

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050125\
 Data File : BF142259.D
 Acq On : 01 May 2025 14:37
 Operator : RC/JU
 Sample : Q1914-14
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FB04282025

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043025.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF142259.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.122	489	498	504	rBV	161141	239649	4.05%	0.763%
2	5.516	558	565	570	rBV	1924405	2516865	42.54%	8.016%
3	6.516	729	735	740	rBV	1222472	1553155	26.25%	4.947%
4	6.904	796	801	806	rBV	1006044	1229013	20.77%	3.914%
5	7.463	890	896	902	rBV	2438417	3360237	56.79%	10.702%
6	8.187	1014	1019	1024	rVB	1310530	1596400	26.98%	5.084%
7	8.404	1051	1056	1057	rBV	101062	115425	1.95%	0.368%
8	8.428	1057	1060	1069	rVB	142916	182285	3.08%	0.581%
9	8.510	1069	1074	1078	rBV3	41844	67438	1.14%	0.215%
10	9.263	1196	1202	1207	rVB	4681451	5916987	100.00%	18.845%
11	9.939	1312	1317	1322	rBV	1332146	1631502	27.57%	5.196%
12	10.728	1445	1451	1456	rBV	2396644	3013254	50.93%	9.597%
13	11.428	1565	1570	1575	rVB	1089395	1337303	22.60%	4.259%
14	11.945	1654	1658	1662	rBV	44829	63252	1.07%	0.201%
15	12.663	1773	1780	1788	rBV	108111	182719	3.09%	0.582%
16	12.739	1788	1793	1805	rVB	71835	122191	2.07%	0.389%
17	13.016	1834	1840	1845	rBV	3564315	4565739	77.16%	14.542%
18	13.804	1960	1974	1998	rBV4	220274	1148233	19.41%	3.657%
19	14.063	2013	2018	2028	rBV	929252	1228671	20.77%	3.913%
20	14.627	2110	2114	2124	rBV3	45723	87817	1.48%	0.280%
21	15.557	2266	2272	2288	rVB	818188	1239513	20.95%	3.948%

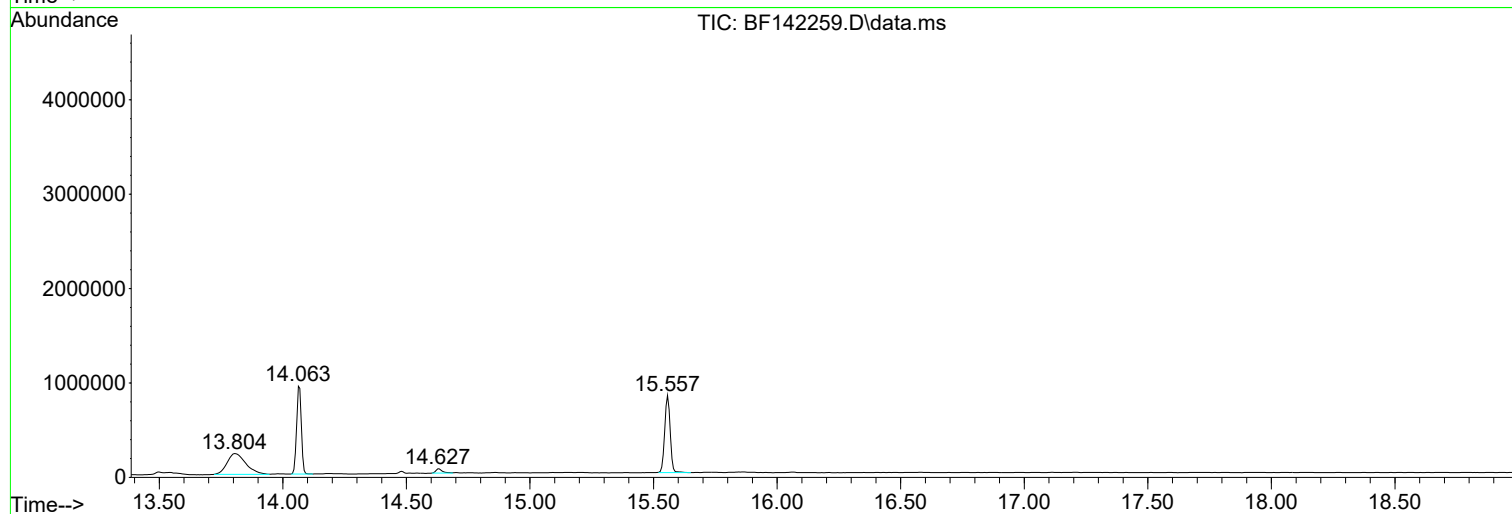
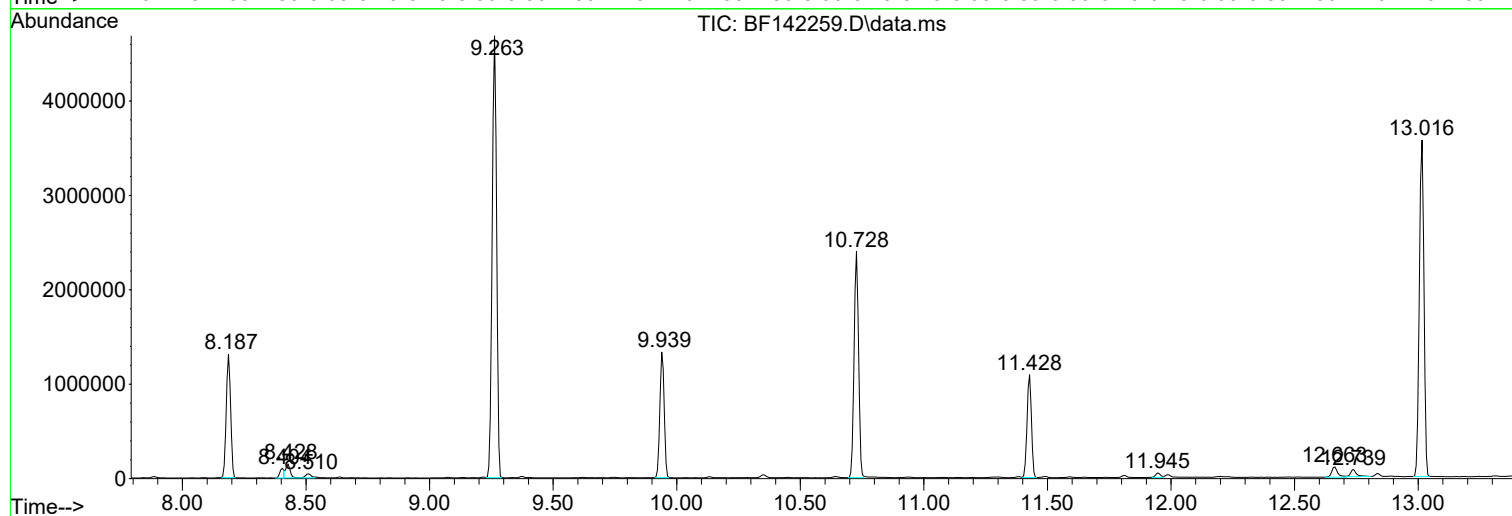
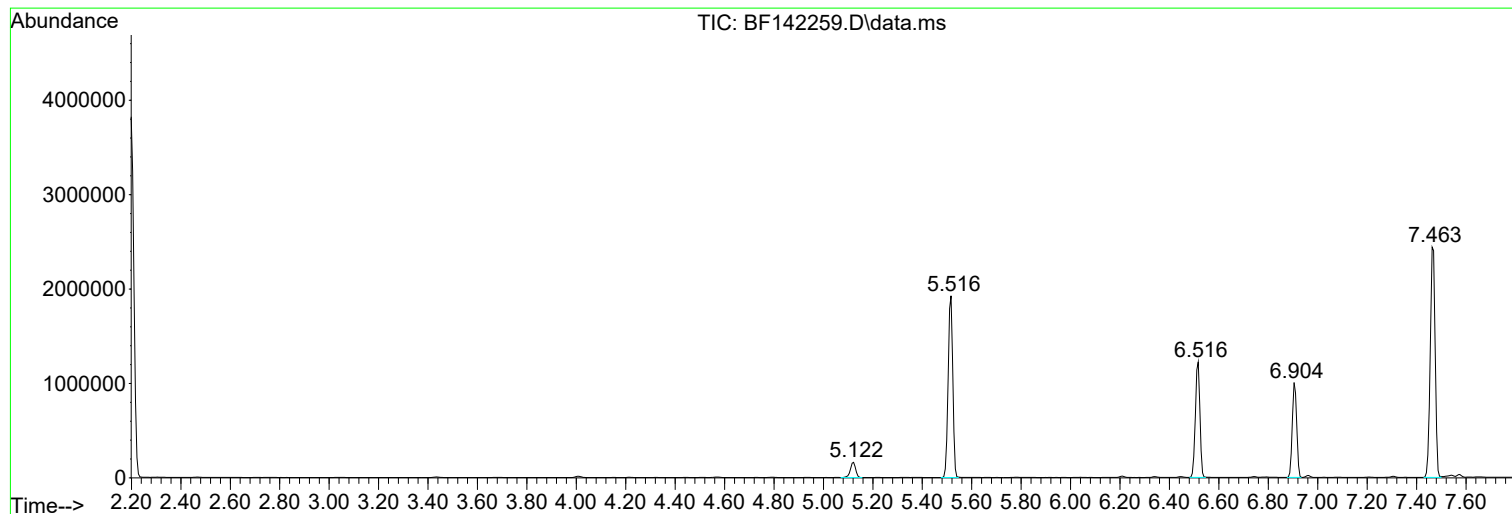
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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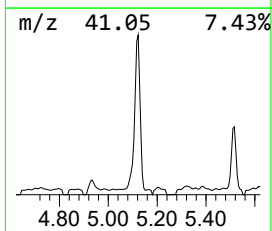
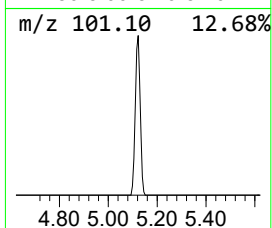
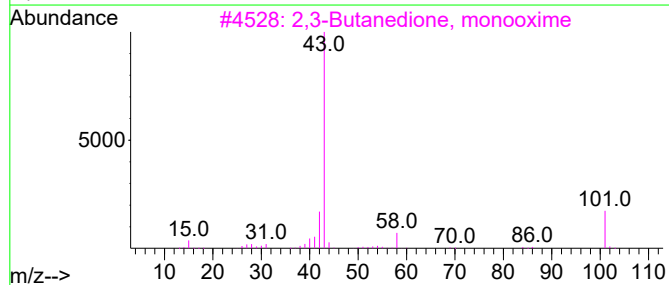
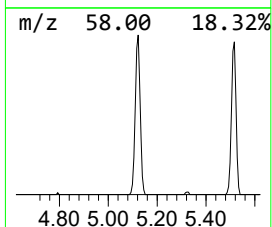
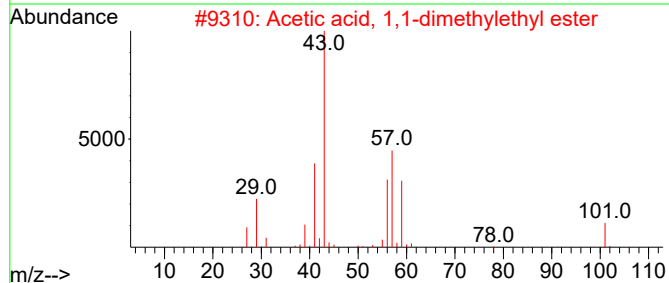
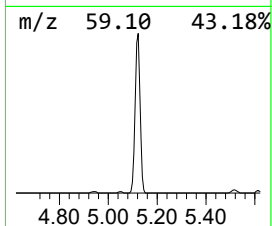
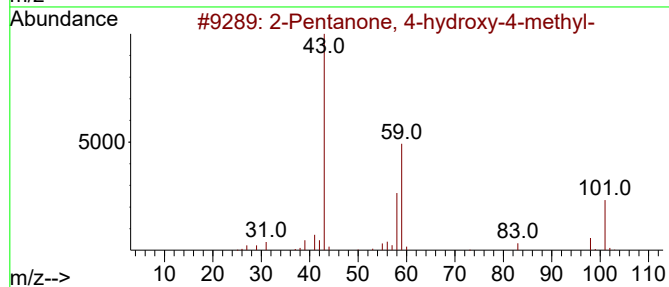
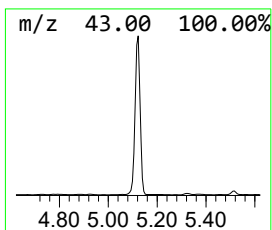
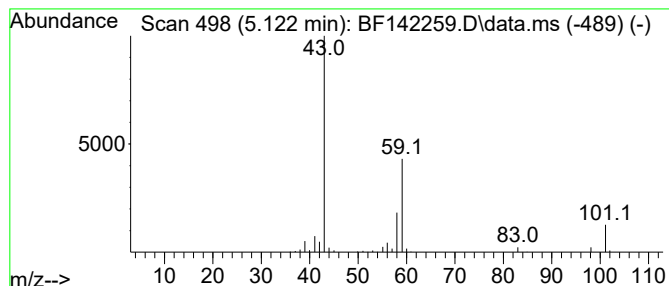
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.122	3.90 ng	239649	1,4-Dichlorobenzene-d4	6.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	83		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9		



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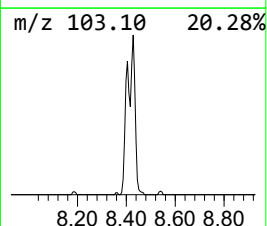
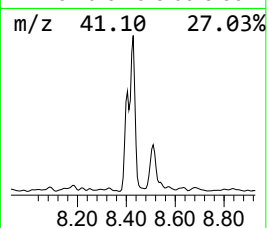
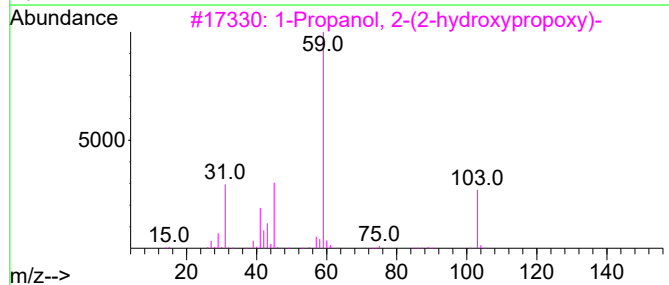
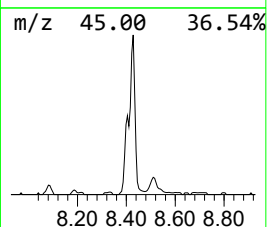
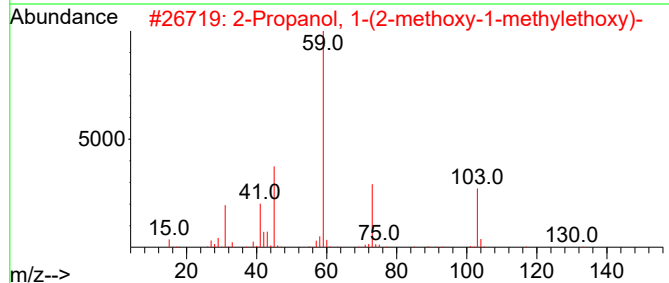
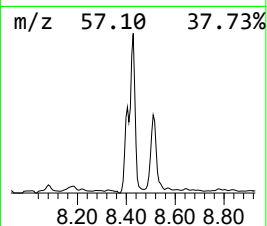
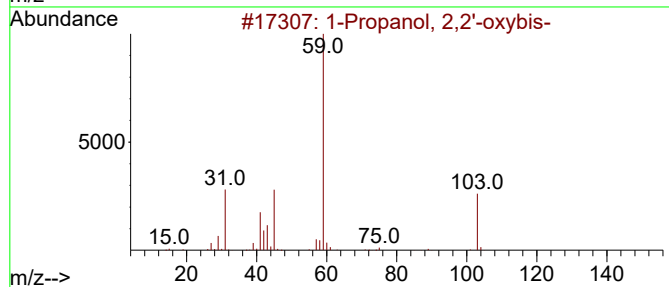
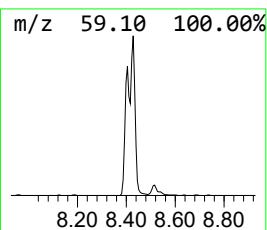
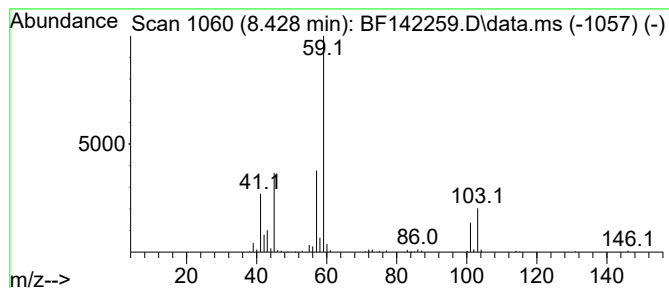
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Peak Number 2 1-Propanol, 2,2'-oxybis- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.428	2.28 ng	182285	Naphthalene-d8	8.187

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	72
2		2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	72
3		1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72
4		Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	64
5		1-Propanol, 3,3'-oxybis-	134	C6H14O3	002396-61-4	64



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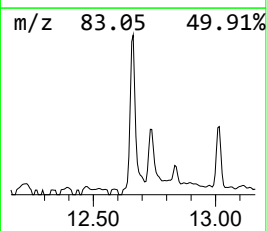
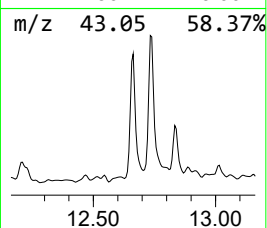
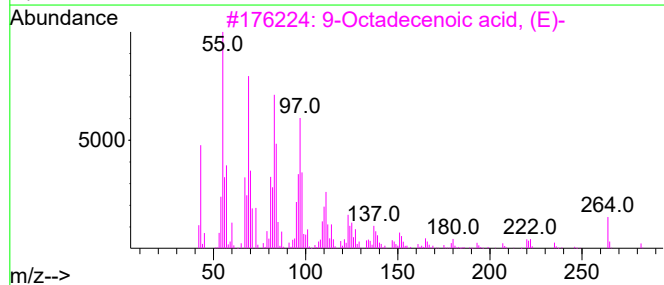
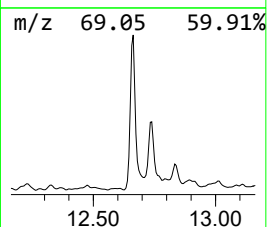
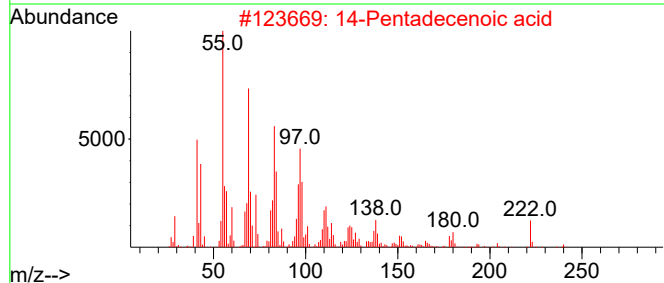
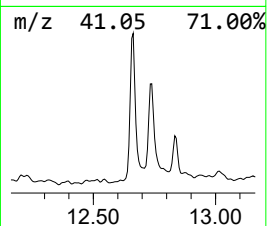
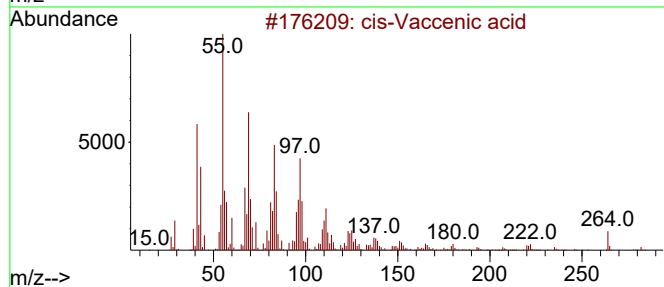
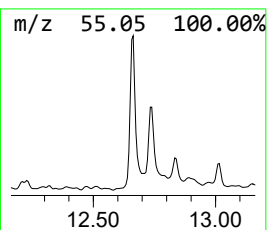
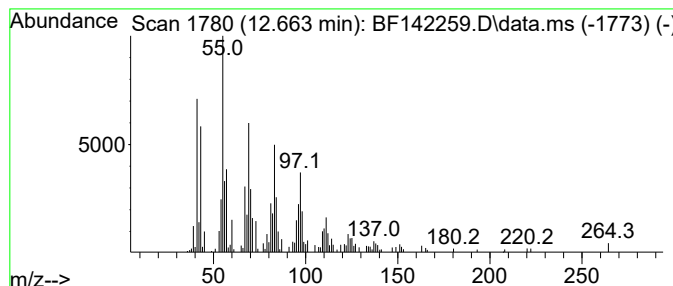
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Peak Number 3 cis-Vaccenic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.663	2.73 ng	182719	Phenanthrene-d10	11.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-Vaccenic acid	282	C18H34O2	000506-17-2	93
2			14-Pentadecenoic acid	240	C15H28O2	017351-34-7	91
3			9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	91
4			(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	90
5			Palmitoleic acid	254	C16H30O2	000373-49-9	90



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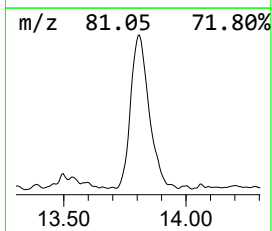
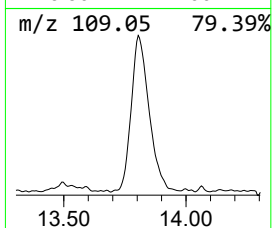
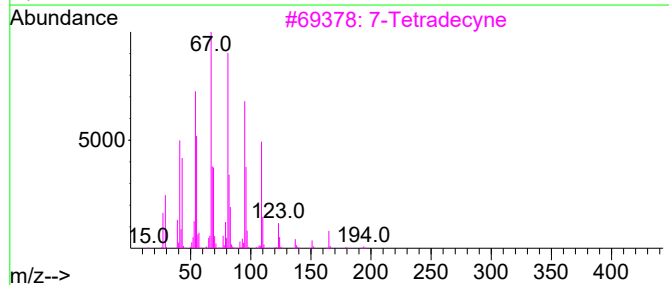
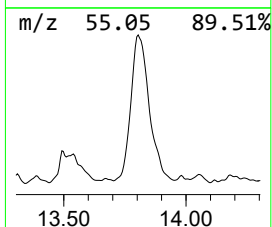
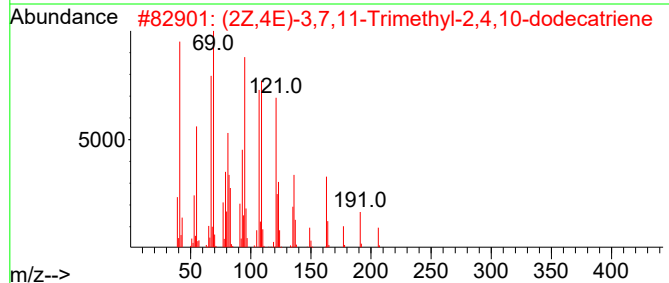
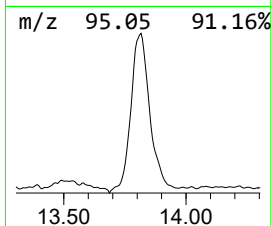
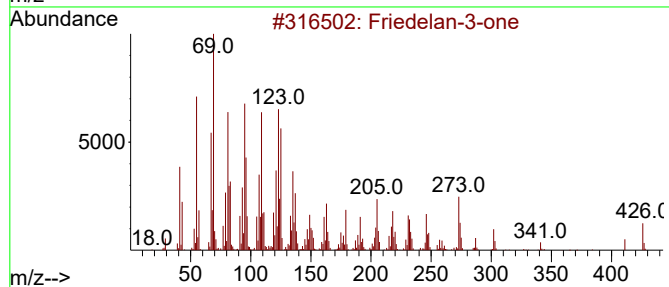
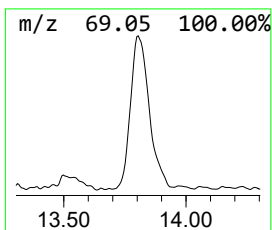
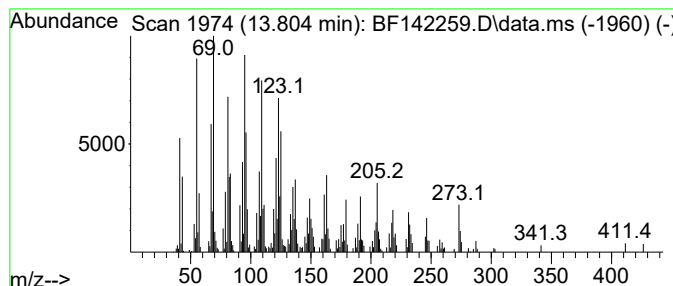
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Peak Number 4 Friedelan-3-one Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.804	18.69 ng	1148230	Chrysene-d12	14.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Friedelan-3-one	426	C30H50O	000559-74-0	62
2			(2Z,4E)-3,7,11-Trimethyl-2,4,10-...	206	C15H26	172549-29-0	58
3			7-Tetradecyne	194	C14H26	035216-11-6	55
4			5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	53
5			Silane, monochloride, methylviny...	218	C10H19ClOSi	1000421-09-7	51



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.122	3.9	ng	239649	1	6.904	1229010	20.0
1-Propanol, 2,2...	8.428	2.3	ng	182285	2	8.187	1596400	20.0
cis-Vaccenic acid	12.663	2.7	ng	182719	4	11.428	1337300	20.0
Friedelan-3-one	13.804	18.7	ng	1148230	5	14.063	1228670	20.0