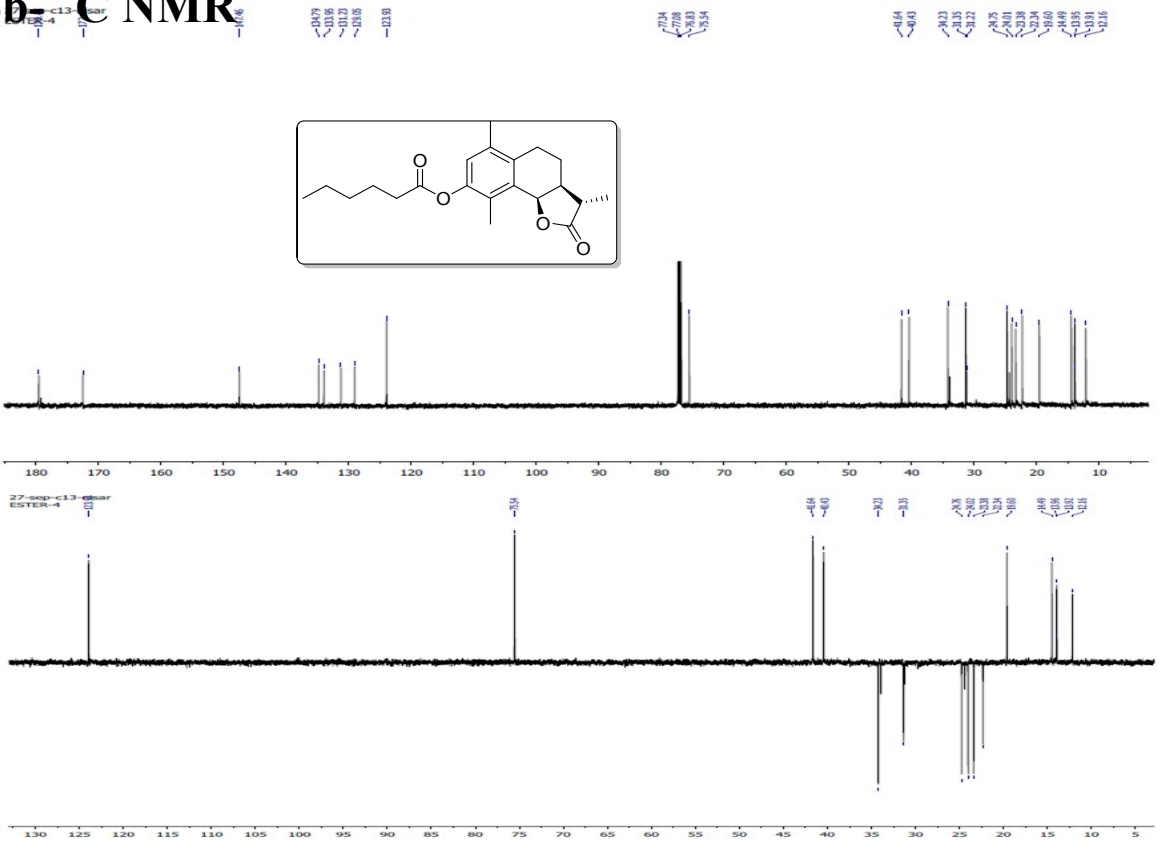
4b-^{1}H NMR



4b-^{13}C NMR



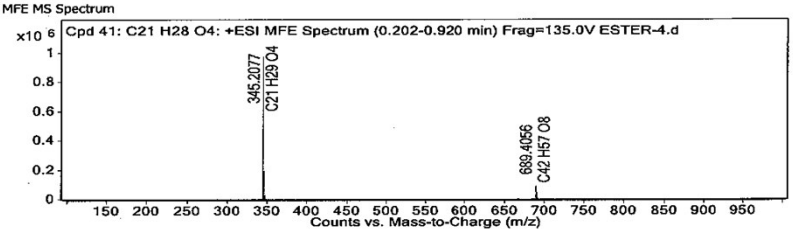
4b-HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 41: C21 H28 O4	0.344	344.2005	C21 H28 O4	C21 H28 O4	-4.99	C21 H28 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 41: C21 H28 O4	345.2077	0.344	Find by Molecular Feature	344.2005

MFE MS Spectrum



MS Spectrum Peak List

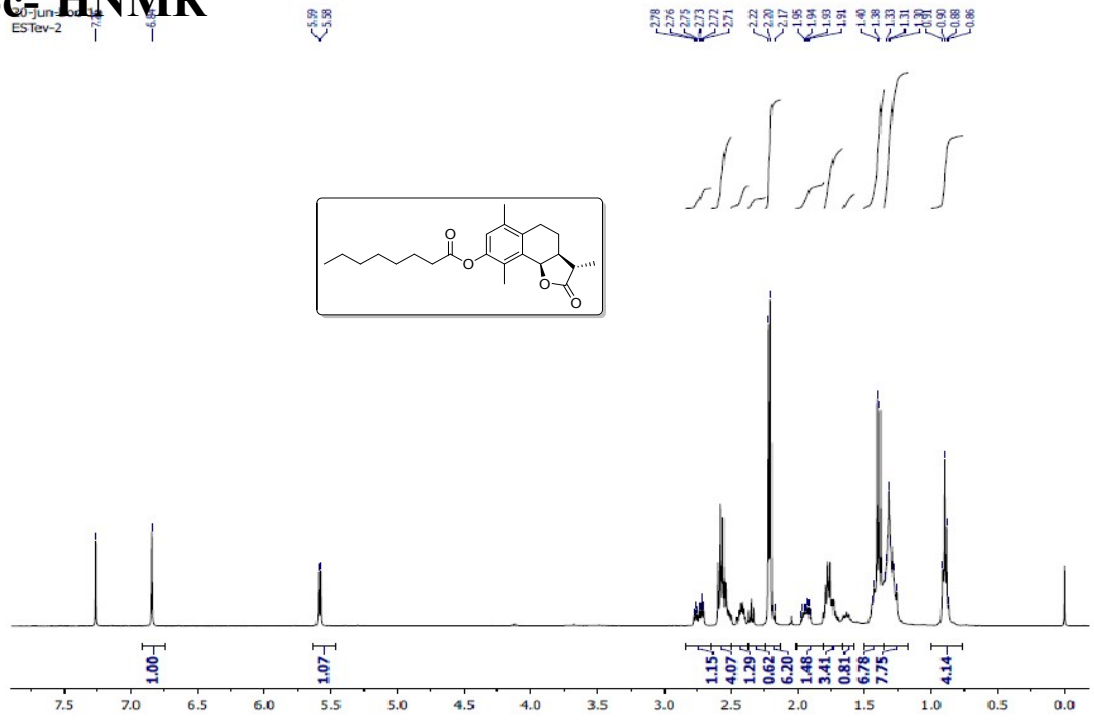
m/z	z	Abund	Formula	Ion
345.2077	1	971585.25	C21 H29 O4	(M+H)+
346.2113	1	191310.58	C21 H29 O4	(M+H)+
347.2138	1	29088.8	C21 H29 O4	(M+H)+
689.4056	1	87788.53	C42 H57 O8	(2M+H)+
690.409	1	41244.23	C42 H57 O8	(2M+H)+

Predicted Isotope Match Table

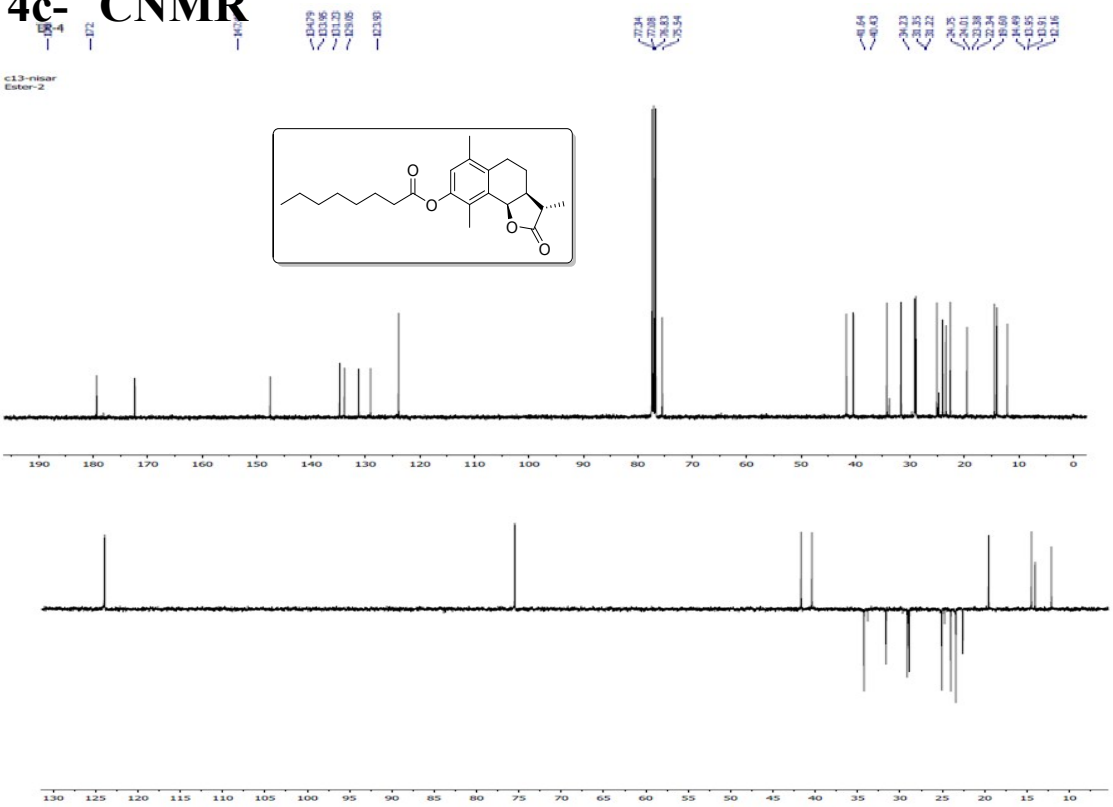
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	345.2077	345.206	-4.89	100	100	81.12	78.74
2	346.2113	346.2094	-5.32	19.69	23.2	15.97	18.27
3	347.2138	347.2122	-4.53	2.99	3.39	2.43	2.67
4	348.2179	348.2149	-8.42	0.5	0.37	0.41	0.29
5	349.2218	349.2176	-11.92	0.09	0.03	0.07	0.03

--- End Of Report ---

4c-^{1}HNMR



4c-^{13}CNMR



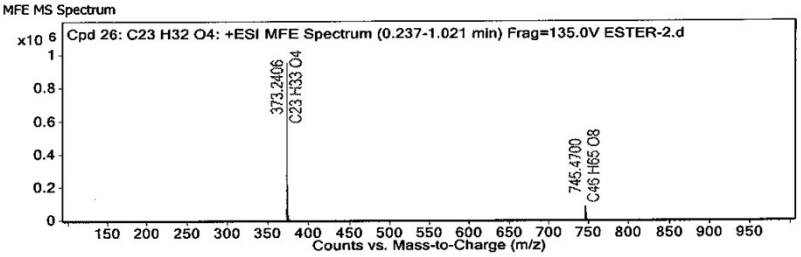
4c-HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 26: C23 H32 O4	0.344	372.2334	C23 H32 O4	C23 H32 O4	-8.95	C23 H32 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 26: C23 H32 O4	373.2406	0.344	Find by Molecular Feature	372.2334

MFE MS Spectrum



MS Spectrum Peak List

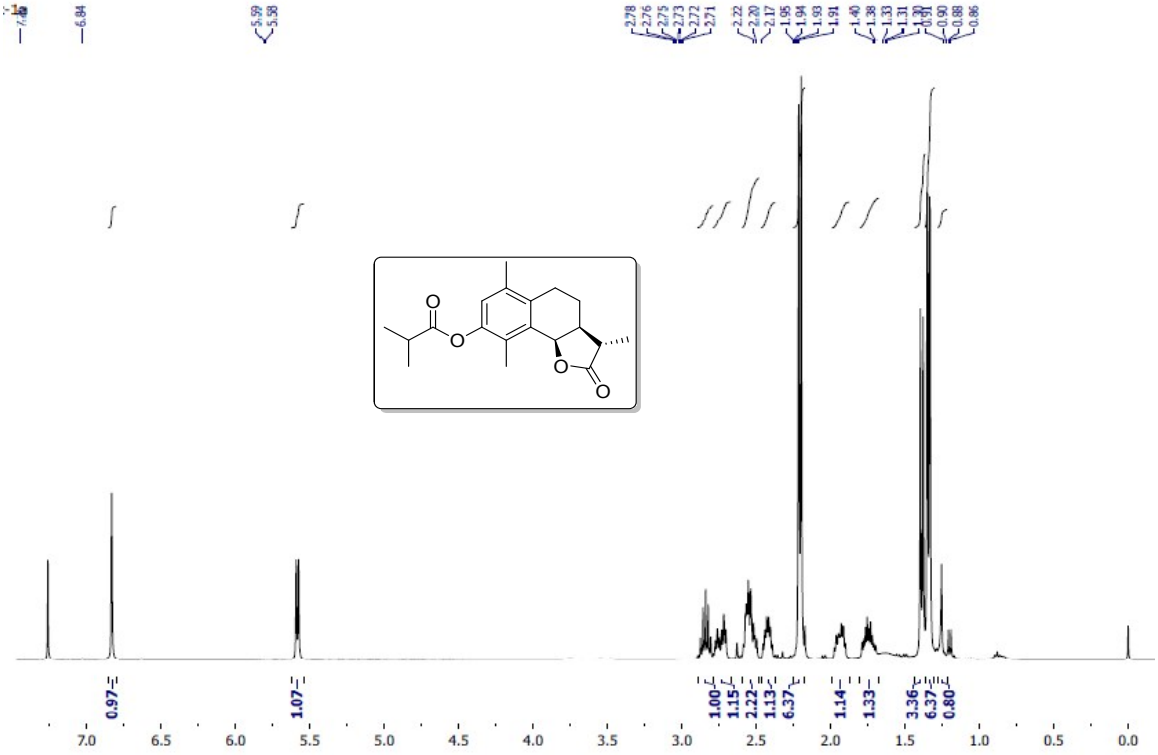
m/z	z	Abund	Formula	Ion
373.2406	1	952065.63	C23 H33 O4	(M+H)+
374.2443	1	215911.33	C23 H33 O4	(M+H)+
375.2469	1	34384.83	C23 H33 O4	(M+H)+
745.47	1	80257.11	C46 H65 O8	(2M+H)+
746.4734	1	44637.95	C46 H65 O8	(2M+H)+

Predicted Isotope Match Table

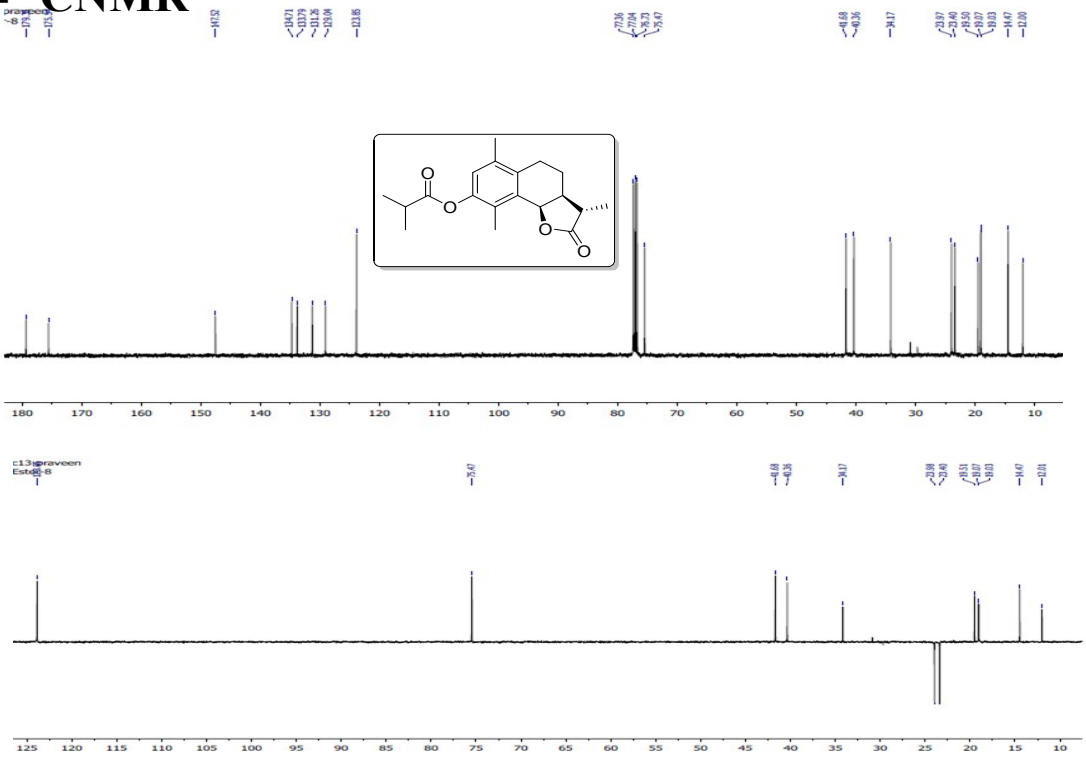
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	373.2406	373.2373	-8.81	100	100	78.8	77.03
2	374.2443	374.2407	-9.49	22.68	25.41	17.87	19.57
3	375.2469	375.2436	-8.72	3.61	3.92	2.85	3.02
4	376.2494	376.2464	-8.15	0.55	0.45	0.44	0.35
5	377.2498	377.2491	-1.94	0.06	0.04	0.05	0.03

--- End Of Report ---

4d-^{1}HNMR



4d-^{13}CNMR



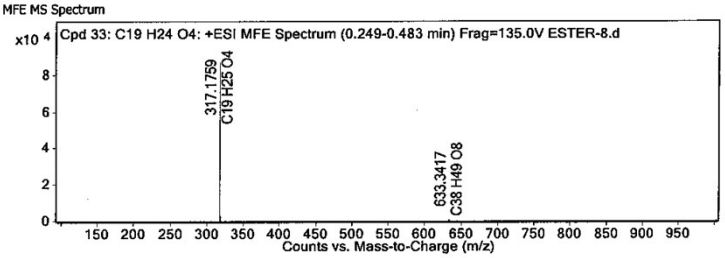
4d-HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 33: C19 H24 O4	0.344	316.1686	C19 H24 O4	C19 H24 O4	-3.7	C19 H24 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 33: C19 H24 O4	317.1759	0.344	Find by Molecular Feature	316.1686

MFE MS Spectrum



MS Spectrum Peak List

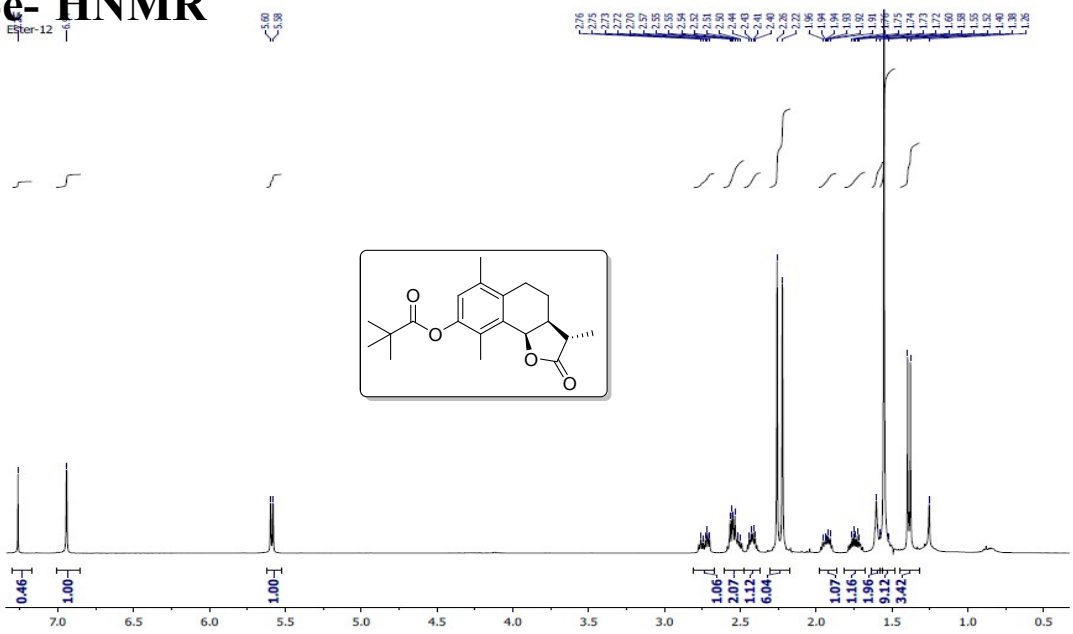
m/z	z	Abund	Formula	Ion
317.1759	1	86736.3	C19 H25 O4	(M+H)+
318.1794	1	16992.7	C19 H25 O4	(M+H)+
319.1825	1	2939.97	C19 H25 O4	(M+H)+
633.3417	1	729.04	C38 H49 O8	(2M+H)+
634.344	1	351.9	C38 H49 O8	(2M+H)+

Predicted Isotope Match Table

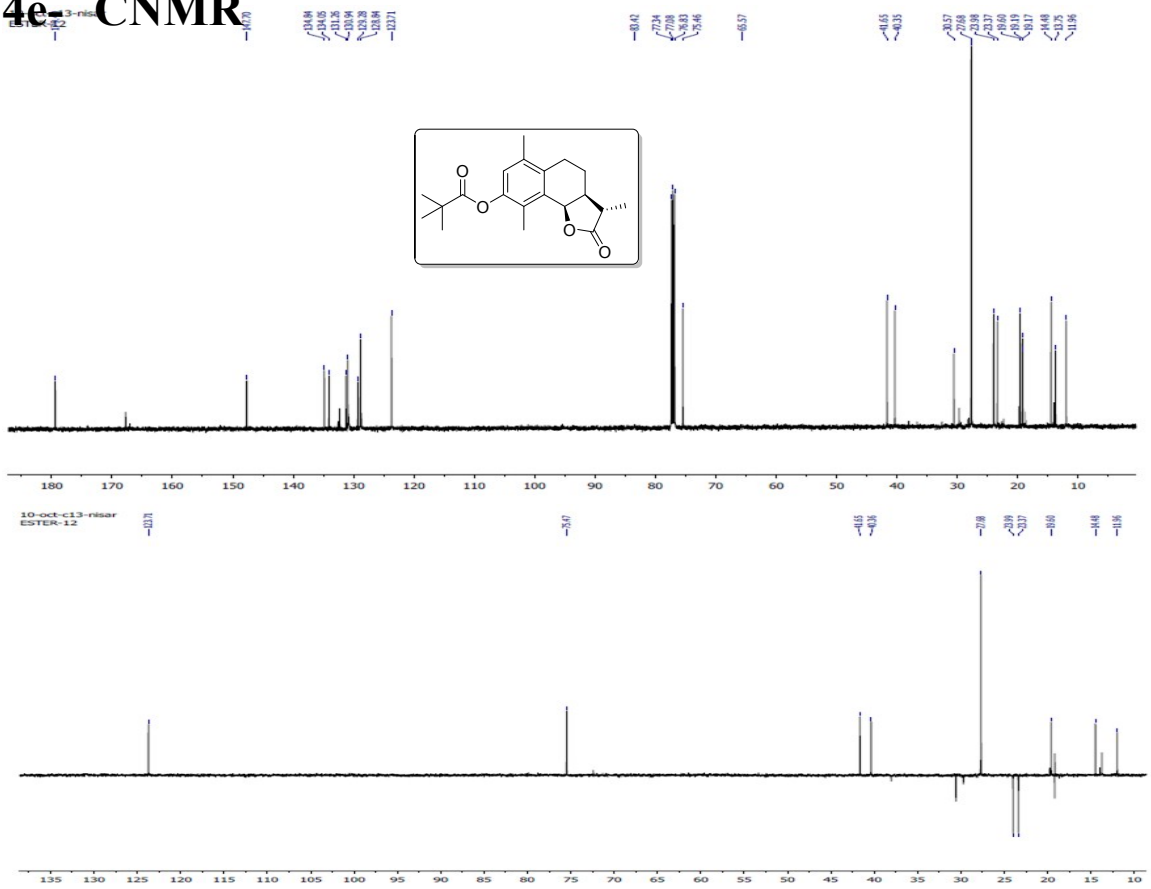
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	317.1759	317.1747	-3.58	100	100	81.31	80.71
2	318.1794	318.1781	-3.95	19.59	20.99	15.93	16.94
3	319.1825	319.1808	-5.24	3.39	2.91	2.76	2.35

--- End Of Report ---

4e-^{1}HNMR



4e-^{13}CNMR



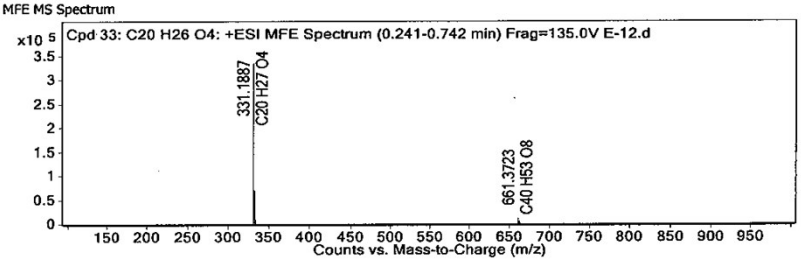
4e-HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 33: C20 H26 O4	0.341	330.1815	C20 H26 O4	C20 H26 O4	4.9	C20 H26 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 33: C20 H26 O4	331.1887	0.341	Find by Molecular Feature	330.1815

MFE MS Spectrum



MS Spectrum Peak List

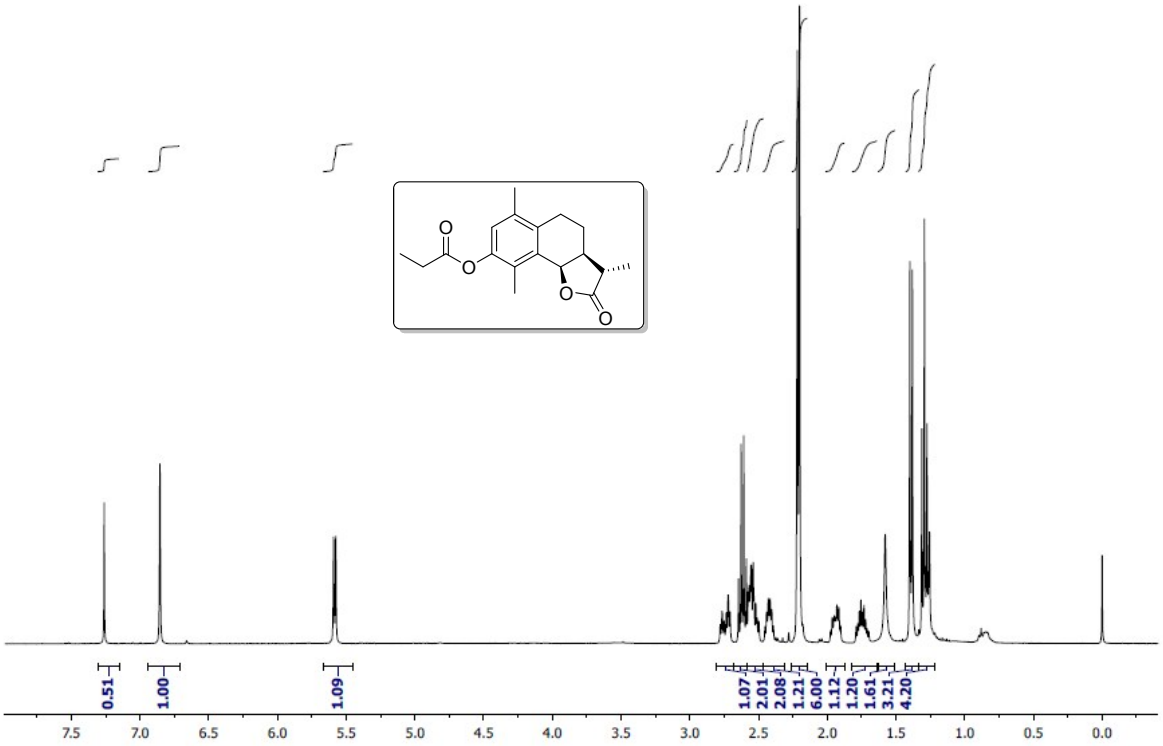
m/z	z	Abund	Formula	Ion
331.1887	1	334444.03	C20 H27 O4	(M+H)+
332.1923	1	70161.08	C20 H27 O4	(M+H)+
333.195	1	10302.89	C20 H27 O4	(M+H)+
661.3723	1	11072.51	C40 H53 O8	(2M+H)+
662.3768	1	5044.16	C40 H53 O8	(2M+H)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	331.1887	331.1904	4.96	100	100	80.16	79.63
2	332.1923	332.1938	4.51	20.98	22.09	16.82	17.59
3	333.195	333.1965	4.53	3.08	3.15	2.47	2.51
4	334.1971	334.1992	6.41	0.69	0.34	0.56	0.27

--- End Of Report ---

4f-^{1}HNMR



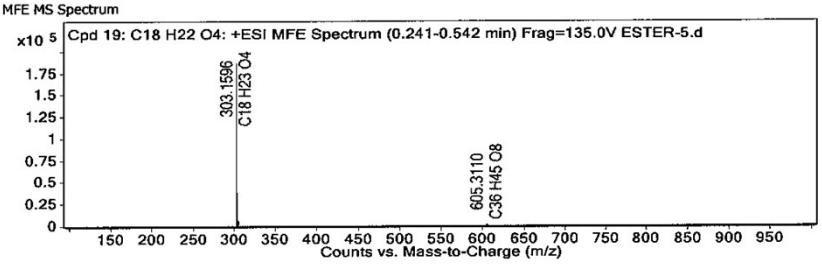
4f-HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 19: C18 H22 O4	0.342	302.1523	C18 H22 O4	C18 H22 O4	-1.62	C18 H22 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 19: C18 H22 O4	303.1596	0.342	Find by Molecular Feature	302.1523

MFE MS Spectrum



MS Spectrum Peak List

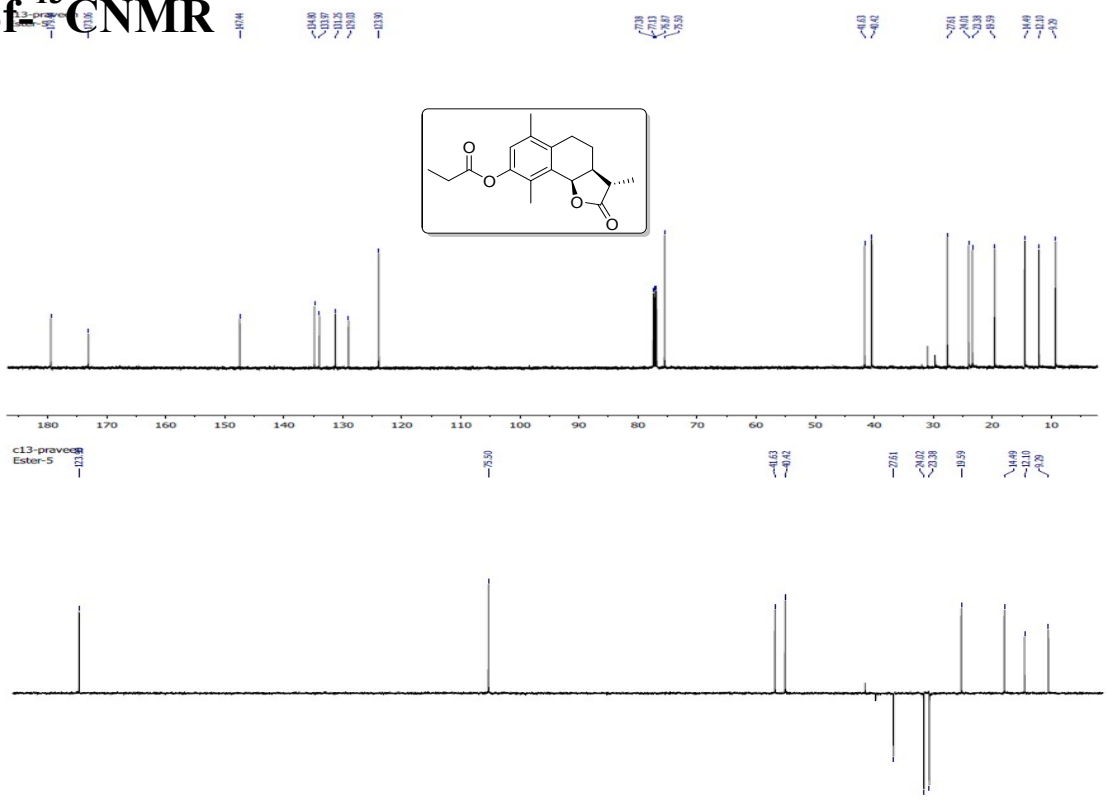
m/z	z	Abund	Formula	Ion
303.1596	1	186029.88	C18 H23 O4	(M+H)+
304.1627	1	37429.66	C18 H23 O4	(M+H)+
305.1659	1	6819.66	C18 H23 O4	(M+H)+
605.311	1	2413.01	C36 H45 O8	(2M+H)+
606.3158	1	883.95	C36 H45 O8	(2M+H)+

Predicted Isotope Match Table

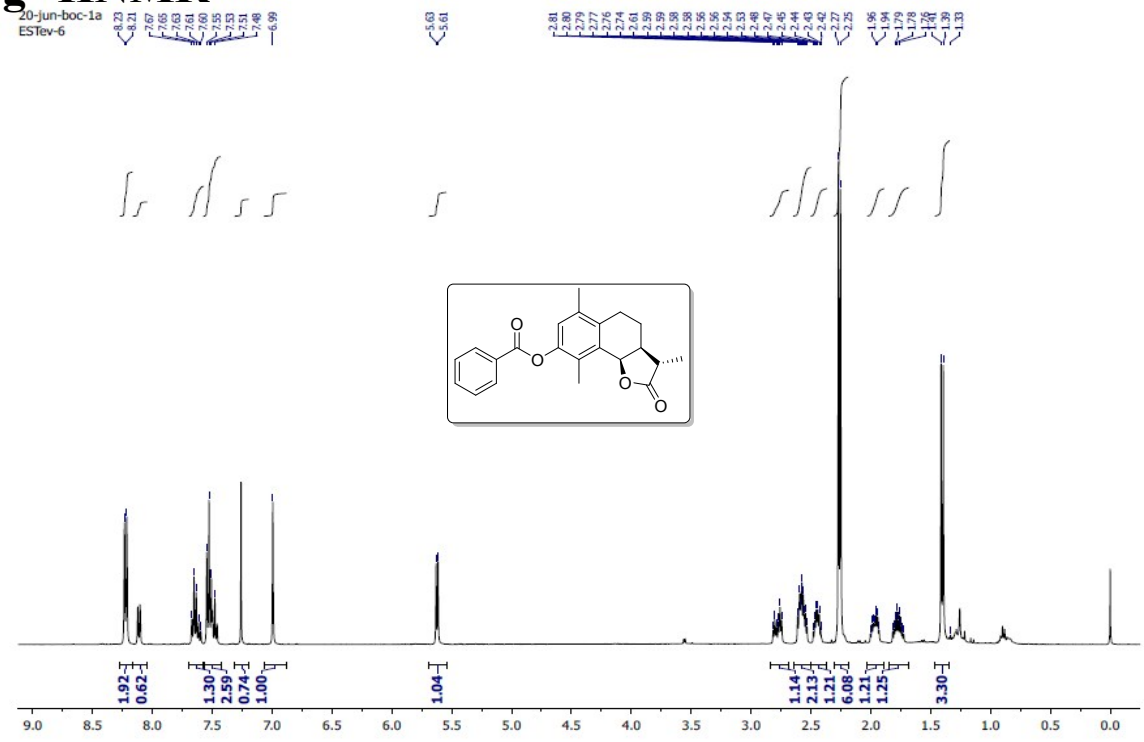
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	303.1596	303.1591	-1.79	100	100	80.78	81.58
2	304.1627	304.1625	-0.56	20.12	19.89	16.25	16.22
3	305.1659	305.1651	-2.54	3.67	2.69	2.96	2.2

--- End Of Report ---

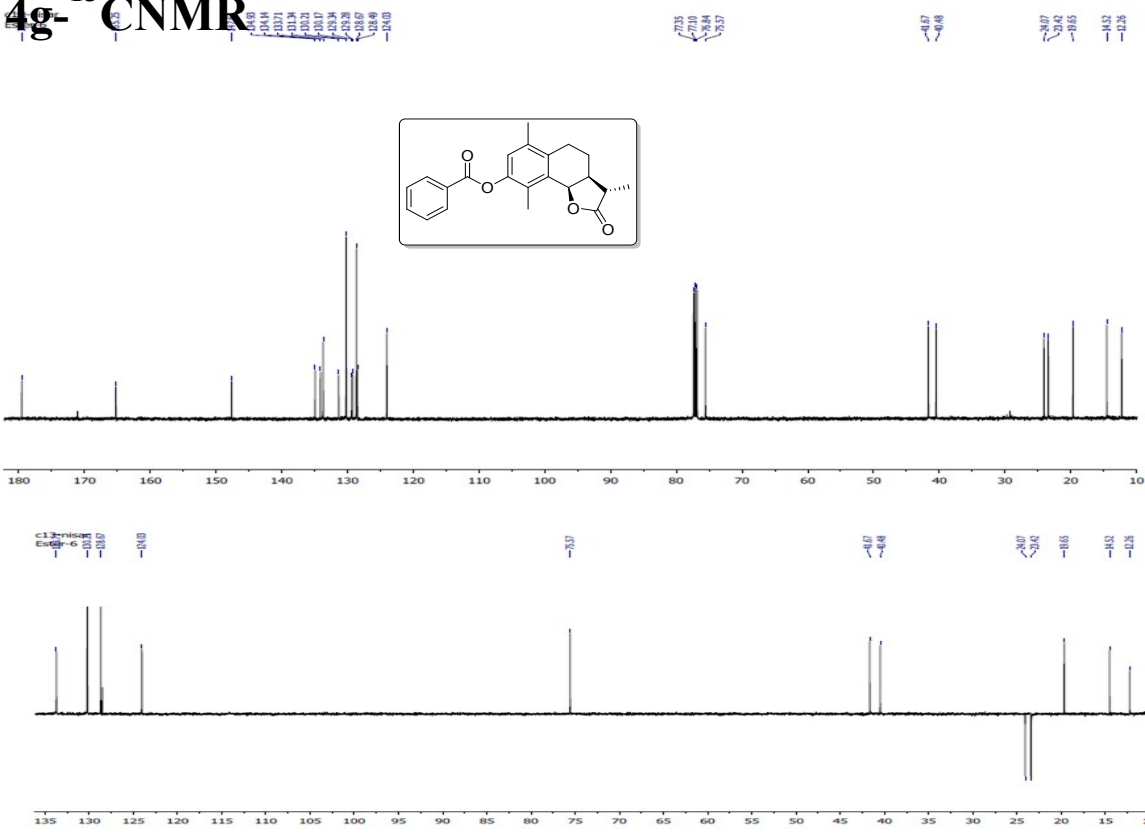
4f-^{13}CNMR



4g-^{1}HNMR



4g- ^{13}CNMR



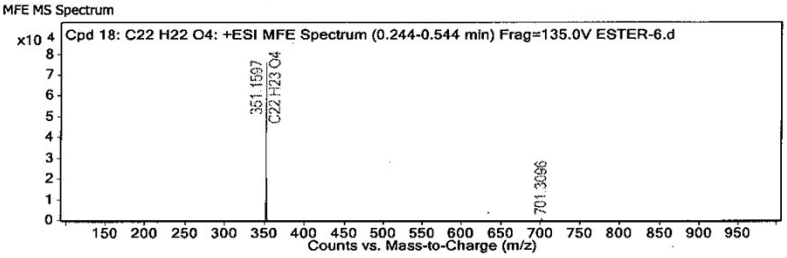
4g-HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 18: C22 H22 O4	0.341	350.1525	C22 H22 O4	C22 H22 O4	-1.91	C22 H22 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 18: C22 H22 O4	351.1597	0.341	Find by Molecular Feature	350.1525

MFE MS Spectrum



MS Spectrum Peak List

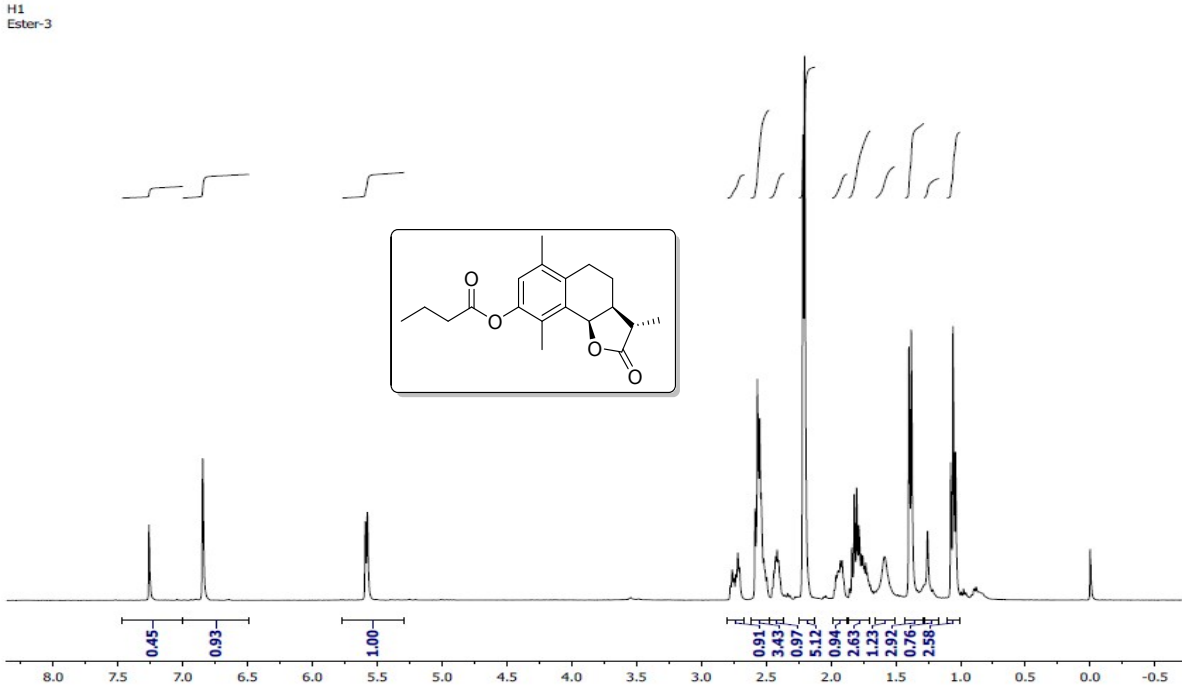
m/z	z	Abund	Formula	Ion
351.1597	1	75530.73	C22 H23 O4	(M+H)+
352.1631	1	20453.84	C22 H23 O4	(M+H)+
353.1665	1	3656.73	C22 H23 O4	(M+H)+
701.3096	1	807.34		(2M+H)+
702.3148	1	583.45		(2M+H)+

Predicted Isotope Match Table

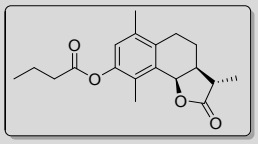
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	351.1597	351.1591	-1.88	100	100	75.44	77.98
2	352.1631	352.1625	-1.7	27.08	24.21	20.43	18.88
3	353.1665	353.1653	-3.33	4.84	3.62	3.65	2.83
4	354.1692	354.168	-3.3	0.63	0.41	0.48	0.32

--- End Of Report ---

4h-^{1}HNMR



4h-^{13}CNMR



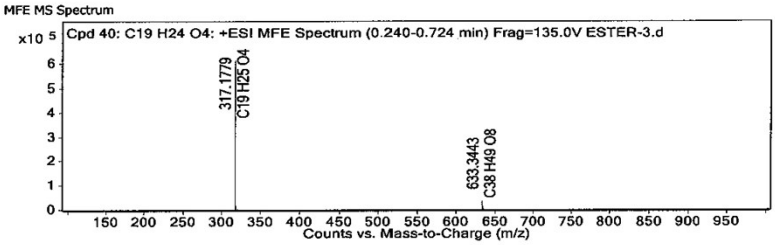
4h-HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 40: C19 H24 O4	0.344	316.1706	C19 H24 O4	C19 H24 O4	-9.8	C19 H24 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 40: C19 H24 O4	317.1779	0.344	Find by Molecular Feature	316.1706

MFE MS Spectrum



MS Spectrum Peak List

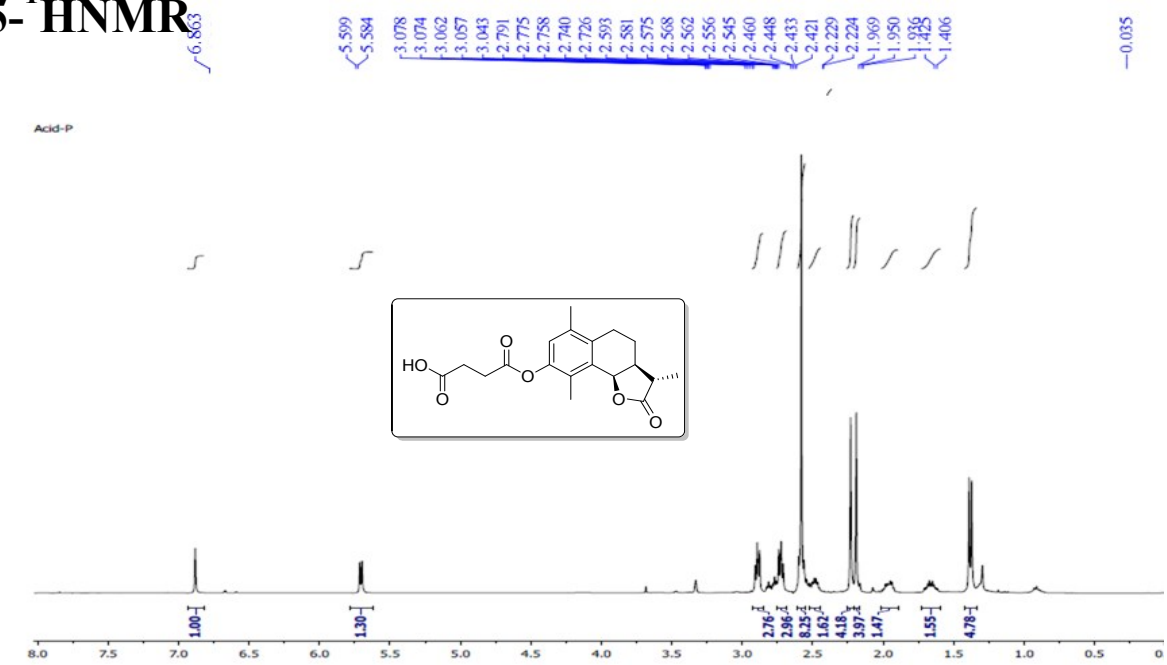
m/z	z	Abund	Formula	Ion
317.1779	1	614381.19	C19 H25 O4	(M+H)+
318.1808	1	115471.52	C19 H25 O4	(M+H)+
319.1834	1	16288.95	C19 H25 O4	(M+H)+
633.3443	1	33324.07	C38 H49 O8	(2M+H)+
634.3478	1	14670.79	C38 H49 O8	(2M+H)+

Predicted Isotope Match Table

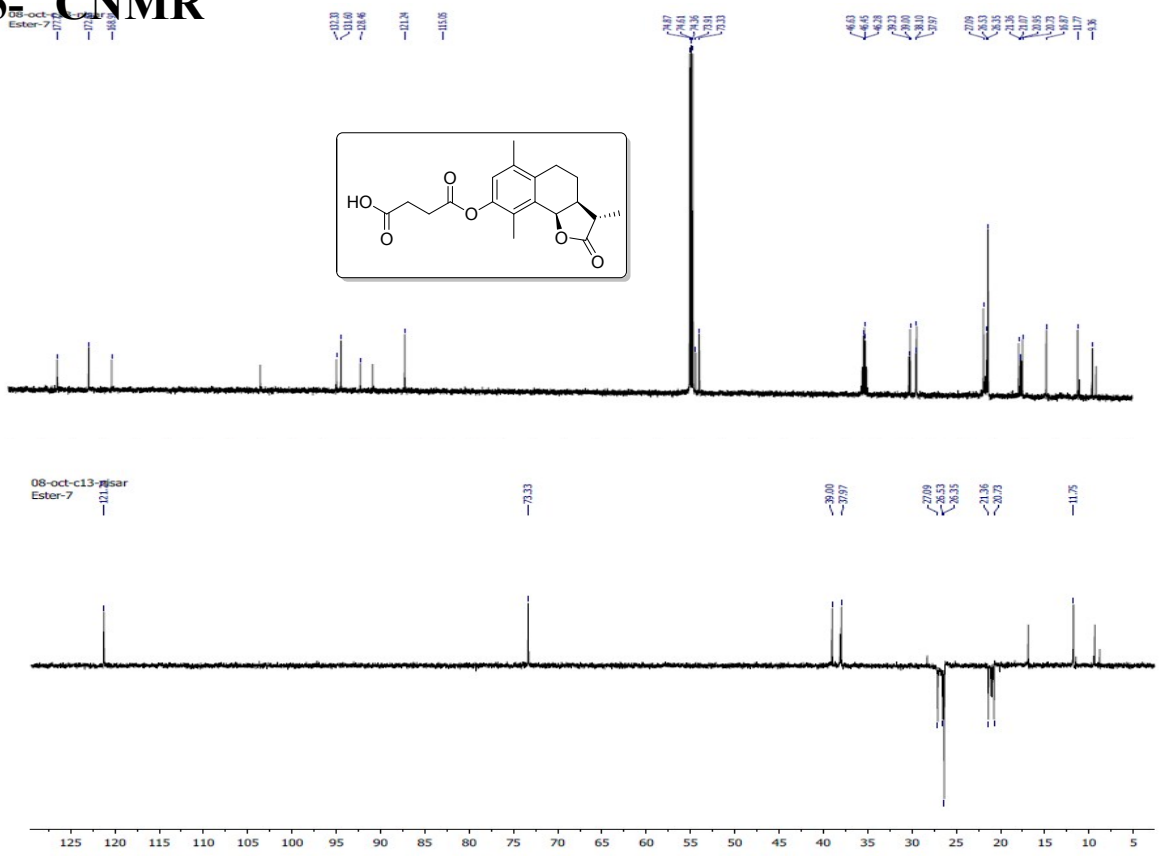
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	317.1779	317.1747	-10.05	100	100	81.99	80.49
2	318.1808	318.1781	-8.41	18.79	20.99	15.41	16.9
3	319.1834	319.1808	-8.22	2.65	2.91	2.17	2.35
4	320.1875	320.1835	-12.59	0.44	0.3	0.36	0.24
5	321.1868	321.1861	-2.12	0.08	0.03	0.06	0.02

--- End Of Report ---

5-^{1}HNMR



5-^{13}CNMR



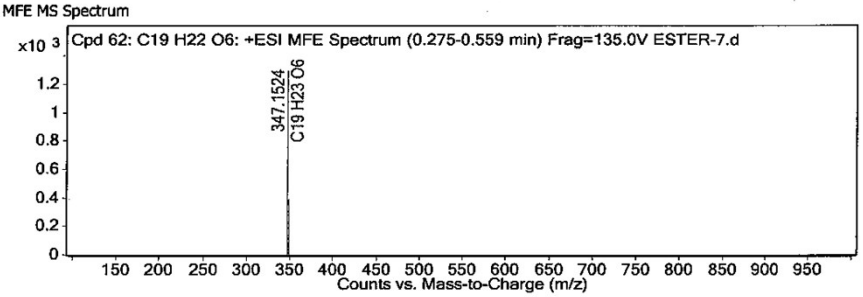
5-HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 62: C19 H22 O6	0.359	346.143	C19 H22 O6	C19 H22 O6	-4.03	C19 H22 O6

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 62: C19 H22 O6	347.1524	0.359	Find by Molecular Feature	346.143

MFE MS Spectrum



MS Spectrum Peak List

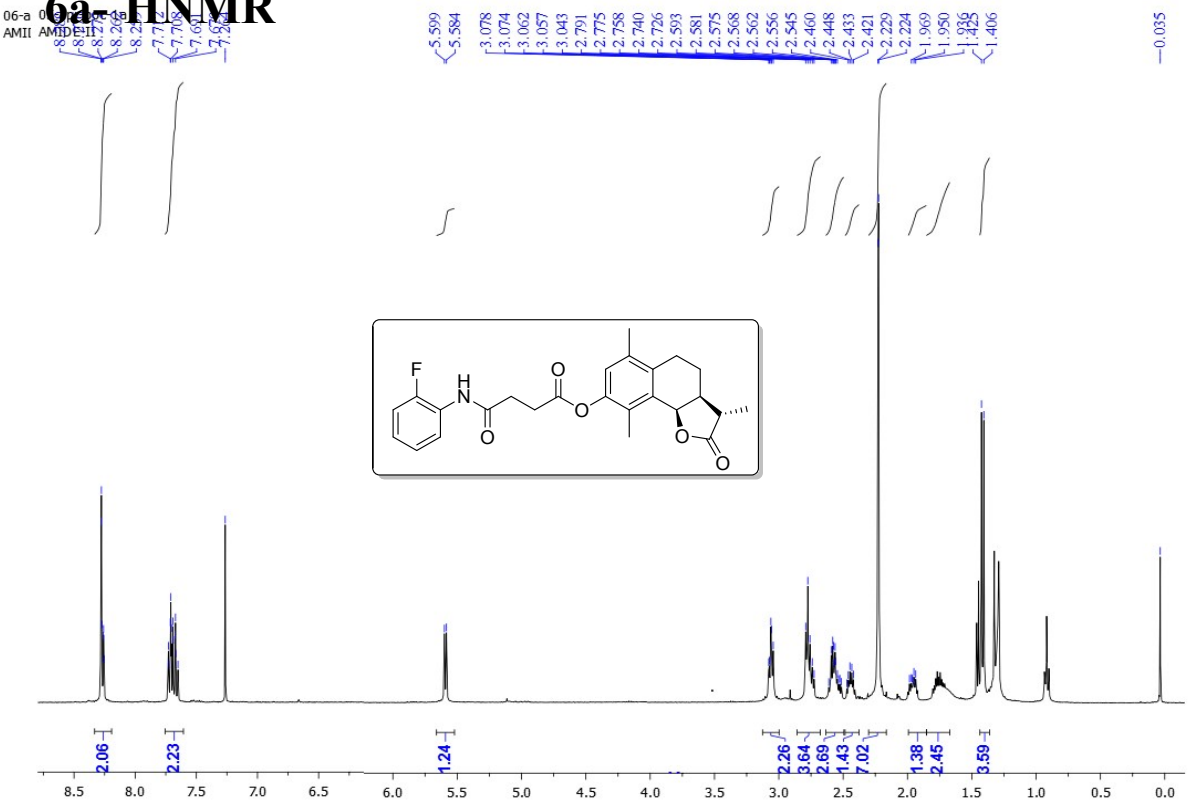
m/z	z	Abund	Formula	Ion
347.1524	1	1293.18	C19 H23 O6	(M+H)+
348.1537	1	387.41	C19 H23 O6	(M+H)+
349.1446	1	239.88	C19 H23 O6	(M+H)+

Predicted Isotope Match Table

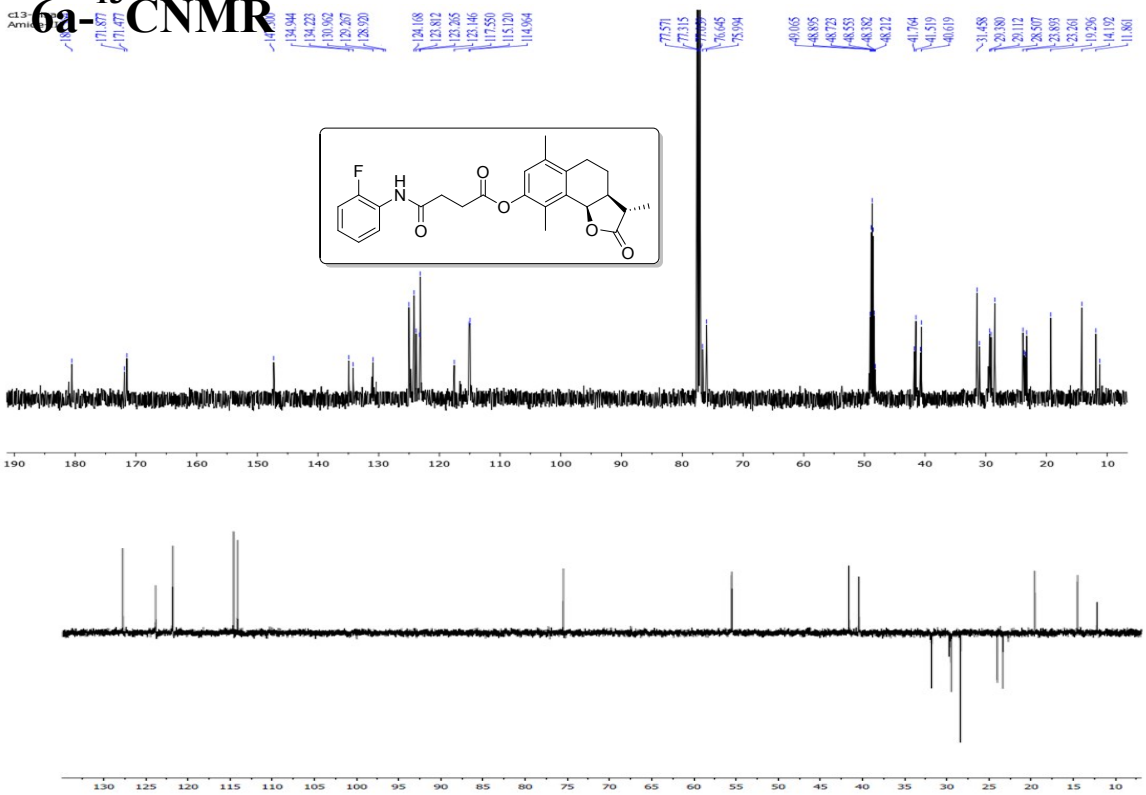
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	347.1524	347.1489	-10.15	100	100	67.34	80.4
2	348.1537	348.1523	-4.05	29.96	21.04	20.17	16.92
3	349.1446	349.1548	29.01	18.55	3.34	12.49	2.68

--- End Of Report ---

6a- ^{1}HNMR



6a-^{13}CNMR



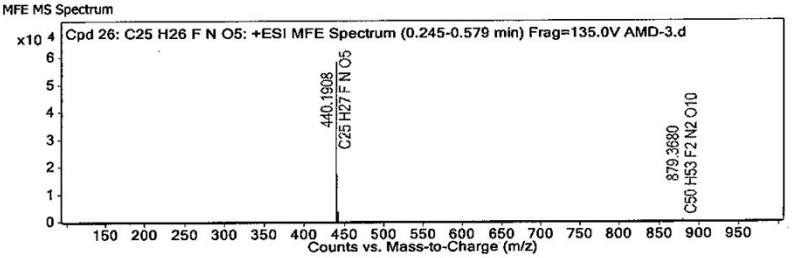
6a-HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 26: C25 H26 F N O5	0.339	439.1835	C25 H26 F N O5	C25 H26 F N O5	-9.08	C25 H26 F N O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 26: C25 H26 F N O5	440.1908	0.339	Find by Molecular Feature	439.1835

MFE MS Spectrum



MS Spectrum Peak List

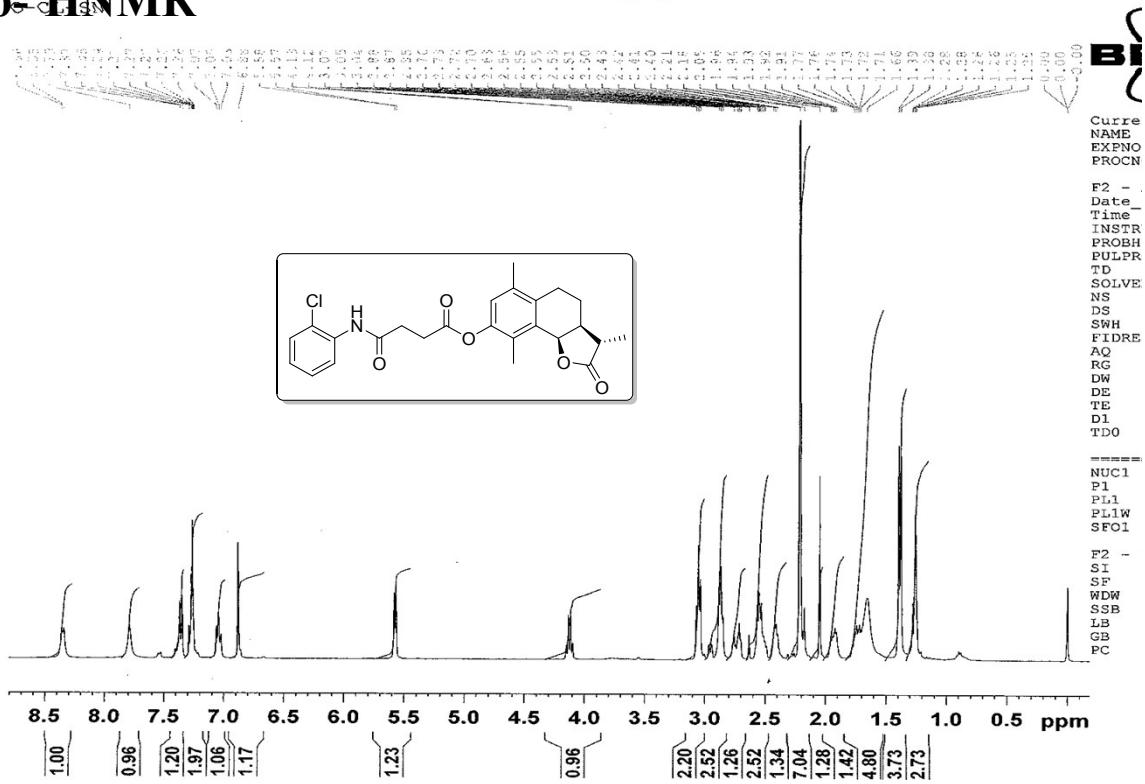
m/z	z	Abund	Formula	Ion
440.1908	1	58052.72	C25 H27 F N O5	(M+H)+
441.1942	1	17473.34	C25 H27 F N O5	(M+H)+
442.1962	1	3446.66	C25 H27 F N O5	(M+H)+
443.1995	1	499.52	C25 H27 F N O5	(M+H)+
879.368	1	712.17	C50 H53 F2 N2 O10	(2M+H)+

Predicted Isotope Match Table

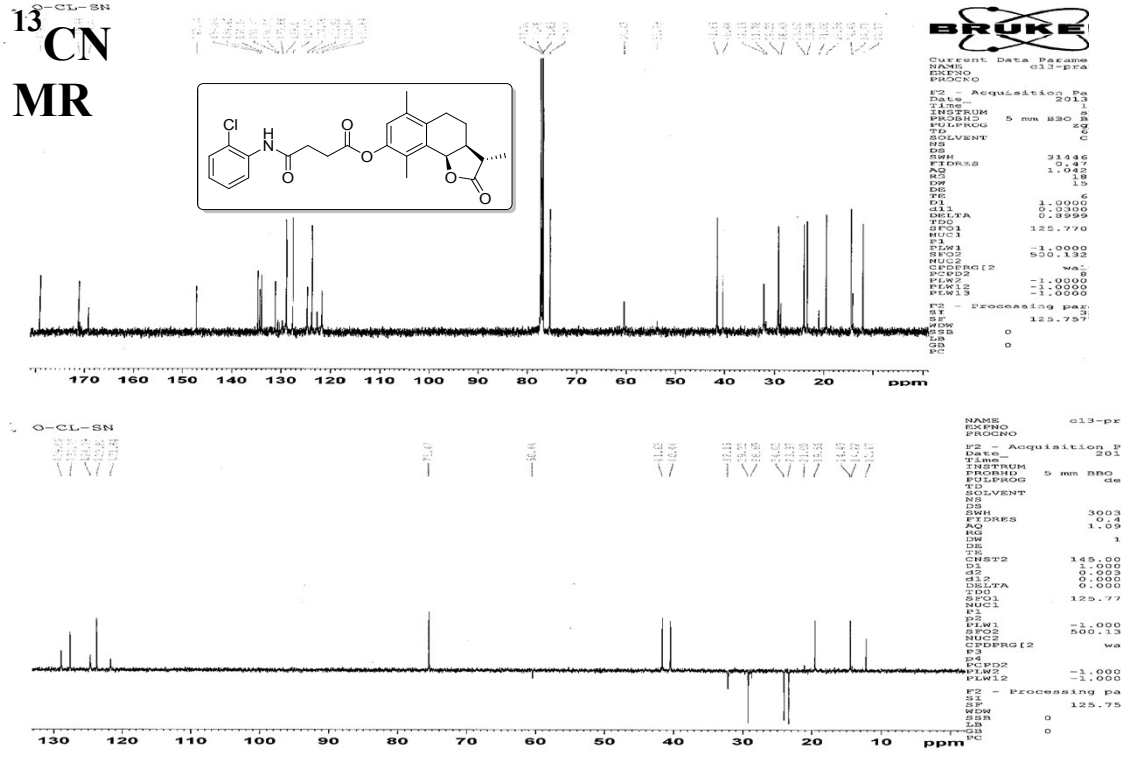
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	440.1908	440.1868	-9.04	100	100	73.05	75.03
2	441.1942	441.1901	-9.38	30.1	27.91	21.99	20.94
3	442.1962	442.1929	-7.57	5.94	4.77	4.34	3.58
4	443.1995	443.1956	-8.81	0.86	0.61	0.63	0.46

--- End Of Report ---

6b- ^{1}HNMR



6b- ^{13}CNMR



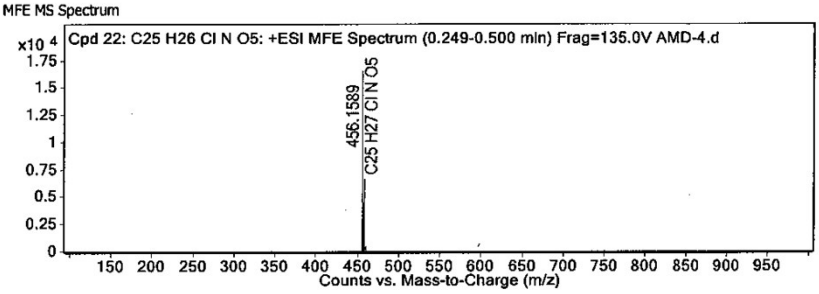
6b-HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 22: C25 H26 Cl N O5	0.338	455.1517	C25 H26 Cl N O5	C25 H26 Cl N O5	-3.75	C25 H26 Cl N O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 22: C25 H26 Cl N O5	456.1589	0.338	Find by Molecular Feature	455.1517

MFE MS Spectrum



MS Spectrum Peak List

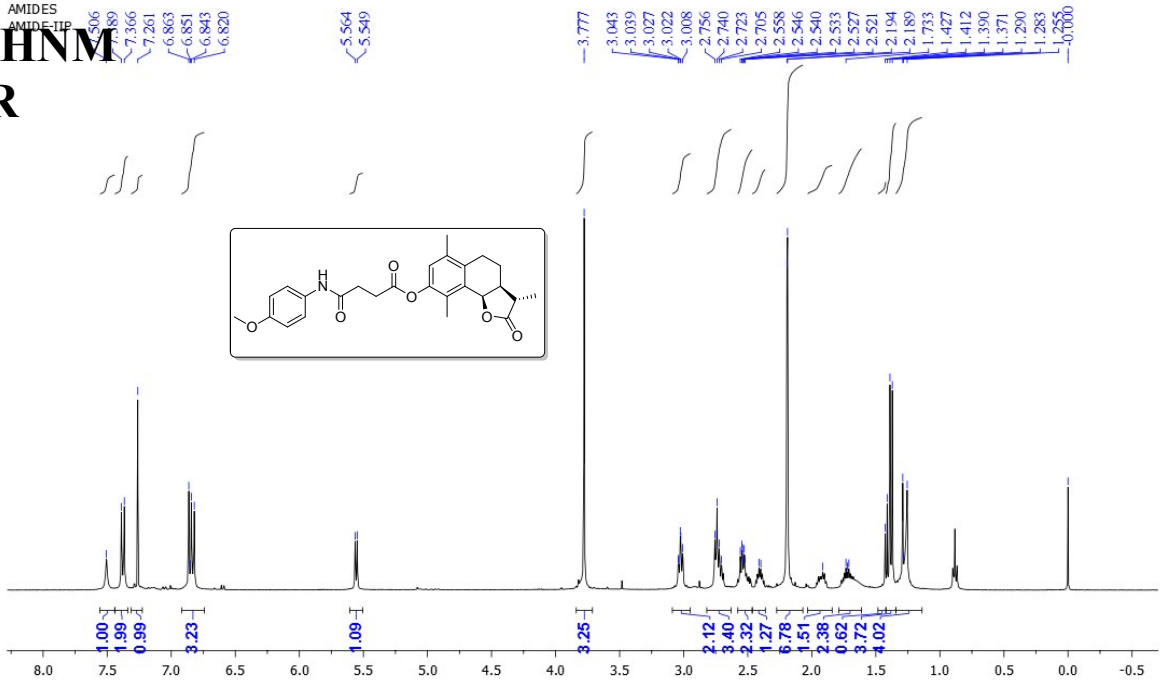
m/z	z	Abund	Formula	Ion
456.1589	1	16546.83	C25 H27 Cl N O5	(M+H)+
457.1622	1	4492.13	C25 H27 Cl N O5	(M+H)+
458.1571	1	6651.85	C25 H27 Cl N O5	(M+H)+
459.1601	1	1729.21	C25 H27 Cl N O5	(M+H)+
460.1649	1	426.22	C25 H27 Cl N O5	(M+H)+

Predicted Isotope Match Table

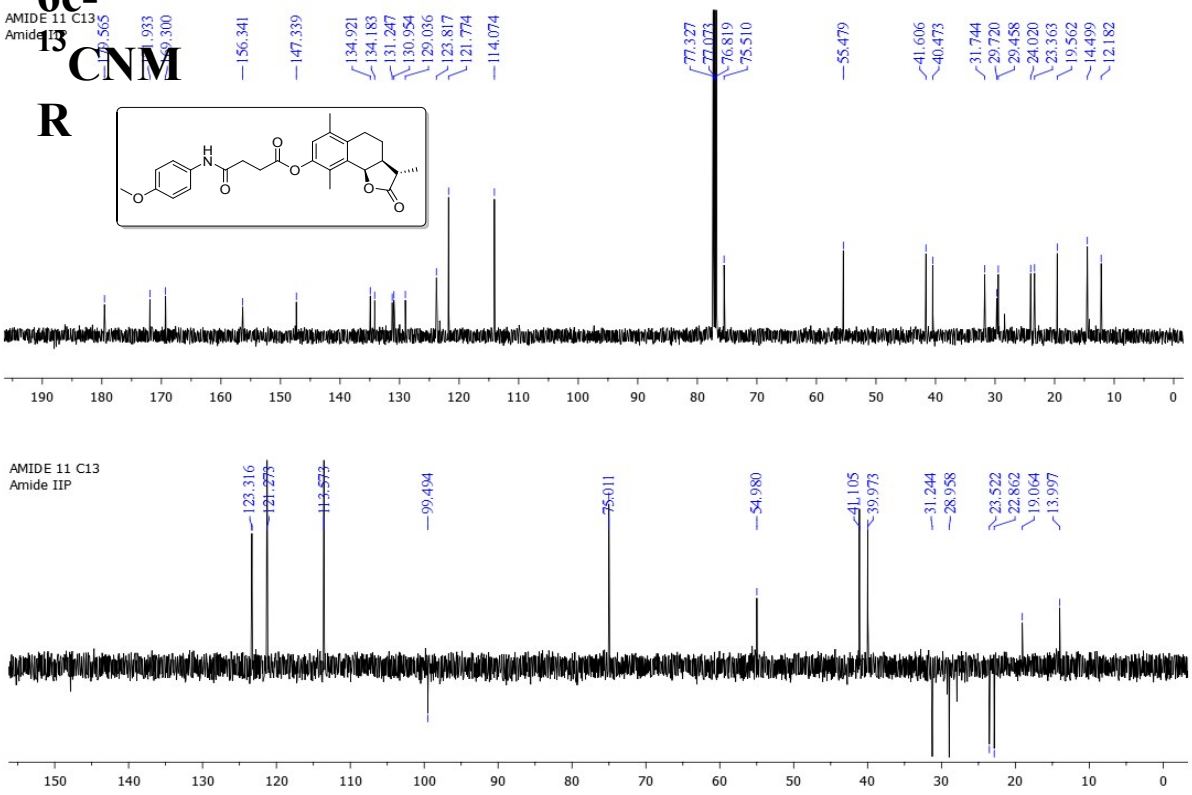
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	456.1589	456.1572	-3.62	100	100	55.44	56.88
2	457.1622	457.1605	-3.7	27.15	27.91	15.05	15.87
3	458.1571	458.1555	-3.54	40.2	36.77	22.29	20.92
4	459.1601	459.1581	-4.36	10.45	9.54	5.79	5.42
5	460.1649	460.1607	-9.05	2.58	1.59	1.43	0.9

--- End Of Report ---

6c-1HNMR



6c-13CNMR



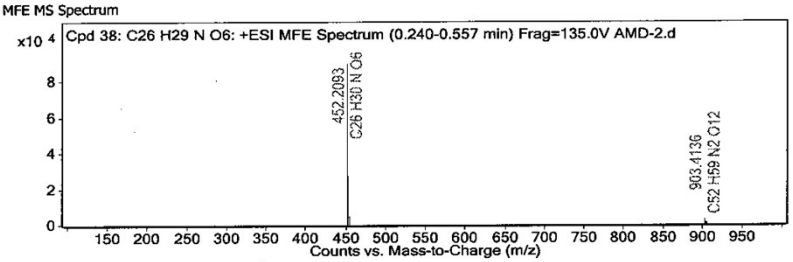
6c-HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 38: C26 H29 N O6	0.341	451.202	C26 H29 N O6	C26 H29 N O6	-5.57	C26 H29 N O6

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 38: C26 H29 N O6	452.2093	0.341	Find by Molecular Feature	451.202

MFE MS Spectrum



MS Spectrum Peak List

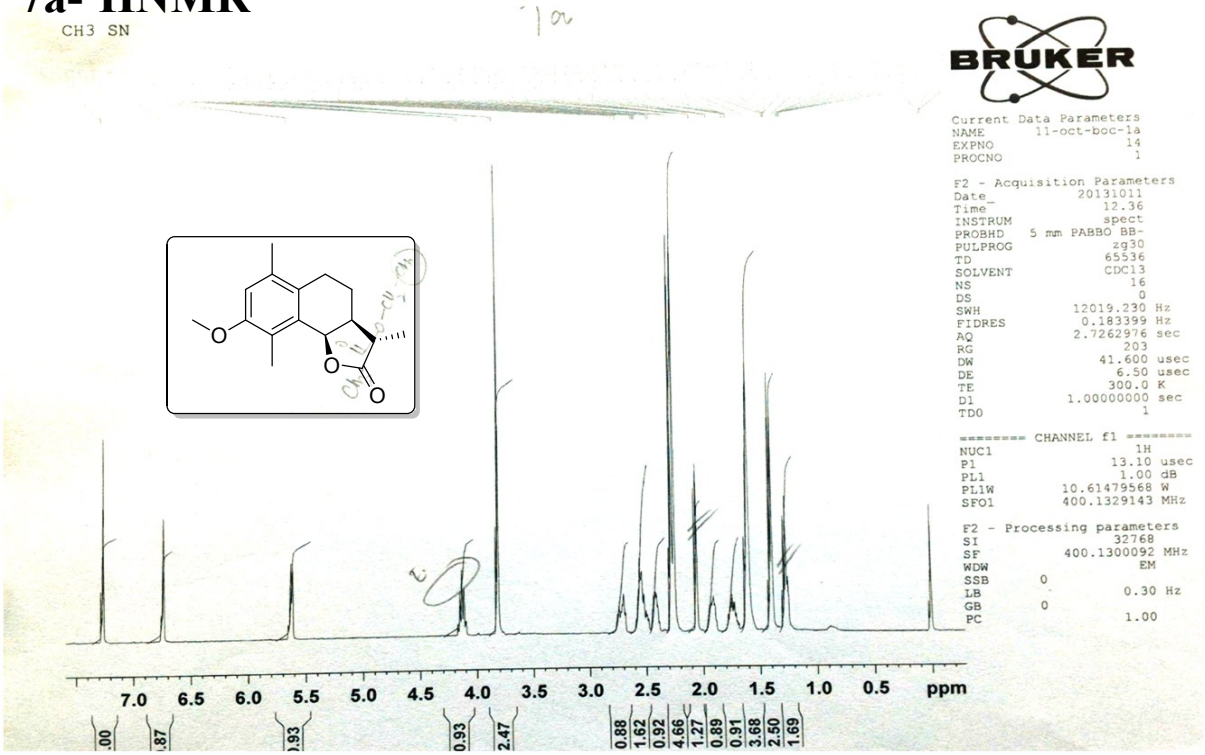
m/z	z	Abund	Formula	Ion
452.2093	1	89683.57	C26 H30 N O6	(M+H)+
453.2126	1	27589.89	C26 H30 N O6	(M+H)+
454.2153	1	5104.69	C26 H30 N O6	(M+H)+
903.4136	1	3224.48	C52 H59 N2 O12	(2M+H)+
904.415	1	1707.49	C52 H59 N2 O12	(2M+H)+

Predicted Isotope Match Table

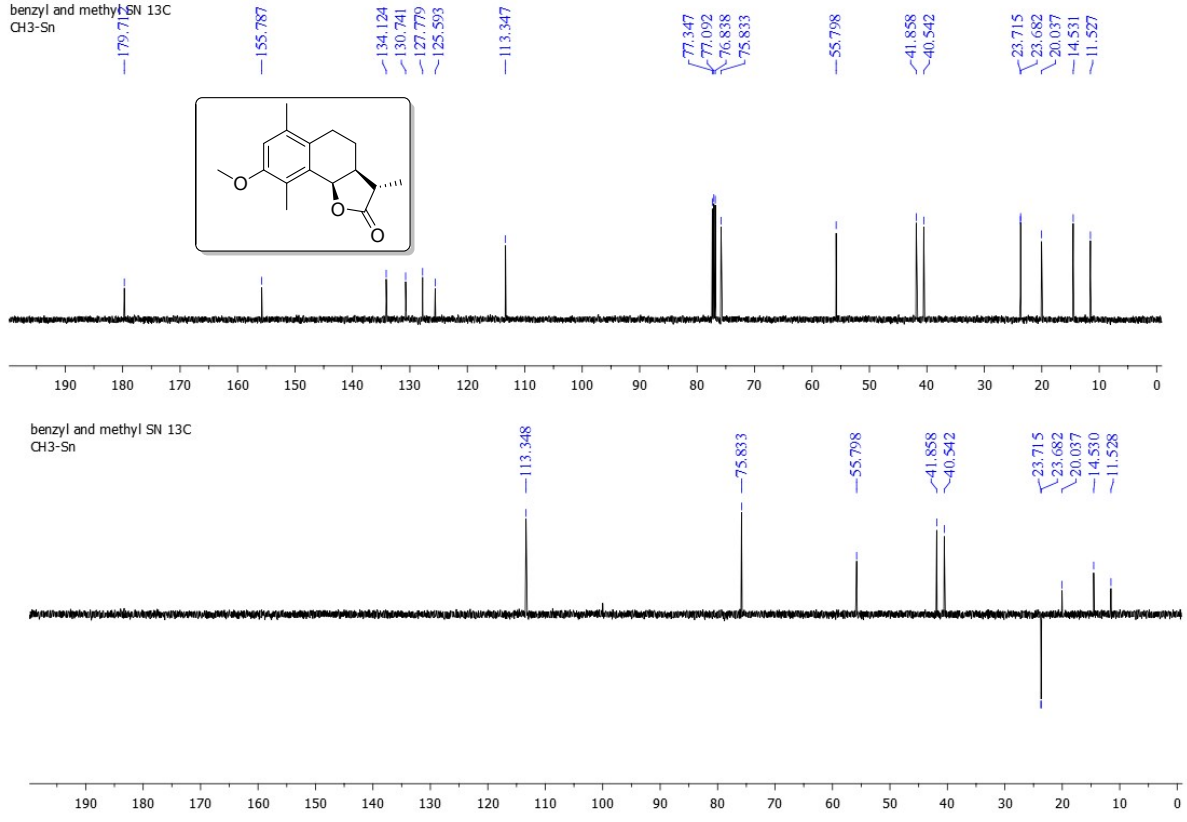
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	452.2093	452.2068	-5.51	100	100	72.47	74.03
2	453.2126	453.2101	-5.45	30.76	29.06	22.3	21.51
3	454.2153	454.2128	-5.42	5.69	5.3	4.13	3.93
4	455.2208	455.2155	-11.65	1.52	0.72	1.1	0.54

--- End Of Report ---

7a-^{1}HNMR



7a-^{13}CNMR



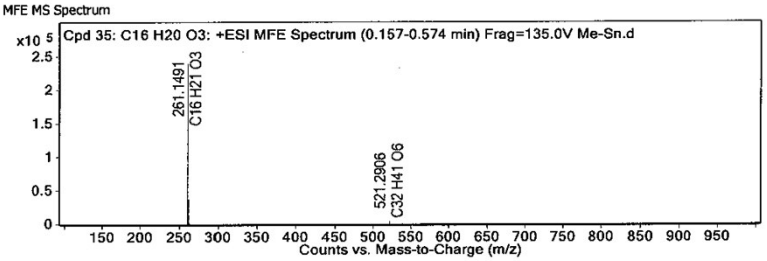
7a- HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 35: C16 H20 O3	0.342	260.1418	C16 H20 O3	C16 H20 O3	-2.16	C16 H20 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 35: C16 H20 O3	261.1491	0.342	Find by Molecular Feature	260.1418

MFE MS Spectrum



MS Spectrum Peak List

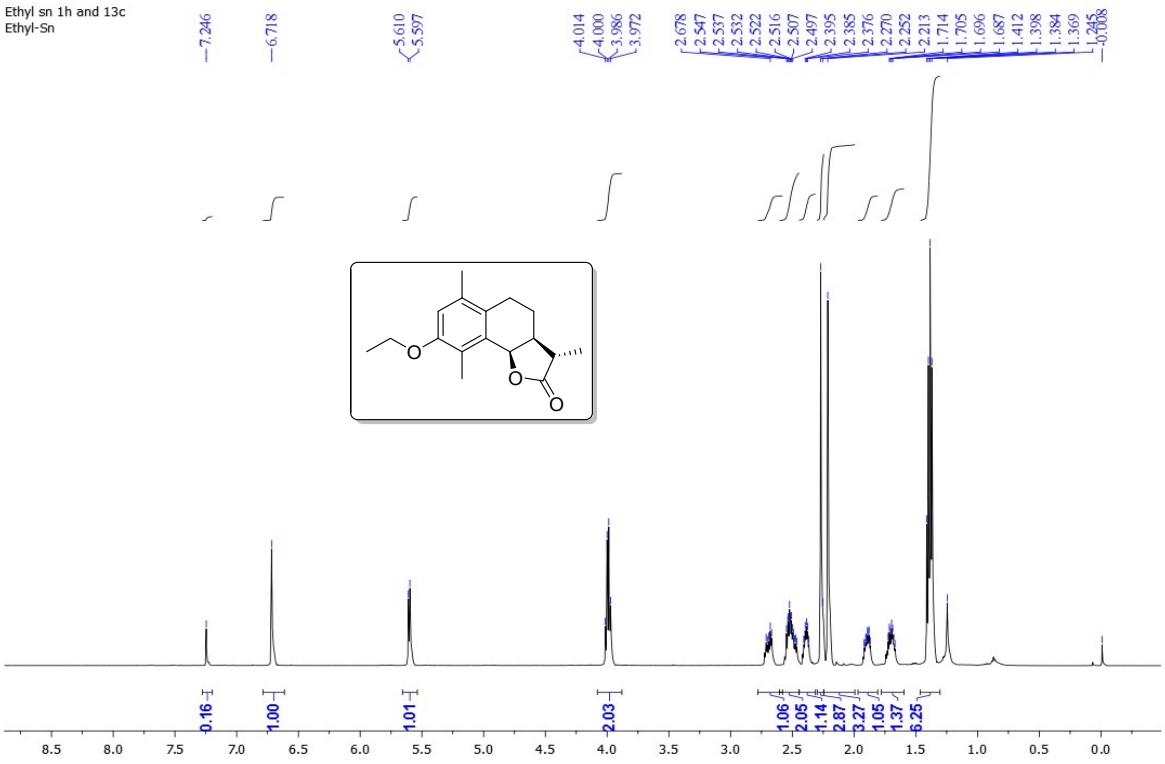
m/z	z	Abund	Formula	Ion
261.1491	1	239147.03	C16 H21 O3	(M+H)+
262.1524	1	37327.34	C16 H21 O3	(M+H)+
263.1557	1	4625.03	C16 H21 O3	(M+H)+
521.2906	1	3571.02	C32 H41 O6	(2M+H)+
522.2935	1	1096.33	C32 H41 O6	(2M+H)+

Predicted Isotope Match Table

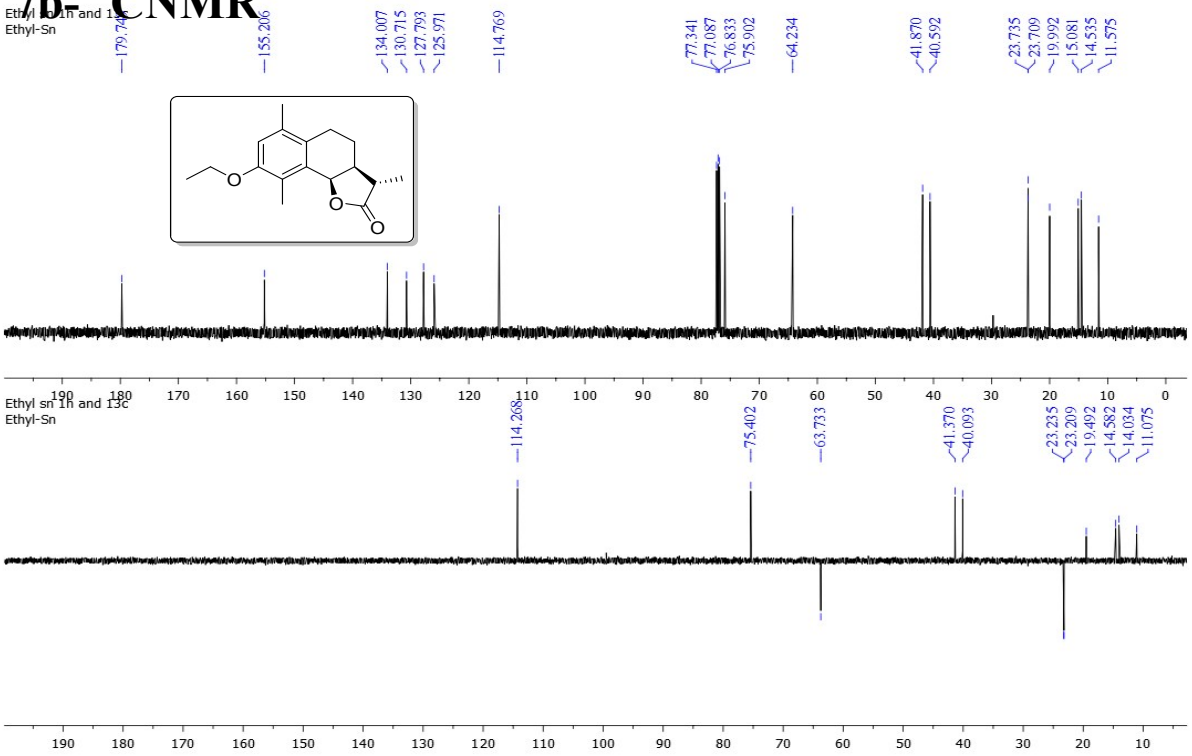
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	261.1491	261.1485	-2.13	100	100	84.84	83.38
2	262.1524	262.1519	-1.99	15.61	17.66	13.24	14.73
3	263.1557	263.1546	-4.28	1.93	2.08	1.64	1.74
4	264.1582	264.1572	-3.77	0.32	0.18	0.27	0.15

--- End Of Report ---

7b- ^{1}HNMR



7b-^{13}CNMR



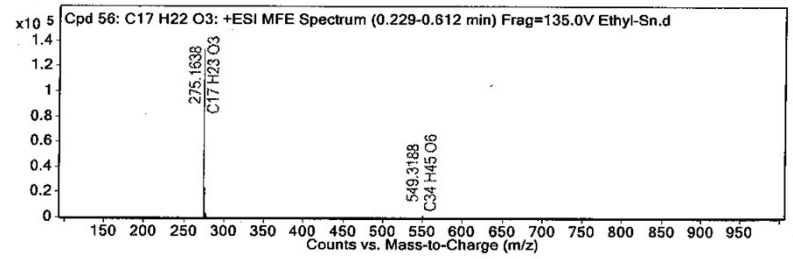
7b-HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 56: C17 H22 O3	0.341	274.1566	C17 H22 O3	C17 H22 O3	1.01	C17 H22 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 56: C17 H22 O3	275.1638	0.341	Find by Molecular Feature	274.1566

MFE MS Spectrum



MS Spectrum Peak List

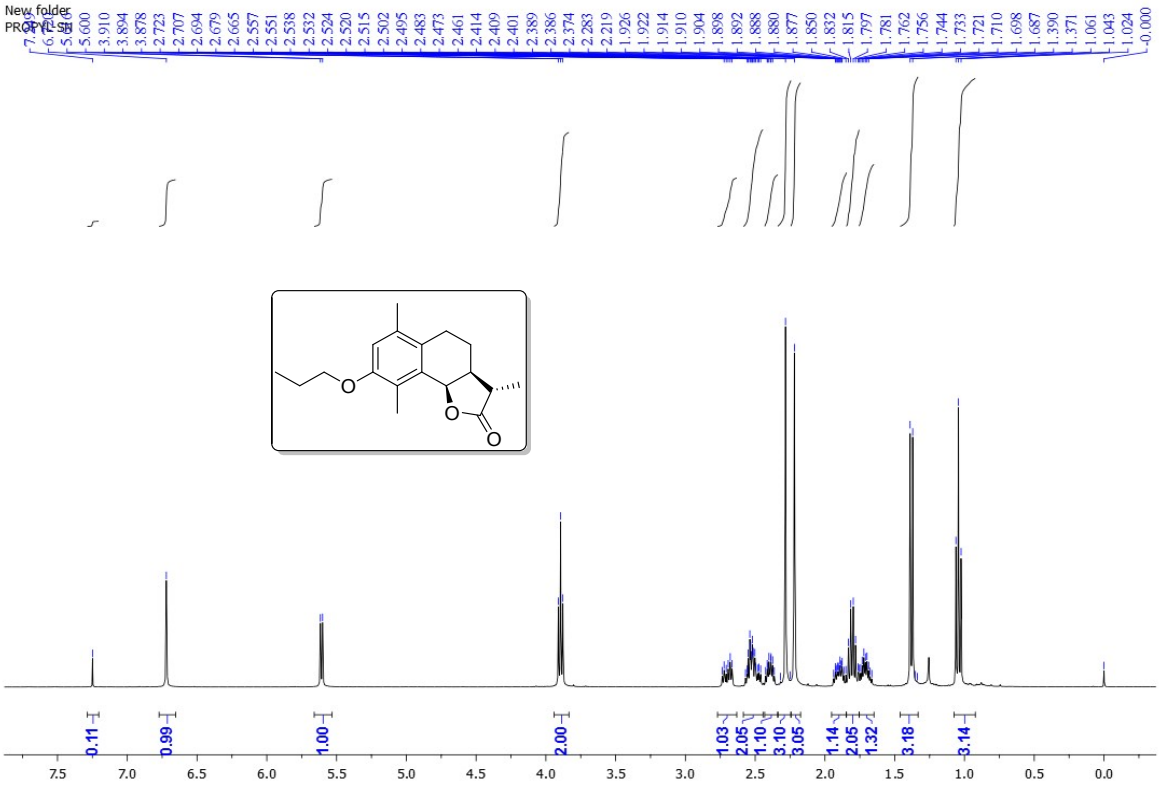
m/z	z	Abund	Formula	Ion
275.1638	1	133000.11	C17 H23 O3	(M+H)+
276.1675	1	23110.87	C17 H23 O3	(M+H)+
277.1706	1	3223.87	C17 H23 O3	(M+H)+
278.1738	1	676.89	C17 H23 O3	(M+H)+
549.3188	1	1699.39	C34 H45 O6	(2M+H)+

Predicted Isotope Match Table

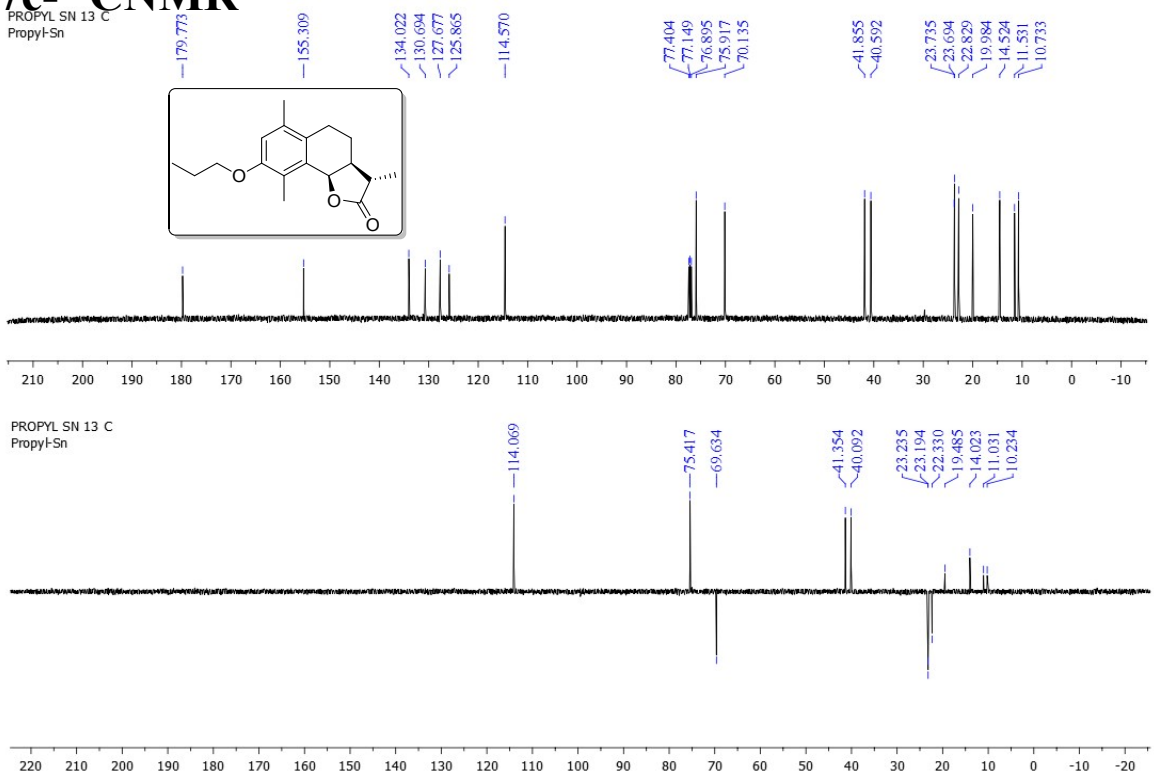
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	275.1638	275.1642	1.23	100	100	83.12	82.47
2	276.1675	276.1676	0.19	17.38	18.77	14.44	15.48
3	277.1706	277.1703	-1.23	2.42	2.28	2.01	1.88
4	278.1738	278.173	-3.02	0.51	0.21	0.42	0.17

--- End Of Report ---

7c-^{1}HNMR



7c-^{13}CNMR



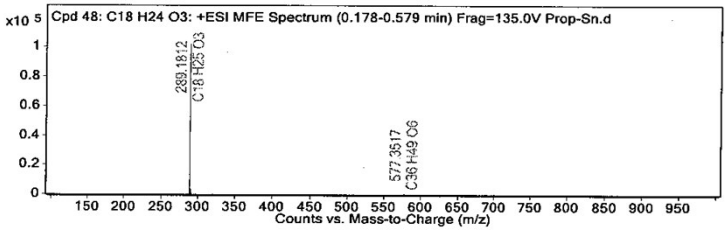
7c-HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 48: C18 H24 O3	0.341	288.1739	C18 H24 O3	C18 H24 O3	-4.76	C18 H24 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 48: C18 H24 O3	289.1812	0.341	Find by Molecular Feature	288.1739

MFE MS Spectrum



MS Spectrum Peak List

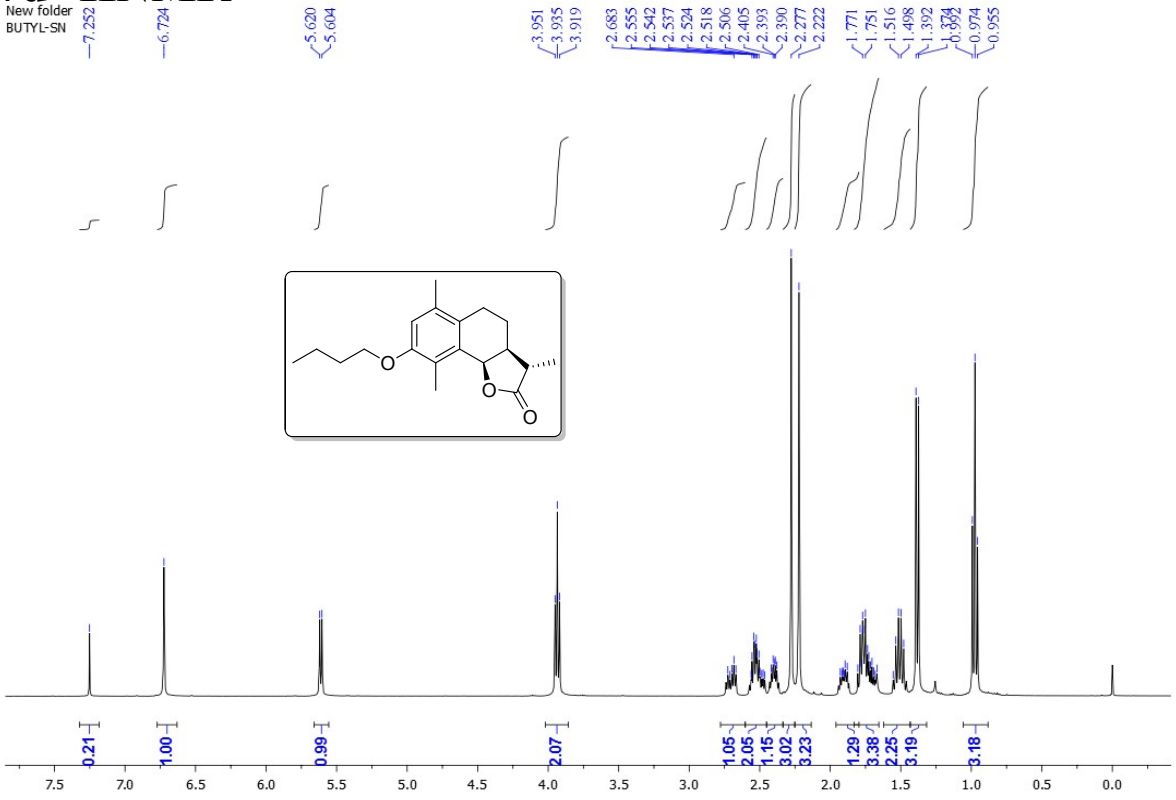
m/z	z	Abund	Formula	Ion
289.1812	1	101849.02	C18 H25 O3	(M+H)+
290.1848	1	22401.21	C18 H25 O3	(M+H)+
291.1877	1	3268.99	C18 H25 O3	(M+H)+
292.1875	1	511.43	C18 H25 O3	(M+H)+
577.3517	1	851.44	C36 H49 O6	(2M+H)+

Predicted Isotope Match Table

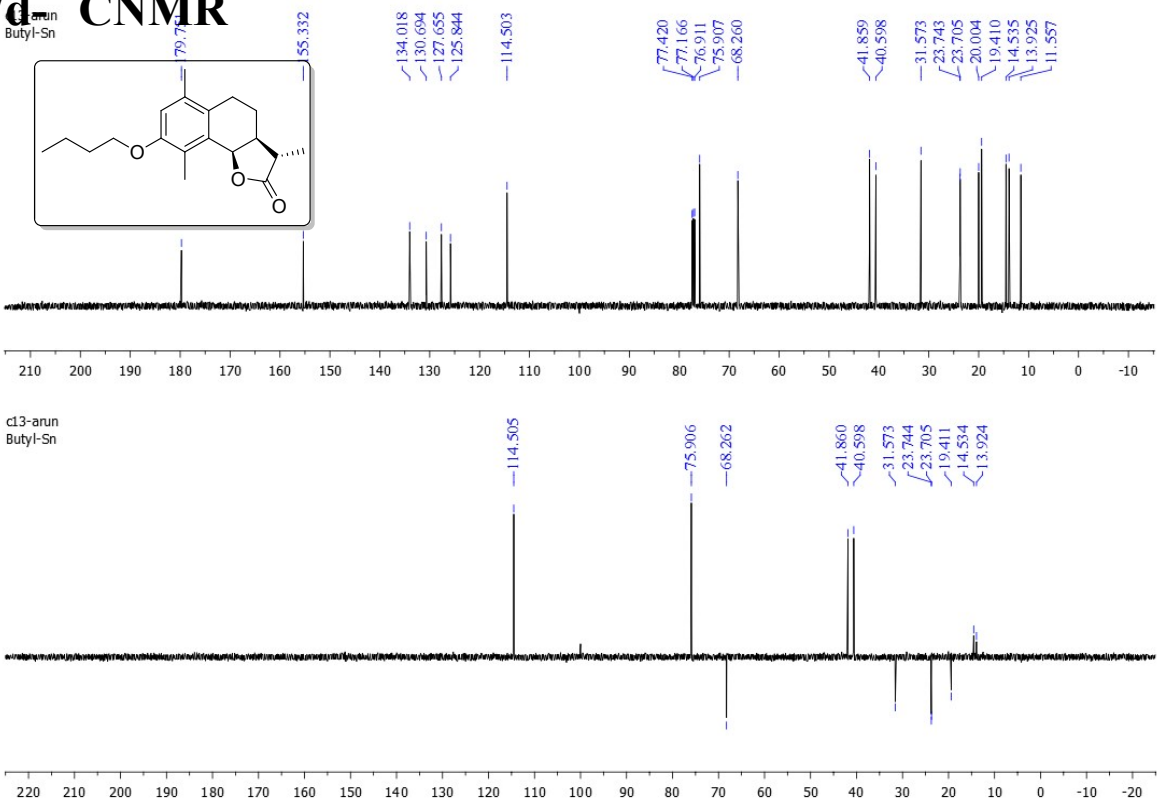
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	289.1812	289.1798	-4.62	100	100	79.55	81.57
2	290.1848	290.1832	-5.29	21.99	19.87	17.5	16.21
3	291.1877	291.186	-5.9	3.21	2.49	2.55	2.03
4	292.1875	292.1887	4.03	0.5	0.23	0.4	0.19

--- End Of Report ---

7d-^{1}HNMR



7d-^{13}CNMR



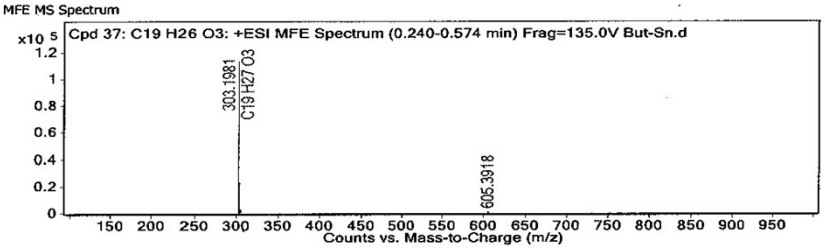
7d-HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 37: C19 H26 O3	0.339	302.1908	C19 H26 O3	C19 H26 O3	-8.68	C19 H26 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 37: C19 H26 O3	303.1981	0.339	Find by Molecular Feature	302.1908

MFE MS Spectrum



MS Spectrum Peak List

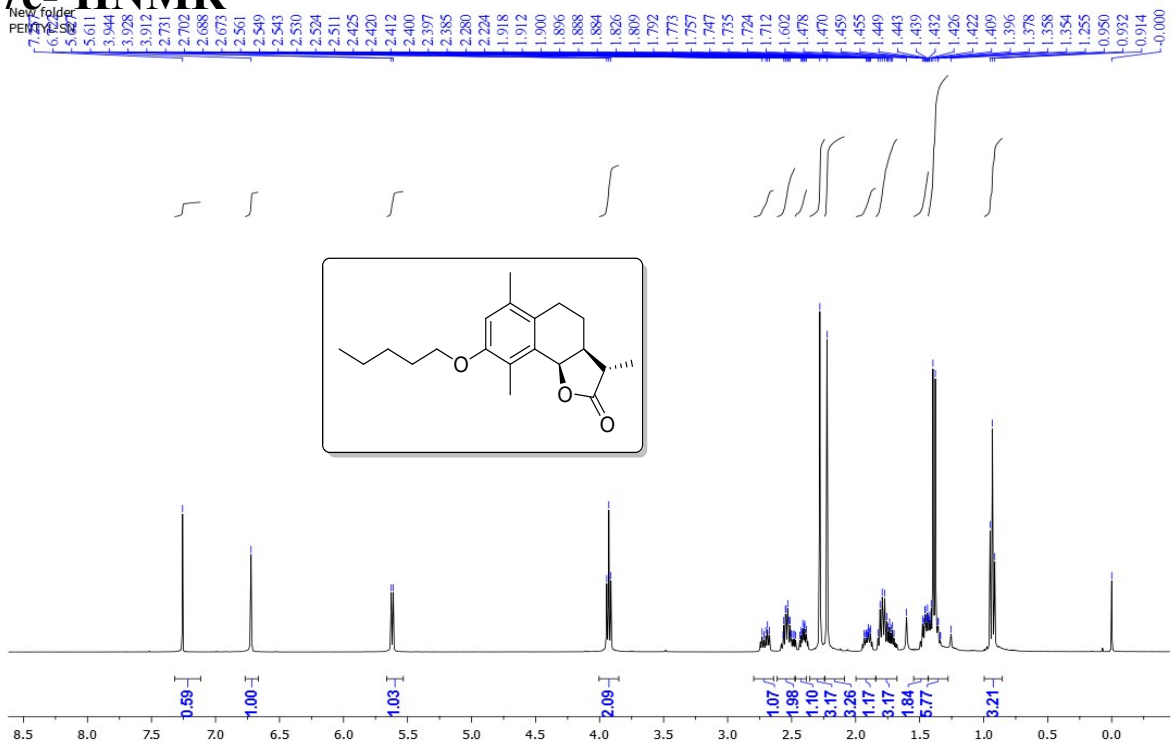
m/z	z	Abund	Formula	Ion
303.1981	1	113229.38	C19 H27 O3	(M+H)+
304.2013	1	23009.65	C19 H27 O3	(M+H)+
305.2039	1	3184.22	C19 H27 O3	(M+H)+
605.3918	1	1108.61		(2M+H)+
606.3932	1	406.07		(2M+H)+

Predicted Isotope Match Table

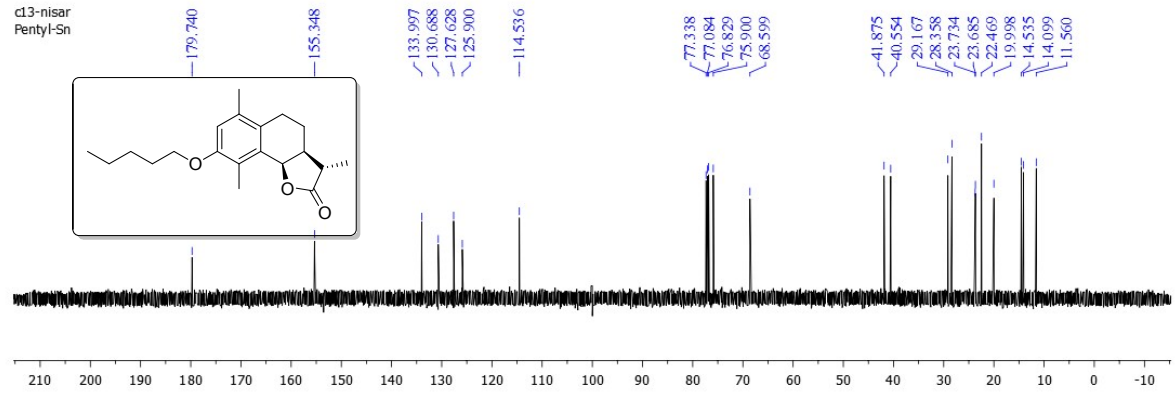
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	303.1981	303.1955	-8.81	100	100	80.99	80.68
2	304.2013	304.1989	-7.98	20.32	20.97	16.46	16.92
3	305.2039	305.2017	-7.36	2.81	2.71	2.28	2.18
4	306.2081	306.2044	-11.92	0.34	0.26	0.28	0.21

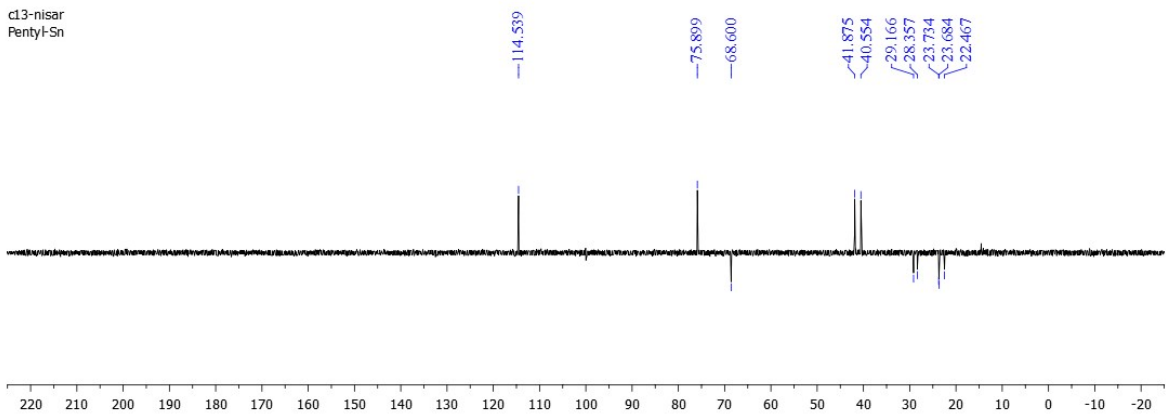
--- End Of Report ---

7e-^{1}HNMR



7e-^{13}CNMR





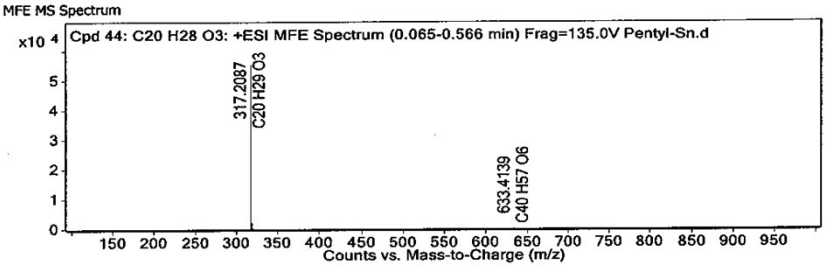
7e- HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 44: C20 H28 O3	0.342	316.2015	C20 H28 O3	C20 H28 O3	7.37	C20 H28 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 44: C20 H28 O3	317.2087	0.342	Find by Molecular Feature	316.2015

MFE MS Spectrum



MS Spectrum Peak List

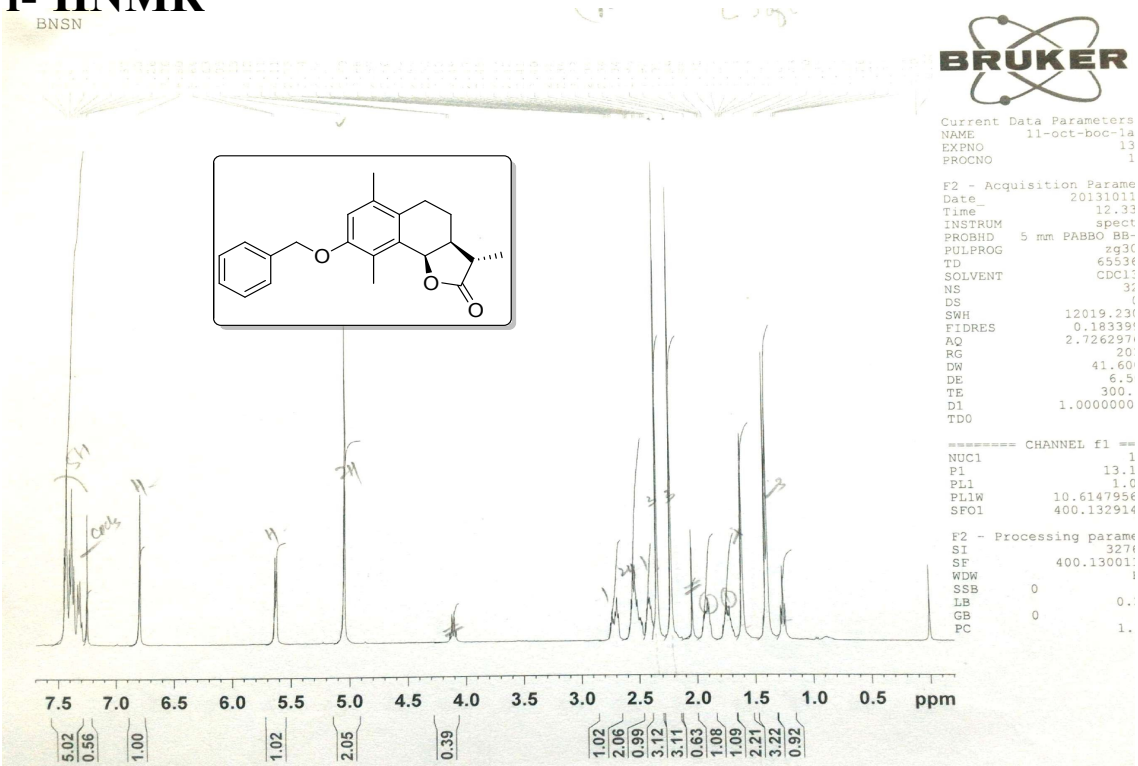
m/z	z	Abund	Formula	Ion
317.2087	1	55312.84	C20 H29 O3	(M+H)+
318.2124	1	13000.19	C20 H29 O3	(M+H)+
319.2166	1	2219.97	C20 H29 O3	(M+H)+
320.2222	1	278.22	C20 H29 O3	(M+H)+
633.4139	1	466.63	C40 H57 O6	(2M+H)+

Predicted Isotope Match Table

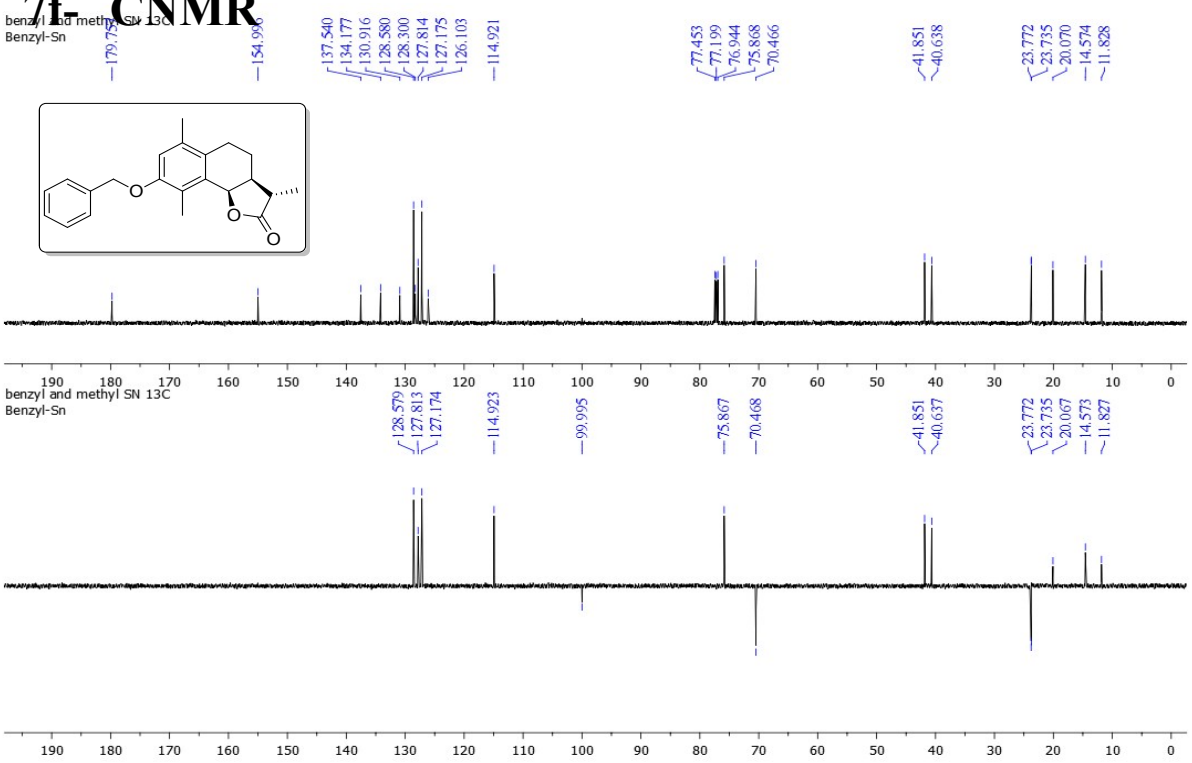
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	317.2087	317.2111	7.73	100	100	78.11	79.8
2	318.2124	318.2145	6.82	23.5	22.08	18.36	17.62
3	319.2166	319.2174	2.56	4.01	2.94	3.14	2.34
4	320.2222	320.2201	-6.53	0.5	0.29	0.39	0.23

--- End Of Report ---

7f- ^{1}HNMR



7f-^{13}CNMR



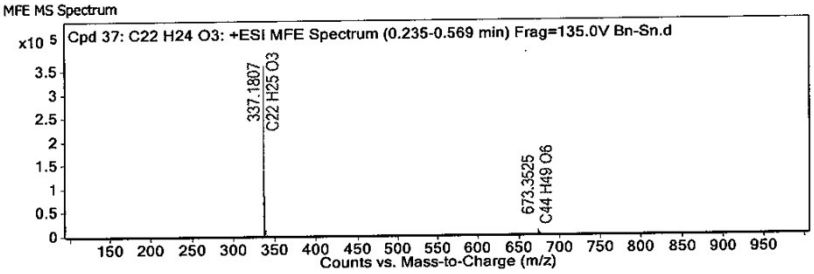
7f-HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 37: C22 H24 O3	0.342	336.1734	C22 H24 O3	C22 H24 O3	-2.48	C22 H24 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 37: C22 H24 O3	337.1807	0.342	Find by Molecular Feature	336.1734

MFE MS Spectrum



MS Spectrum Peak List

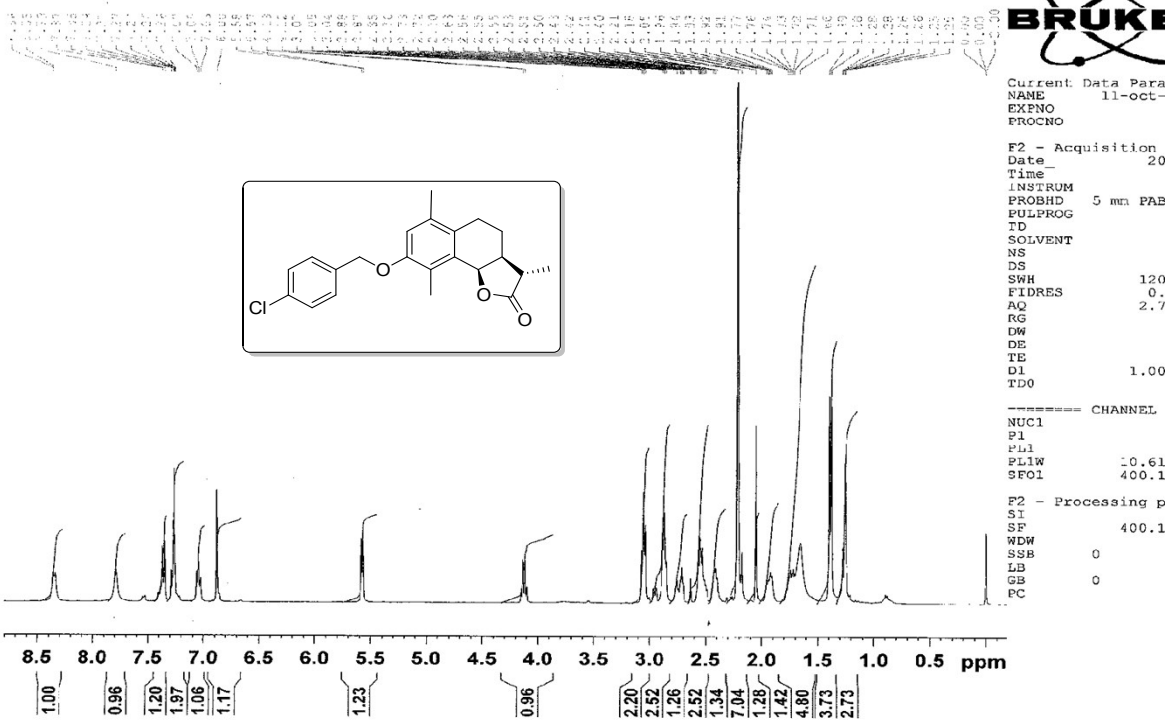
m/z	z	Abund	Formula	Ion
337.1807	1	360433.63	C22 H25 O3	(M+H)+
338.1838	1	82600.91	C22 H25 O3	(M+H)+
339.1869	1	12149.19	C22 H25 O3	(M+H)+
673.3525	1	11205.7	C44 H49 O6	(2M+H)+
674.3558	1	6455.44	C44 H49 O6	(2M+H)+

Predicted Isotope Match Table

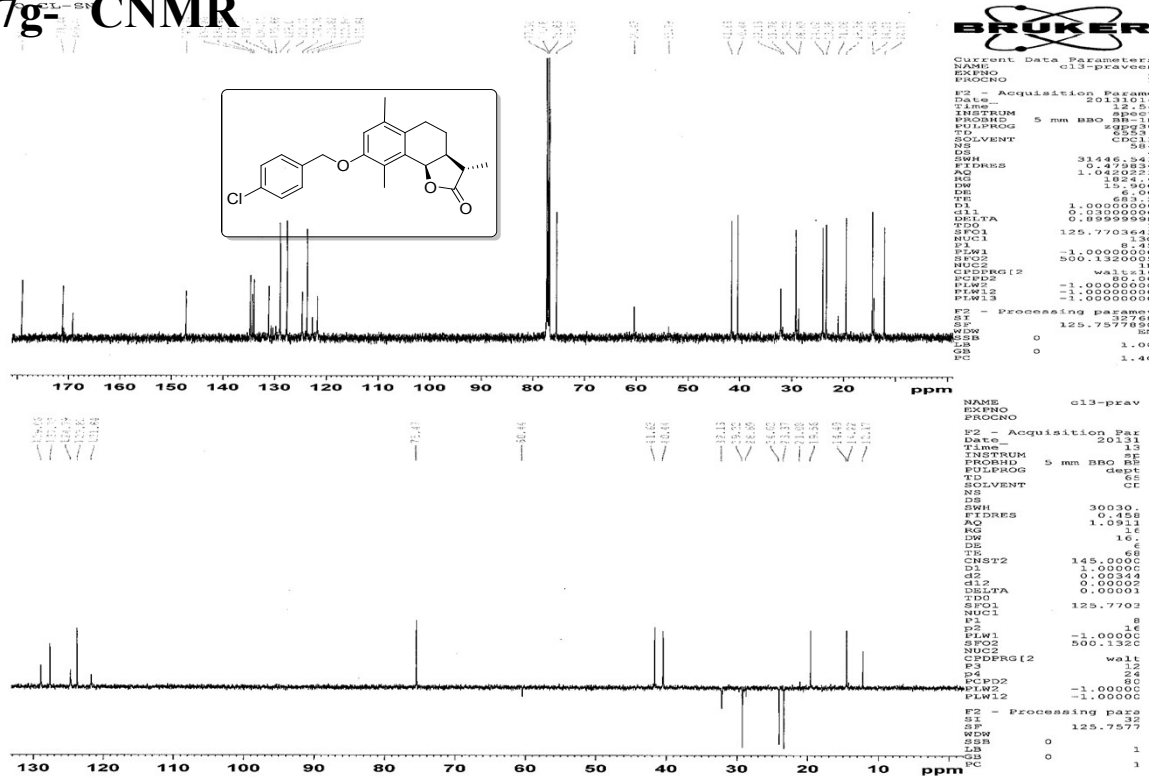
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	337.1807	337.1798	-2.63	100	100	78.95	78.15
2	338.1838	338.1832	-1.78	22.92	24.2	18.09	18.91
3	339.1869	339.1862	-2.28	3.37	3.42	2.66	2.67
4	340.1899	340.1889	-2.87	0.38	0.35	0.3	0.28

--- End Of Report ---

7g- ^{1}HNMR



7g- ^{13}CNMR



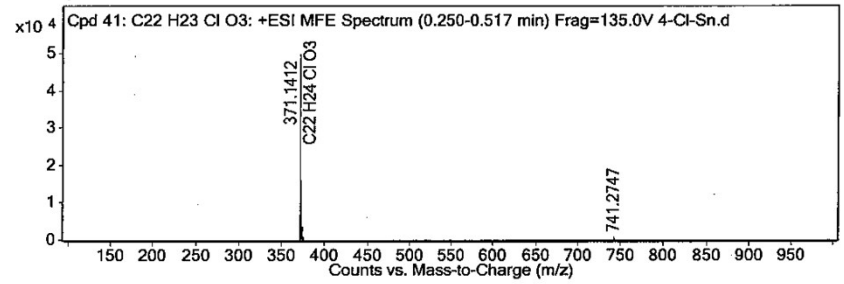
7g-HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 41: C22 H23 Cl O3	0.341	370.134	C22 H23 Cl O3	C22 H23 Cl O3	-1.17	C22 H23 Cl O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 41: C22 H23 Cl O3	371.1412	0.341	Find by Molecular Feature	370.134

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
371.1412	1	49728.36	C22 H24 Cl O3	(M+H)+
372.1446	1	14165.91	C22 H24 Cl O3	(M+H)+
373.1395	1	15888.38	C22 H24 Cl O3	(M+H)+
374.1419	1	3672.21	C22 H24 Cl O3	(M+H)+
741.2747	1	902.98		(2M+H)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	371.1412	371.1408	-0.96	100	100	59.07	59.24
2	372.1446	372.1442	-0.93	28.49	24.18	16.83	14.33
3	373.1395	373.1388	-1.89	31.95	35.41	18.87	20.98
4	374.1419	374.1417	-0.52	7.38	8.09	4.36	4.79
5	375.147	375.1444	-6.87	1.47	1.12	0.87	0.66

--- End Of Report ---