Electronic Supplementary Material (ESI) for RSC Advances.

Synthesis and anti-proliferative evaluation of novel 3,4-dihydro-2H-1,3-oxazine derivatives of bakuchiol

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CONTENTS:

Section A: General experimental procedure

General methods:

All the reagents and solvents for synthesis were purchased from Sigma-Aldrich. All the chemical reactions were monitored by TLC on silica gel 60 F_{254} plates (E. Merck) using 2% ceric ammonium sulphate solution as spraying reagent for detection of spots. Purification of all derivatives was carried out by column chromatography using silica gel 60-120 mesh as stationary phase. All NMR spectra were recorded on Bruker DPX 400 and DPX 500 instruments using $CDCl_3$ as the solvent taking TMS as the internal standard. The chemical shifts are expressed in δ and coupling constant in Hertz. High Resolution Mass Spectra (HRMS) were recorded on Agilent Technologies 6540 instrument. IR recorded on an FT-IR Bruker (270-30) spectrophotometer.

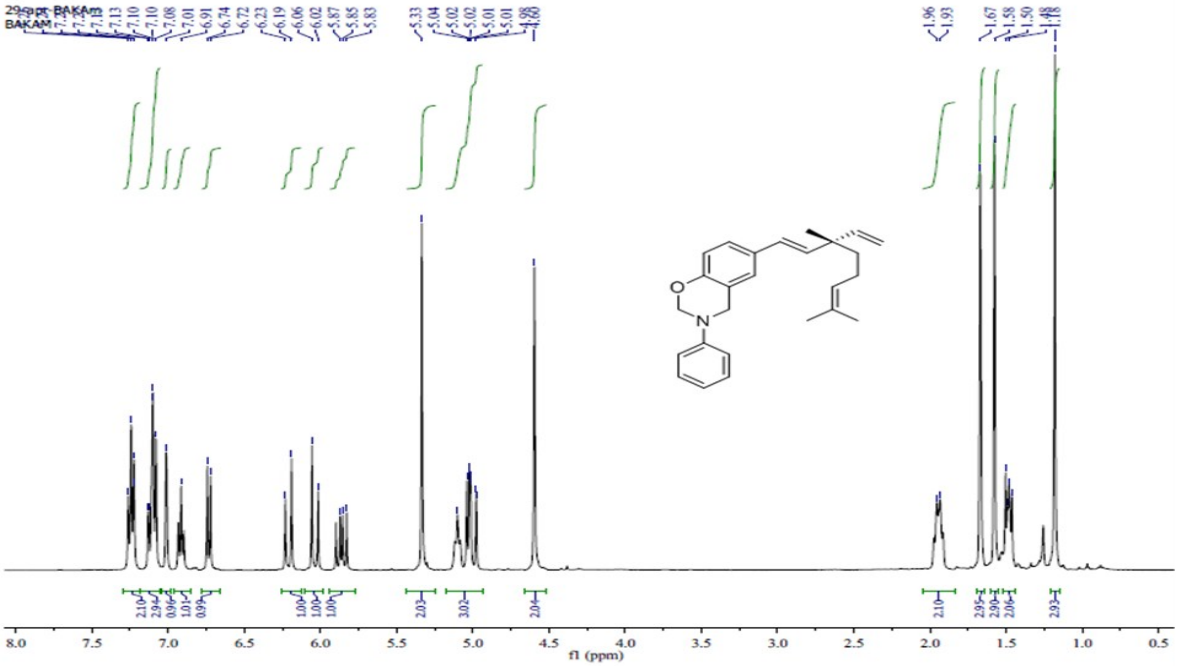
General procedure

Compounds **2-26** were synthesized by portion wise addition of respective primary amine (0.39 mmol) in 3ml of tetrahydrofuran containing 37% aqueous formaldehyde (0.78 mmol) followed by the addition of methanolic solution of bakuchiol (100mg, 0.39mmol). The reaction mixture was heated under reflux for 2-8 hours till the completion (monitored by TLC analysis). Workup of the reaction was done by diluting the reaction mixture with ice-cold water and extracting it with ethyl acetate (3 times).The combined organic layers were dried over sodium sulphate and concentrated on rotavapour. The crude product obtained was purified by column chromatography on silica gel 60-120 mesh with EtoAc: Hexane (1: 50) as the eluent to afford the desired pure products **2-26** in 80-85% yield.

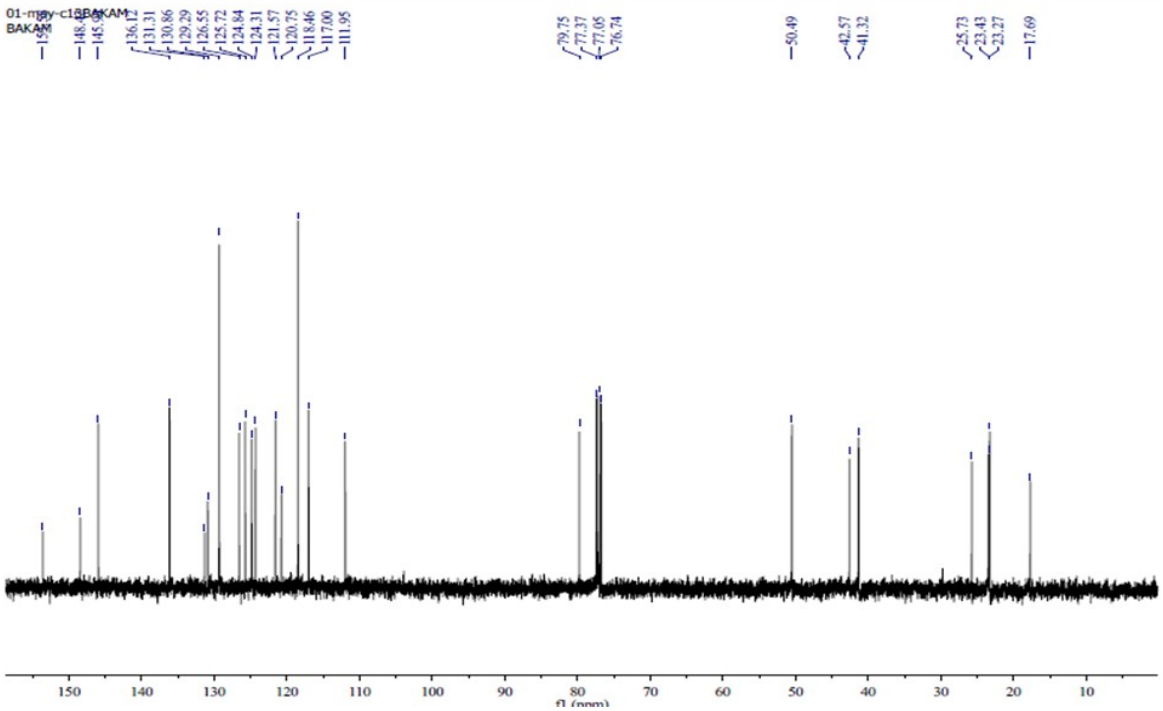
Section B: ^{1}H NMR, ^{13}C NMR, DEPT135 and HRMS spectra of compounds 2-26

3,4-dihydro-6-(3,7-dimethyl-3-vinylocta-1,6-dienyl)-3-phenyl-2H-benzo[e][1,3]oxazine (2)

2 - ^{1}HNMR



2 – ^{13}C NMR



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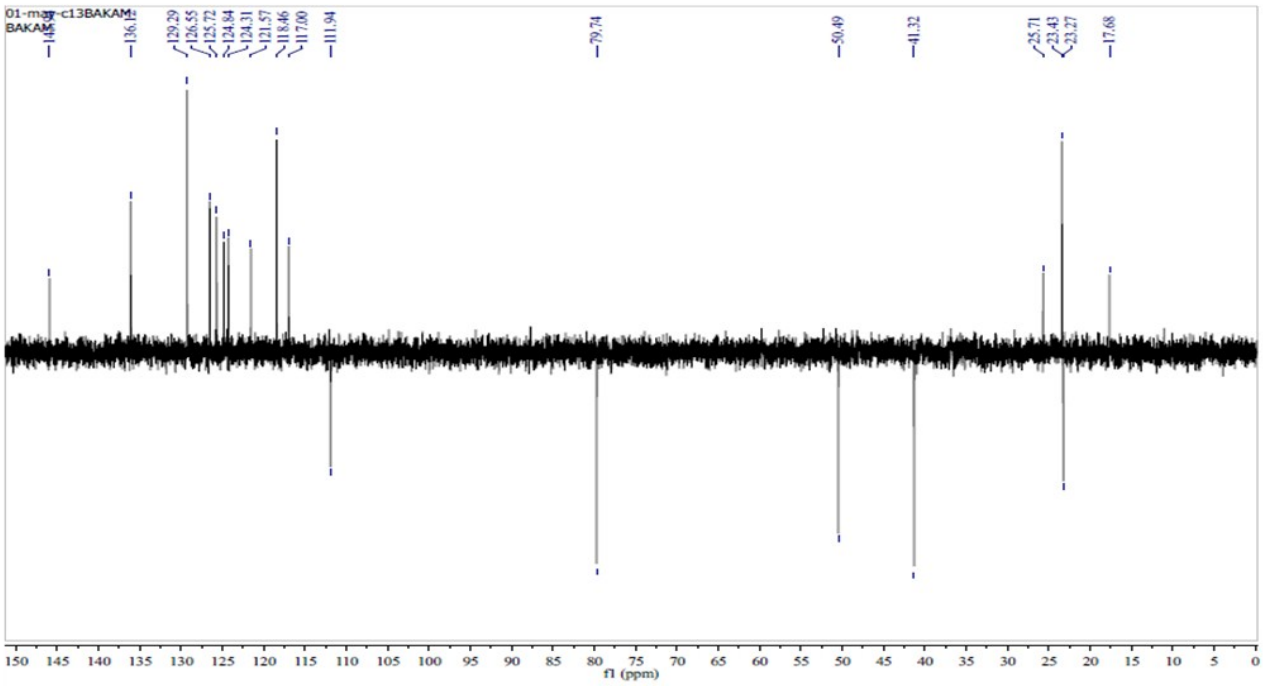


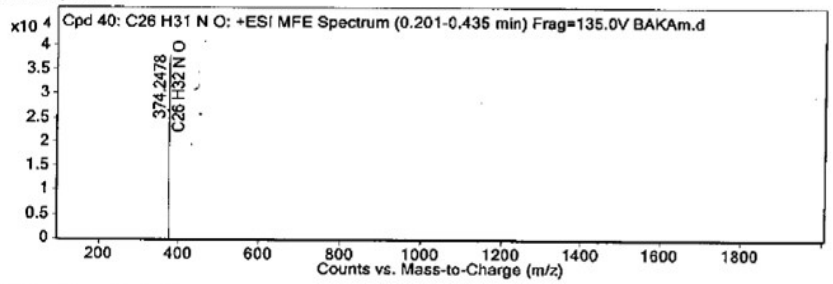
2 - HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 40: C26 H31 N O	0.266	373.2403	C26 H31 N O	C26 H31 N O	0.67	C26 H31 N O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 40: C26 H31 N O	374.2478	0.266	Find by Molecular Feature	373.2403

MFE MS Spectrum



MS Spectrum Peak List

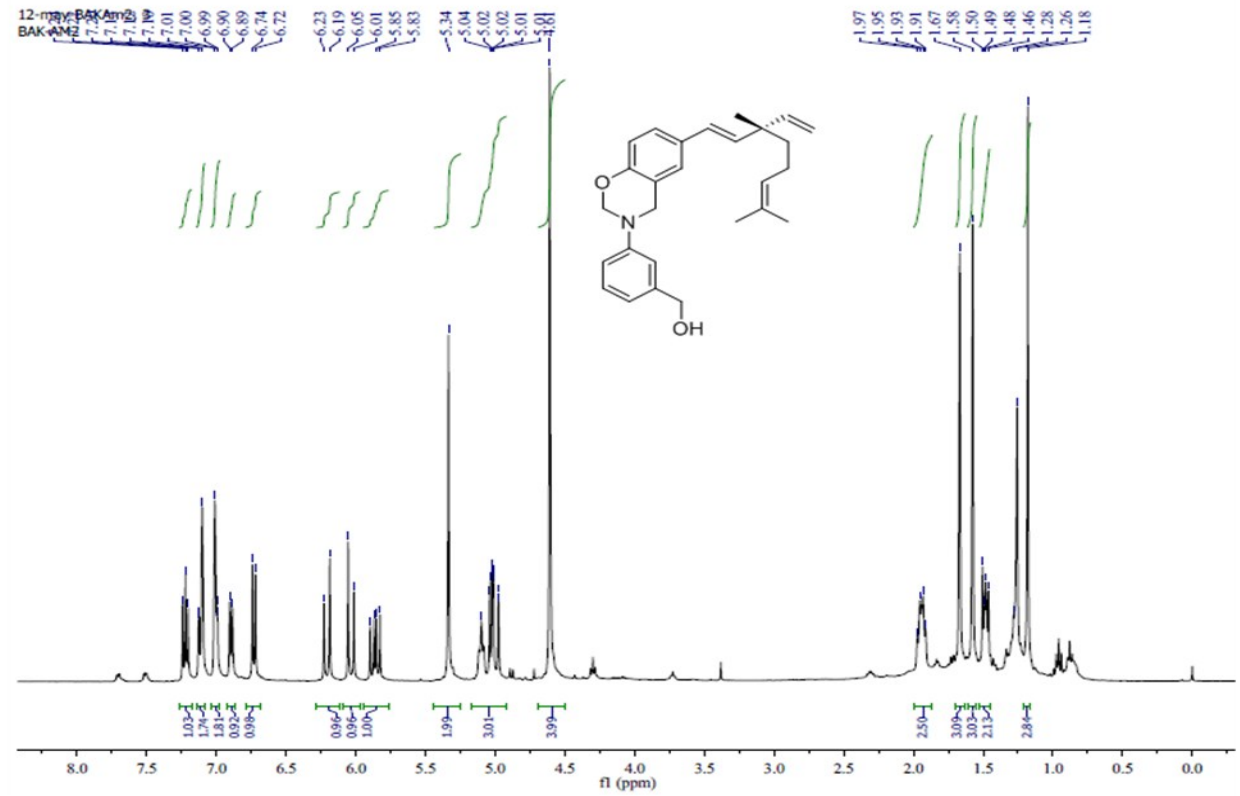
m/z	z	Abund	Formula	Ion
374.2478	1	38039.36	C26 H32 N O	(M+H)+
375.2506	1	10830.28	C26 H32 N O	(M+H)+
376.2522	1	1952.6	C26 H32 N O	(M+H)+
377.2602	1	286.67	C26 H32 N O	(M+H)+

Predicted Isotope Match Table

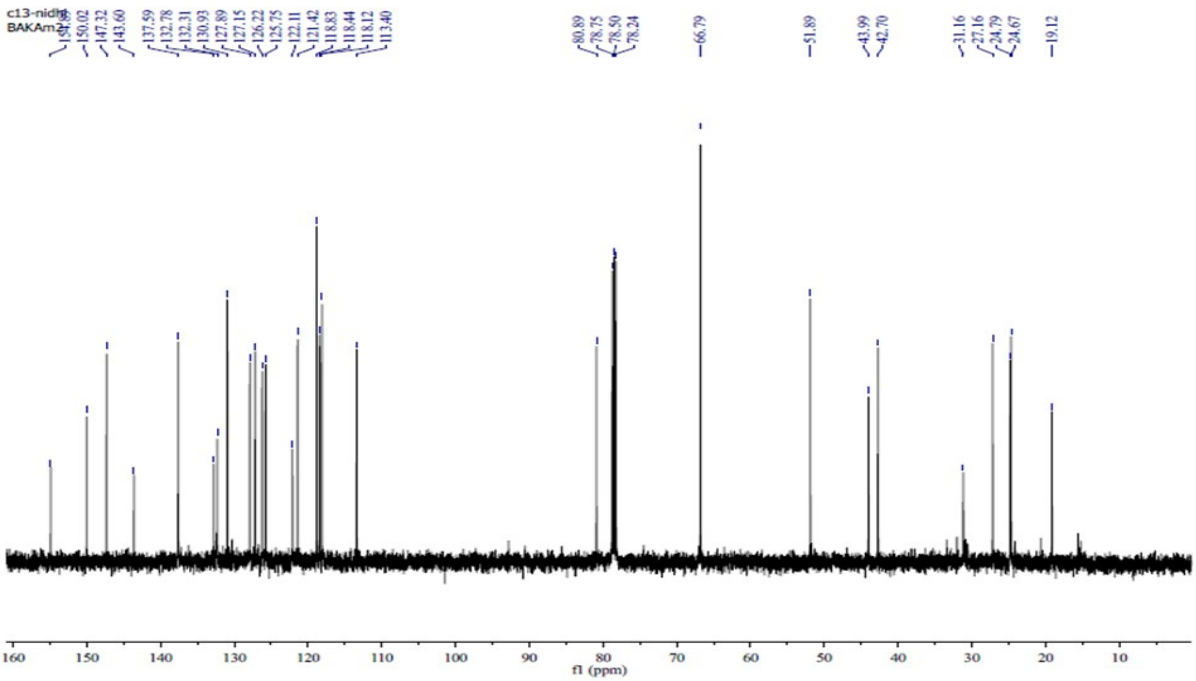
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	374.2478	374.2478	0.2	100	100	74.43	74.89
2	375.2506	375.2512	1.6	28.47	28.89	21.19	21.64
3	376.2522	376.2544	5.78	5.13	4.23	3.82	3.17
4	377.2602	377.2574	-7.19	0.75	0.42	0.56	0.31

3-(6-(3,7-dimethyl-3-vinylocta-1,6-dienyl)-2H-benzo[e][1,3]oxazin-3(4H)-yl) phenyl)methanol (3)

3 - ^{1}HNMR



3 – ^{13}C NMR



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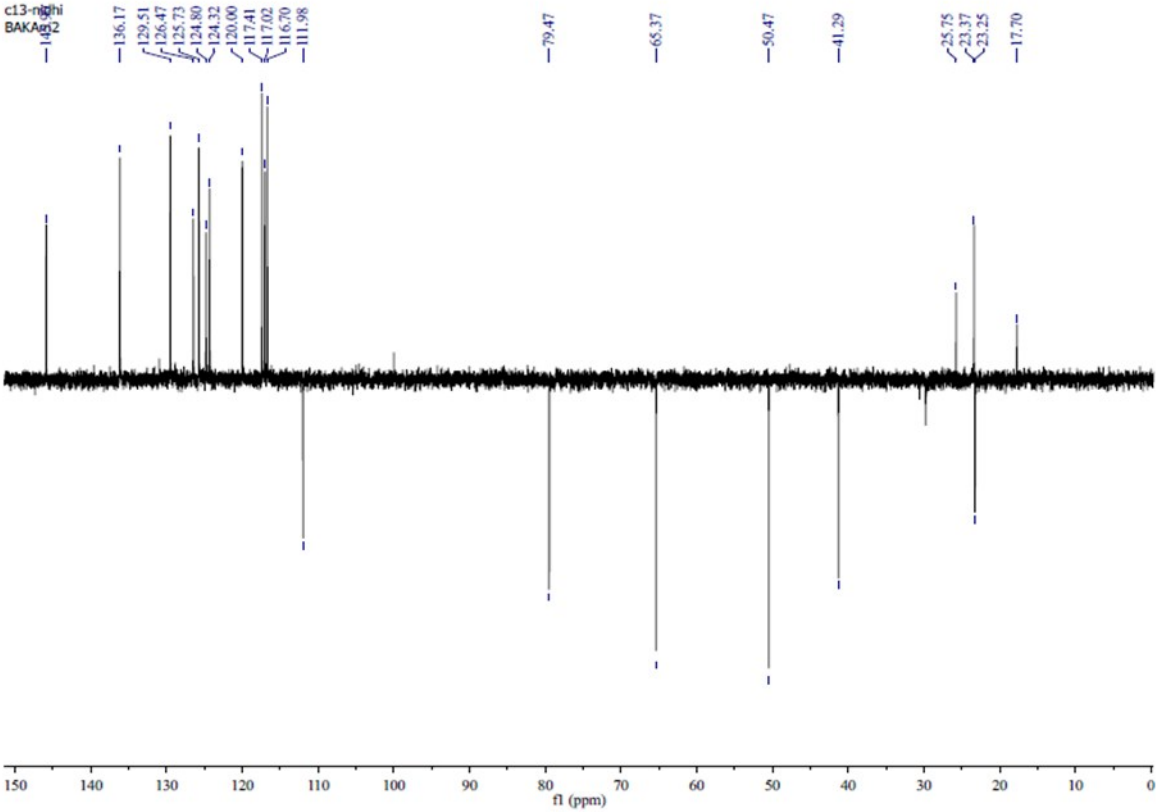


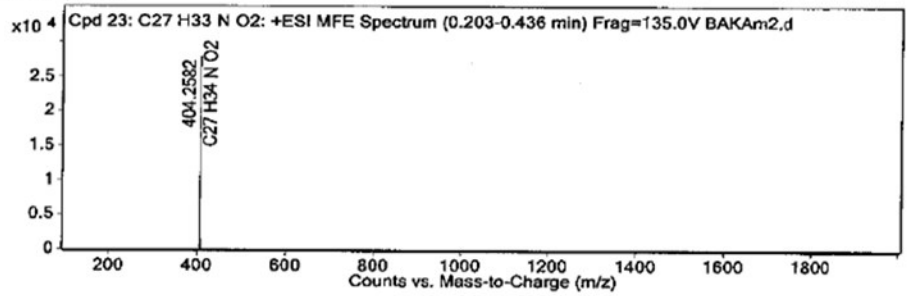
3 - HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 23: C27 H33 N O2	0.264	403.2506	C27 H33 N O2	C27 H33 N O2	1.27	C27 H33 N O2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 23: C27 H33 N O2	404.2582	0.264	Find by Molecular Feature	403.2506

MFE MS Spectrum



MS Spectrum Peak List

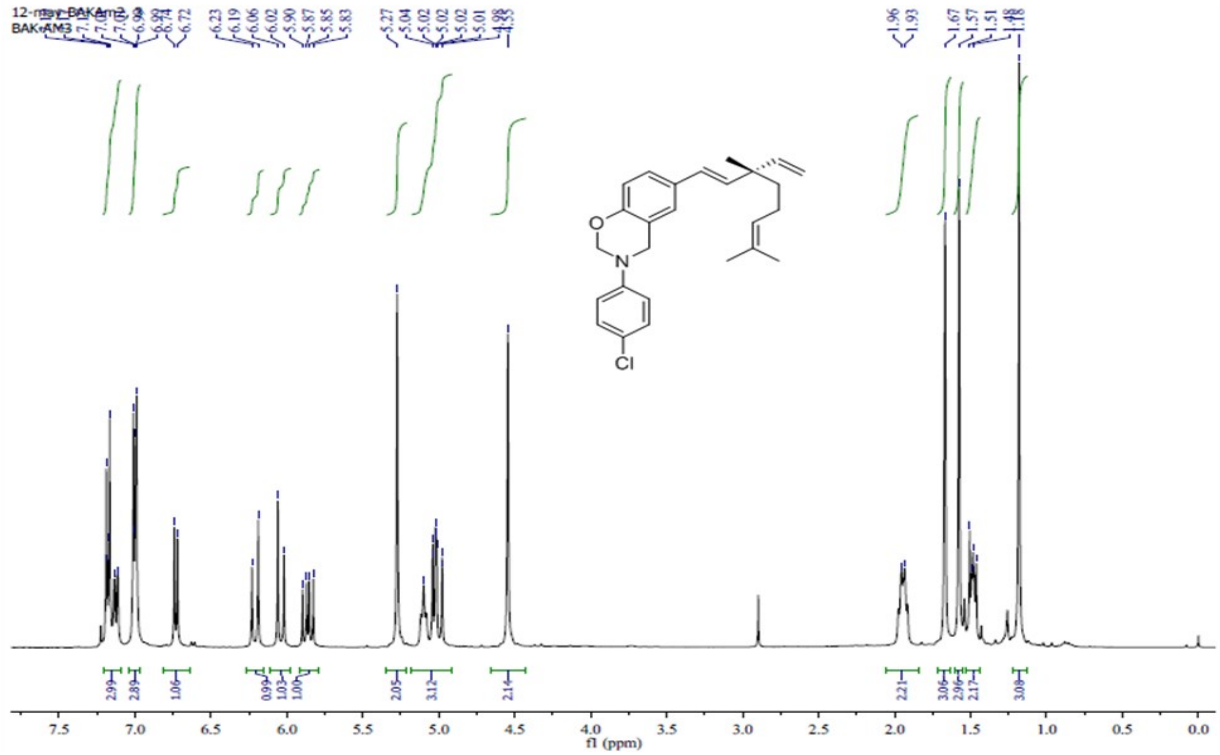
m/z	z	Abund	Formula	Ion
404.2582	1	27915.57	C27 H34 N O2	(M+H)+
405.2607	1	7608.7	C27 H34 N O2	(M+H)+
406.2645	1	1530.77	C27 H34 N O2	(M+H)+
407.2539	1	295.98	C27 H34 N O2	(M+H)+

Predicted Isotope Match Table

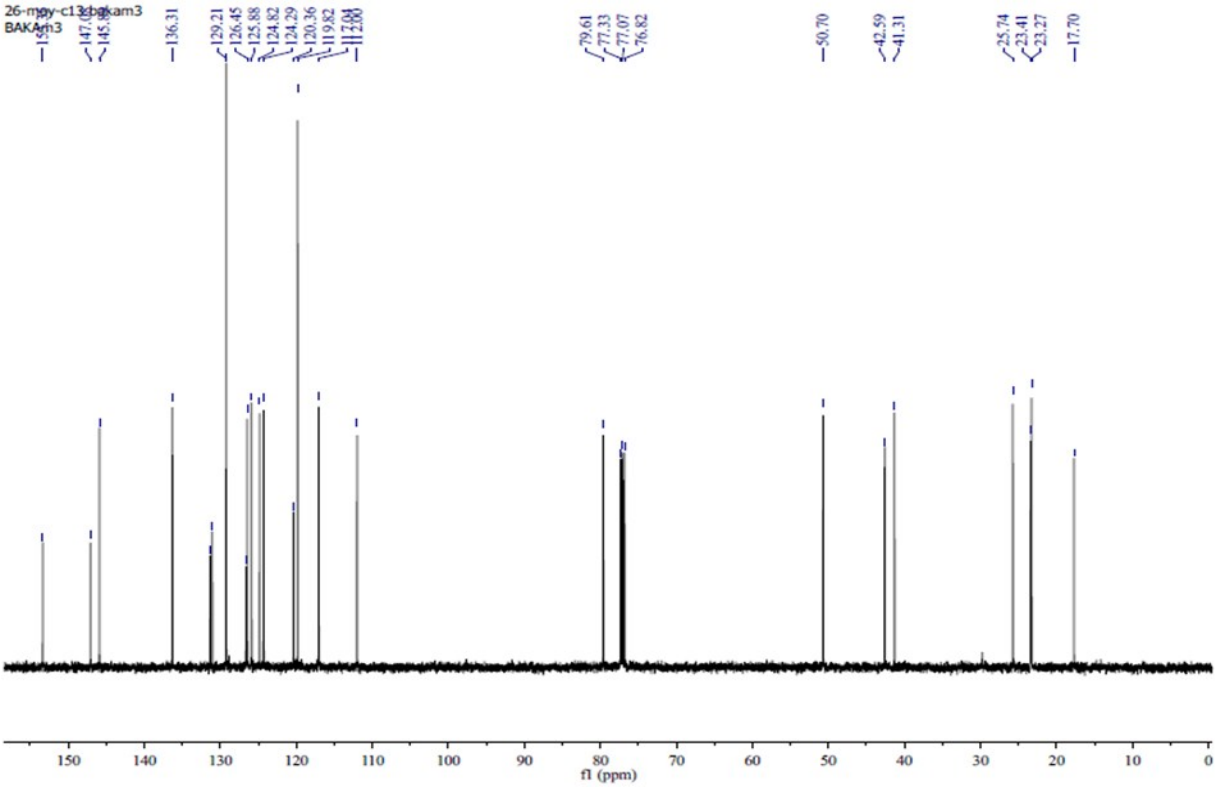
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	404.2582	404.2584	0.61	100	100	74.74	73.9
2	405.2607	405.2617	2.45	27.26	30.04	20.37	22.19
3	406.2645	406.2648	0.87	5.48	4.76	4.1	3.52
4	407.2539	407.2678	34.06	1.06	0.53	0.79	0.39

3-(4-chlorophenyl)-3,4-dihydro-6-(3,7-dimethyl-3-vinylocta-1,6-dienyl)-2H-benzo[e][1,3]oxazine(4)

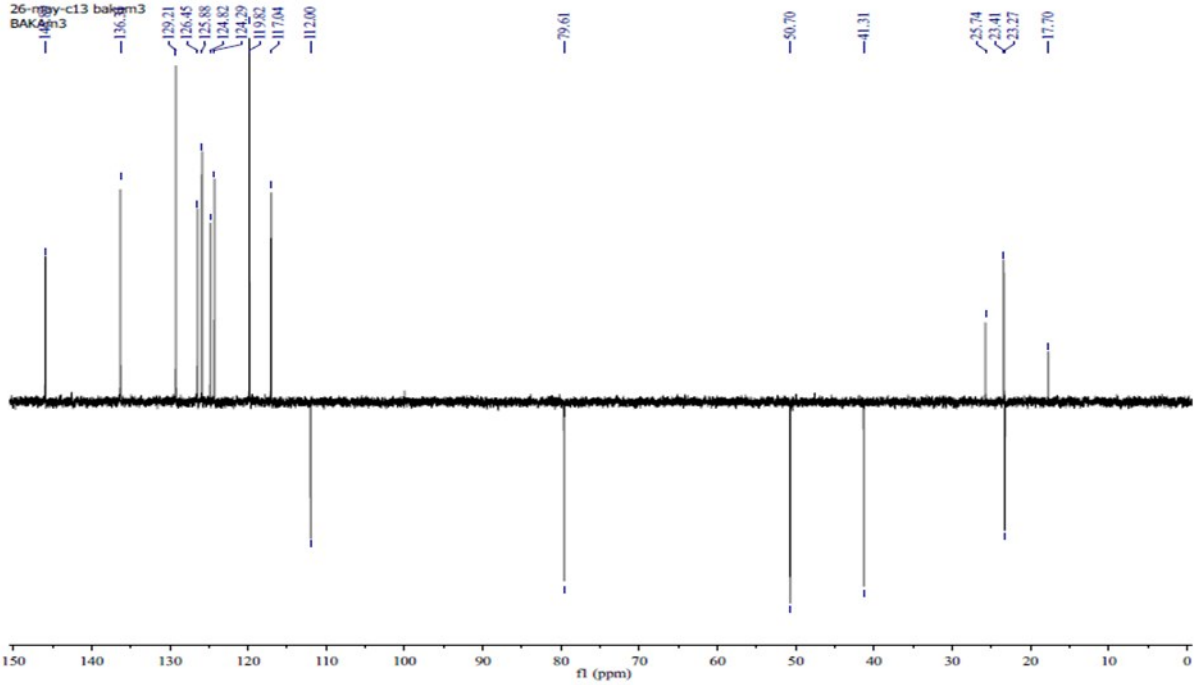
4 - ^{1}HNMR



4 – ^{13}C NMR



DEPT-4



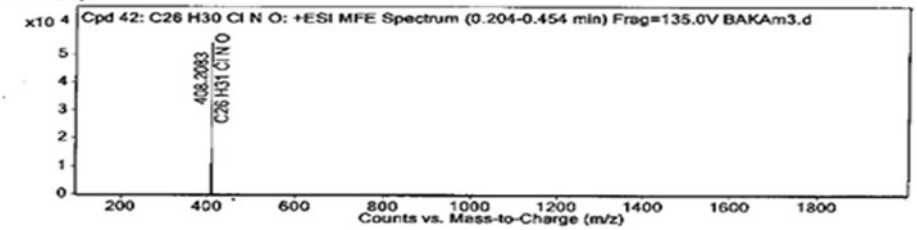
4 - HRMS

Compound Table

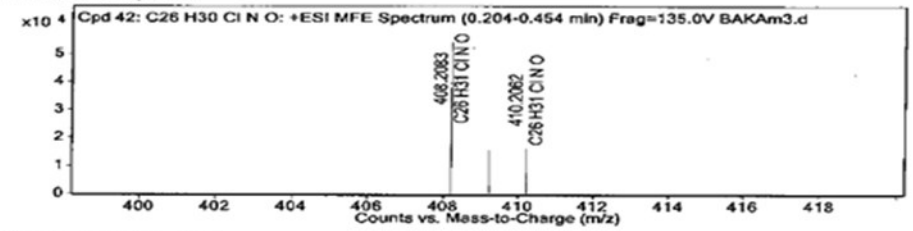
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 42: C26 H30 Cl N O	0.267	407.2009	C26 H30 Cl N O	C26 H30 Cl N O	1.71	C26 H30 Cl N O

Compound Label	m/z	RT	Algorithm	Mass
Cpd 42: C26 H30 Cl N O	408.2083	0.267	Find by Molecular Feature	407.2009

MFE MS Spectrum



MFE MS Zoomed Spectrum



MS Spectrum Peak List

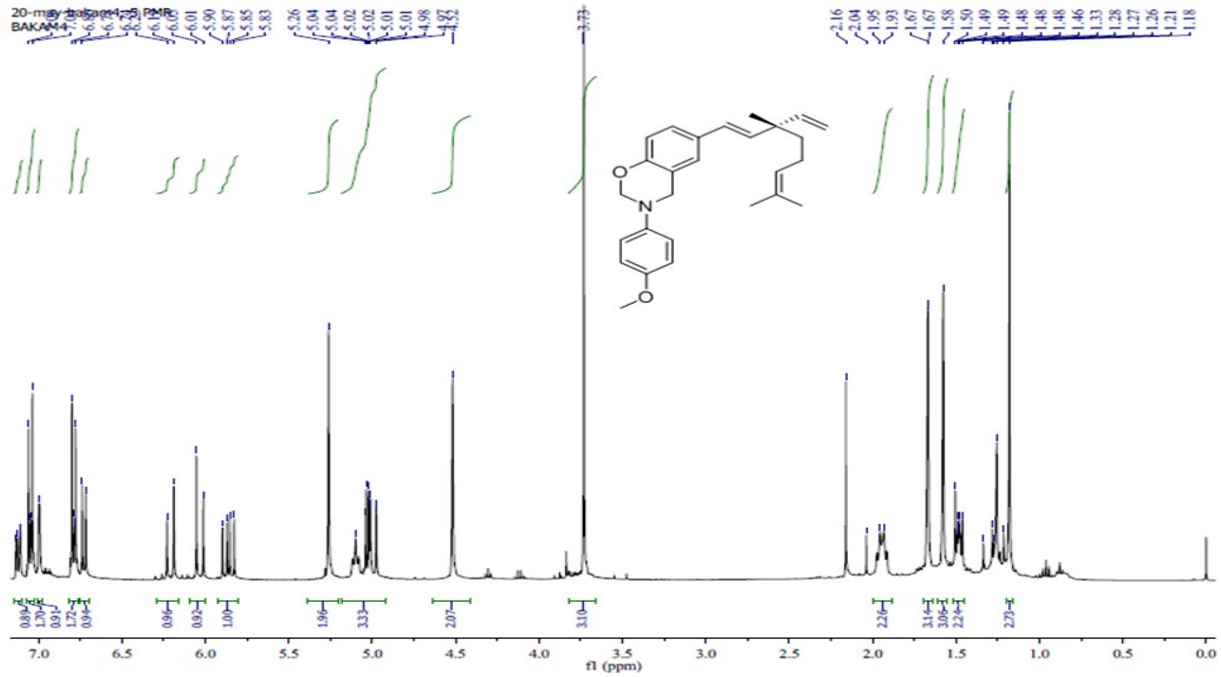
m/z	z	Abund	Formula	Ion
408.2083	1	53981.57	C26 H31 Cl N O	(M+H)+
409.2112	1	15755.09	C26 H31 Cl N O	(M+H)+
410.2062	1	16357.71	C26 H31 Cl N O	(M+H)+

Predicted Isotope Match Table

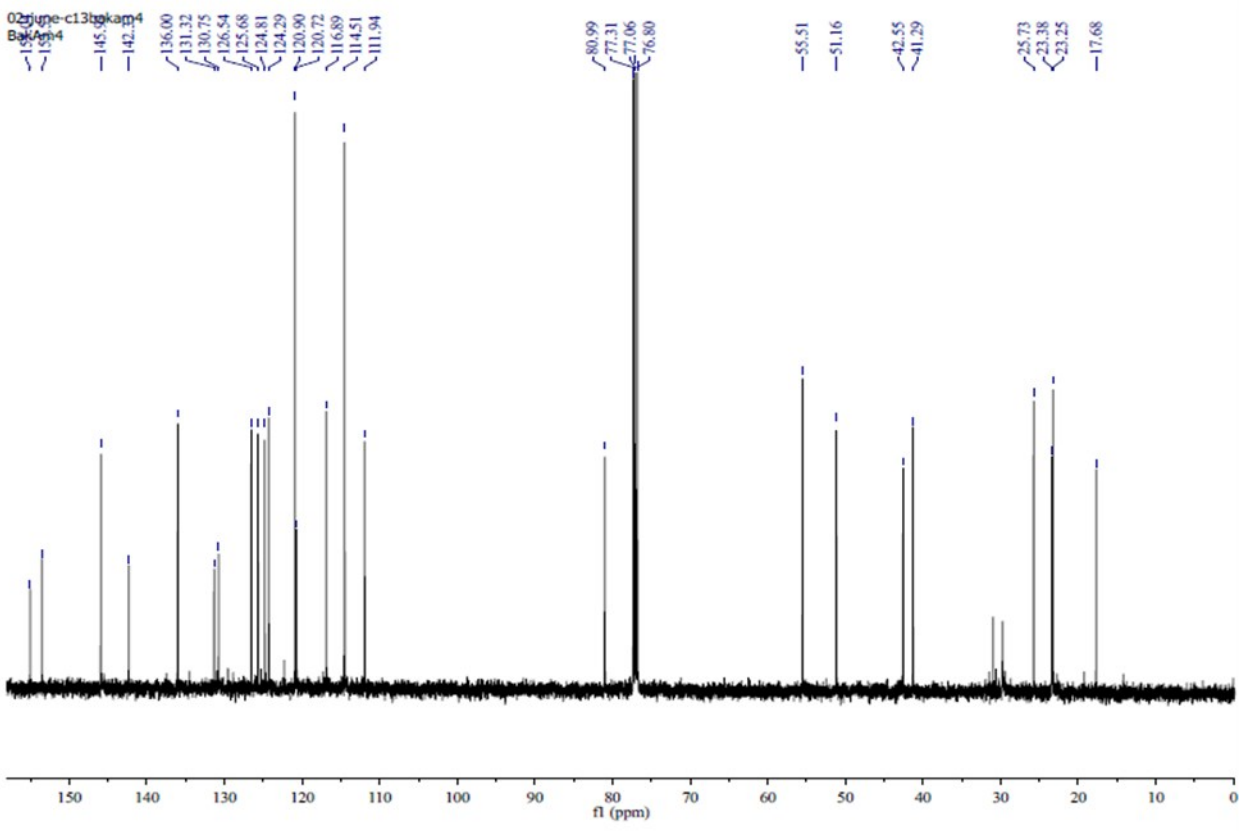
Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	408.2083	408.2089	1.48	100	100	62.7	60.57
2	409.2112	409.2122	2.28	29.19	28.88	18.3	17.49
3	410.2062	410.207	1.9	30.3	36.22	19	21.94

3,4-dihydro-3-(4-methoxyphenyl)-6-(3,7-dimethyl-3-vinylocta-1,6-dienyl)-2H-benzo[e][1,3]oxazine (5)

5 - ^{1}H NMR



5 – ^{13}C NMR



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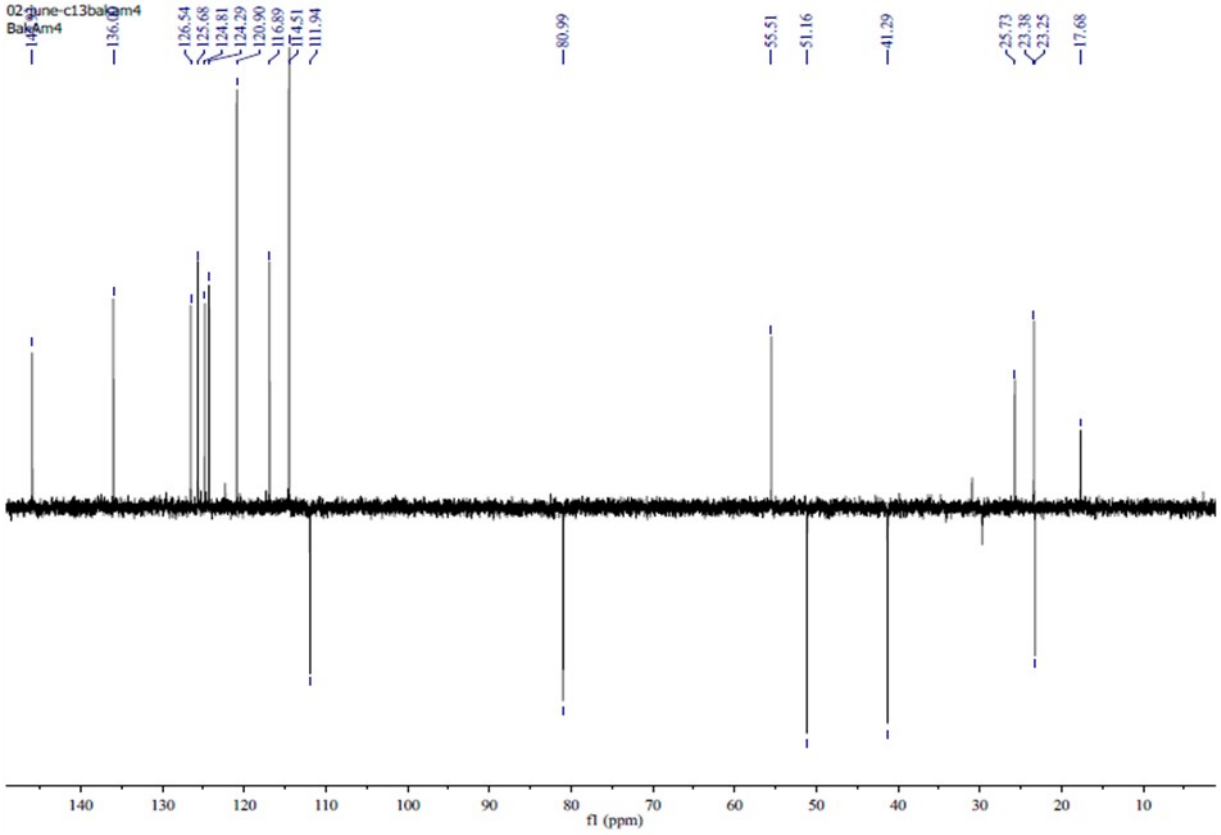


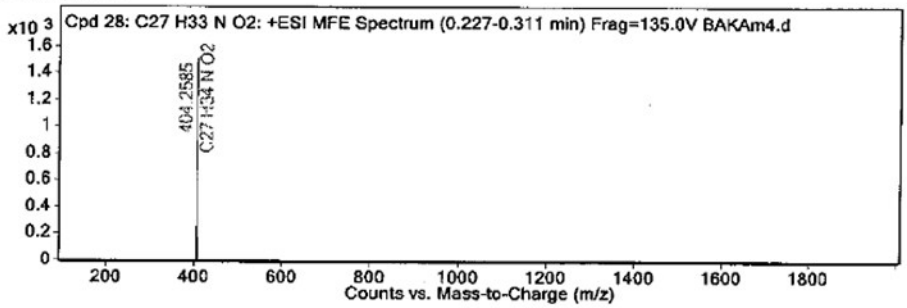
5 - HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 28: C27 H33 N O2	0.273	403.2511	C27 H33 N O2	C27 H33 N O2	-0.03	C27 H33 N O2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 28: C27 H33 N O2	404.2585	0.273	Find by Molecular Feature	403.2511

MFE MS Spectrum



MS Spectrum Peak List

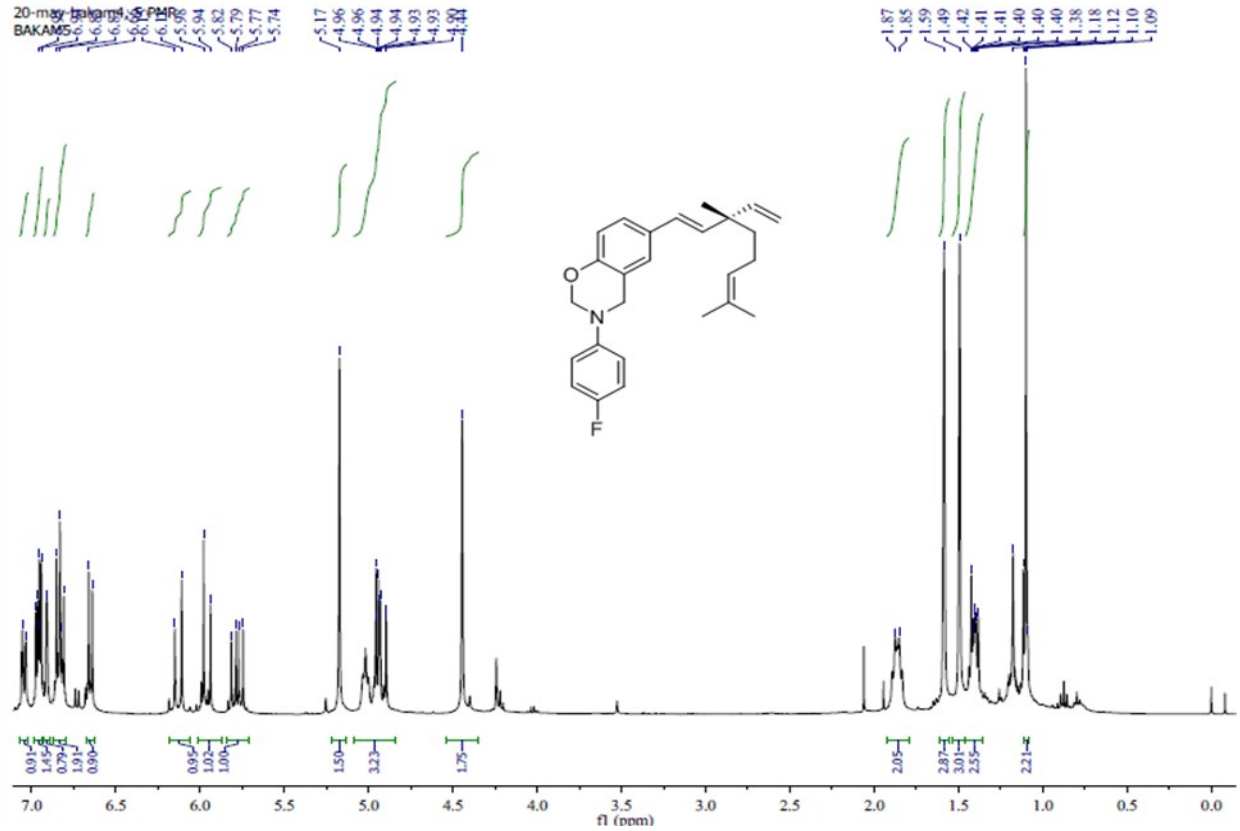
m/z	z	Abund	Formula	Ion
404.2585	1	1514.91	C27 H34 N O2	(M+H)+
405.2596	1	484.4	C27 H34 N O2	(M+H)+
406.2703	1	166.07	C27 H34 N O2	(M+H)+

Predicted Isotope Match Table

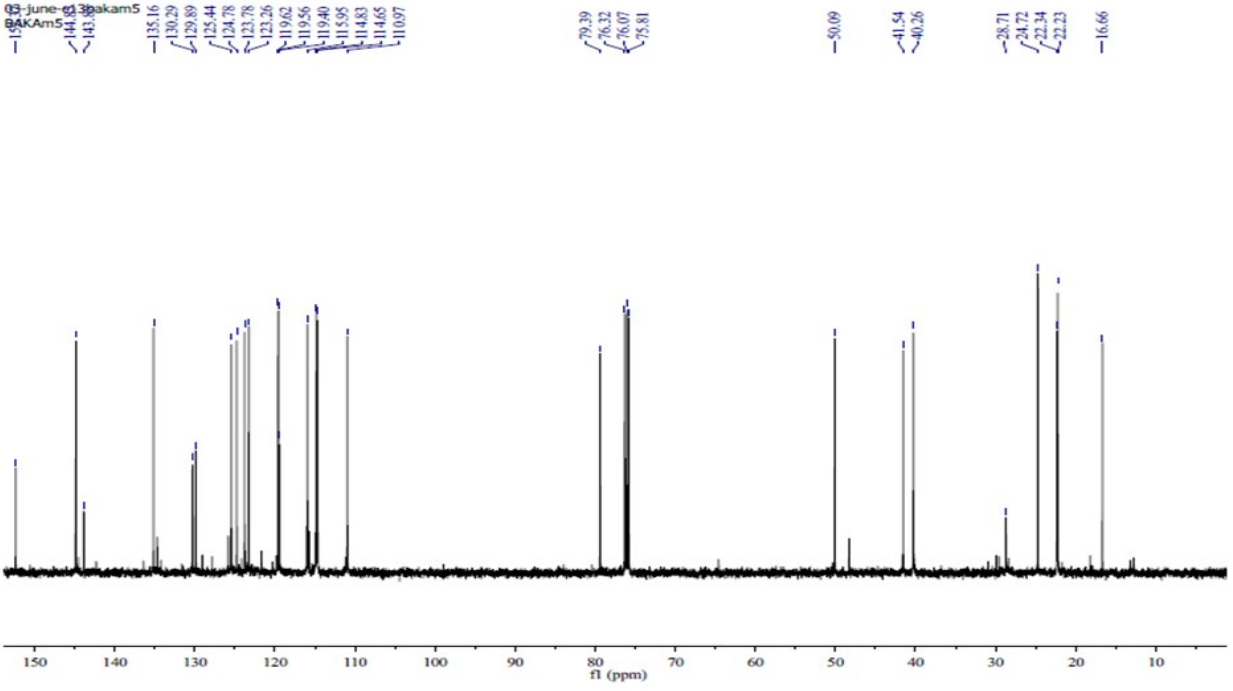
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	404.2585	404.2584	-0.27	100	100	69.96	74.19
2	405.2596	405.2617	5.33	31.98	30.04	22.37	22.28
3	406.2703	406.2648	-13.36	10.96	4.76	7.67	3.53

3-(4-fluorophenyl)-3,4-dihydro-6-(3,7-dimethyl-3-vinylocta-1,6-dienyl)-2H-benzo[e][1,3]oxazine(6)

6 - ^{1}H NMR



6 – ^{13}C NMR



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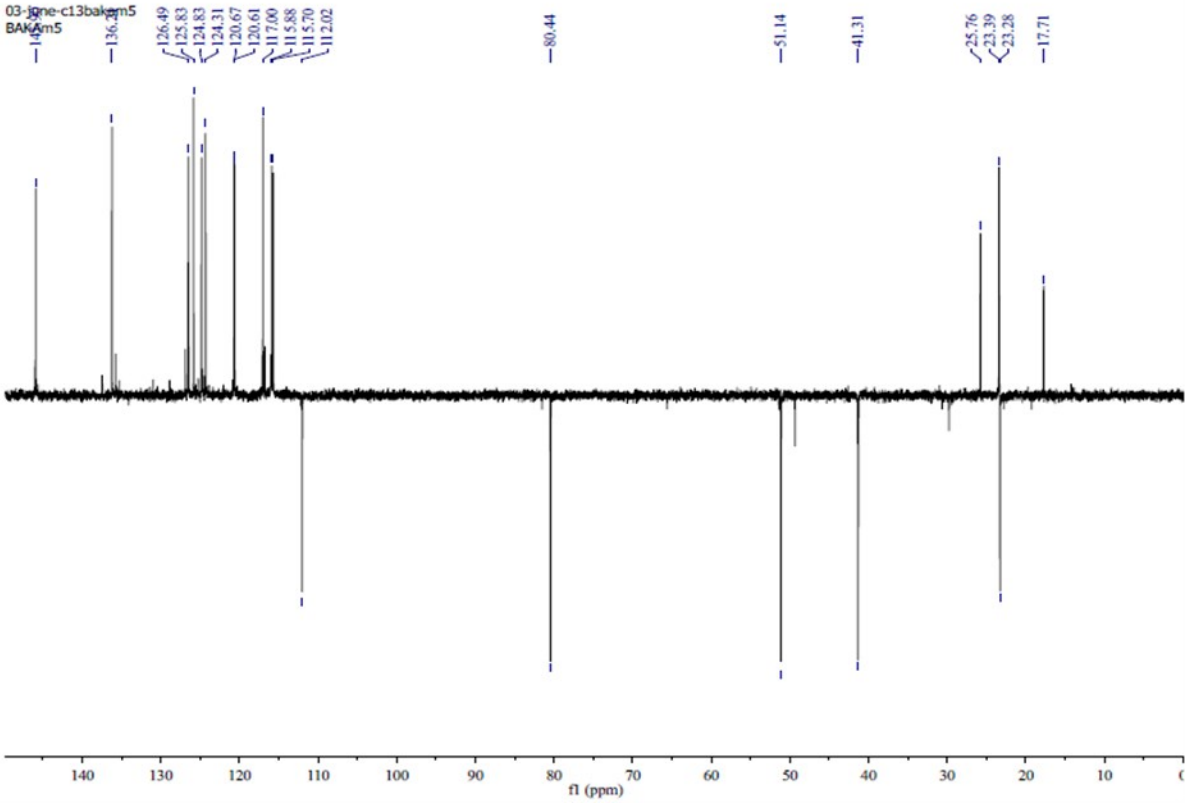


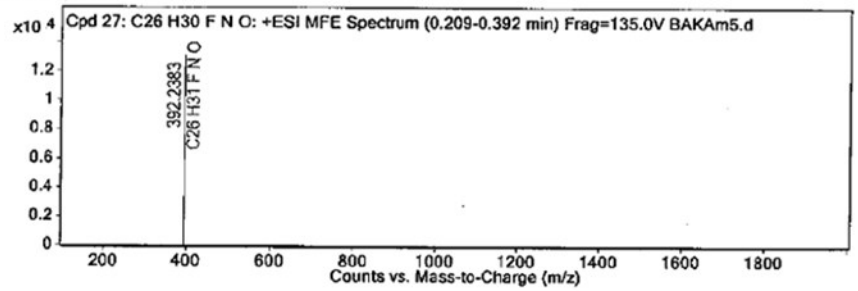
6 - HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 27: C26 H30 F N O	0.266	391.2305	C26 H30 F N O	C26 H30 F N O	1.72	C26 H30 F N O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 27: C26 H30 F N O	392.2383	0.266	Find by Molecular Feature	391.2305

MFE MS Spectrum



MS Spectrum Peak List

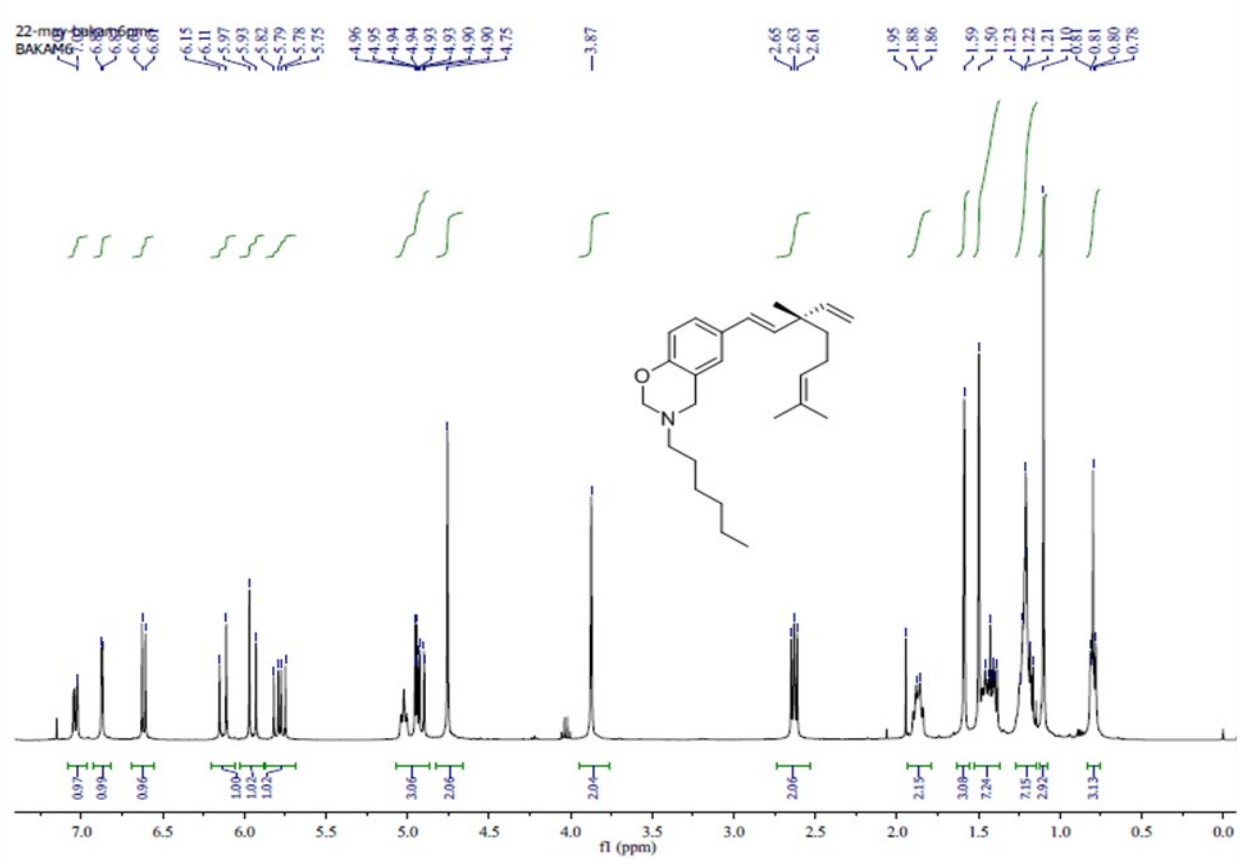
m/z	z	Abund	Formula	Ion
392.2383	1	13130.8	C26 H31 F N O	(M+H)+
393.2417	1	3059.76	C26 H31 F N O	(M+H)+
394.236	1	1116.6	C26 H31 F N O	(M+H)+

Predicted Isotope Match Table

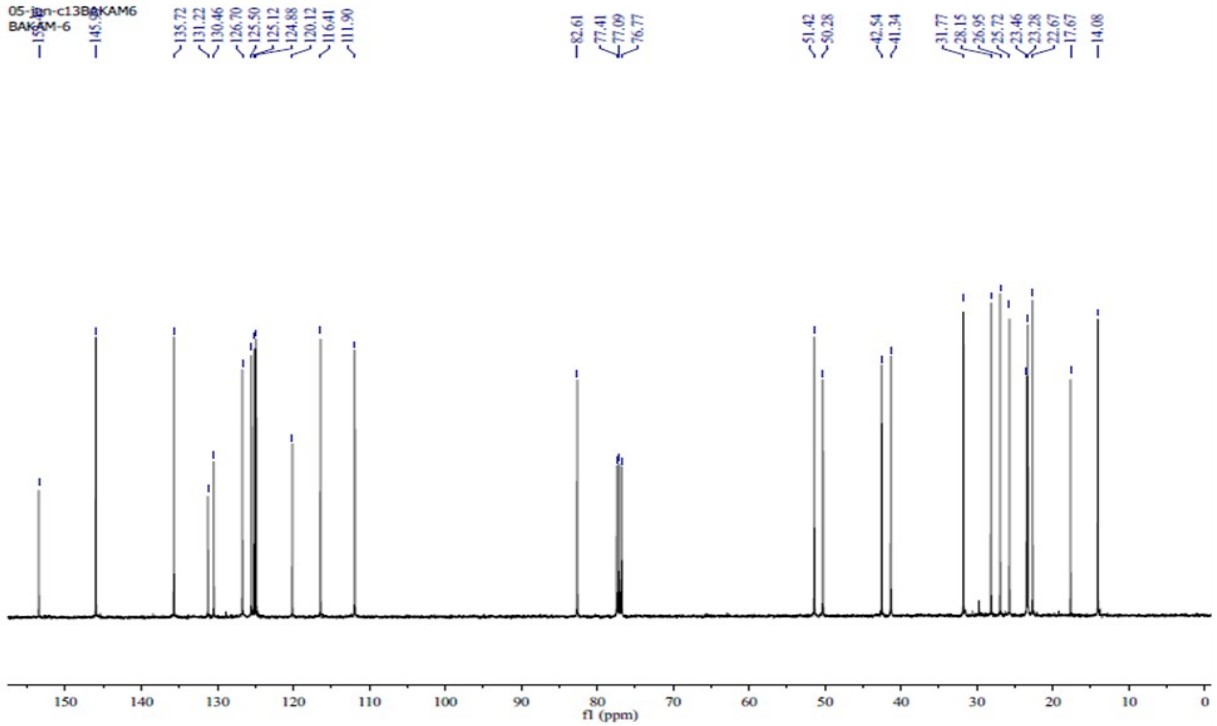
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	392.2383	392.2384	0.32	100	100	75.87	75.13
2	393.2417	393.2417	0.07	23.3	28.88	17.68	21.7
3	394.236	394.2449	22.59	8.5	4.22	6.45	3.17

3-hexyl-3,4-dihydro-6-(3,7-dimethyl-3-vinylocta-1,6-dienyl)-2H-benzo[e][1, 3]oxazine (7)

7 - ^{1}HNMR



7– ^{13}C NMR



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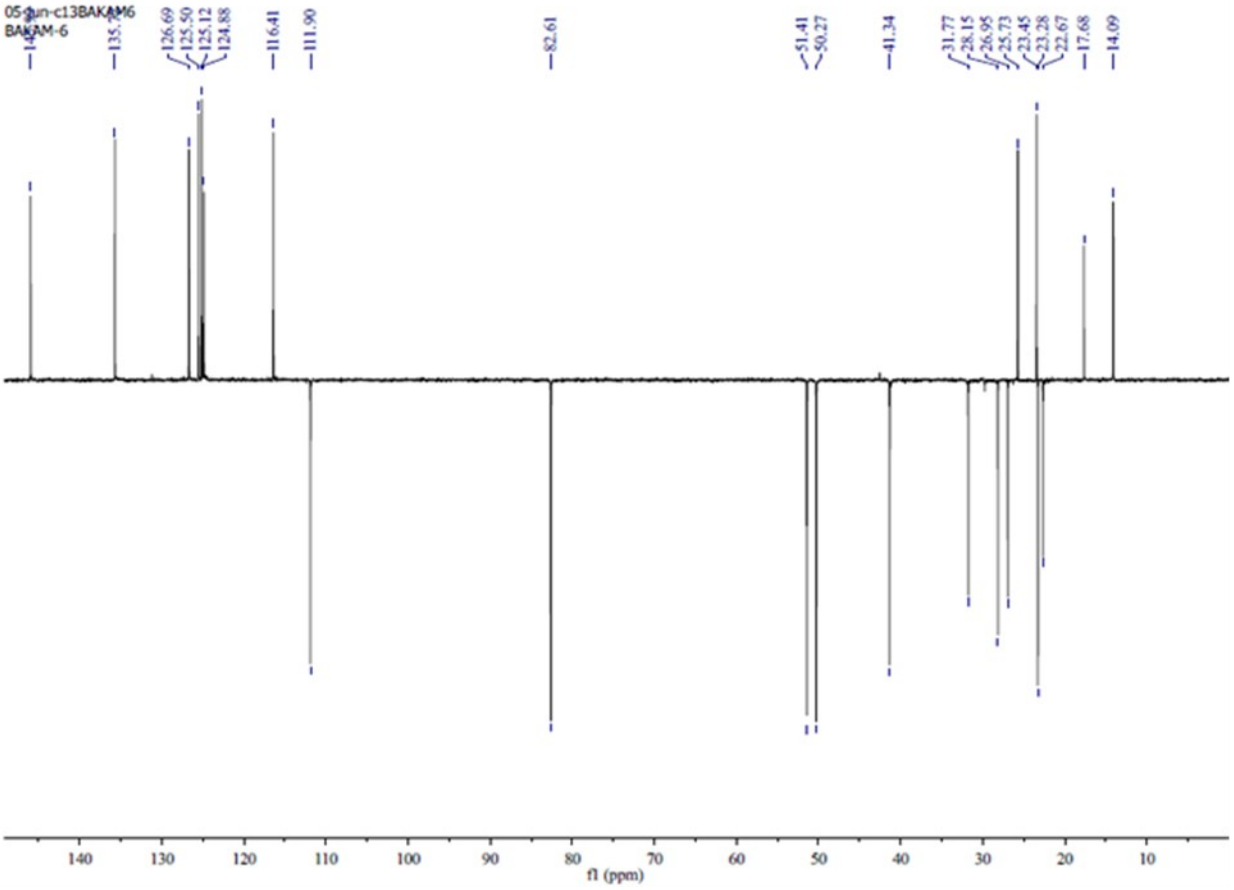


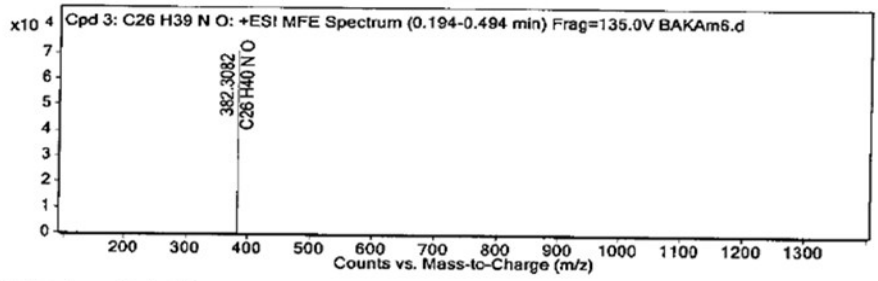
7 - HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 3: C26 H39 N O	0.247	381.3009	C26 H39 N O	C26 H39 N O	6.06	C26 H39 N O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 3: C26 H39 N O	382.3082	0.247	Find by Molecular Feature	381.3009

MFE MS Spectrum



MS Spectrum Peak List

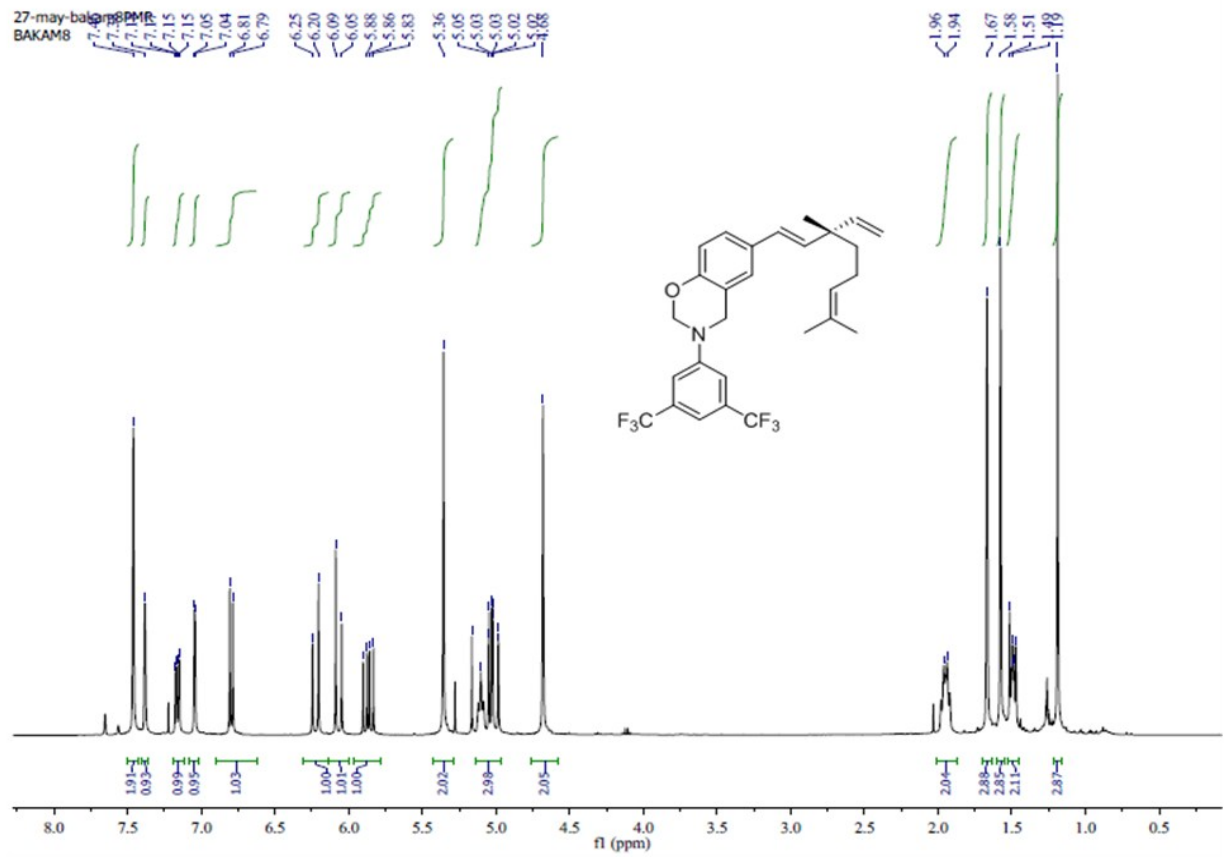
m/z	z	Abund	Formula	Ion
382.3082	1	70958.67	C26 H40 N O	(M+H)+
383.3112	1	21317.11	C26 H40 N O	(M+H)+

Predicted Isotope Match Table

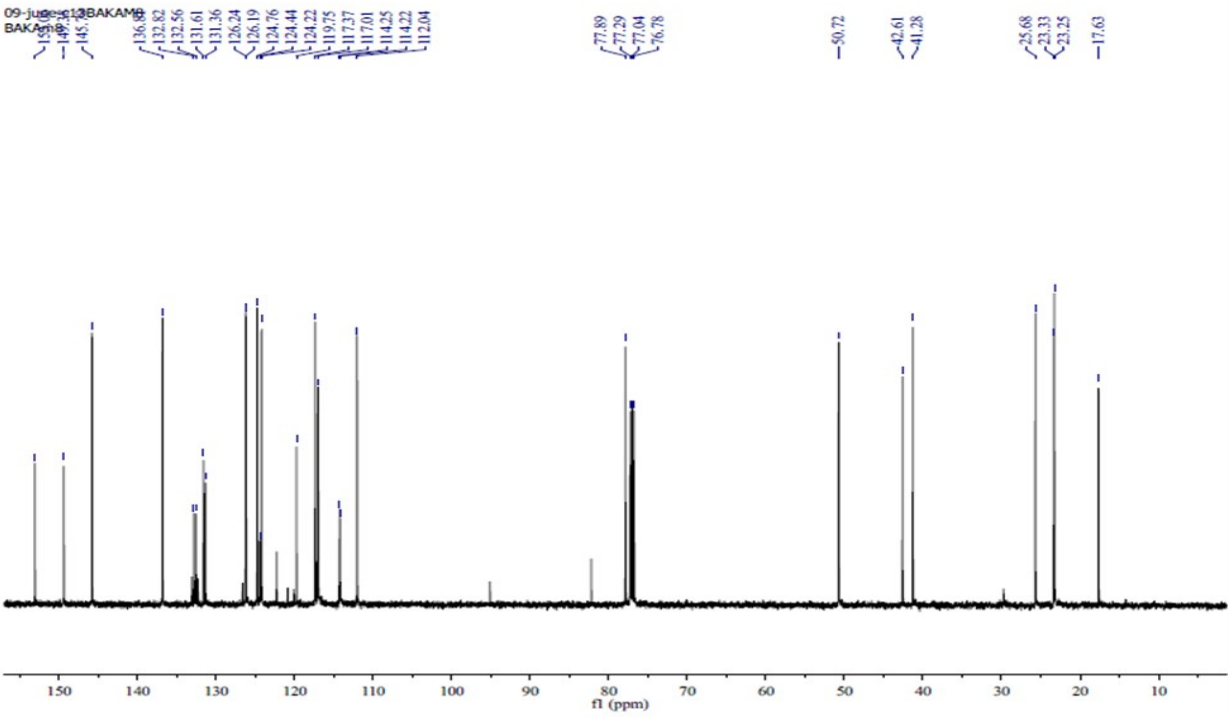
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	382.3082	382.3104	5.83	100	100	76.9	77.53
2	383.3112	383.3138	6.74	30.04	28.98	23.1	22.47

3-(3,5-bis(trifluoromethyl)phenyl)-3,4-dihydro-6-(3,7-dimethyl-3-vinylocta-1,6-dienyl)-2H-benzo[e][1,3]oxazine (8)

8- ^{1}HNMR



8- ^{13}CNMR



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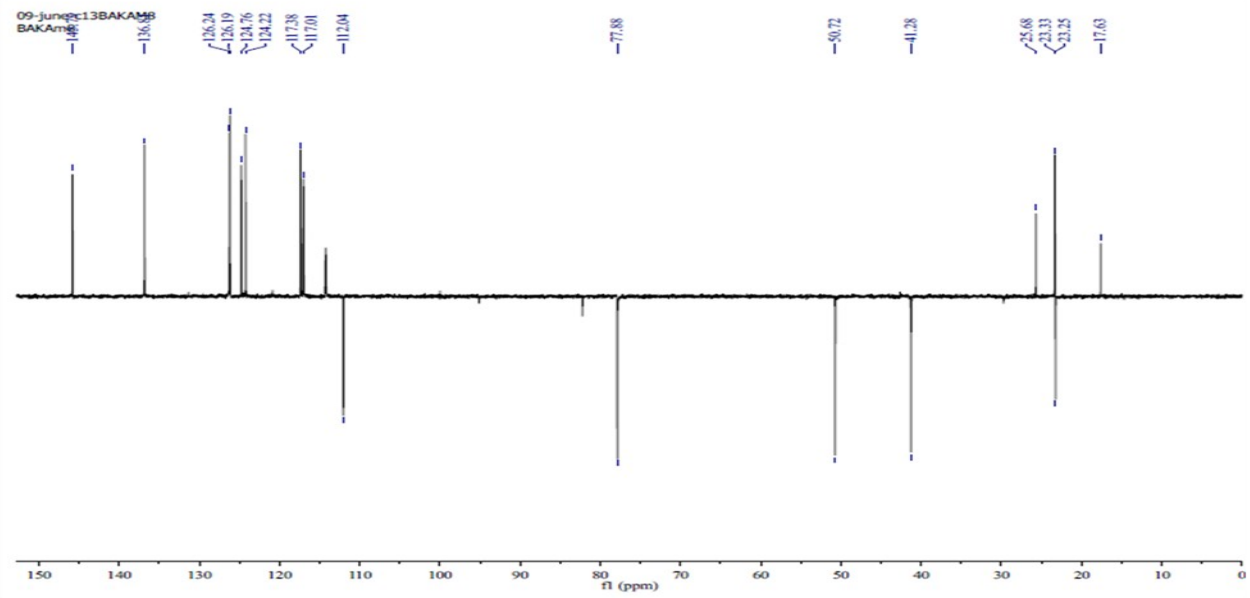


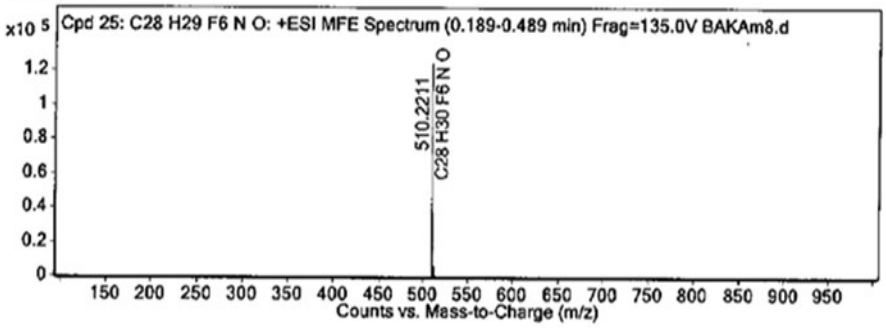
8- HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 25: C28 H29 F6 N O	0.269	509.2137	C28 H29 F6 N O	C28 H29 F6 N O	3.23	C28 H29 F6 N O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 25: C28 H29 F6 N O	510.2211	0.269	Find by Molecular Feature	509.2137

MFE MS Spectrum



MS Spectrum Peak List

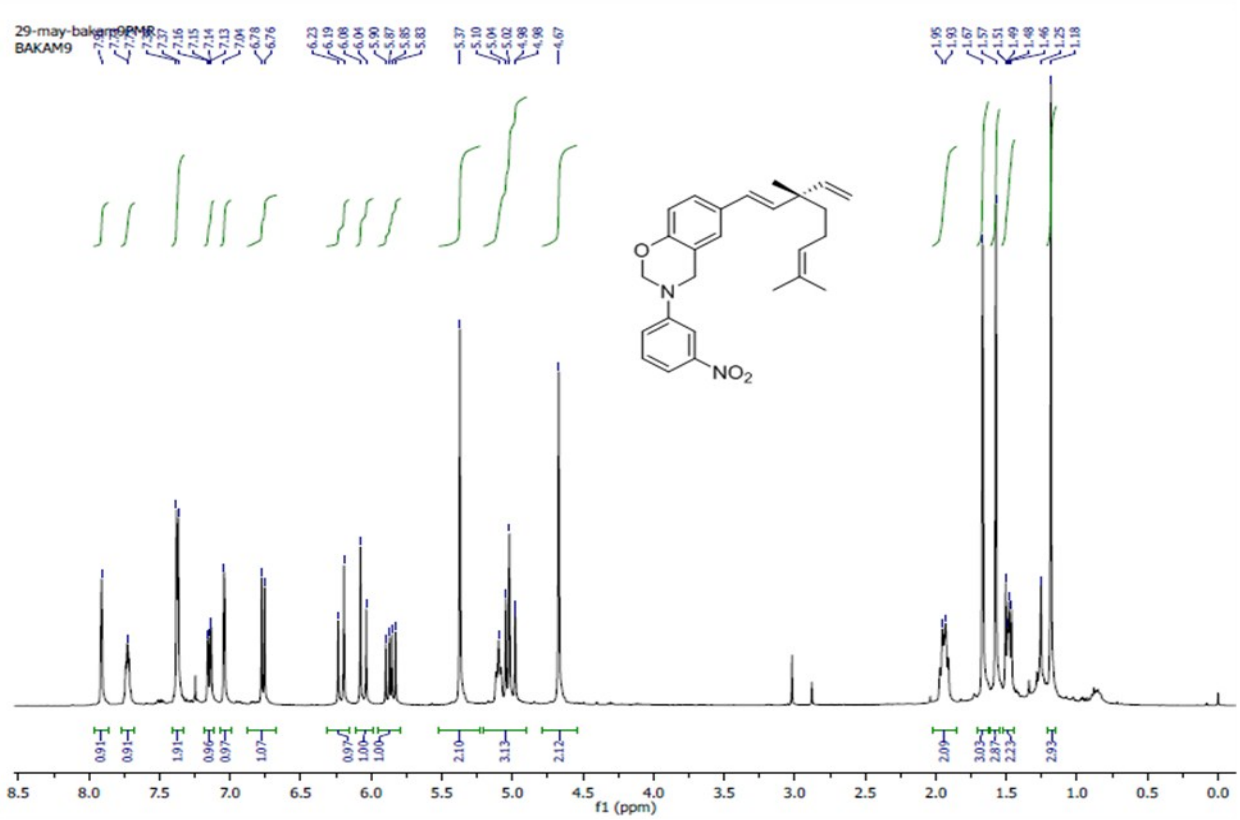
m/z	z	Abund	Formula	Ion
510.2211	1	124293.93	C28 H30 F6 N O	(M+H)+
511.2241	1	37413.97	C28 H30 F6 N O	(M+H)+
512.2263	1	6533.87	C28 H30 F6 N O	(M+H)+
513.2273	1	914.86	C28 H30 F6 N O	(M+H)+

Predicted Isotope Match Table

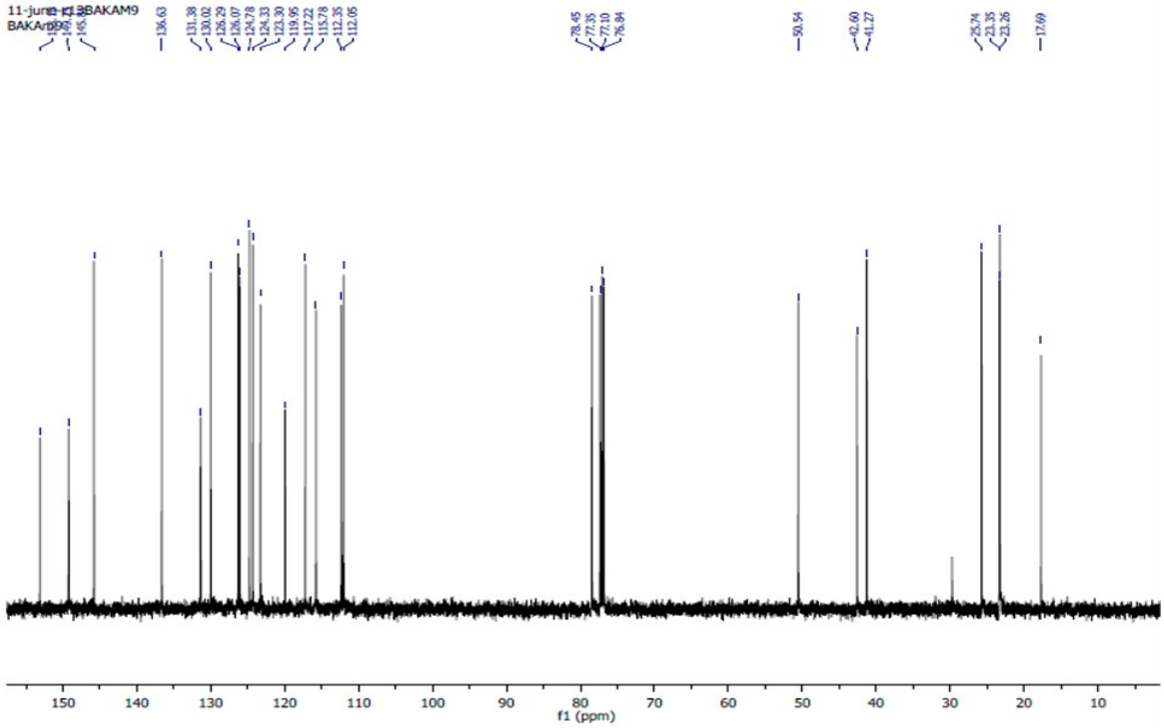
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	510.2211	510.2226	2.95	100	100	73.48	73.31
2	511.2241	511.2259	3.59	30.1	31.03	22.12	22.75
3	512.2263	512.2291	5.48	5.26	4.86	3.86	3.56
4	513.2273	513.2323	9.62	0.74	0.51	0.54	0.38

3,4-dihydro-6-(3,7-dimethyl-3-vinylocta-1,6-dienyl)-3-(3-nitrophenyl)-2H-benzo[e][1,3]oxazine (9)

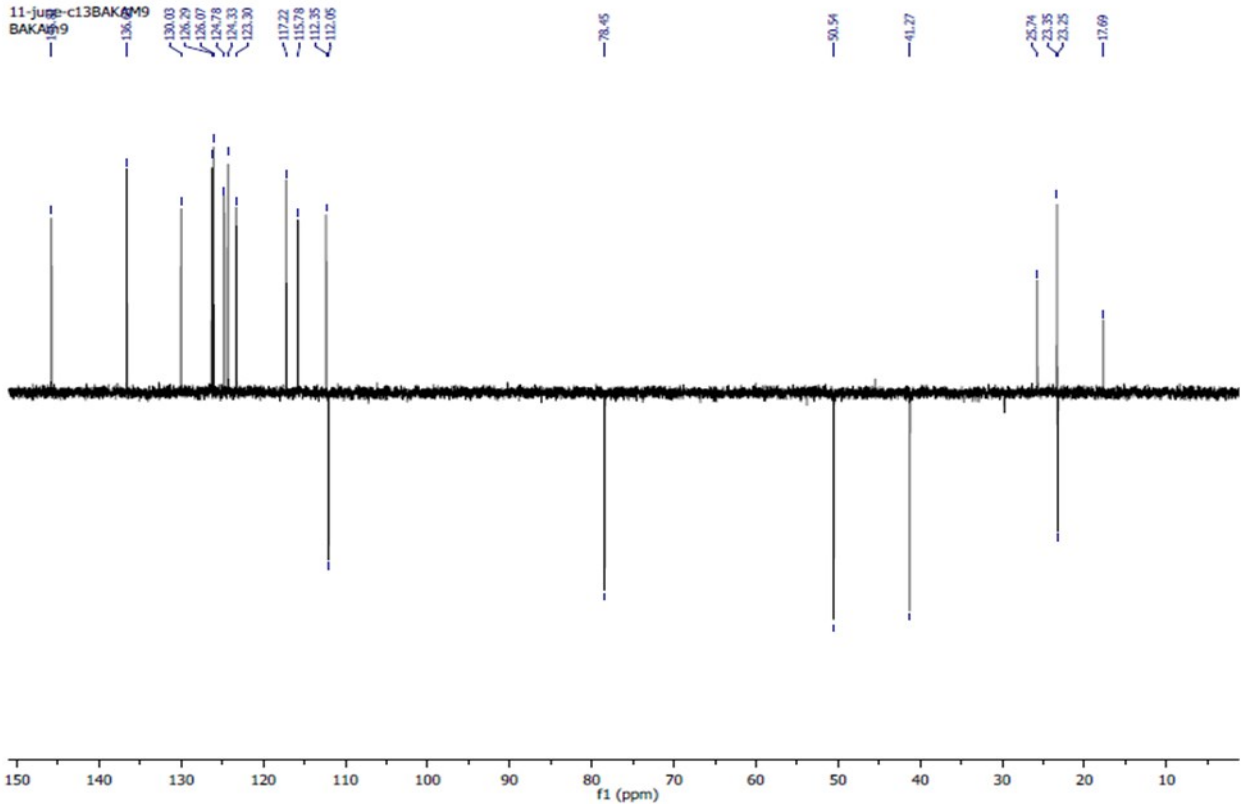
9- ^{1}HNMR



9– ^{13}C NMR



DEPT-9



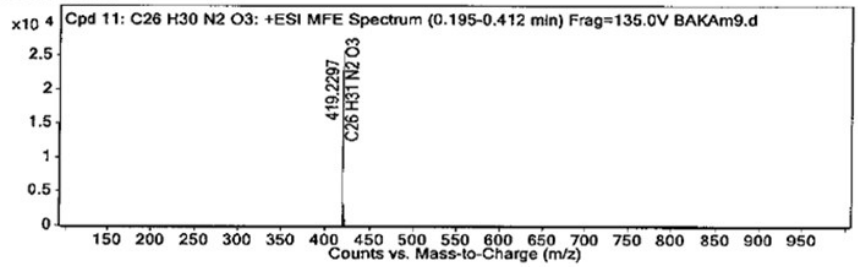
9- HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 11: C26 H30 N2 O3	0.264	418.2209	C26 H30 N2 O3	C26 H30 N2 O3	11.45	C26 H30 N2 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 11: C26 H30 N2 O3	419.2297	0.264	Find by Molecular Feature	418.2209

MFE MS Spectrum



MS Spectrum Peak List

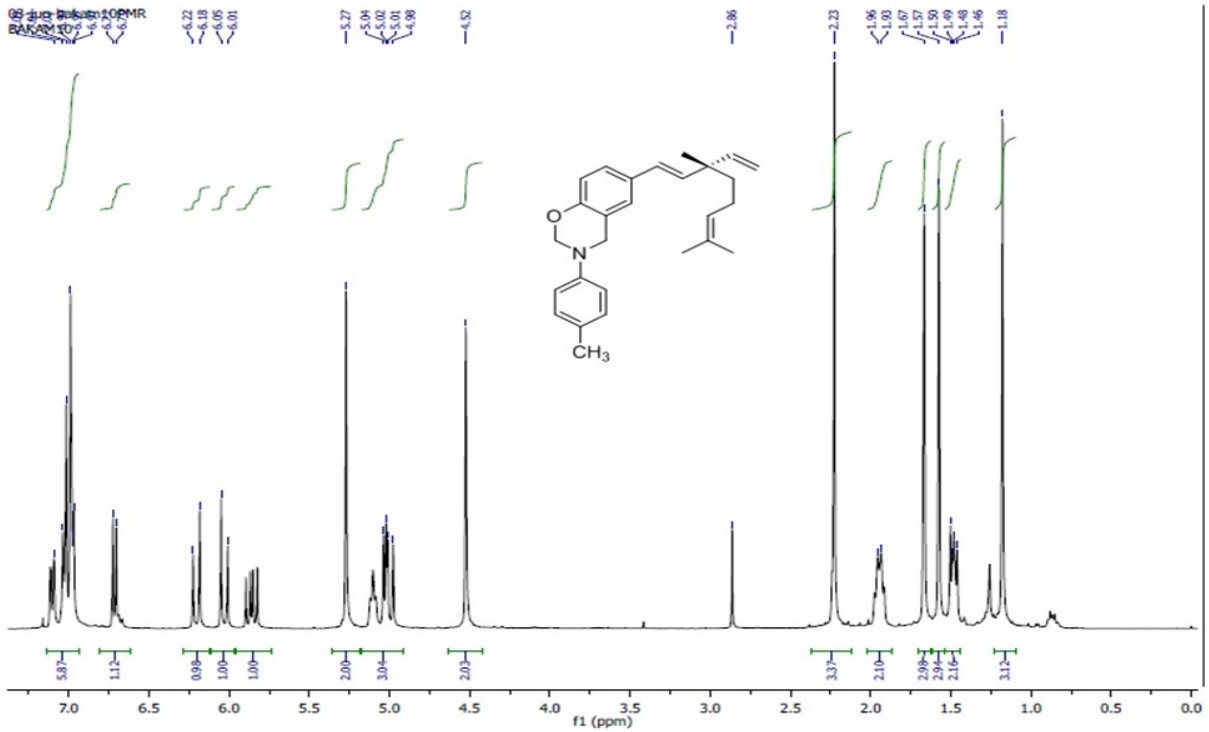
m/z	z	Abund	Formula	Ion
419.2297	1	25620.66	C26 H31 N2 O3	(M+H)+
420.233	1	8251.12	C26 H31 N2 O3	(M+H)+
421.2166	1	3089.11	C26 H31 N2 O3	(M+H)+
422.2137	1	840.94	C26 H31 N2 O3	(M+H)+

Predicted Isotope Match Table

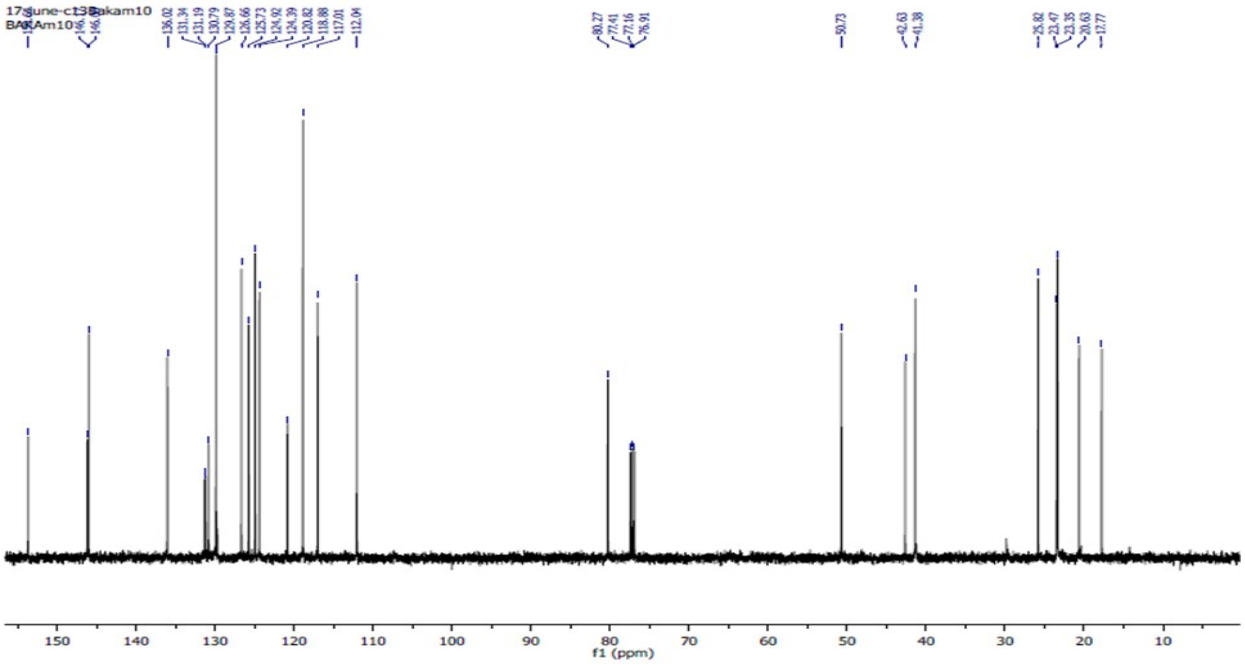
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	419.2297	419.2329	7.71	100	100	67.92	74.27
2	420.233	420.2362	7.56	32.2	29.32	21.87	21.78
3	421.2166	421.2391	53.36	11.74	4.76	7.98	3.54
4	422.2137	422.2419	66.73	3.28	0.56	2.23	0.41

3,4-dihydro-6-(3,7-dimethyl-3-vinylocta-1,6-dienyl)-3-p-tolyl-2H-benzo[e][1,3]oxazine (10)

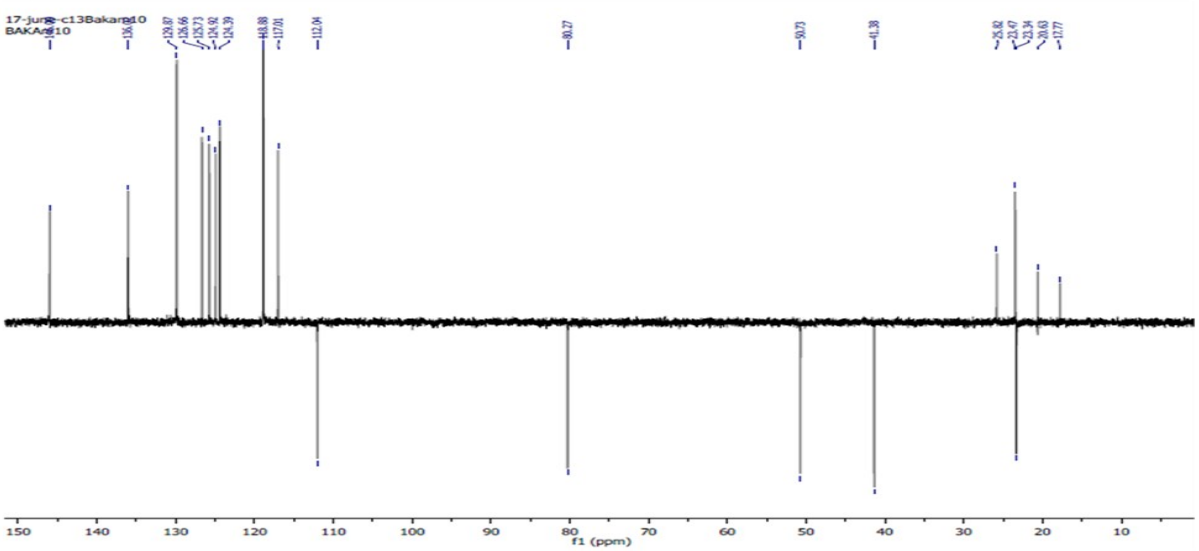
10 - ^{1}HNMR



10 – ^{13}C NMR



DEPT-10



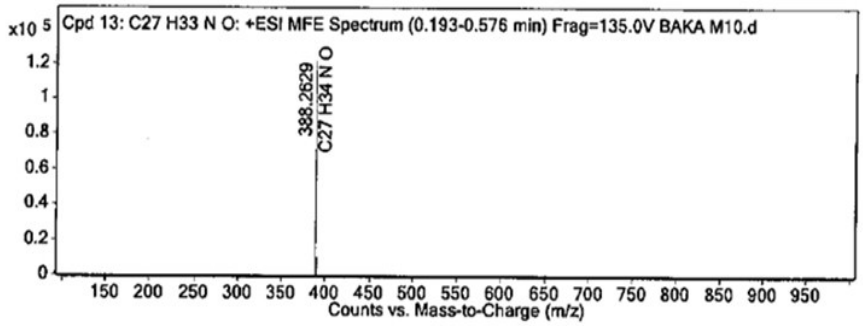
10 - HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 13: C27 H33 N O	0.271	387.2558	C27 H33 N O	C27 H33 N O	1.03	C27 H33 N O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 13: C27 H33 N O	388.2629	0.271	Find by Molecular Feature	387.2558

MFE MS Spectrum



MS Spectrum Peak List

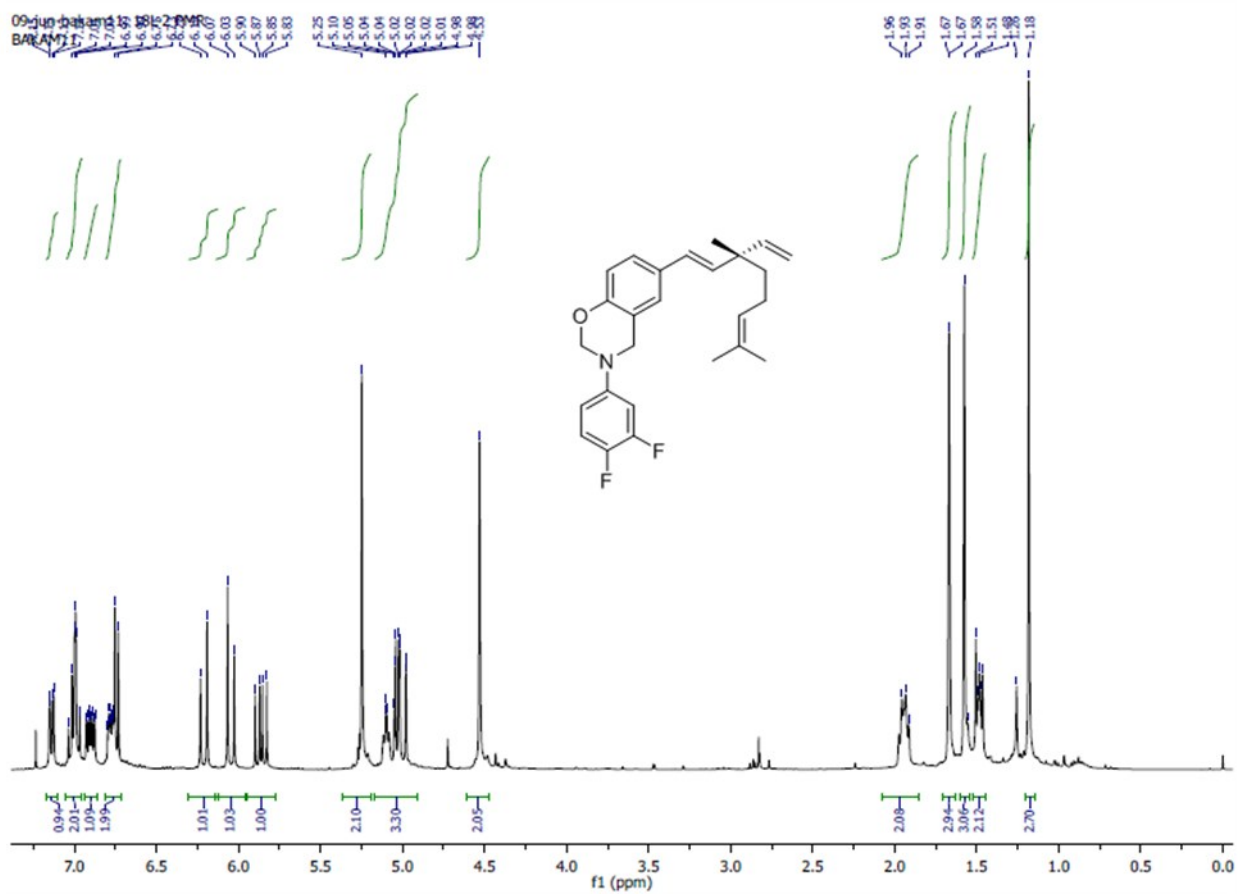
m/z	z	Abund	Formula	Ion
388.2629	1	121266.14	C27 H34 N O	(M+H)+
389.2659	1	35055.15	C27 H34 N O	(M+H)+
390.2735	1	10270.61	C27 H34 N O	(M+H)+

Predicted Isotope Match Table

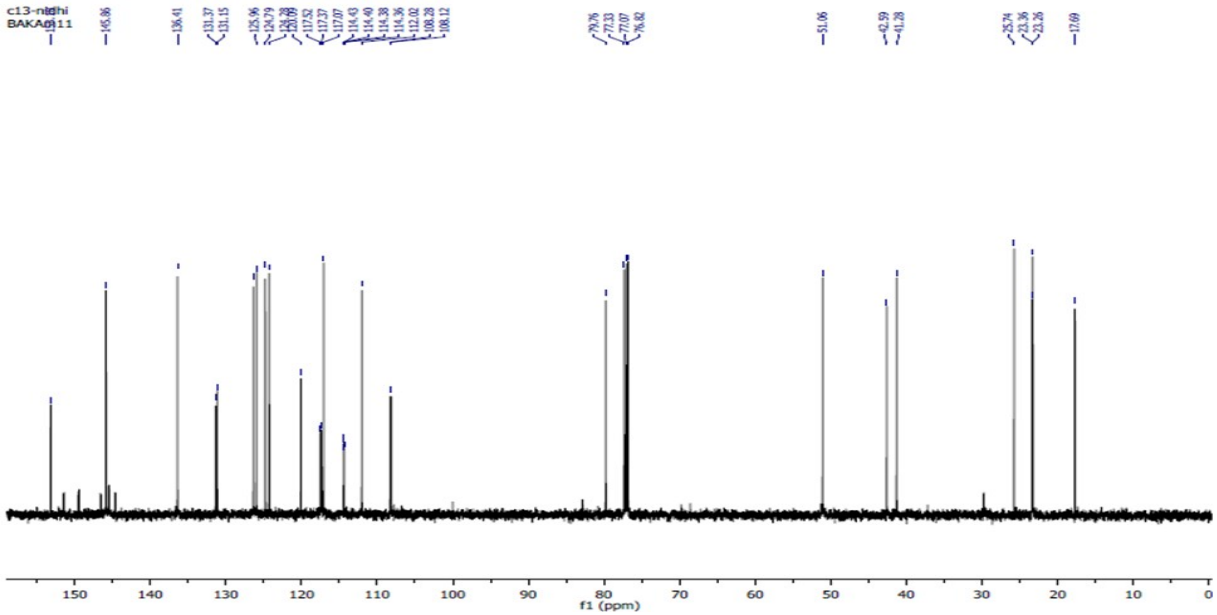
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	388.2629	388.2635	1.47	100	100	72.79	74.33
2	389.2659	389.2668	2.43	28.91	30	21.04	22.3
3	390.2735	390.27	-8.92	8.47	4.55	6.17	3.38

3-(3,4-difluorophenyl)-3,4-dihydro-6-(3,7-dimethyl-3-vinylocta-1,6-dienyl)-2H-benzo[e][1,3]oxazine(11)

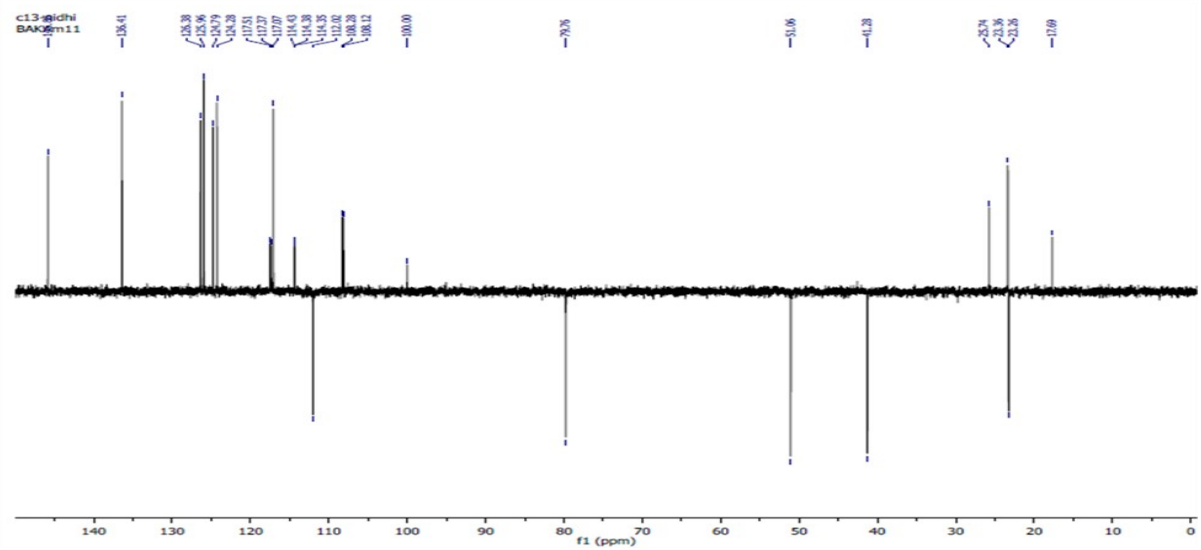
11 - ^{1}HNMR



11 – ^{13}C NMR



DEPT-11



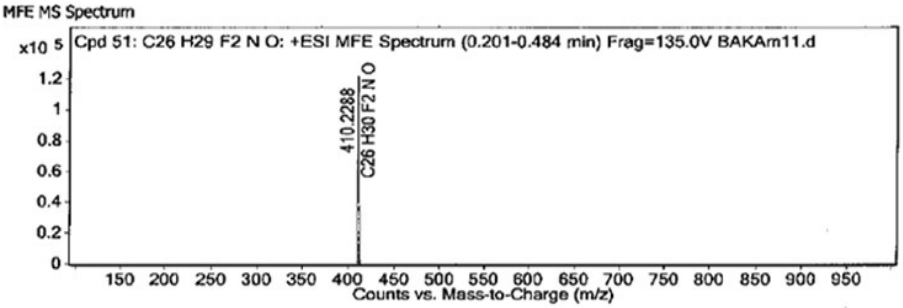
11-HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 51: C26 H29 F2 N O	0.268	409.222	C26 H29 F2 N O	C26 H29 F2 N O	-0.76	C26 H29 F2 N O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 51: C26 H29 F2 N O	410.2288	0.268	Find by Molecular Feature	409.222

MFE MS Spectrum



MS Spectrum Peak List

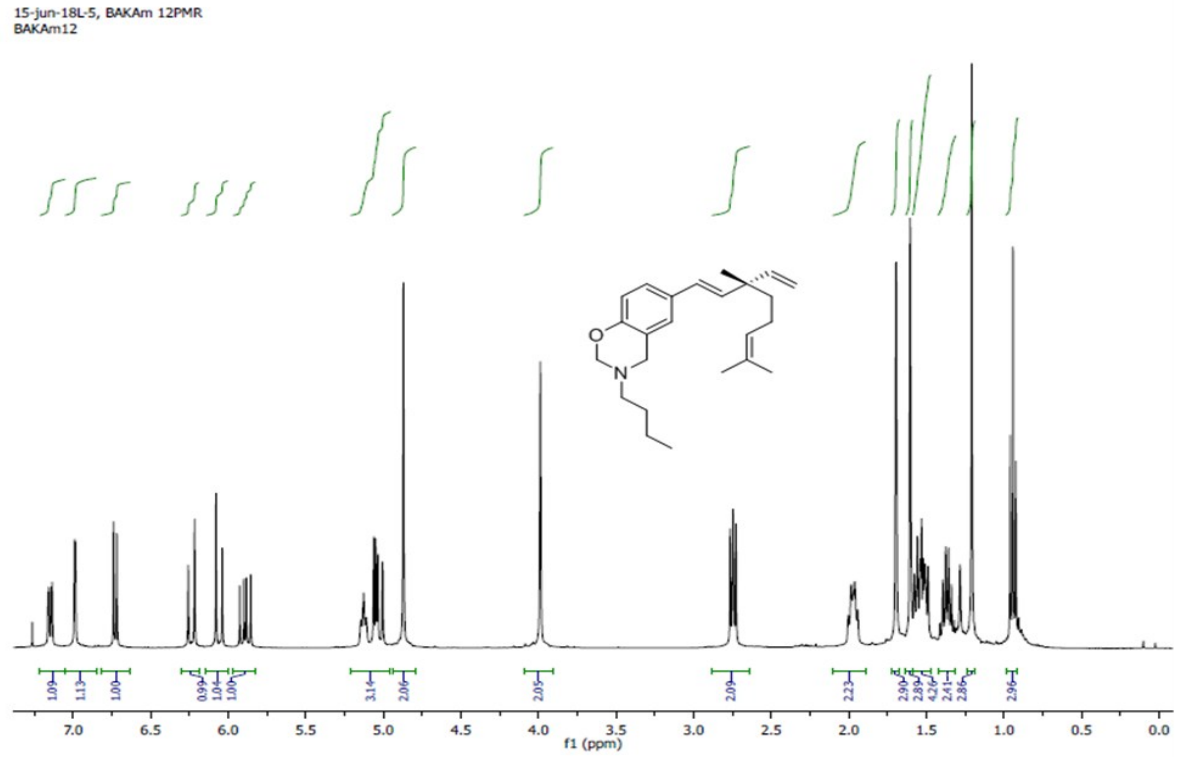
m/z	z	Abund	Formula	Ion
410.2288	1	121927.48	C26 H30 F2 N O	(M+H)+
411.232	1	38612.93	C26 H30 F2 N O	(M+H)+
412.2403	1	12537.41	C26 H30 F2 N O	(M+H)+
413.2483	1	2704.3	C26 H30 F2 N O	(M+H)+
414.2654	1	181.54	C26 H30 F2 N O	(M+H)+

Predicted Isotope Match Table

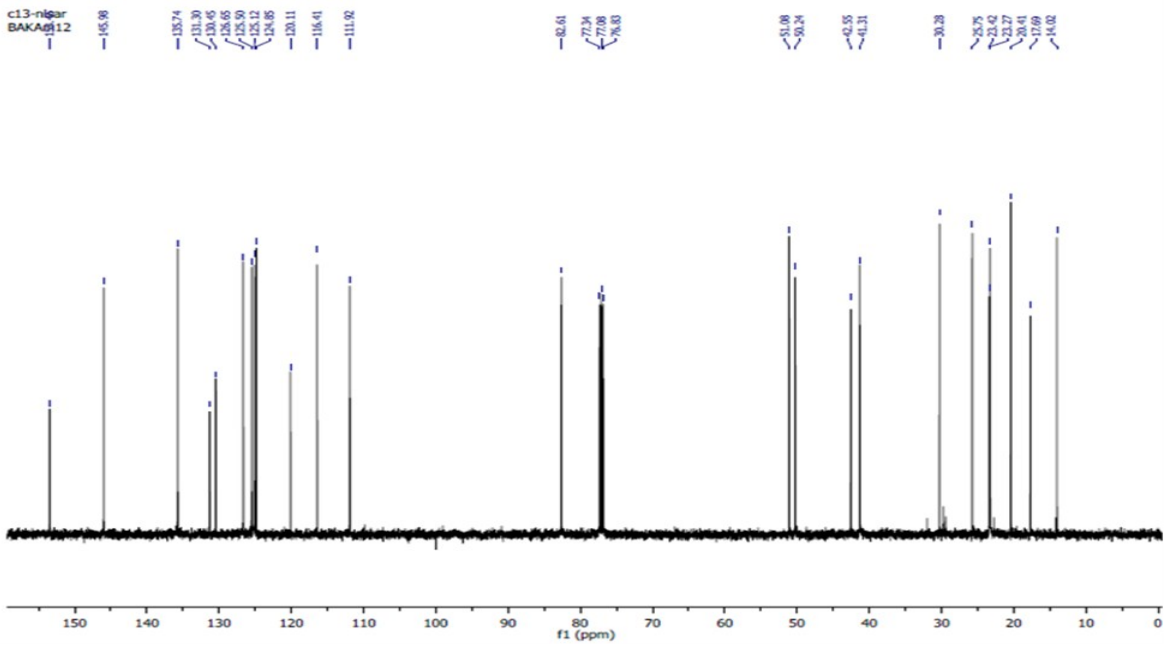
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	410.2288	410.229	0.4	100	100	69.29	74.89
2	411.232	411.2323	0.71	31.67	28.87	21.94	21.62
3	412.2403	412.2355	-11.53	10.28	4.22	7.13	3.16
4	413.2483	413.2386	-23.45	2.22	0.42	1.54	0.31
5	414.2654	414.2416	-57.33	0.15	0.03	0.1	0.02

3-butyl-3,4-dihydro-6-(3,7-dimethyl-3-vinylocta-1,6-dienyl)-2H-benzo[e][1,3]oxazine (12)

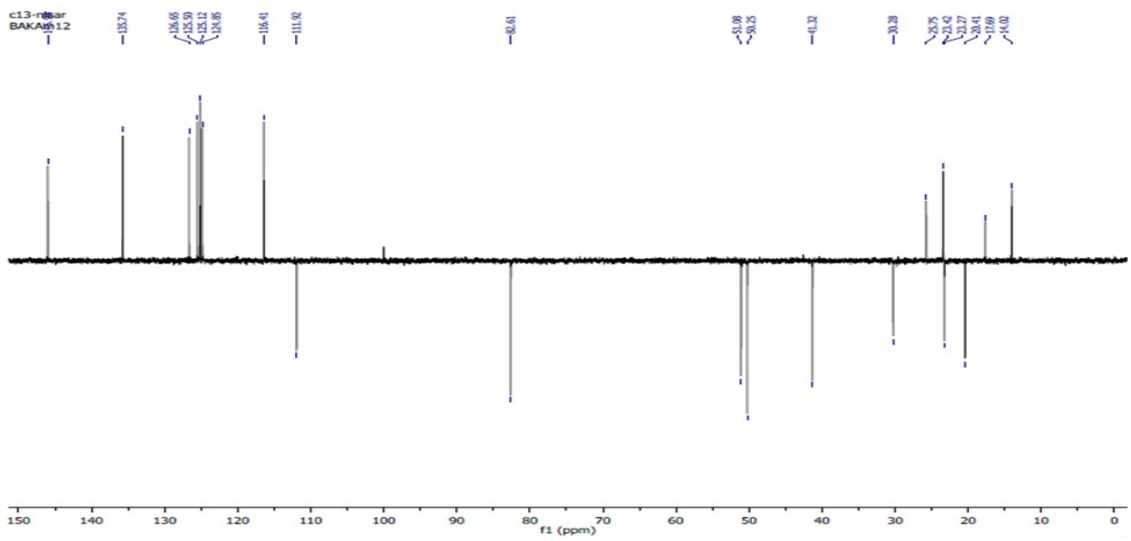
12 - ^{1}HNMR



12 – ^{13}C NMR



DEPT-12



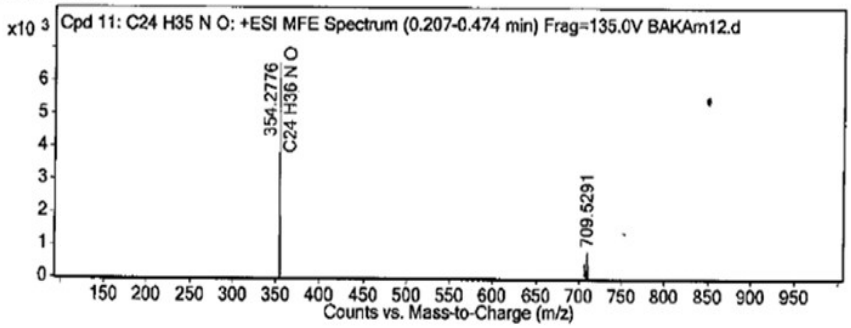
12-HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 11: C24 H35 N O	0.264	353.27	C24 H35 N O	C24 H35 N O	5.23	C24 H35 N O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 11: C24 H35 N O	354.2776	0.264	Find by Molecular Feature	353.27

MFE MS Spectrum



MS Spectrum Peak List

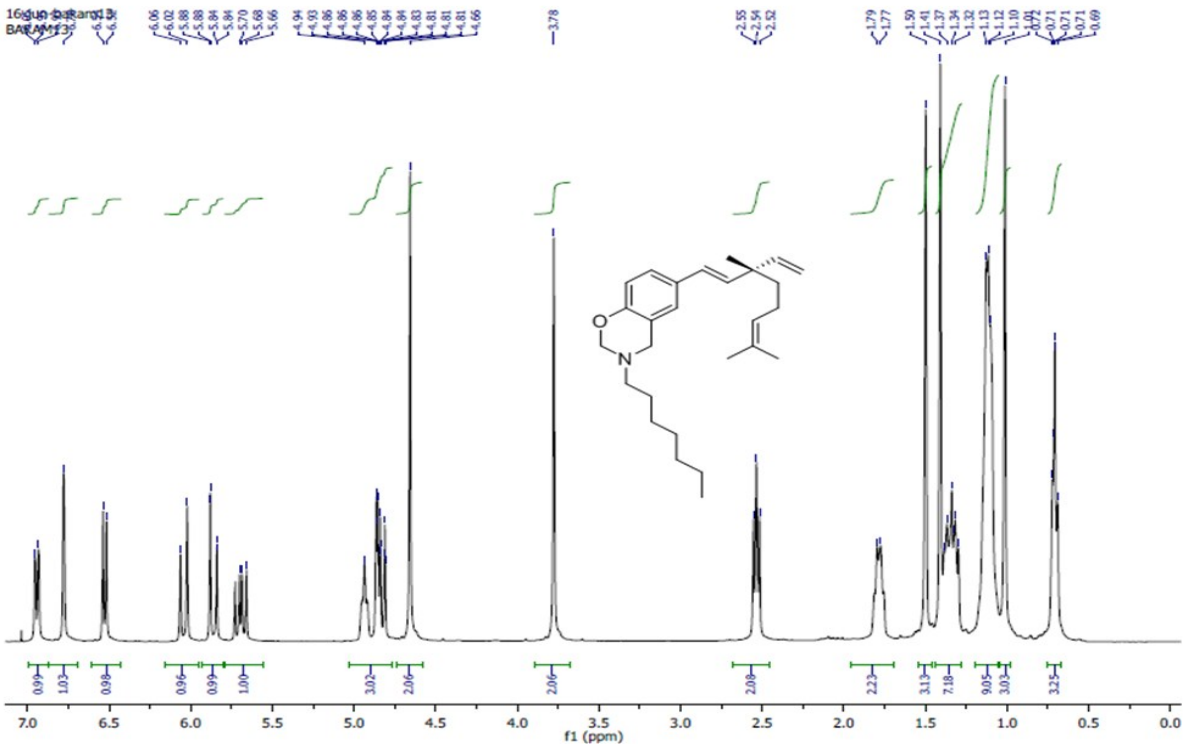
m/z	z	Abund	Formula	Ion
354.2776	1	6563.48	C24 H36 N O	(M+H)+
355.2794	1	1854.37	C24 H36 N O	(M+H)+
707.5488	1	448.81		(2M+H)+
708.5362	1	244.92		(2M+H)+
709.5291	1	811.65		(2M+H)+
710.5318	1	409.94		(2M+H)+

Predicted Isotope Match Table

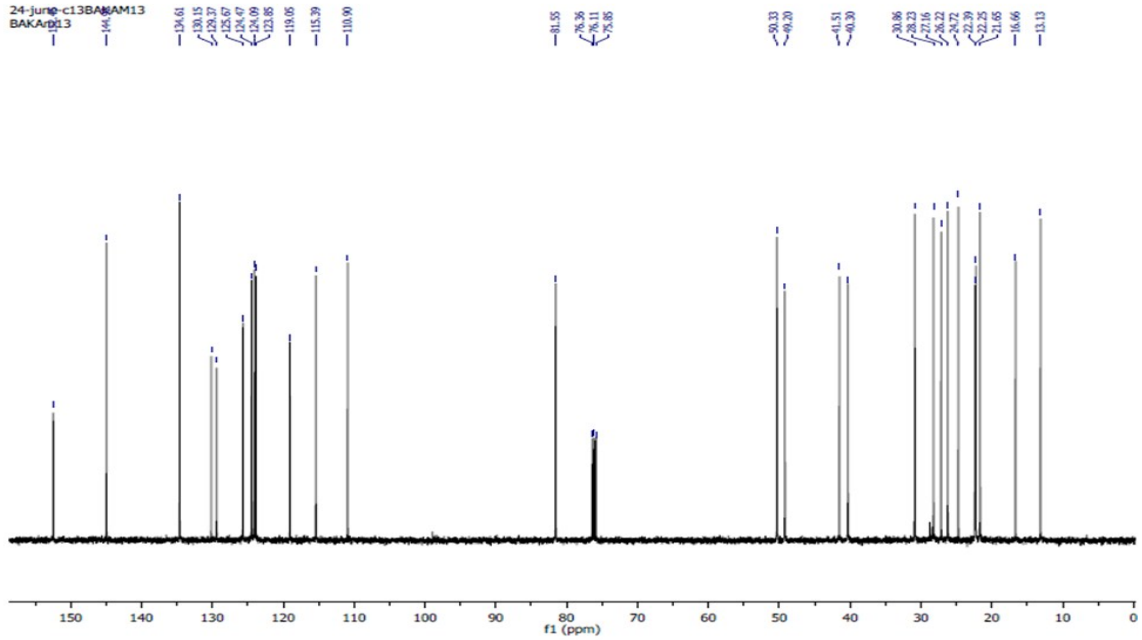
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	354.2776	354.2791	4.28	100	100	77.97	78.88
2	355.2794	355.2825	8.49	28.25	26.78	22.03	21.12

3-heptyl-3,4-dihydro-6-(3,7-dimethyl-3-vinylocta-1,6-dienyl)-2H-benzo[e][1,3]oxazine (13).

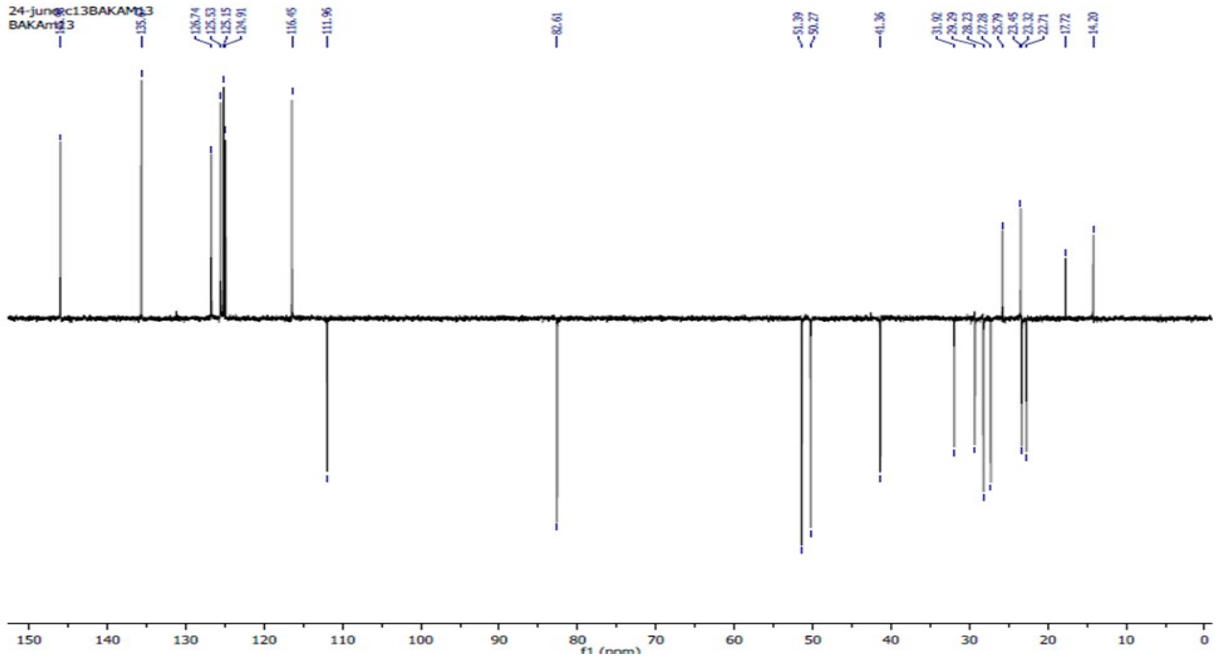
13-^{1}HNMR



13 – ^{13}C NMR



DEPT-13



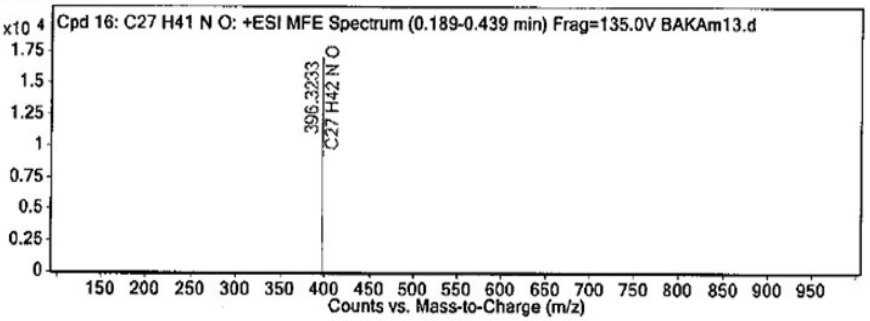
13-HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 16: C27 H41 N O	0.267	395.3162	C27 H41 N O	C27 H41 N O	6.74	C27 H41 N O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 16: C27 H41 N O	396.3233	0.267	Find by Molecular Feature	395.3162

MFE MS Spectrum



MS Spectrum Peak List

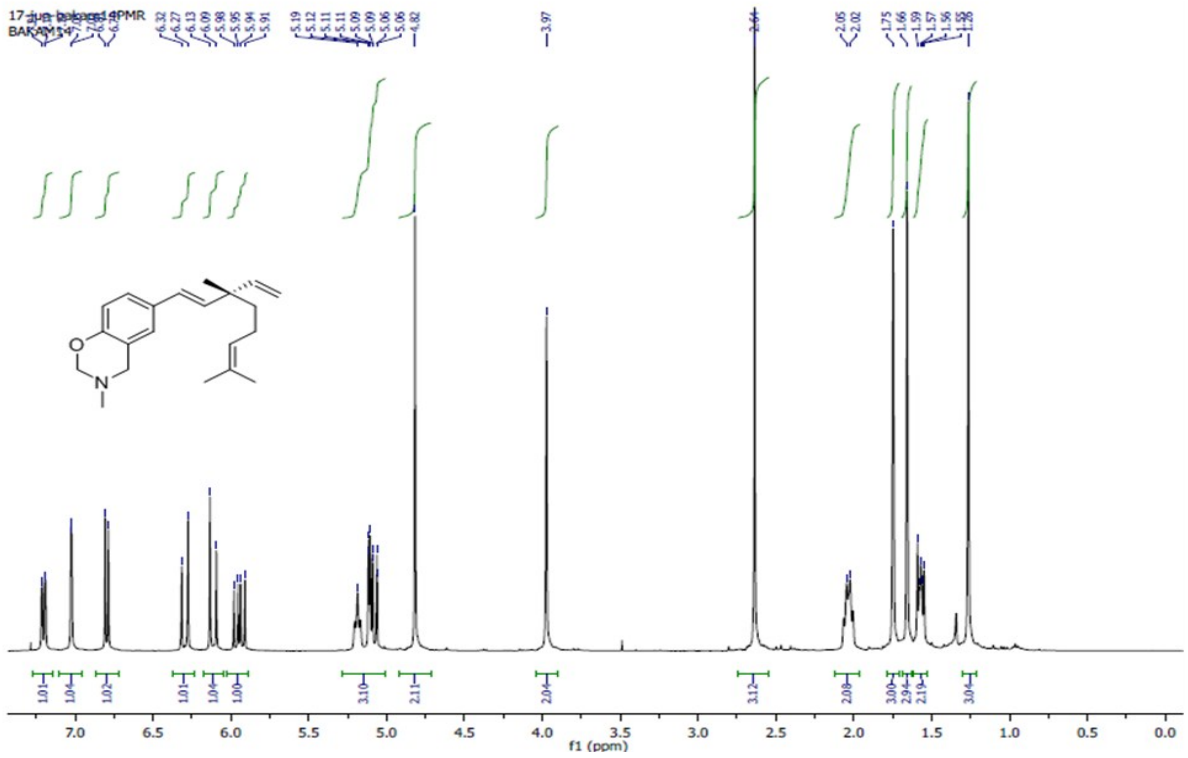
m/z	z	Abund	Formula	Ion
396.3233	1	16942.43	C27 H42 N O	(M+H)+
397.3271	1	4689.58	C27 H42 N O	(M+H)+

Predicted Isotope Match Table

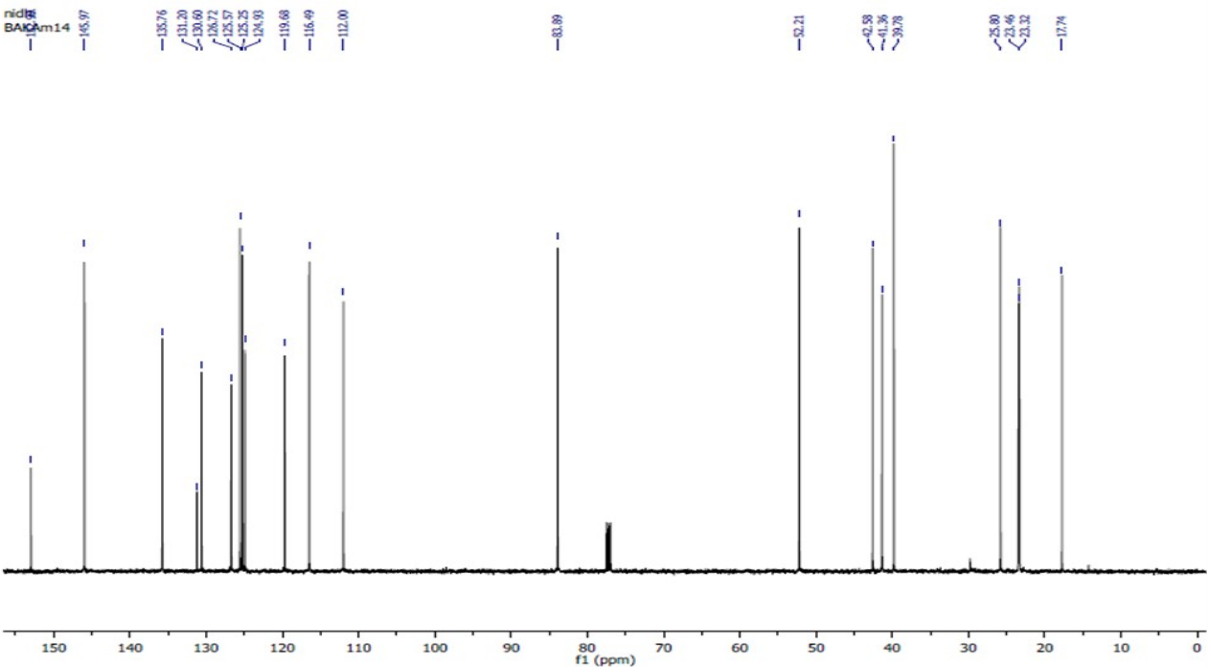
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	396.3233	396.3261	6.99	100	100	78.32	76.87
2	397.3271	397.3294	5.74	27.68	30.09	21.68	23.13

3,4-dihydro-3-methyl-6-(3,7-dimethyl-3-vinylocta-16-dienyl)-2H-benzo[e][1,3]oxazine (14).

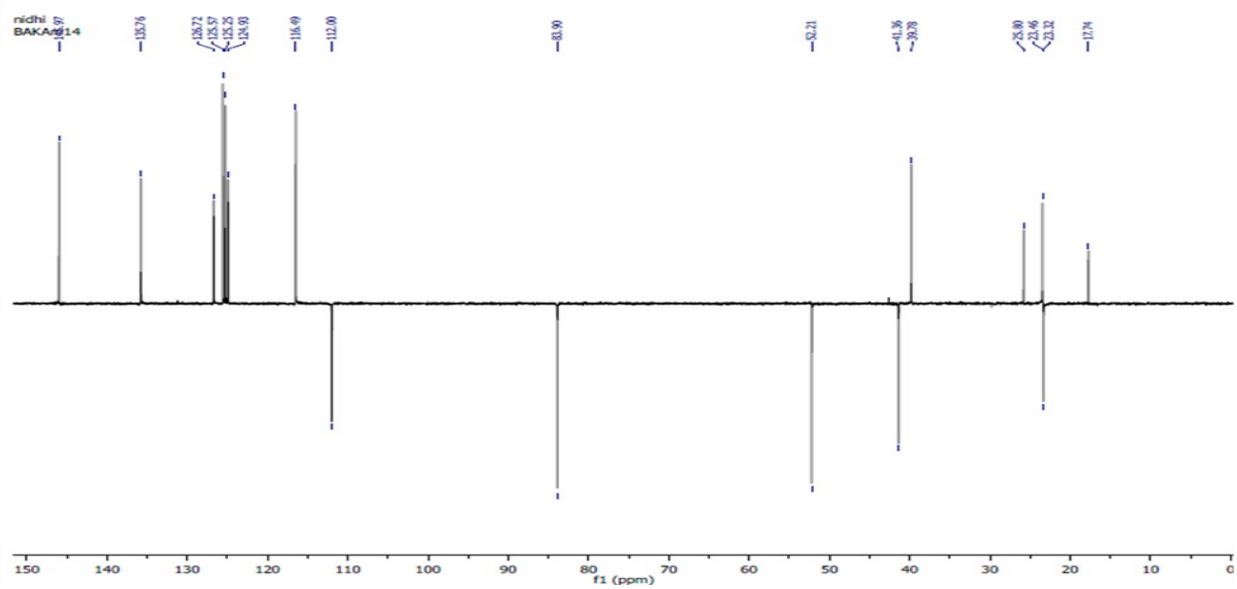
14-^{1}HNMR



14 – ^{13}C NMR



DEPT-14



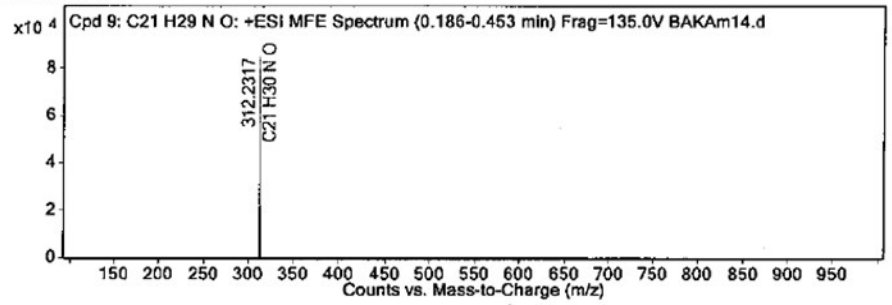
14-HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 9: C21 H29 N O	0.268	311.2243	C21 H29 N O	C21 H29 N O	1.96	C21 H29 N O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 9: C21 H29 N O	312.2317	0.268	Find by Molecular Feature	311.2243

MFE MS Spectrum



MS Spectrum Peak List

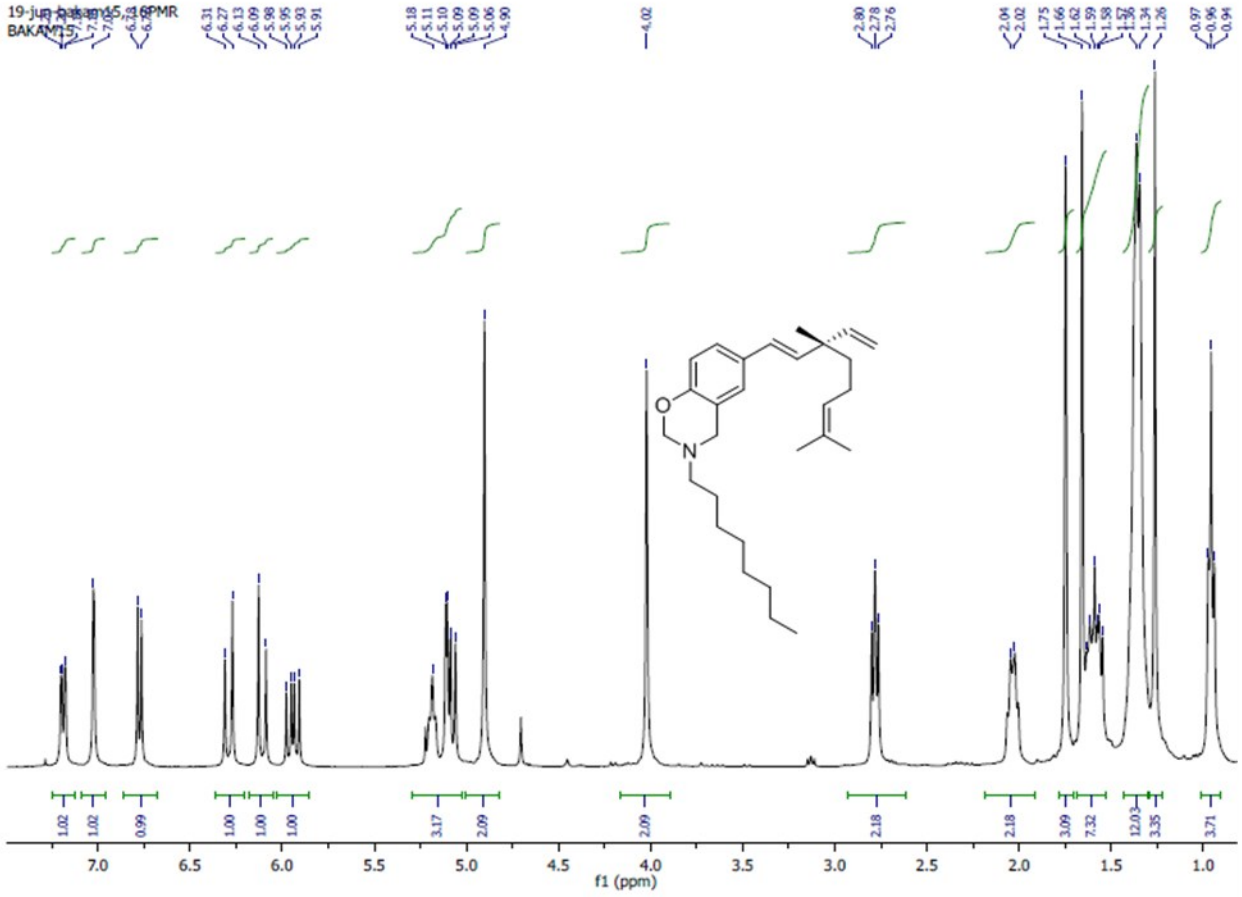
m/z	z	Abund	Formula	Ion
312.2317	1	84580.12	C21 H30 N O	(M+H)+
313.235	1	21718.47	C21 H30 N O	(M+H)+
314.2348	1	4493.36	C21 H30 N O	(M+H)+

Predicted Isotope Match Table

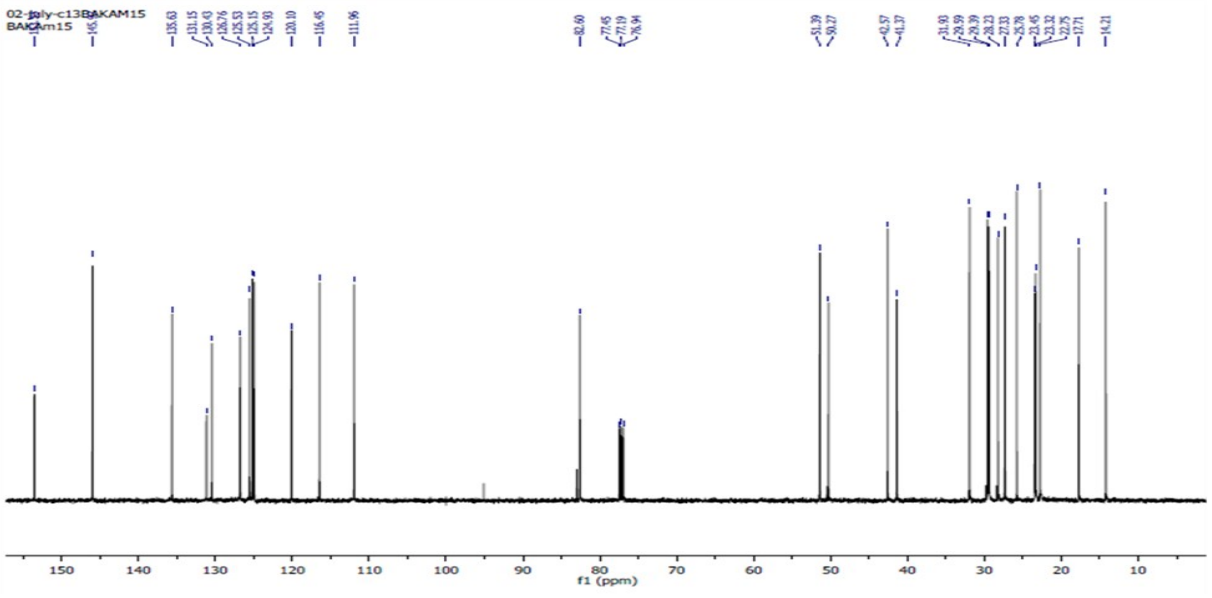
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	312.2317	312.2322	1.5	100	100	76.34	79.18
2	313.235	313.2355	1.57	25.68	23.46	19.6	18.58
3	314.2348	314.2386	12.21	5.31	2.83	4.06	2.24

3,4-dihydro-6-(3,7-dimethyl-3-vinylocta-1,6-dienyl)-3-octyl-2H-benzo[e][1,3]oxazine (15)

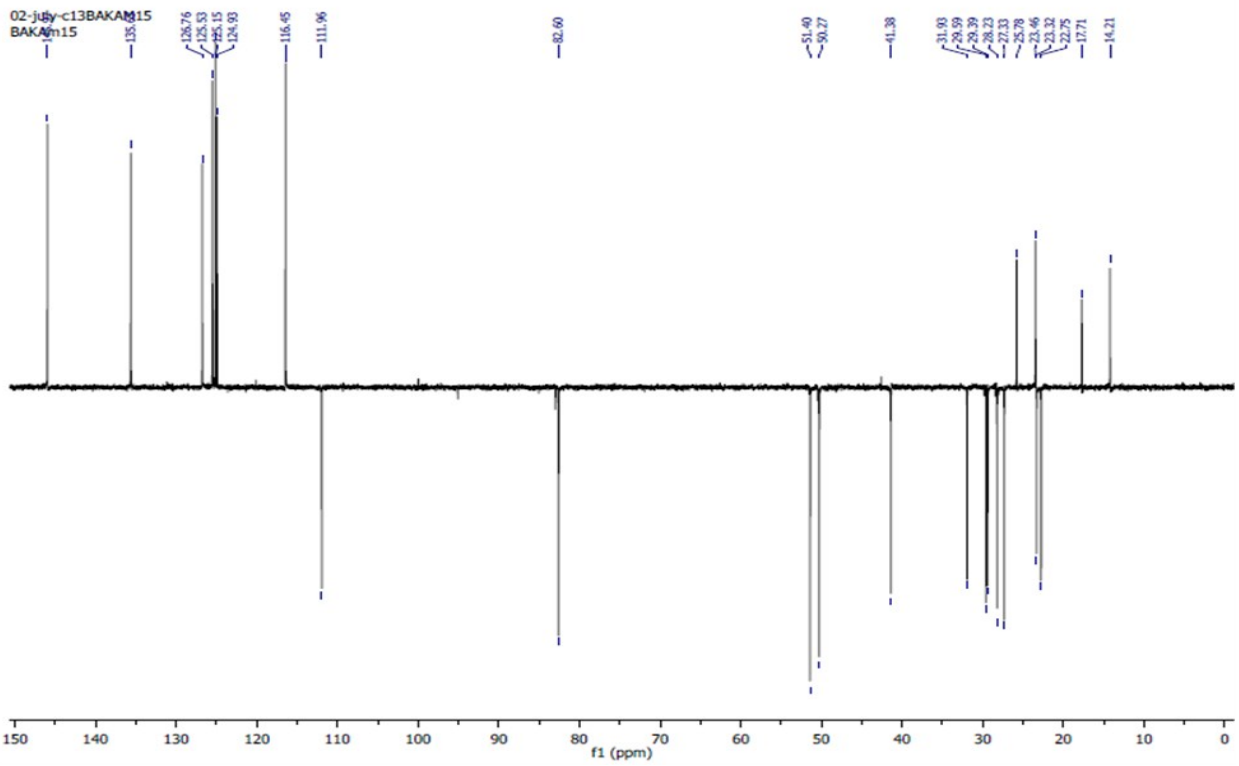
15-^{1}HNMR



15 – ^{13}C NMR



DEPT-15



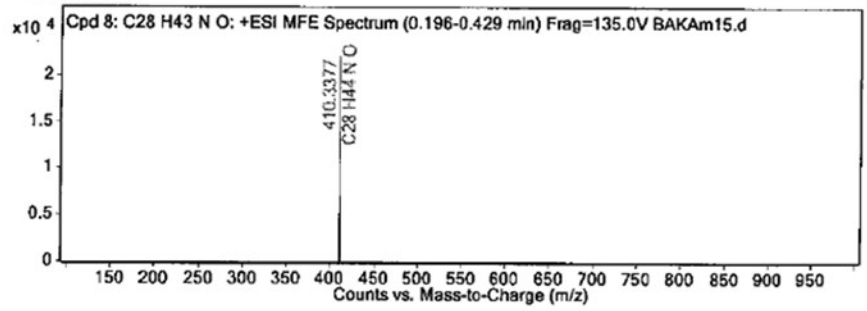
15-HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 8: C28 H43 N O	0.262	409.3299	C28 H43 N O	C28 H43 N O	11.24	C28 H43 N O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 8: C28 H43 N O	410.3377	0.262	Find by Molecular Feature	409.3299

MFE MS Spectrum



MS Spectrum Peak List

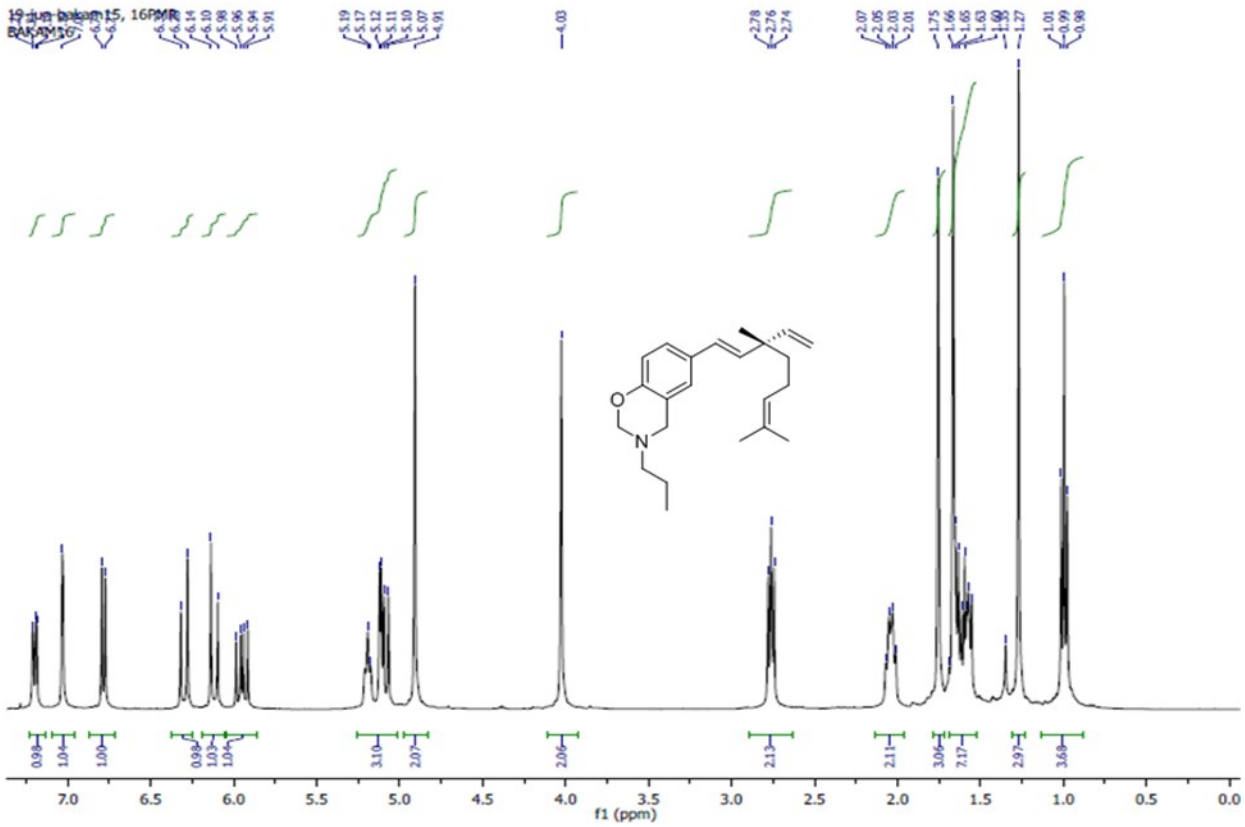
m/z	z	Abund	Formula	Ion
410.3377	1	22054.04	C28 H44 N O	(M+H)+
411.3386	1	6941.43	C28 H44 N O	(M+H)+

Predicted Isotope Match Table

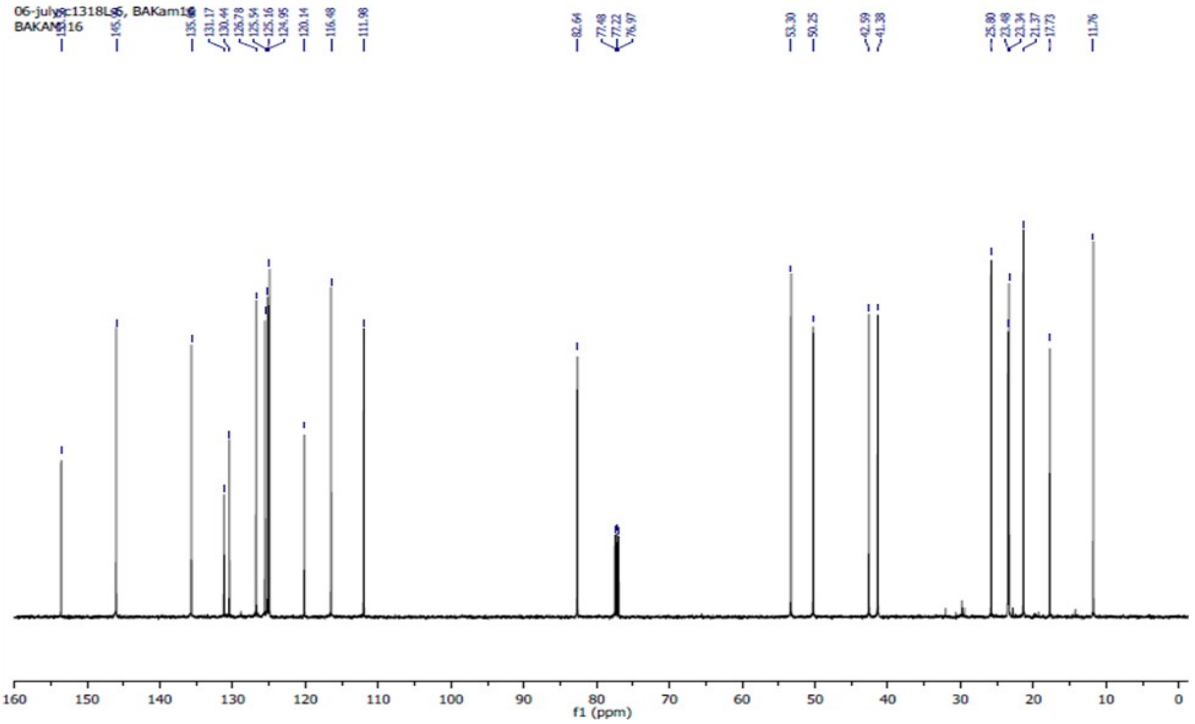
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	410.3377	410.3417	9.82	100	100	76.06	76.22
2	411.3386	411.3451	15.61	31.47	31.19	23.94	23.78

3,4-dihydro-6-(3,7-dimethyl-3-vinylocta-1,6-dienyl)-3propyl-2H-benzo[e][1,3]oxazine (16).

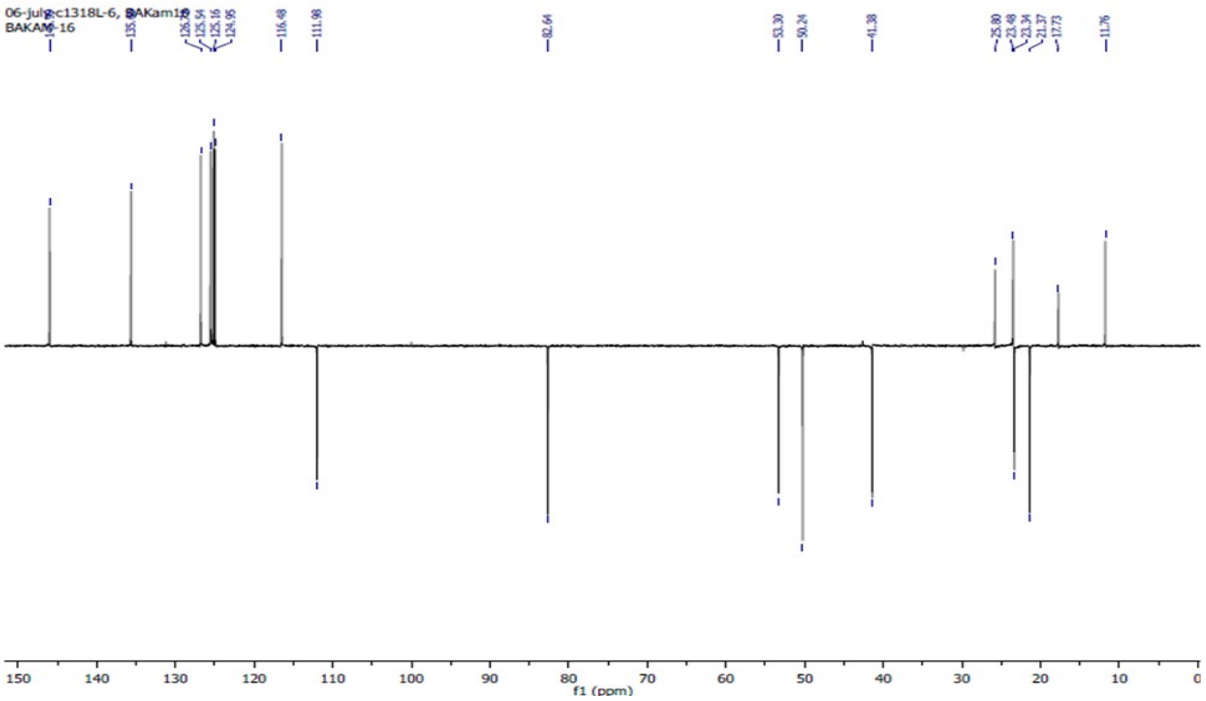
16-^{1}HNMR



16 – ^{13}C NMR



DEPT-16



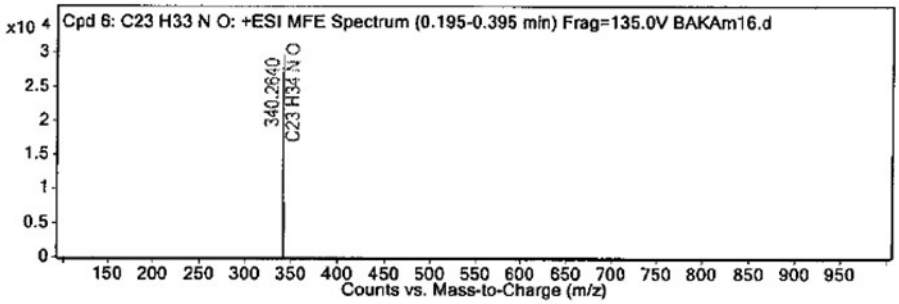
16-HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 6: C23 H33 N O	0.255	339.2565	C23 H33 N O	C23 H33 N O	-0.88	C23 H33 N O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 6: C23 H33 N O	340.264	0.255	Find by Molecular Feature	339.2565

MFE MS Spectrum



MS Spectrum Peak List

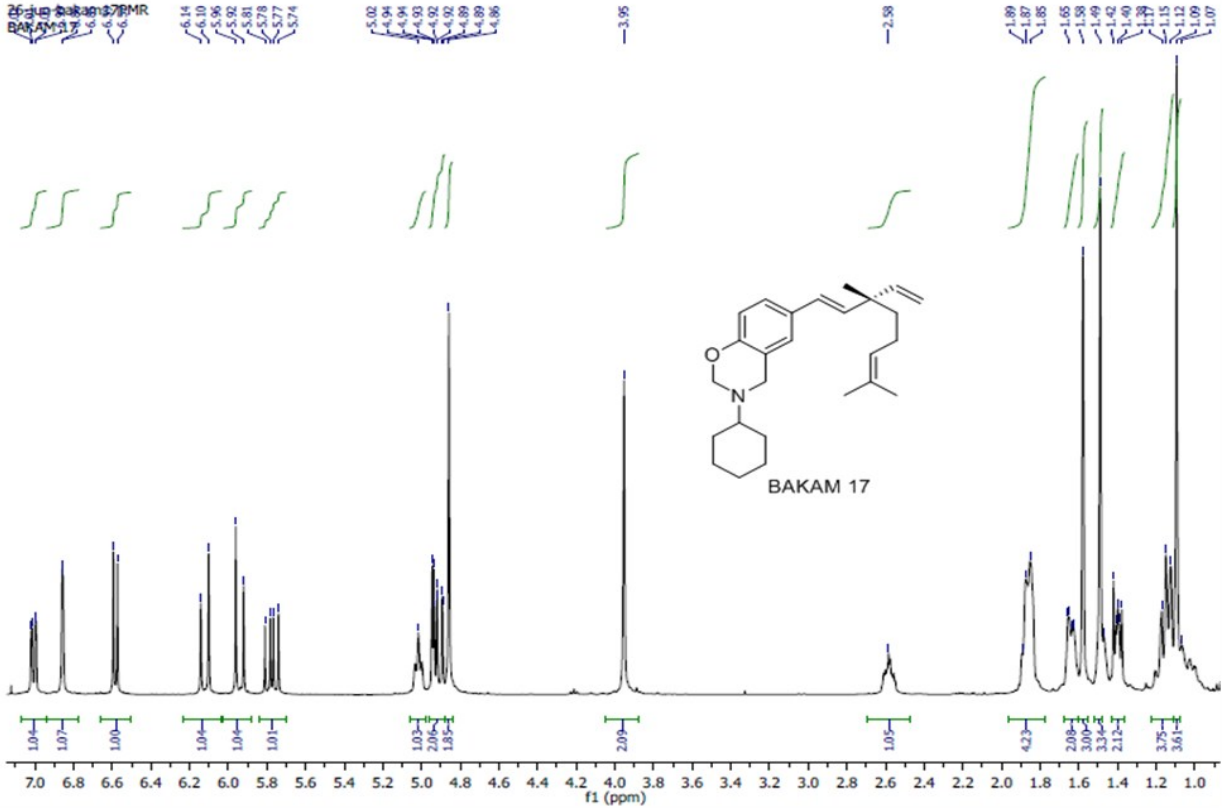
m/z	z	Abund	Formula	Ion
340.264	1	29639.15	C23 H34 N O	(M+H)+
341.2665	1	8112.12	C23 H34 N O	(M+H)+

Predicted Isotope Match Table

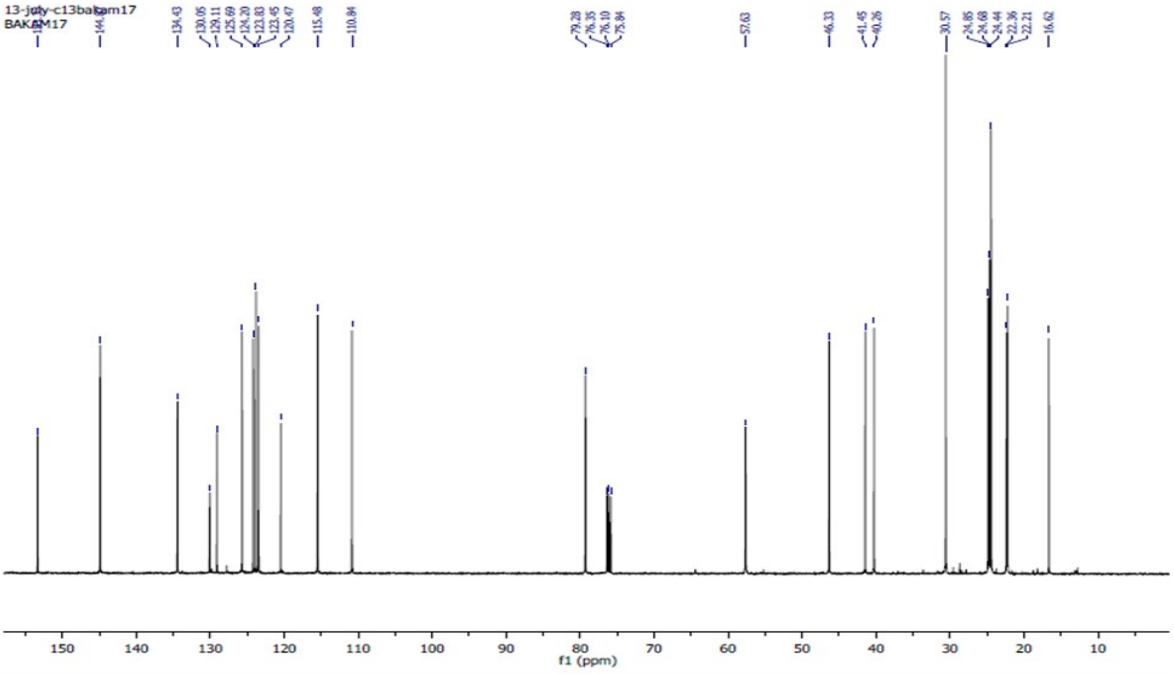
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	340.264	340.2635	-1.37	100	100	78.51	79.57
2	341.2665	341.2668	0.94	27.37	25.67	21.49	20.43

3-cyclohexyl-3,4-dihydro-6-(3,7-dimethyl-3-vinylocta-1,6-dienyl)-2H-benzo[e][1,3]oxazine(17)

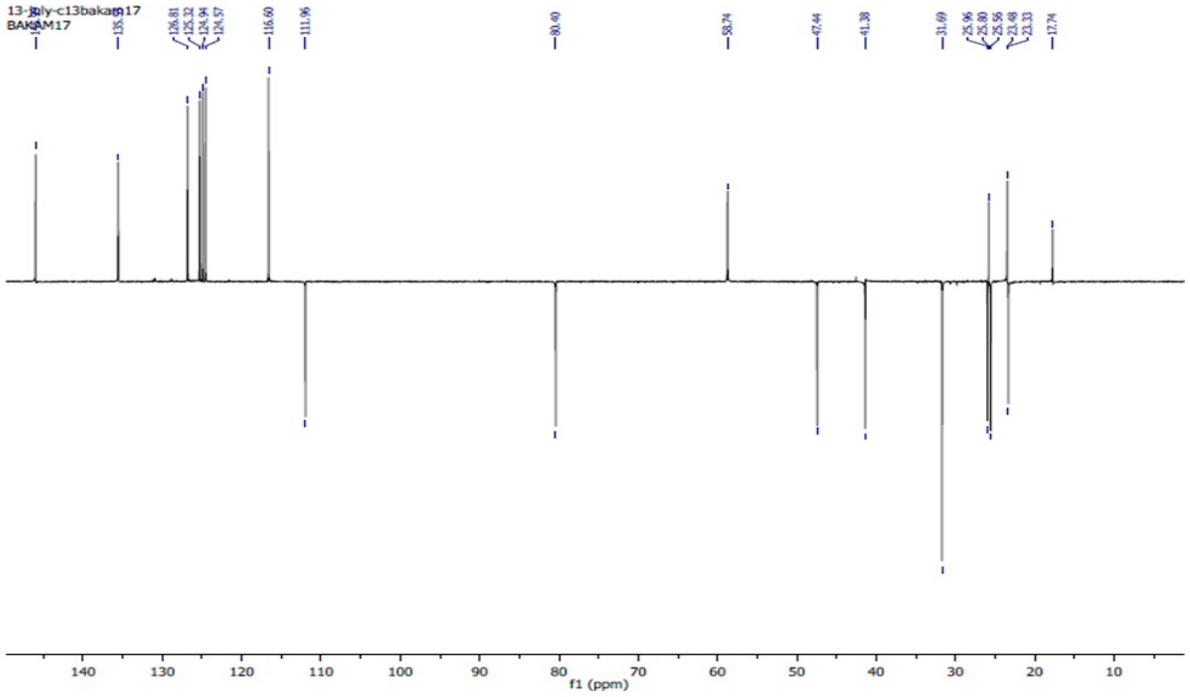
17-^{1}HNMR



17 – ^{13}C NMR



DEPT-17



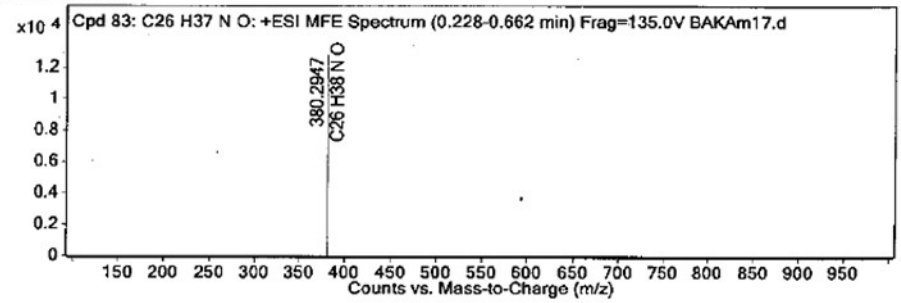
17-HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 83: C26 H37 N O	0.364	379.2876	C26 H37 N O	C26 H37 N O	-0.23	C26 H37 N O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 83: C26 H37 N O	380.2947	0.364	Find by Molecular Feature	379.2876

MFE MS Spectrum



MS Spectrum Peak List

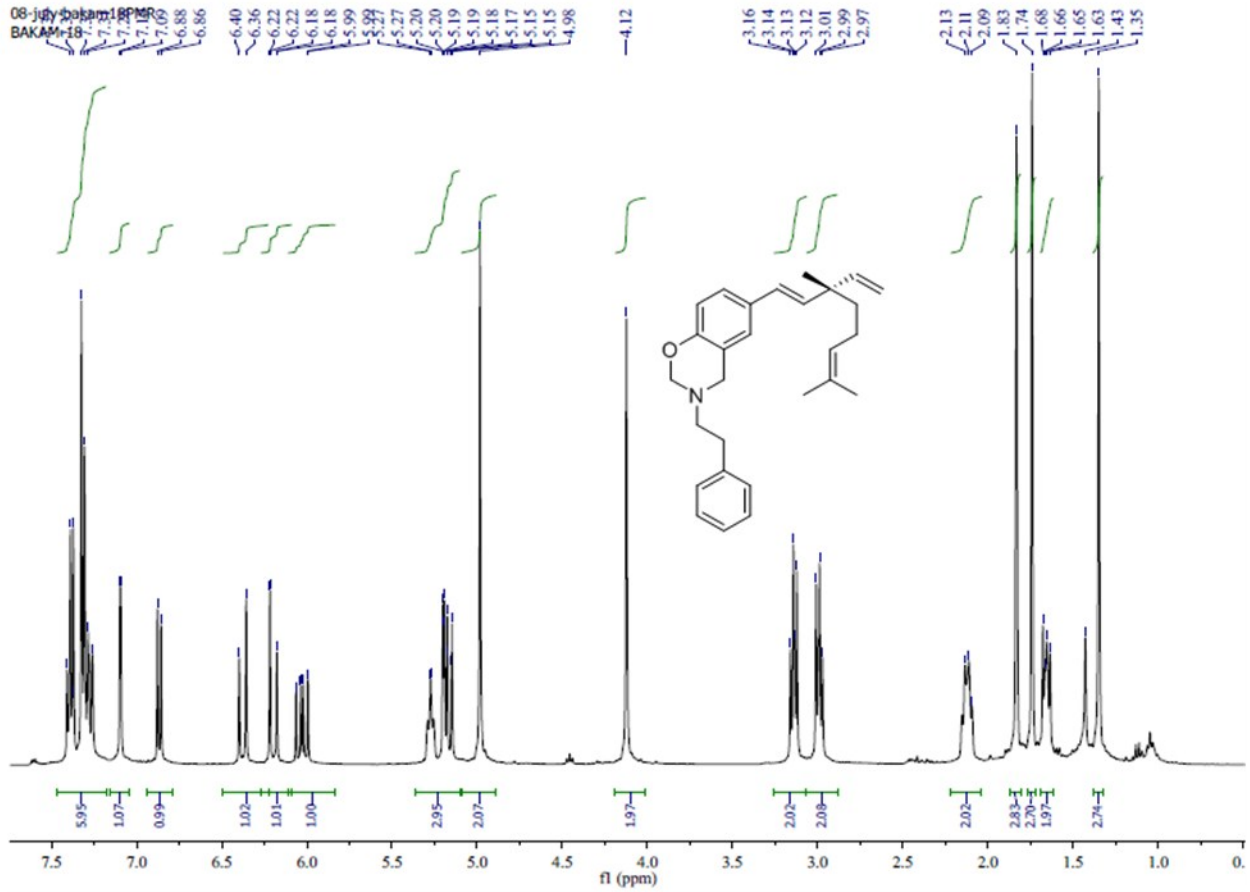
m/z	z	Abund	Formula	Ion
380.2947	1	12866.17	C26 H38 N O	(M+H)+
381.2987	1	4319.7	C26 H38 N O	(M+H)+

Predicted Isotope Match Table

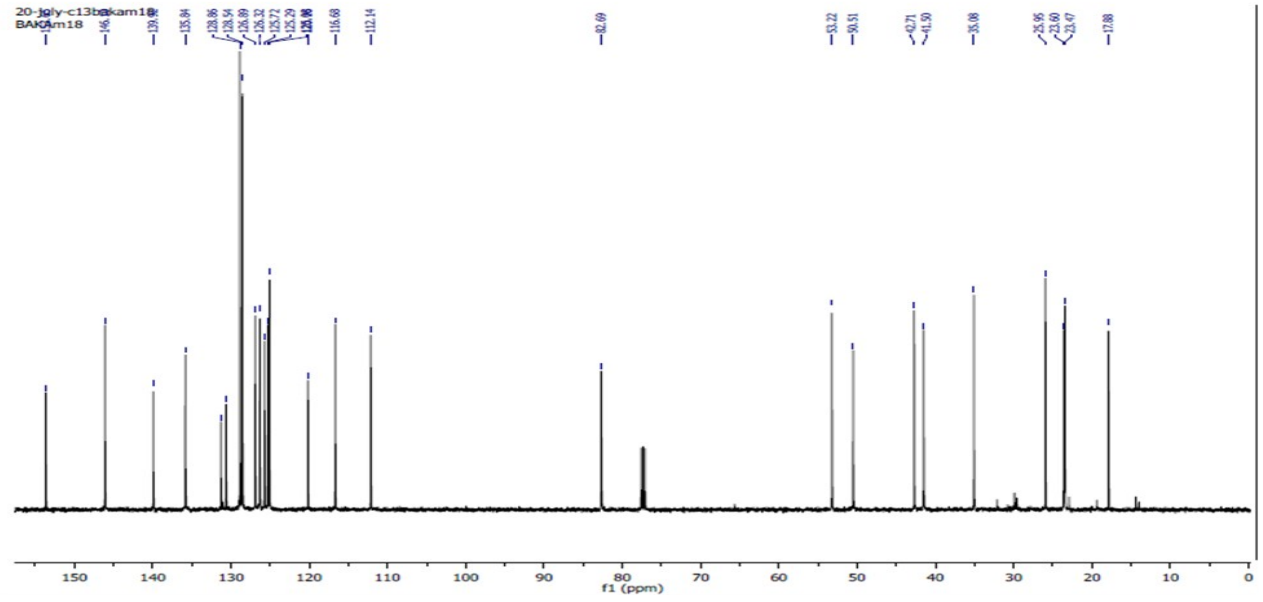
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	380.2947	380.2948	0.22	100	100	74.86	77.54
2	381.2987	381.2981	-1.54	33.57	28.96	25.14	22.46

3,4-dihydro-6-(3,7-dimethyl-3-vinylocta-1,6-dienyl)-3-phenethyl-2H-benzo[e][1,3]oxazine (18)

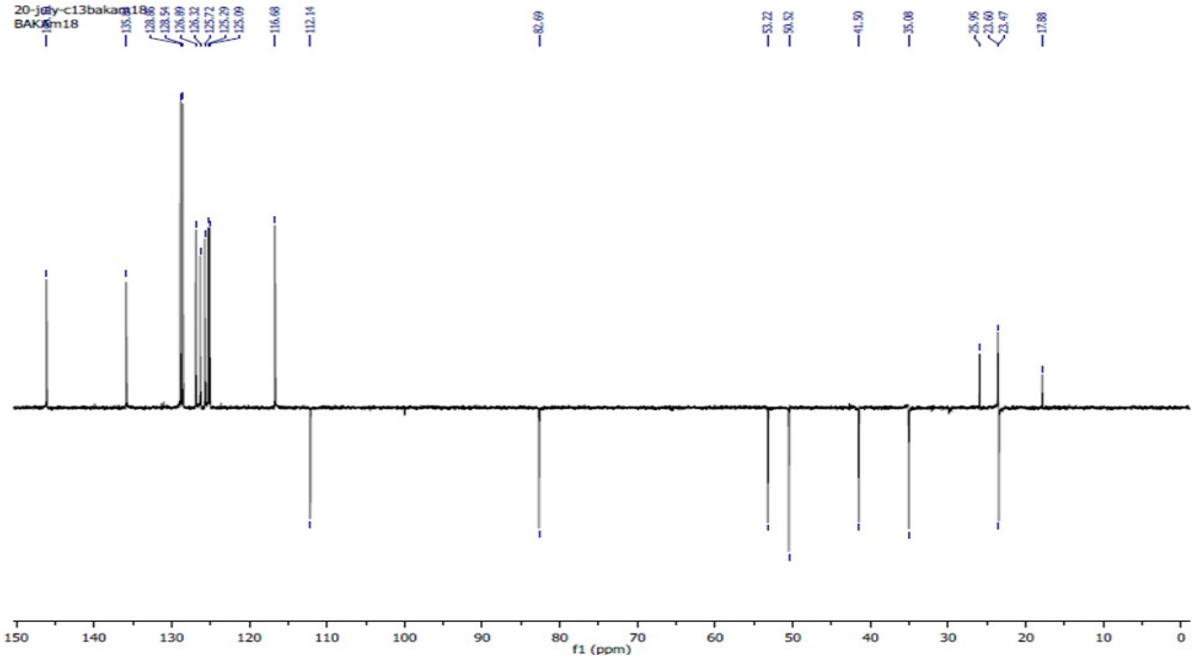
18-^{1}HNMR



18 - ^{13}CNMR



DEPT- 18



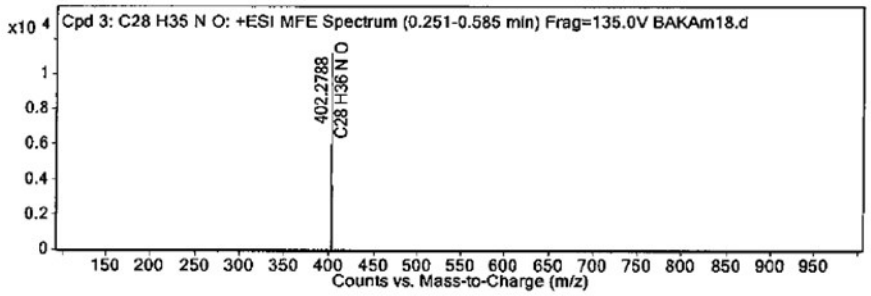
18-HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 3: C28 H35 N O	0.315	401.2715	C28 H35 N O	C28 H35 N O	0.96	C28 H35 N O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 3: C28 H35 N O	402.2788	0.315	Find by Molecular Feature	401.2715

MFE MS Spectrum



MS Spectrum Peak List

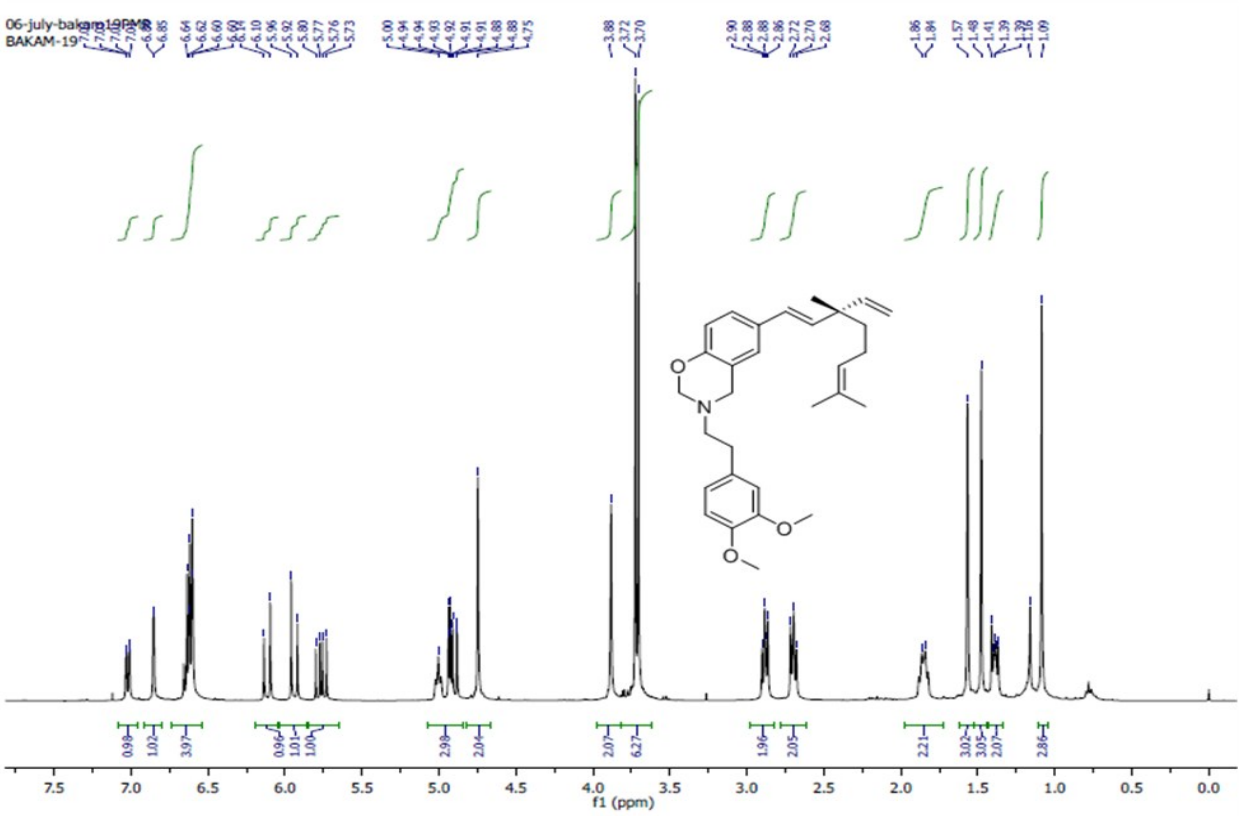
m/z	z	Abund	Formula	Ion
402.2788	1	11184.95	C28 H36 N O	(M+H)+
403.282	1	3654.15	C28 H36 N O	(M+H)+

Predicted Isotope Match Table

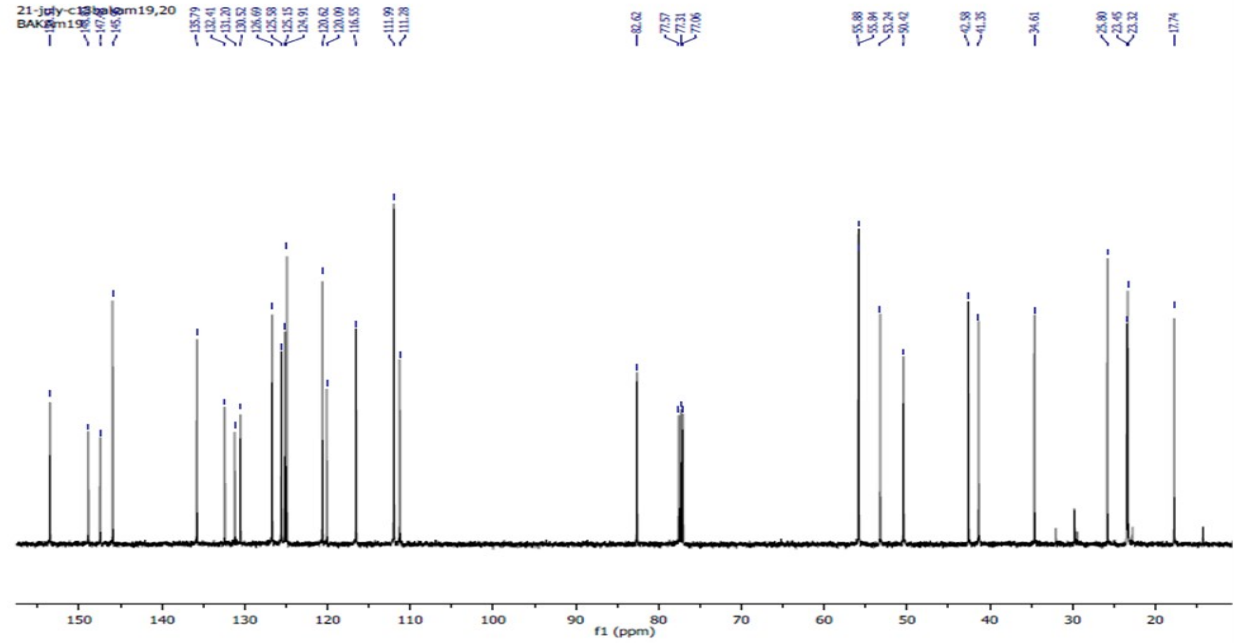
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	402.2788	402.2791	0.92	100	100	75.37	76.28
2	403.282	403.2825	1.08	32.67	31.1	24.63	23.72

3-(3,4-dimethoxyphenethyl)-3,4-dihydro-6-(3,7-dimethyl-3-vinylocta-1,6-dienyl)-2H-benzo[e][1,3]oxazine (19)

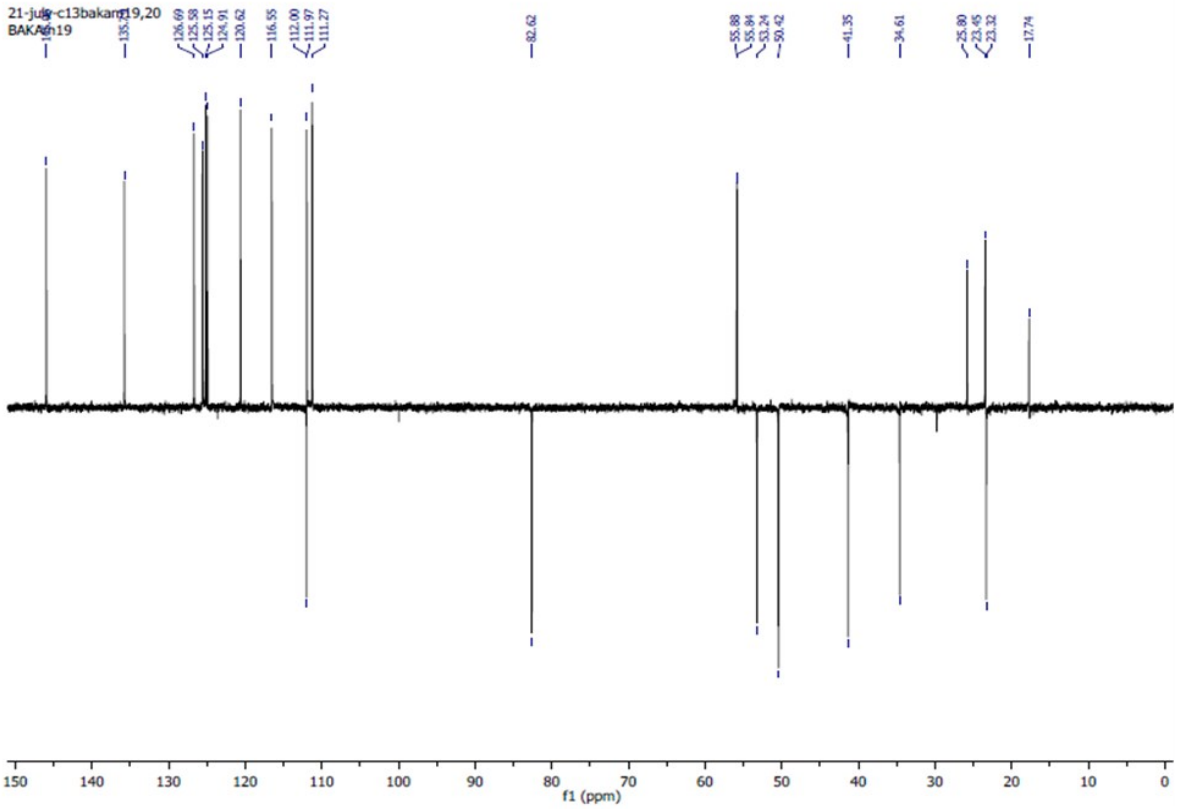
19-^{1}HNMR



19 - ^{13}C NMR



DEPT- 19



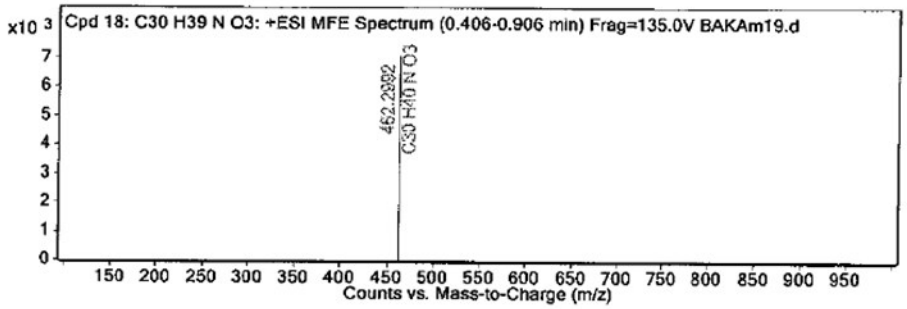
19-HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 18: C30 H39 N O3	0.528	461.2921	C30 H39 N O3	C30 H39 N O3	2	C30 H39 N O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 18: C30 H39 N O3	462.2992	0.528	Find by Molecular Feature	461.2921

MFE MS Spectrum



MS Spectrum Peak List

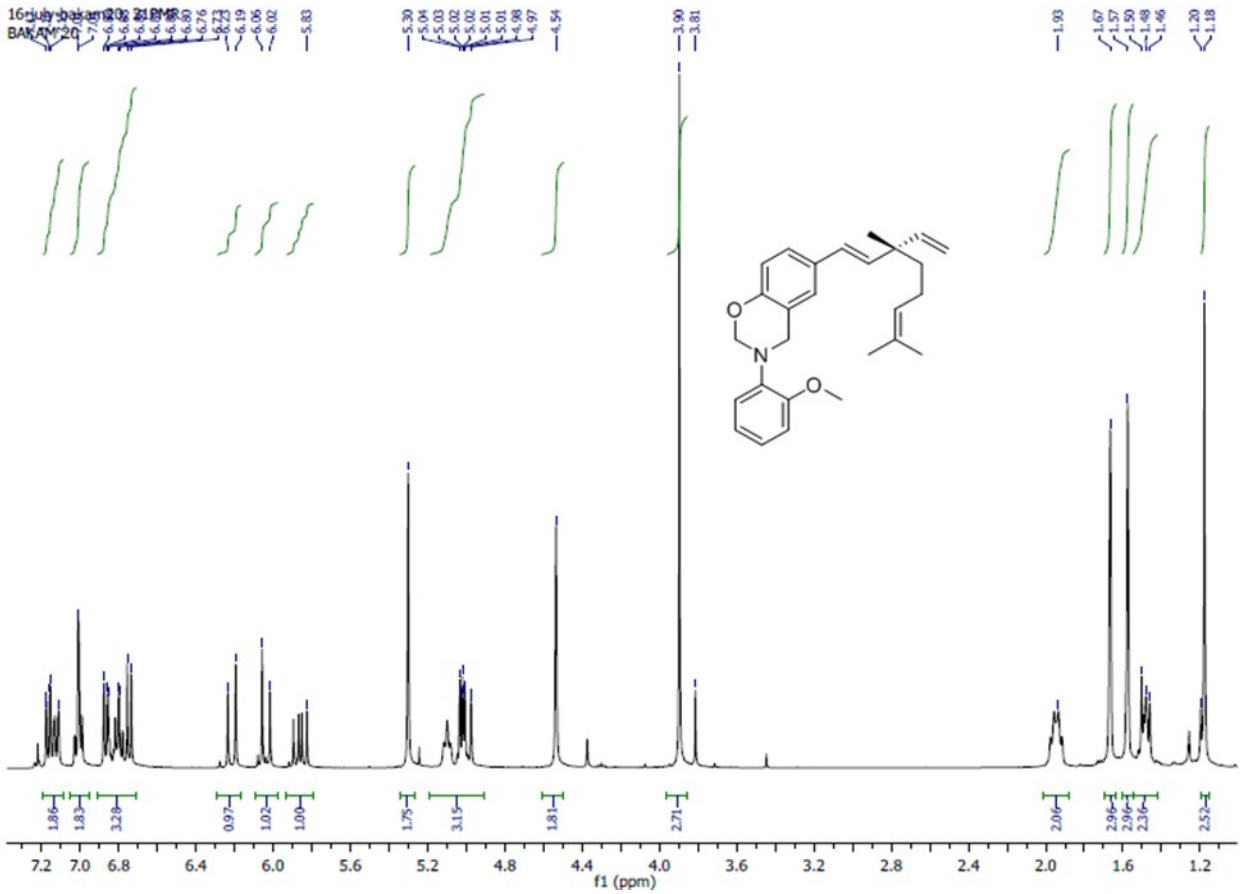
m/z	z	Abund	Formula	Ion
462.2992	1	7066.21	C30 H40 N O3	(M+H)+
463.3031	1	2498.26	C30 H40 N O3	(M+H)+

Predicted Isotope Match Table

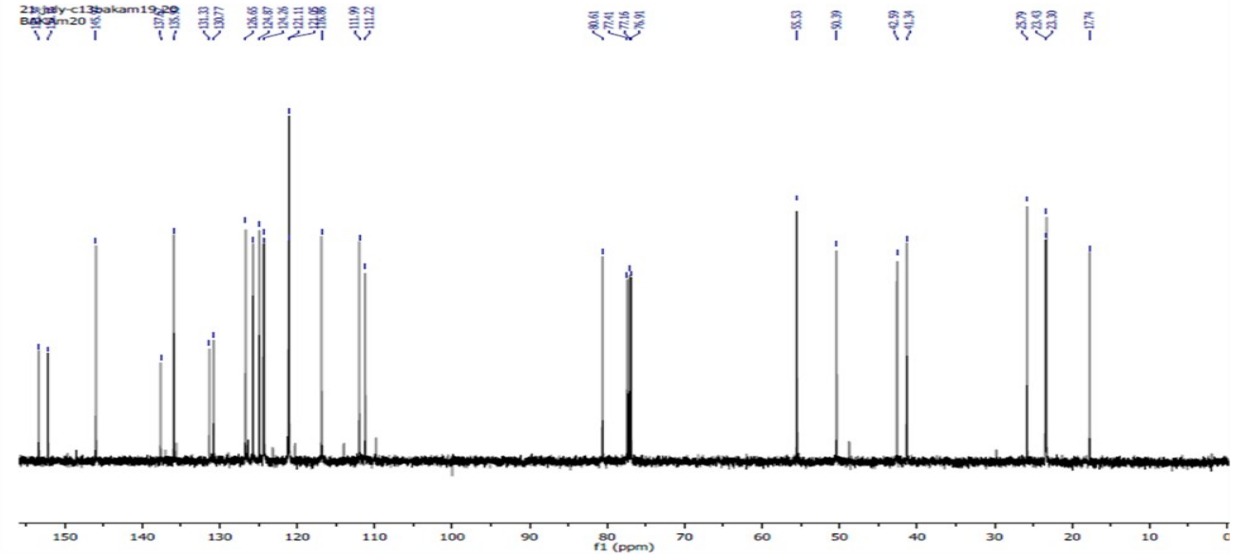
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	462.2992	462.3003	2.33	100	100	73.88	74.97
2	463.3031	463.3036	1.02	35.36	33.39	26.12	25.03

3,4-dihydro-3-(2-methoxyphenyl)-6-(3,7-dimethyl-3-vinylocta-1,6-dienyl)-2H-benzo[e][1,3]oxazine (20)

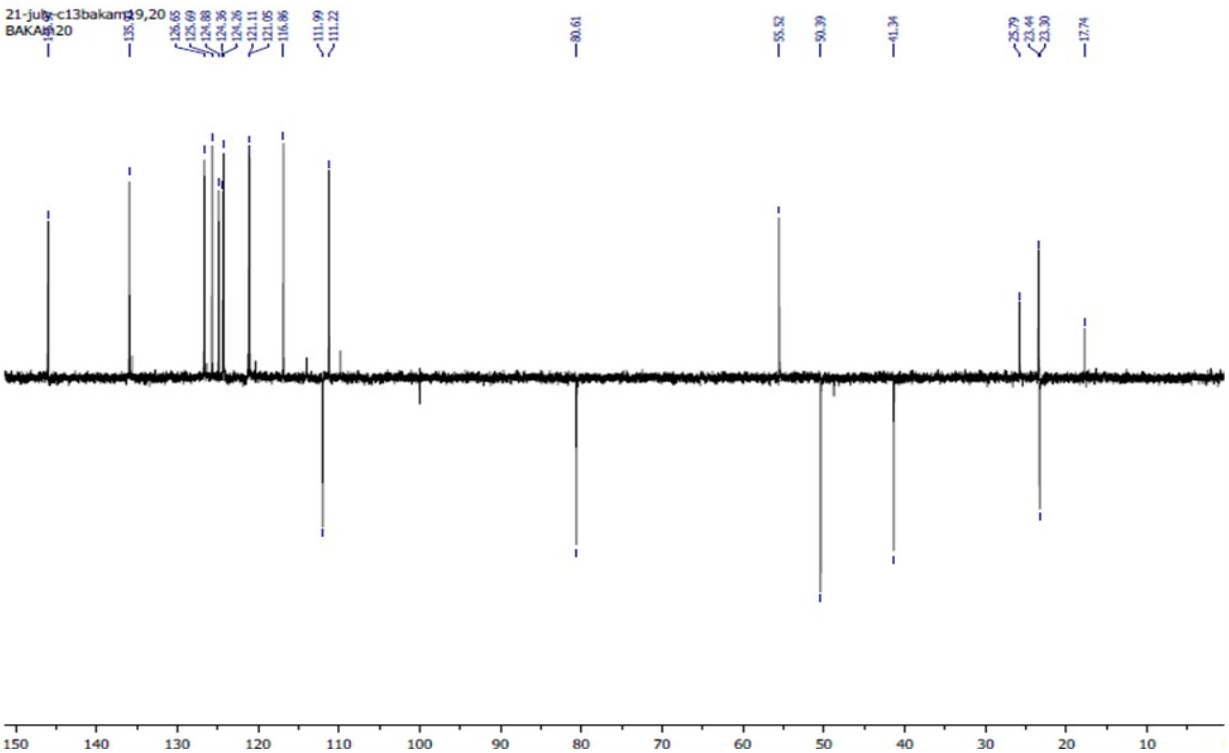
20-^{1}HNMR



20- ^{13}C NMR



DEPT- 20



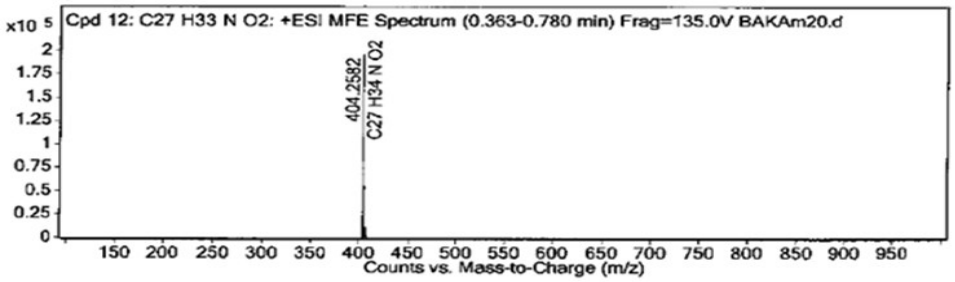
20 -HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 12: C27 H33 N O2	0.519	403.251	C27 H33 N O2	C27 H33 N O2	0.37	C27 H33 N O2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 12: C27 H33 N O2	404.2582	0.519	Find by Molecular Feature	403.251

MFE MS Spectrum



MS Spectrum Peak List

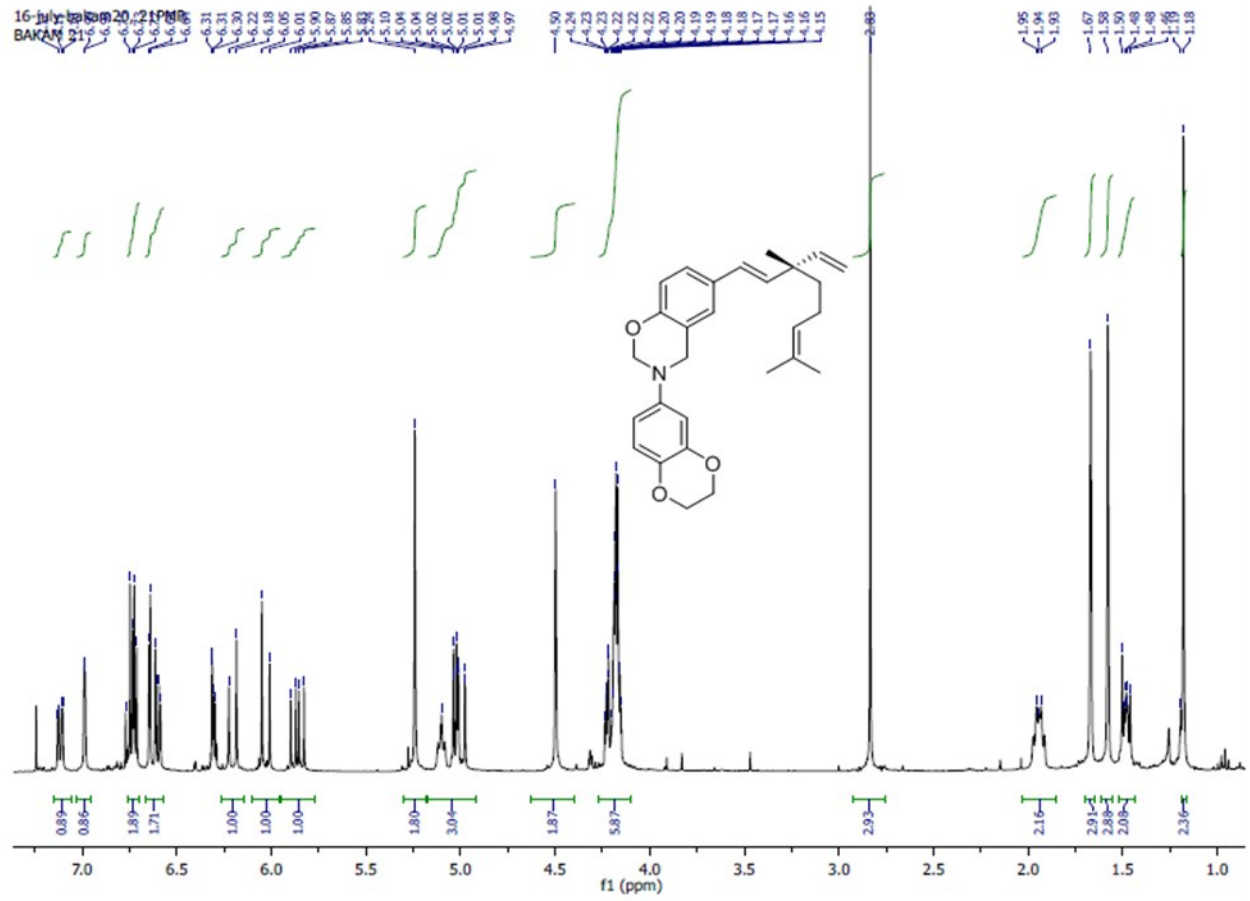
m/z	z	Abund	Formula	Ion
404.2582	1	196469.95	C27 H34 N O2	(M+H)+
405.2618	1	55146.48	C27 H34 N O2	(M+H)+
406.2646	1	11701.7	C27 H34 N O2	(M+H)+
407.2677	1	1823.6	C27 H34 N O2	(M+H)+

Predicted Isotope Match Table

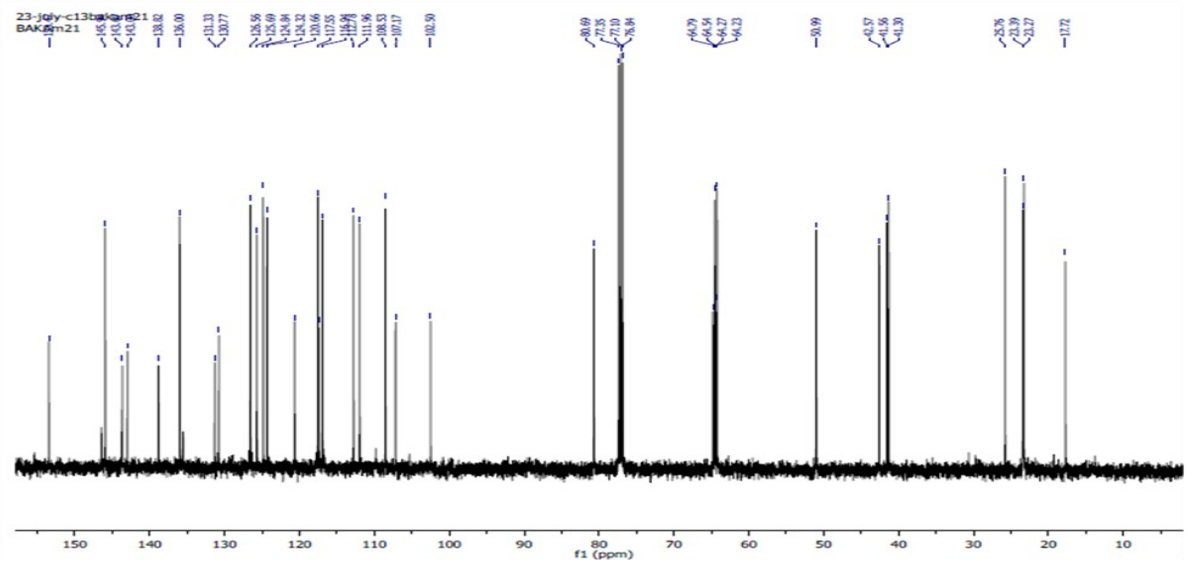
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	404.2582	404.2584	0.51	100	100	74.1	73.9
2	405.2618	405.2617	-0.14	28.07	30.04	20.8	22.19
3	406.2646	406.2648	0.47	5.96	4.76	4.41	3.52
4	407.2677	407.2678	0.23	0.93	0.53	0.69	0.39

3,4-dihydro-3-(2,3-dihydrobenzo[1,4]dioxin-6-yl)-6-(3,7-dimethyl-3-vinylocta-1,6-dienyl)-2H-benzo[e][1,3]oxazine (21)

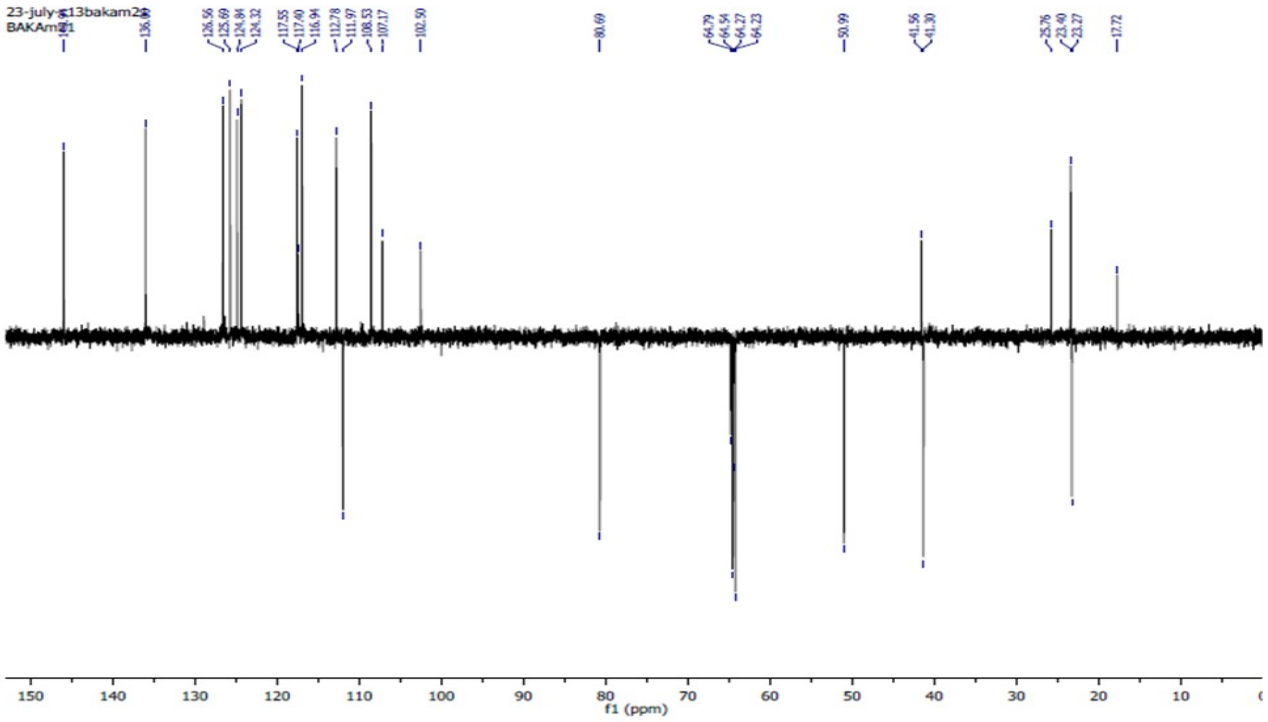
21-^{1}HNMR



21- ^{13}C NMR



DEPT- 21



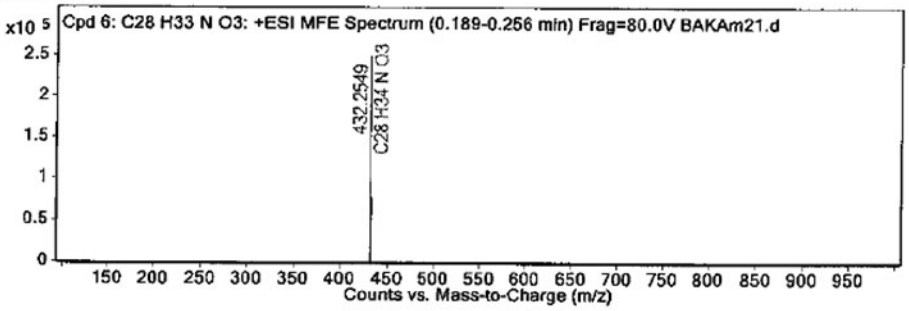
21 -HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 6: C28 H33 N O3	0.241	431.2475	C28 H33 N O3	C28 H33 N O3	-3.39	C28 H33 N O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 6: C28 H33 N O3	432.2549	0.241	Find by Molecular Feature	431.2475

MFE MS Spectrum



MS Spectrum Peak List

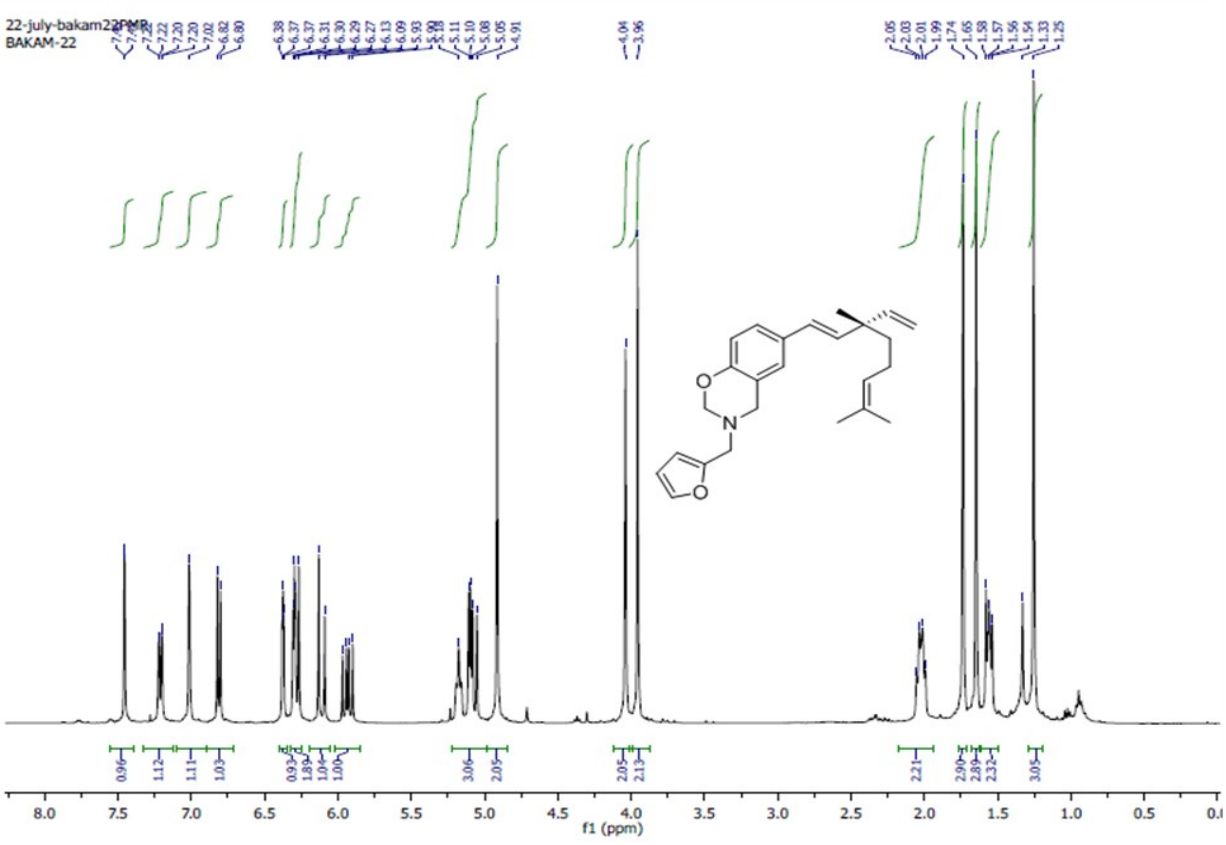
m/z	z	Abund	Formula	Ion
432.2549	1	247852.38	C28 H34 N O3	(M+H)+
433.2578	1	78987.55	C28 H34 N O3	(M+H)+

Predicted Isotope Match Table

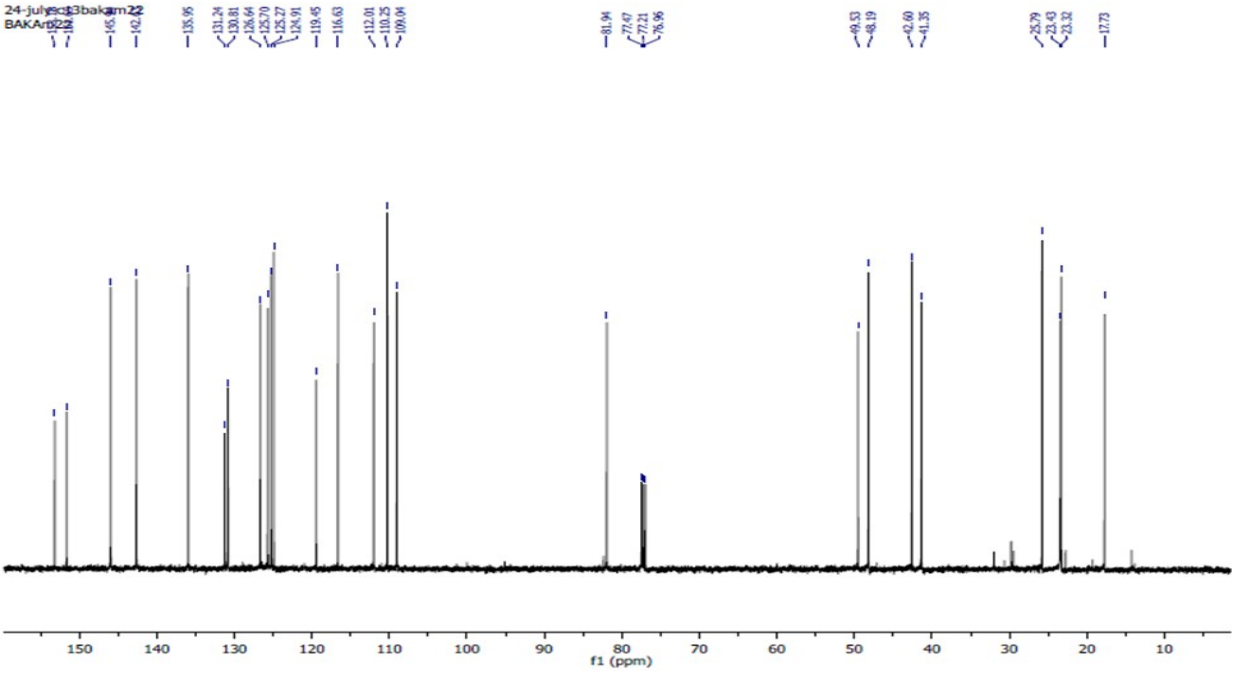
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	432.2549	432.2533	-3.63	100	100	75.83	76.25
2	433.2578	433.2566	-2.61	31.87	31.15	24.17	23.75

3-((furan-2-yl)methyl)-3,4-dihydro)-6-(3,7-dimethyl-3-vinylocta-1,6-dienyl)-2H-benzo[e][1,3]oxazine (22)

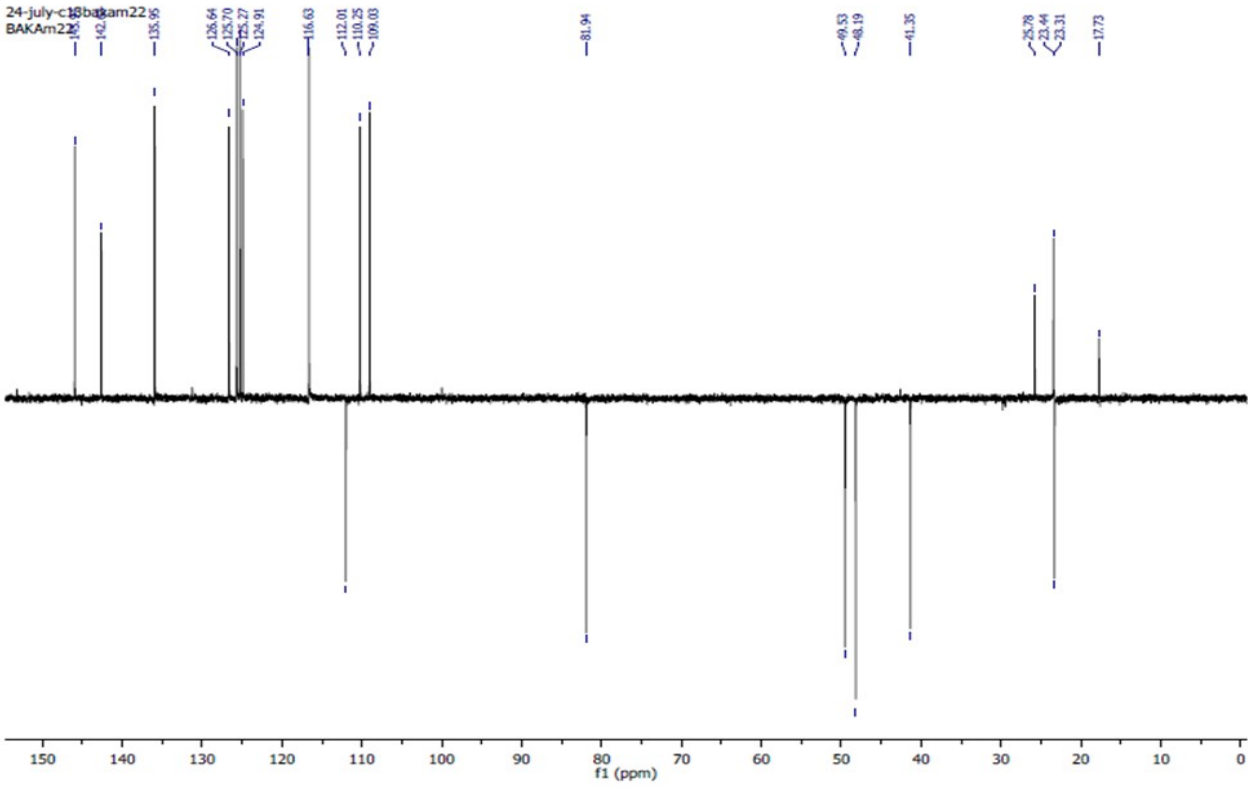
22-^{1}HNMR



22- ^{13}C NMR



DEPT- 22



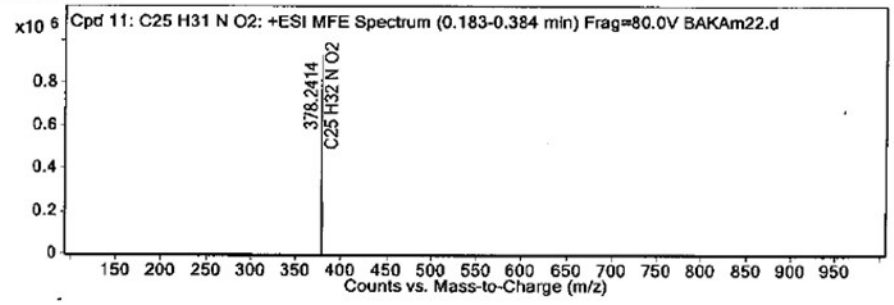
22 -HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 11: C25 H31 N O2	0.255	377.2342	C25 H31 N O2	C25 H31 N O2	3.42	C25 H31 N O2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 11: C25 H31 N O2	378.2414	0.255	Find by Molecular Feature	377.2342

MFE MS Spectrum



MS Spectrum Peak List

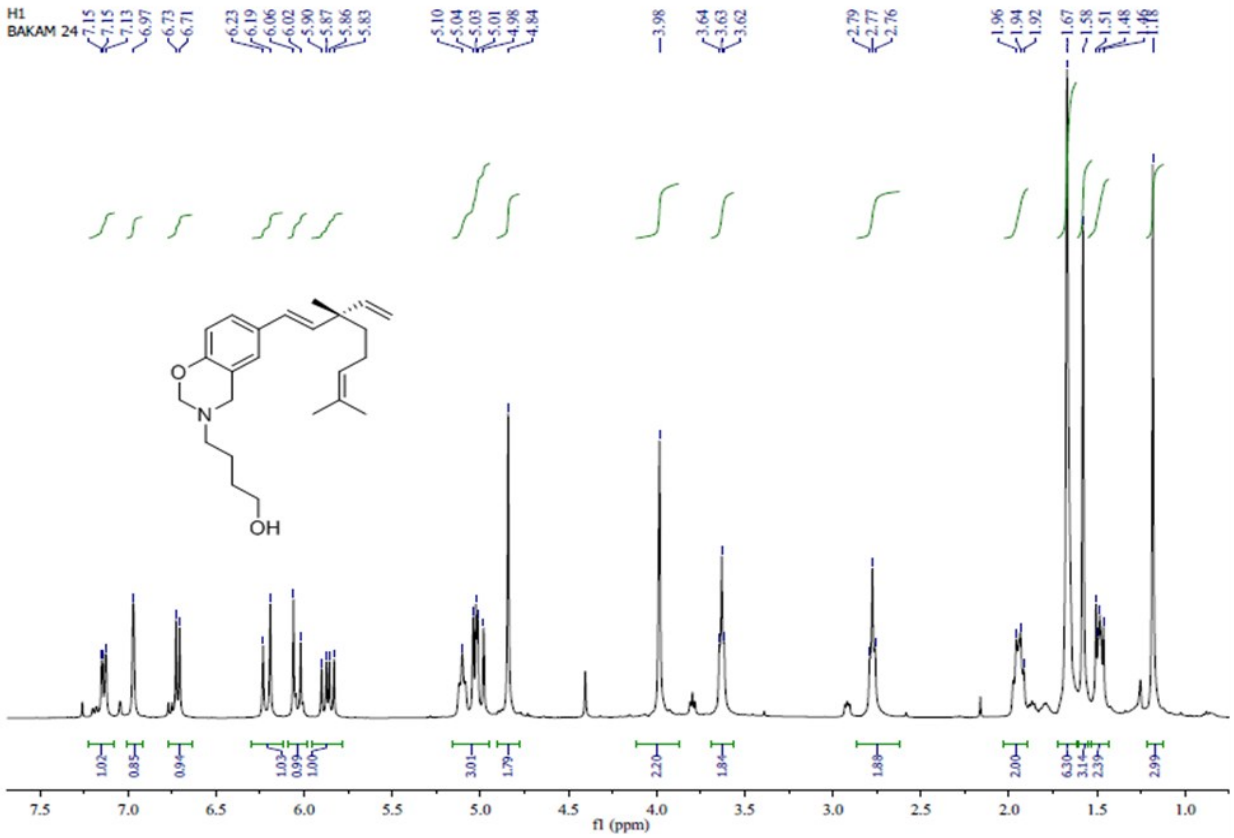
m/z	z	Abund	Formula	Ion
378.2414	1	932569.69	C25 H32 N O2	(M+H)+
379.245	1	242507.36	C25 H32 N O2	(M+H)+

Predicted Isotope Match Table

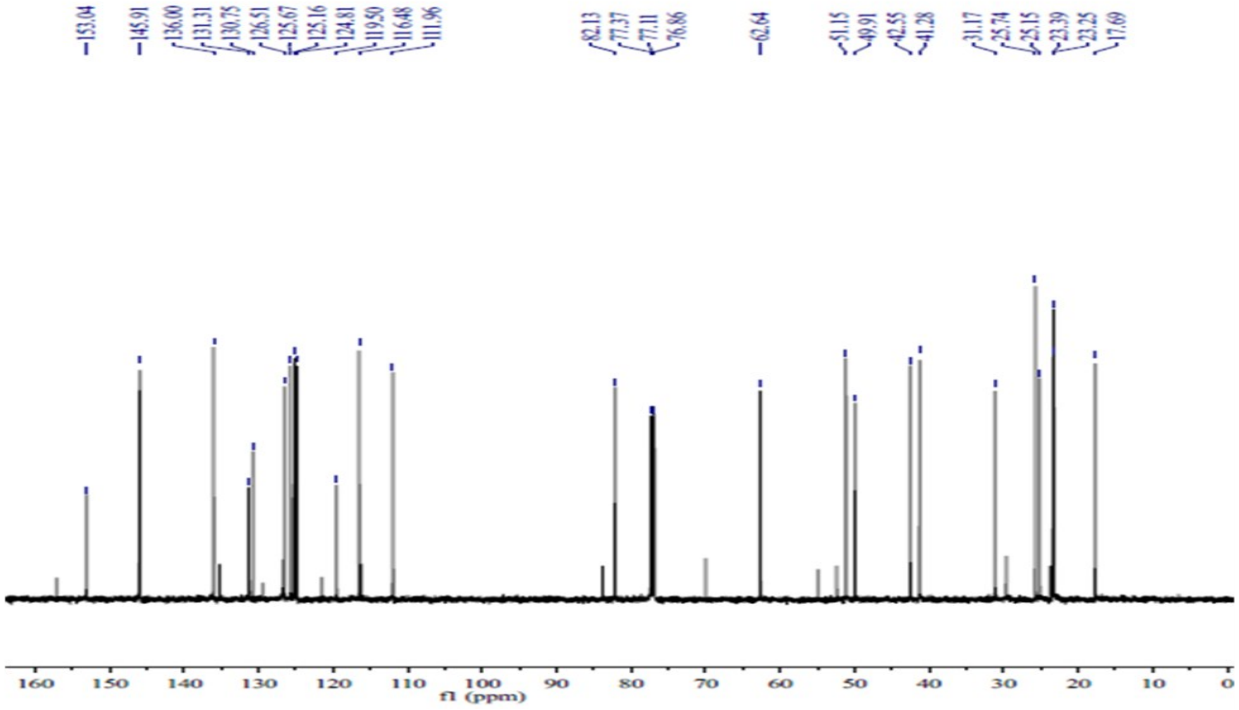
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	378.2414	378.2428	3.59	100	100	79.36	78.22
2	379.245	379.2461	2.72	26	27.85	20.64	21.78

4-(6-(3,7-dimethyl-3-vinylocta-1,6-dienyl)-2H-benzo[e][1,3]oxazin-3(4H)-yl) butan-1-ol (23)

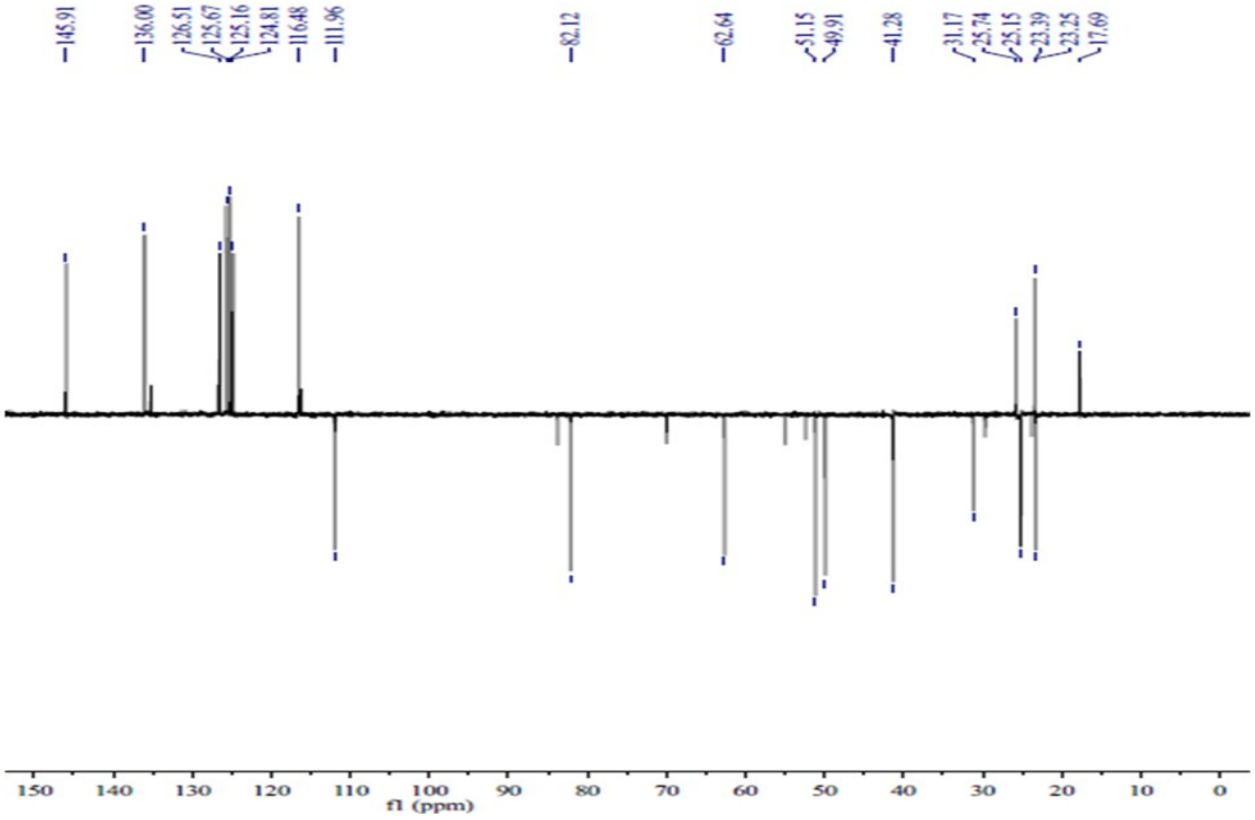
23-^{1}HNMR



23- ^{13}C NMR



DEPT- 23



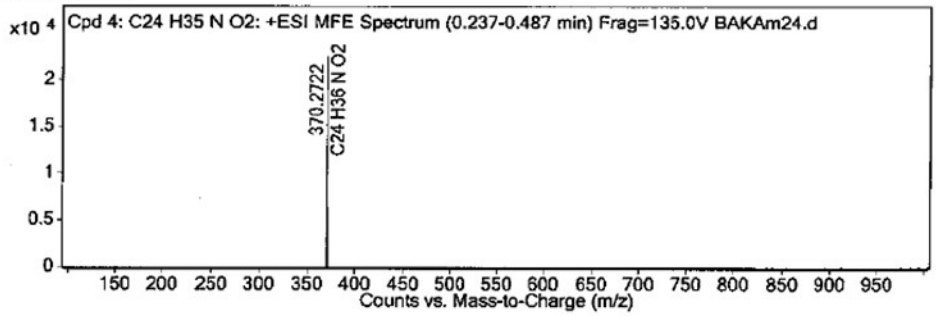
23 -HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C24 H35 N O2	0.328	369.265	C24 H35 N O2	C24 H35 N O2	4.71	C24 H35 N O2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 4: C24 H35 N O2	370.2722	0.328	Find by Molecular Feature	369.265

MFE MS Spectrum



MS Spectrum Peak List

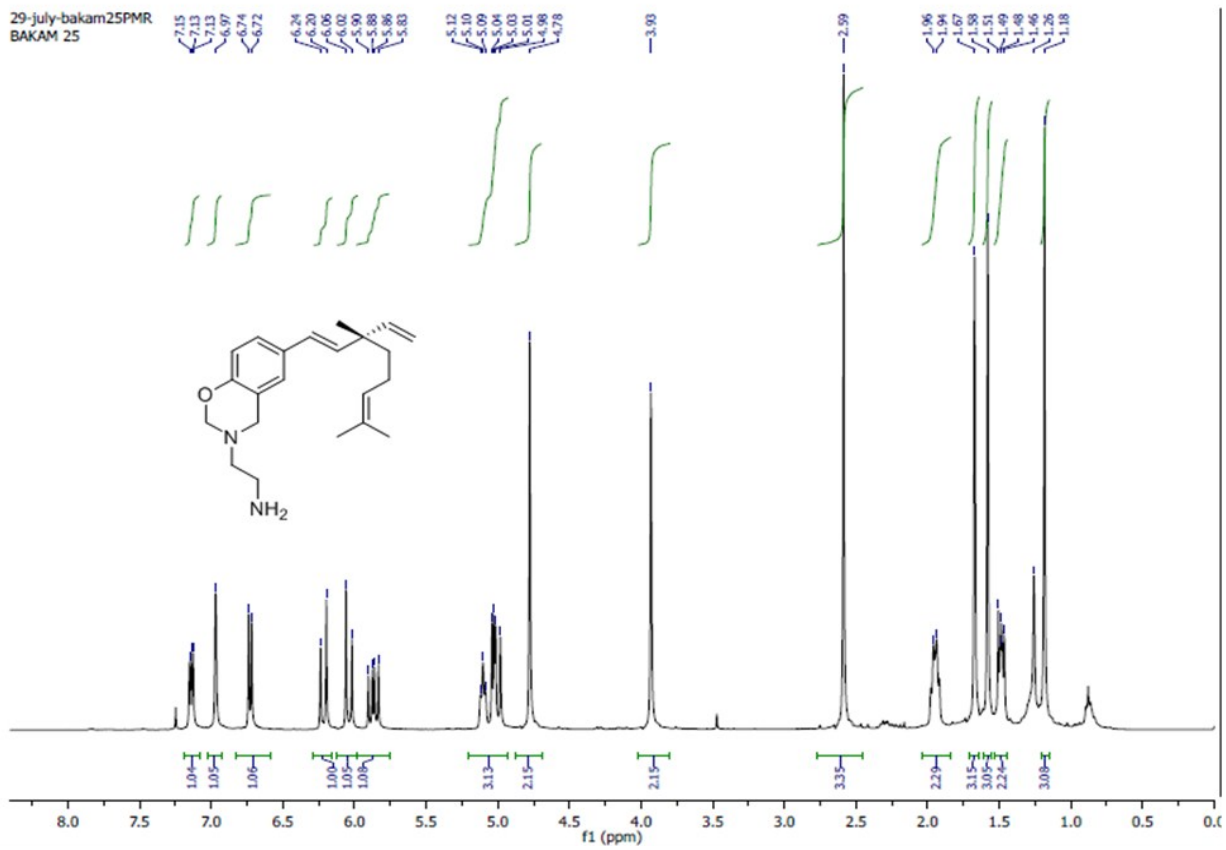
m/z	z	Abund	Formula	Ion
370.2722	1	22514.18	C24 H36 N O2	(M+H)+
371.276	1	6447.44	C24 H36 N O2	(M+H)+

Predicted Isotope Match Table

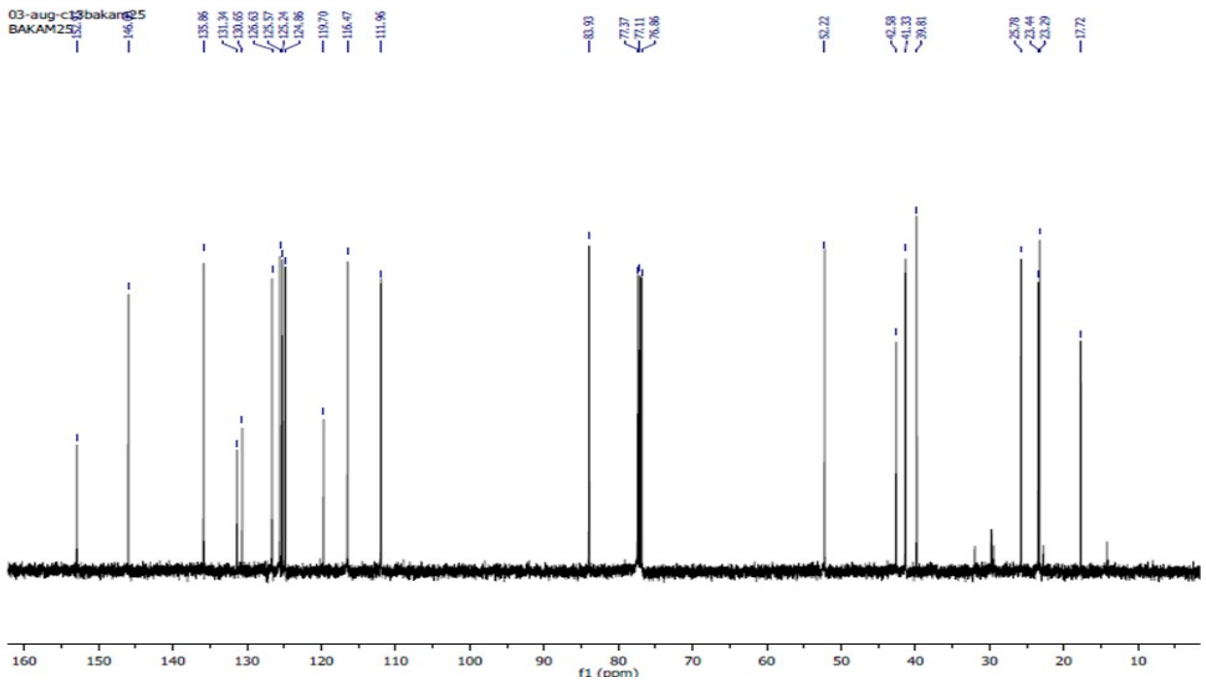
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	370.2722	370.2741	5	100	100	77.74	78.86
2	371.276	371.2774	3.63	28.64	26.81	22.26	21.14

2-(6-(3,7-dimethyl-3-vinylocta-1,6-dienyl)-2H-benzo[e][1,3]oxazin-3(4H)-yl) ethanamine (24)

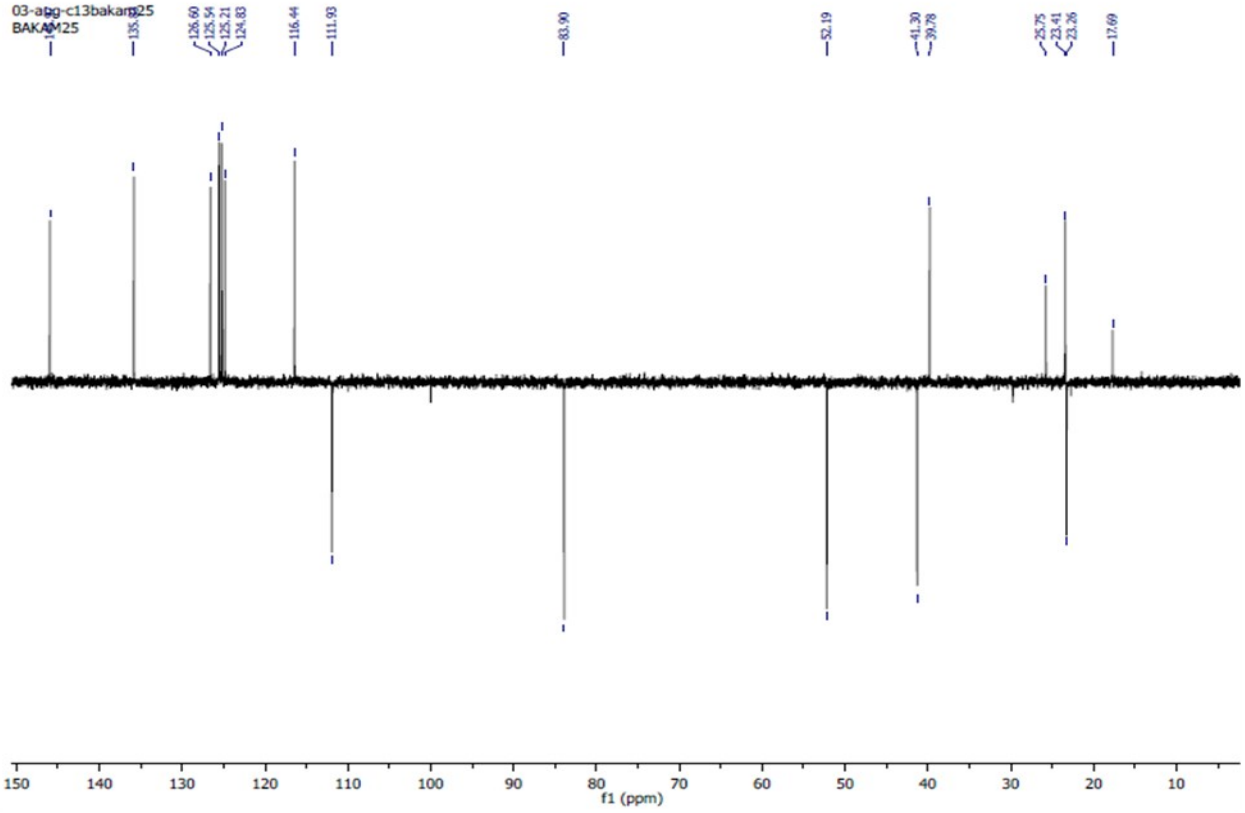
24-^{1}HNMR



24- ^{13}C NMR



DEPT- 24



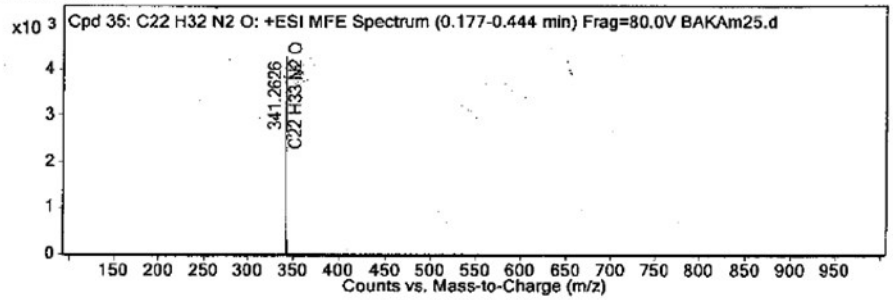
24-HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 35: C22 H32 N2 O	0.27	340.2541	C22 H32 N2 O	C22 H32 N2 O	-7.88	C22 H32 N2 O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 35: C22 H32 N2 O	341.2626	0.27	Find by Molecular Feature	340.2541

MFE MS Spectrum



MS Spectrum Peak List

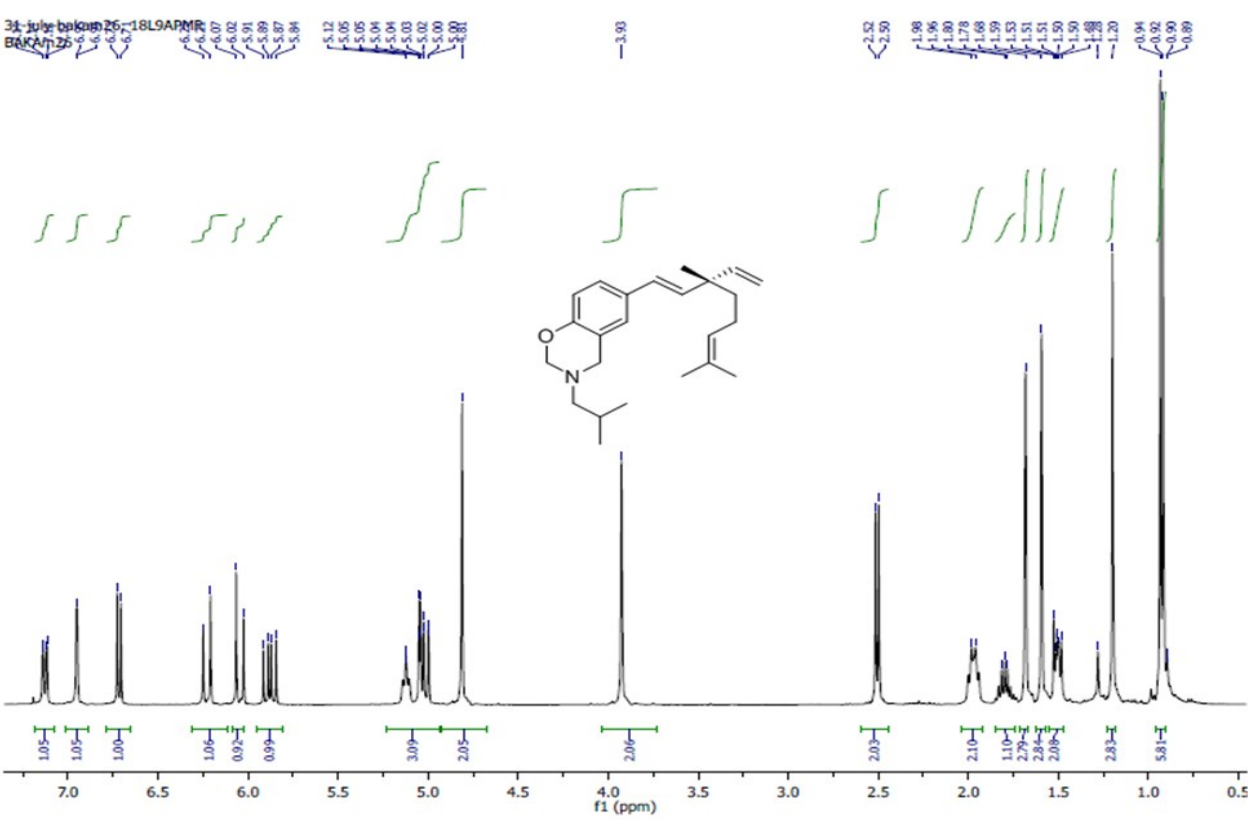
m/z	z	Abund	Formula	Ion
341.2626	1	4279.28	C22 H33 N2 O	(M+H)+
342.2637	1	1013.24	C22 H33 N2 O	(M+H)+
343.2539	1	301.82	C22 H33 N2 O	(M+H)+

Predicted Isotope Match Table

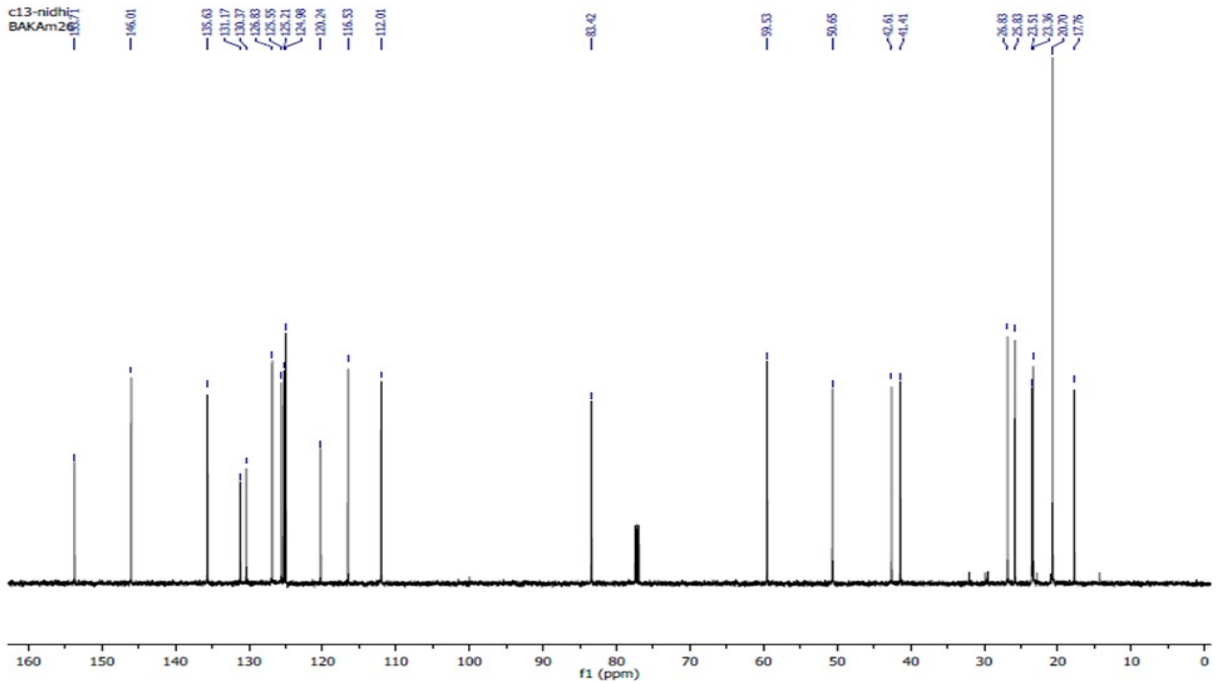
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	341.2626	341.2587	-11.35	100	100	76.49	78.05
2	342.2637	342.262	-5.13	23.68	24.94	18.11	19.47
3	343.2539	343.265	32.49	7.05	3.19	5.4	2.49

3,4-dihydro-3-isobutyl-6-(3,7-dimethyl-3-vinylocta-1,6-dienyl)-2H-benzo[e][1,3]oxazine (25)

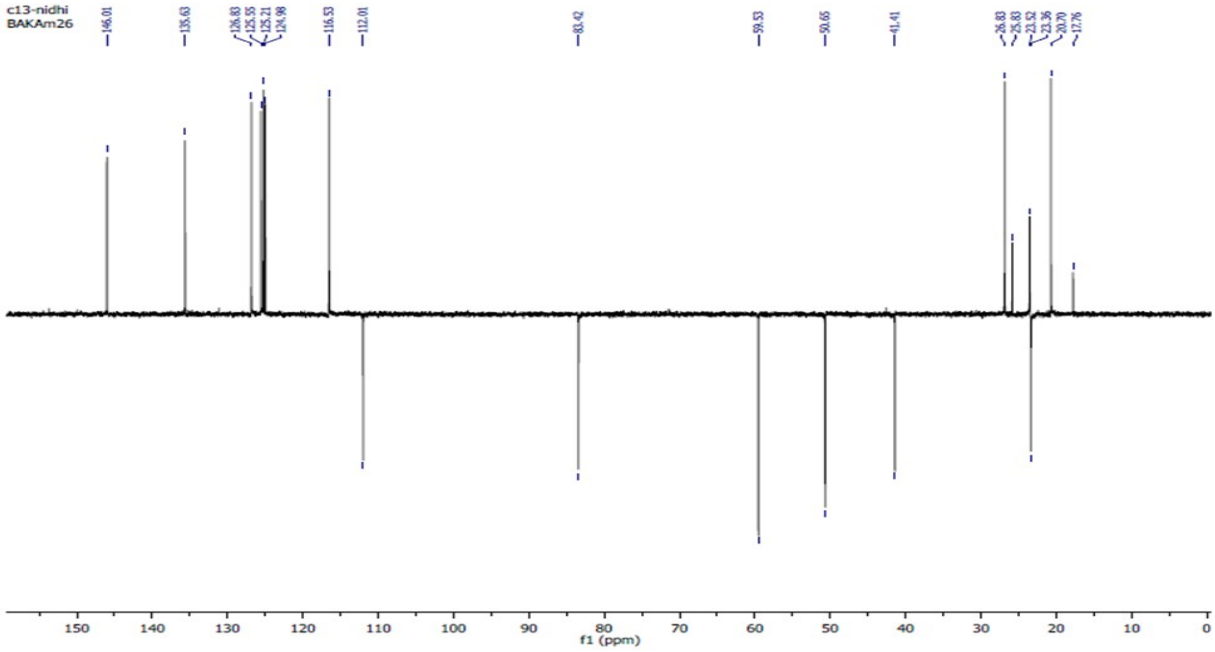
25-^{1}HNMR



25- ^{13}C NMR



DEPT- 25



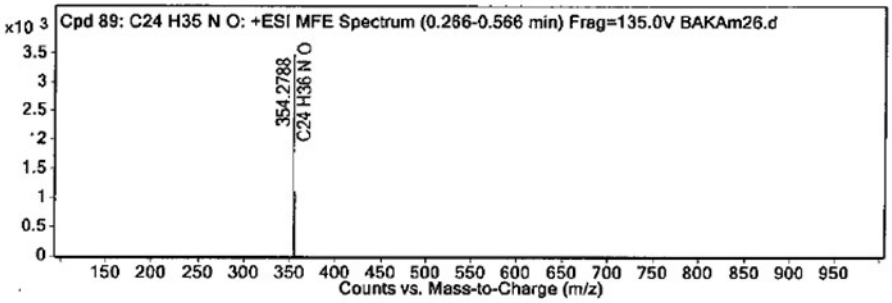
25-HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 89: C24 H35 N O	0.367	353.2714	C24 H35 N O	C24 H35 N O	1.32	C24 H35 N O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 89: C24 H35 N O	354.2788	0.367	Find by Molecular Feature	353.2714

MFE MS Spectrum



MS Spectrum Peak List

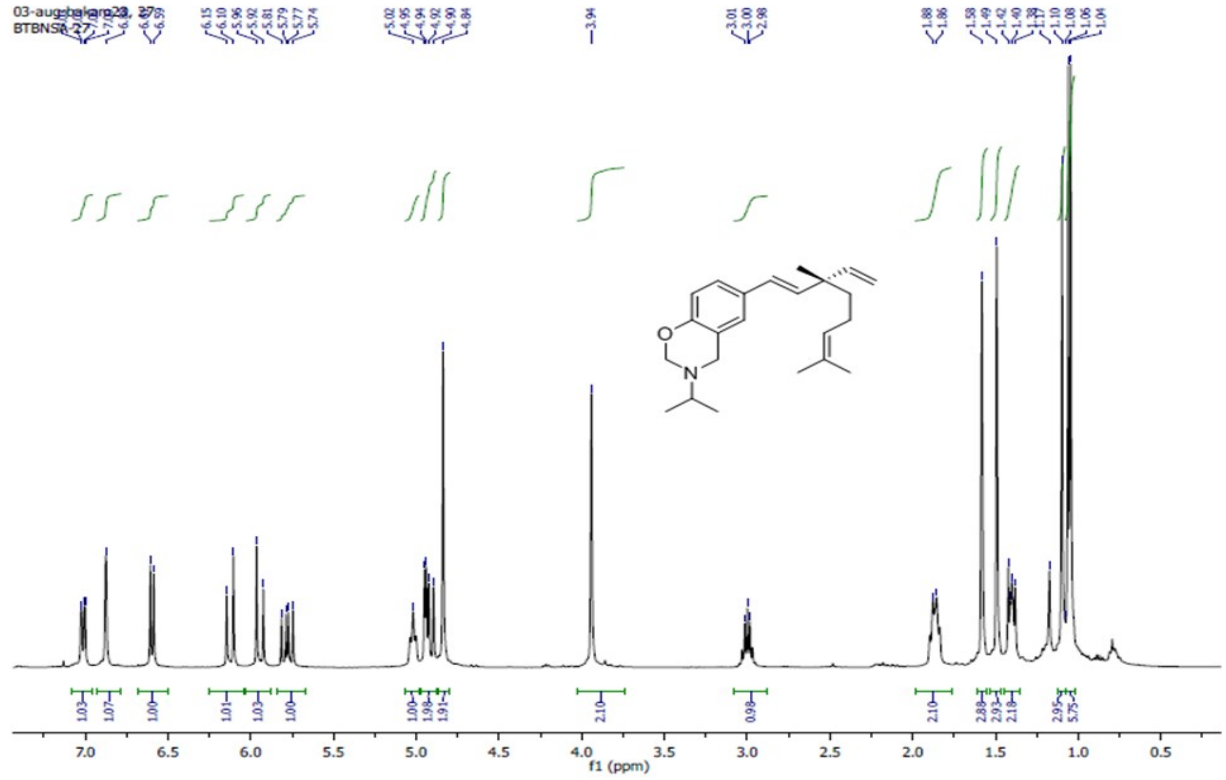
m/z	z	Abund	Formula	Ion
354.2788	1	3470.52	C24 H36 N O	(M+H)+
355.2817	1	1109.91	C24 H36 N O	(M+H)+

Predicted Isotope Match Table

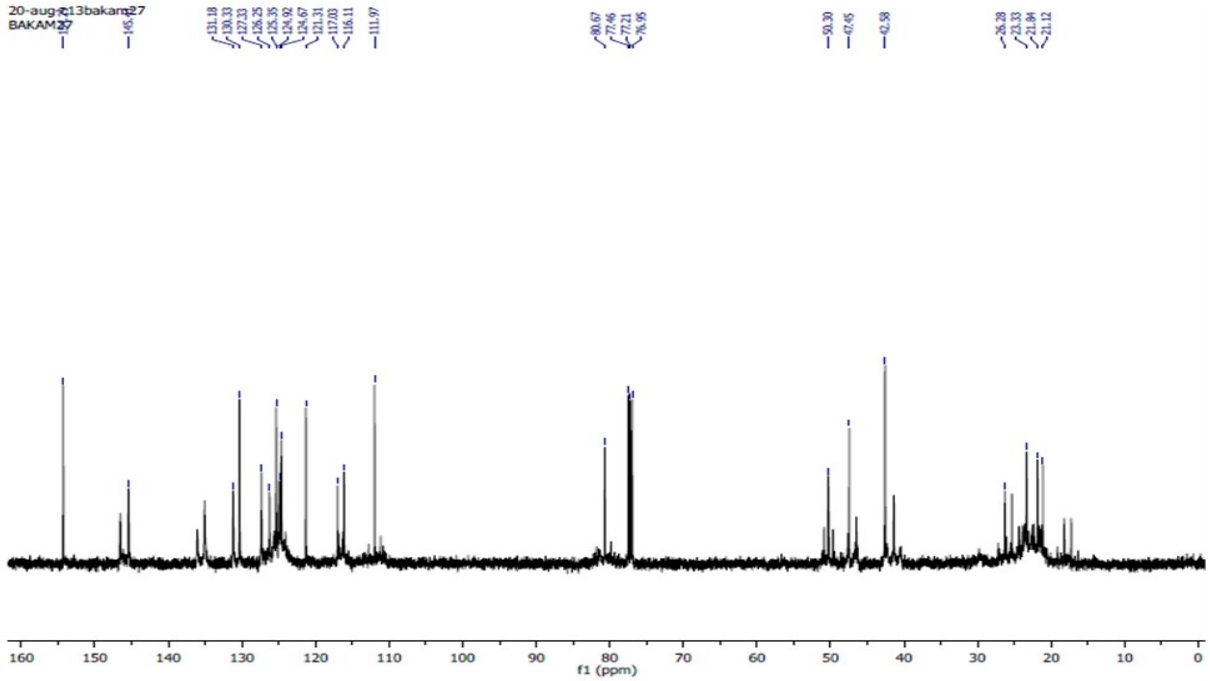
Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	354.2788	354.2791	1.03	100	100	75.77	78.88
2	355.2817	355.2825	2.23	31.98	26.78	24.23	21.12

3,4-dihydro-3-isopropyl-6-(3,7-dimethyl-3-vinylocta-1,6-dienyl)-2H-benzo[e][1,3]oxazine (26)

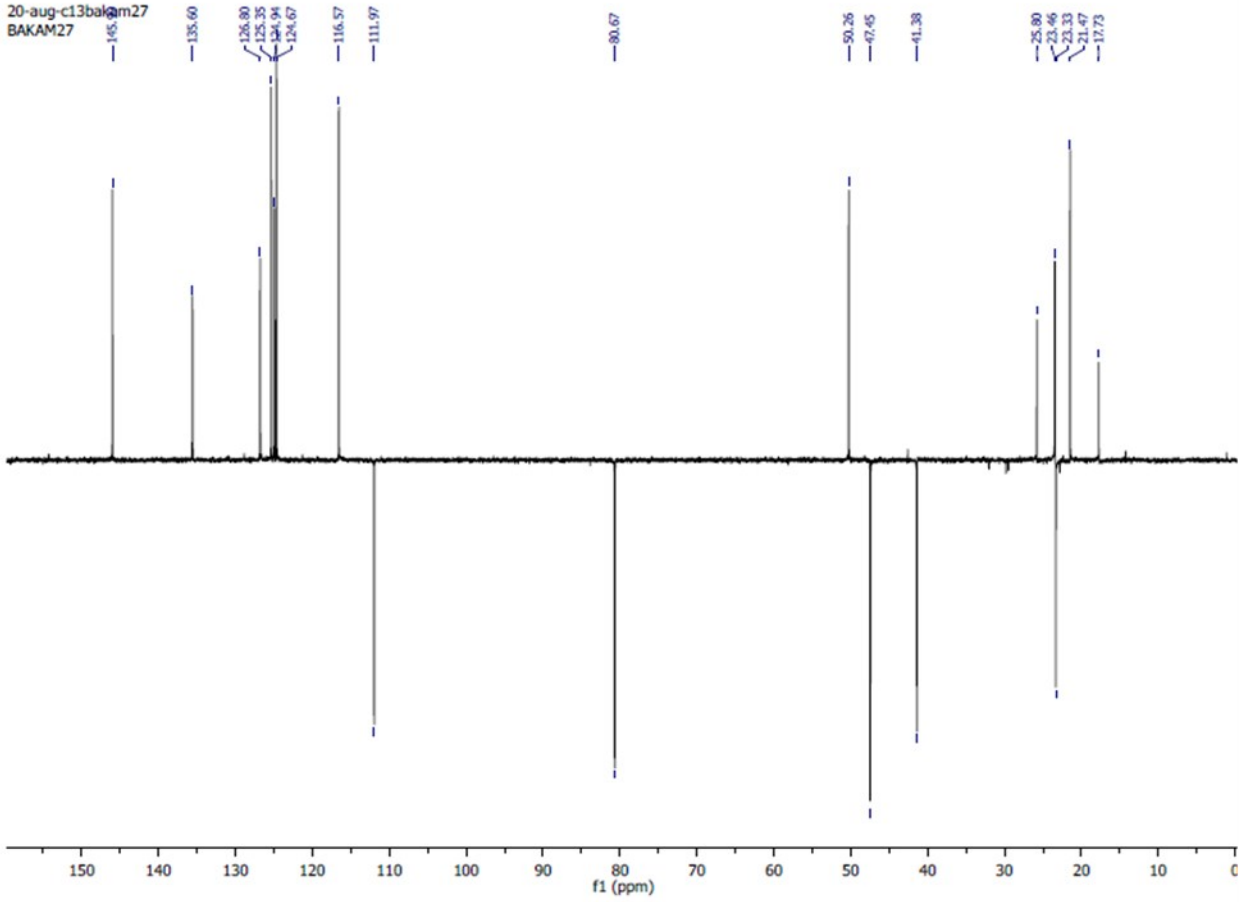
26-^{1}HNMR



26- ^{13}C NMR



DEPT- 26



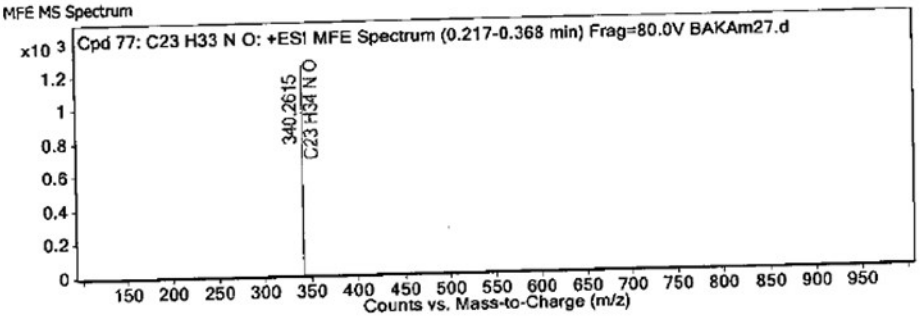
26-HRMS

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 77: C23 H33 N O	0.283	339.2543	C23 H33 N O	C23 H33 N O	5.72	C23 H33 N O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 77: C23 H33 N O	340.2615	0.283	Find by Molecular Feature	339.2543

MFE MS Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
340.2615	1	1252.26	C23 H34 N O	(M+H)+

Predicted Isotope Match Table

Isotope	*m/z*	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	340.2615	340.2635	5.71	100	100	100	100