

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022624\
 Data File : BF137391.D
 Acq On : 26 Feb 2024 18:04
 Operator : CG\JU
 Sample : P1538-10
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20241103-AMENDED-COMPOSITE-35N-N-4-02

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-BF022324.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137391.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.069	491	507	510	rBV	7636664	24613221	100.00%	49.210%
2	5.416	562	566	582	rBV	1699537	1621543	6.59%	3.242%
3	6.416	732	736	749	rBV	2555505	2778794	11.29%	5.556%
4	6.781	795	798	806	rBV	1582216	1286476	5.23%	2.572%
5	7.339	889	893	909	rBV	2592548	2543416	10.33%	5.085%
6	7.498	916	920	925	rBV	1105382	1071457	4.35%	2.142%
7	8.057	1012	1015	1034	rVB	1925574	1770059	7.19%	3.539%
8	9.139	1195	1199	1202	rBV	5037257	4367654	17.75%	8.732%
9	9.816	1310	1314	1317	rBV	2160823	1772937	7.20%	3.545%
10	10.604	1444	1448	1455	rBV	613088	566883	2.30%	1.133%
11	10.727	1466	1469	1475	rBV	355966	359711	1.46%	0.719%
12	11.174	1541	1545	1549	rBV	248456	272151	1.11%	0.544%
13	11.304	1564	1567	1571	rBV	1662233	1492723	6.06%	2.984%
14	12.904	1835	1839	1849	rBV	3581108	3205580	13.02%	6.409%
15	13.957	2015	2018	2022	rBV	1080972	1103222	4.48%	2.206%
16	15.439	2265	2270	2279	rVV	885322	1190580	4.84%	2.380%

Sum of corrected areas: 50016407

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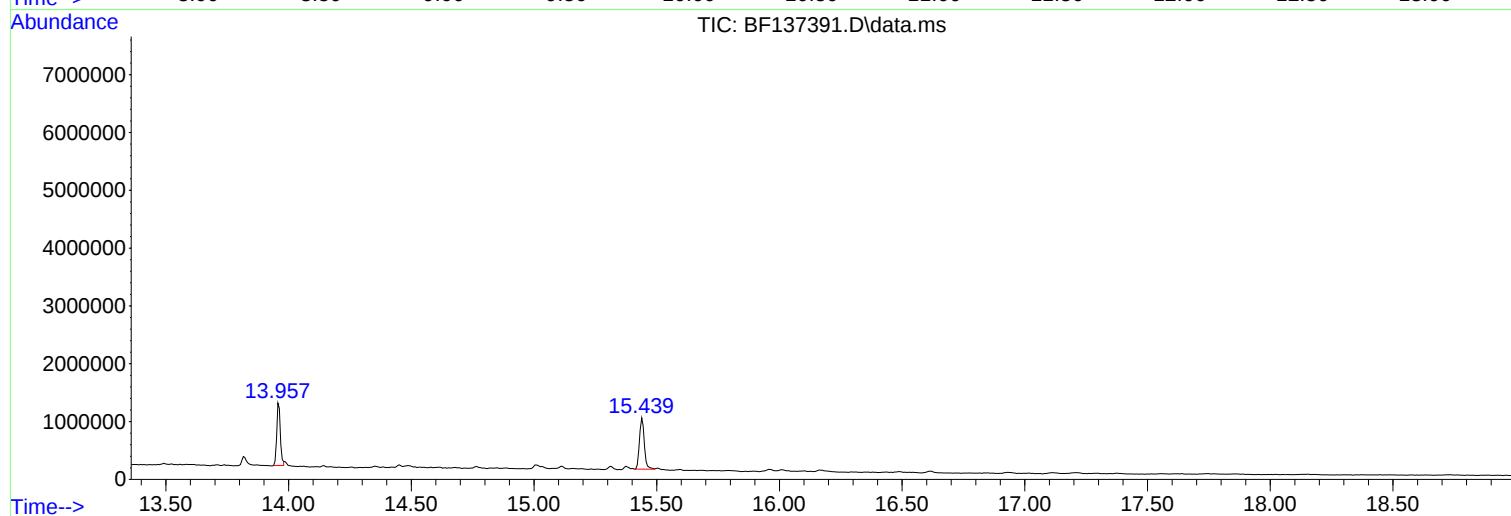
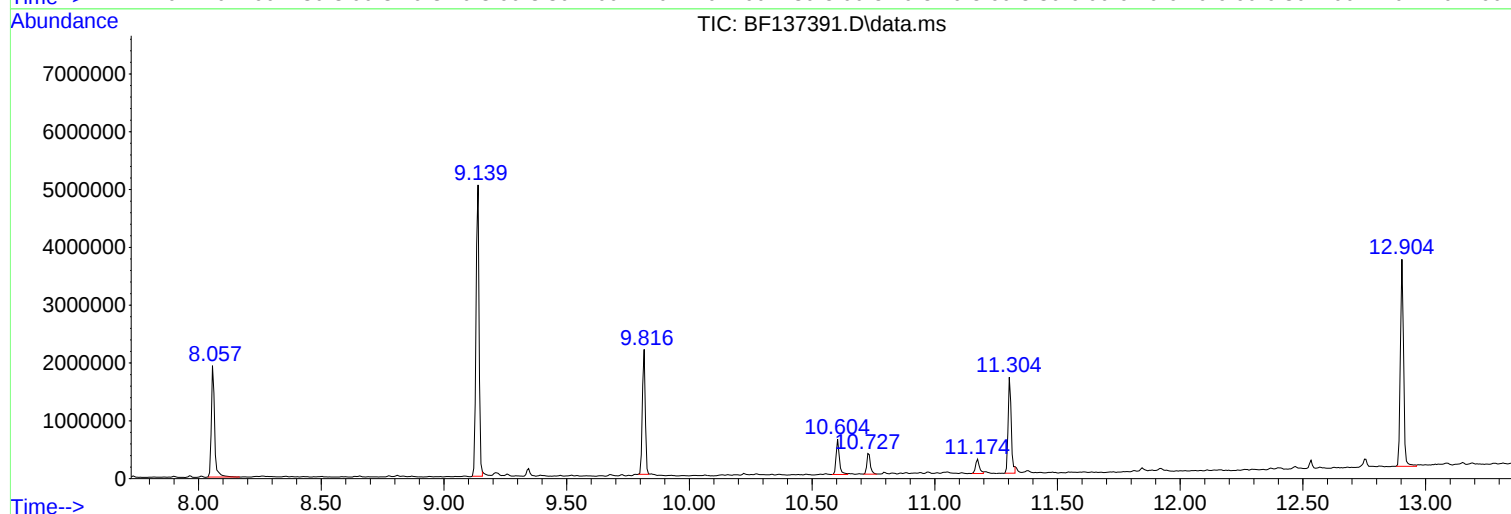
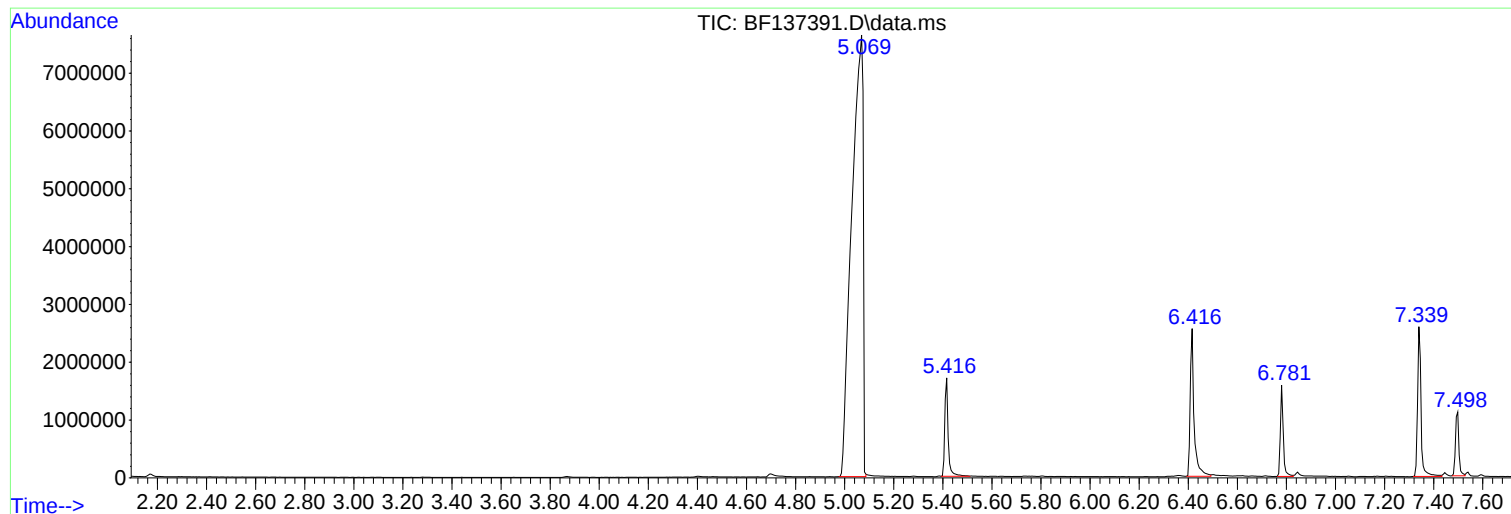
ClientSampleId :

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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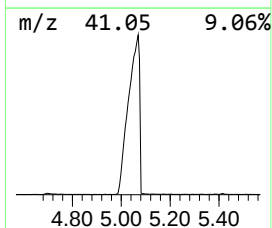
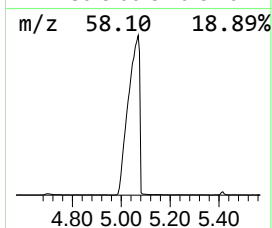
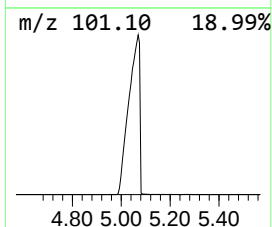
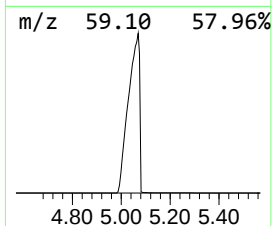
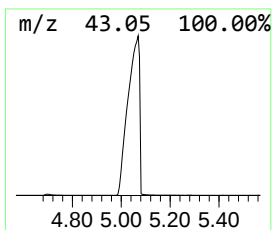
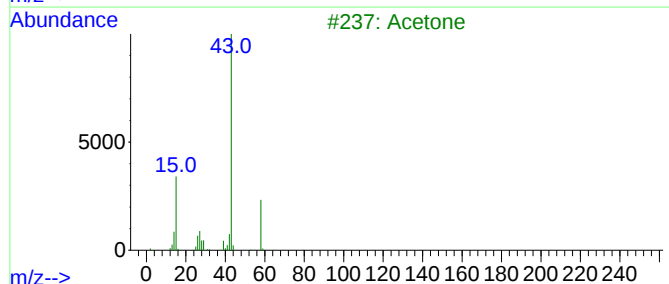
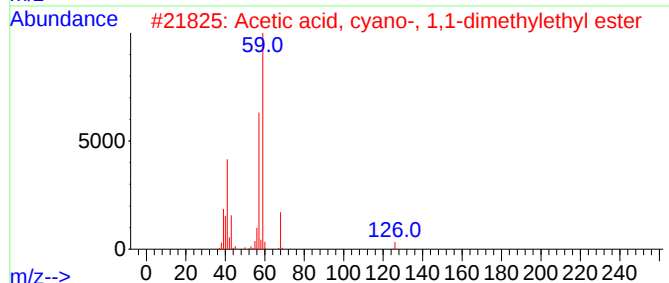
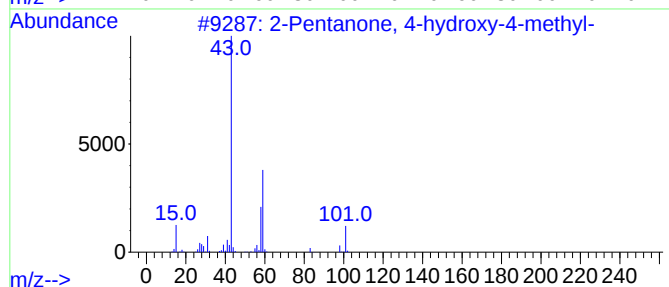
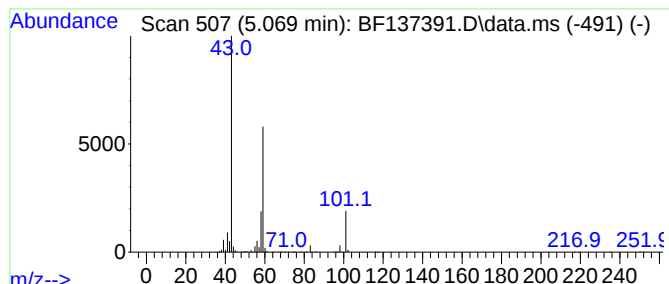
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.069	382.65 ng	24613200	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37		
3	Acetone	58	C3H6O	000067-64-1	12		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10		



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L

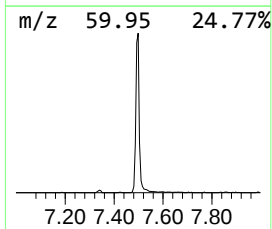
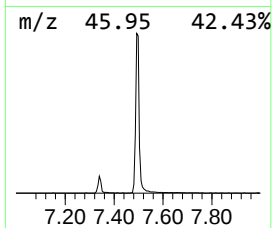
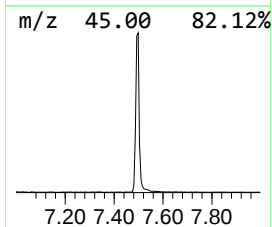
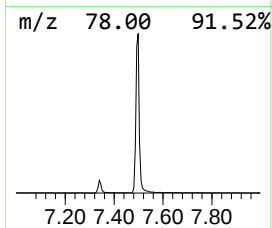
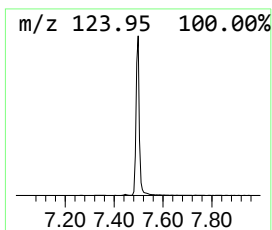
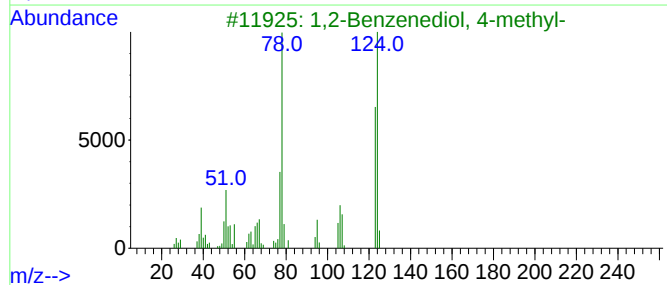
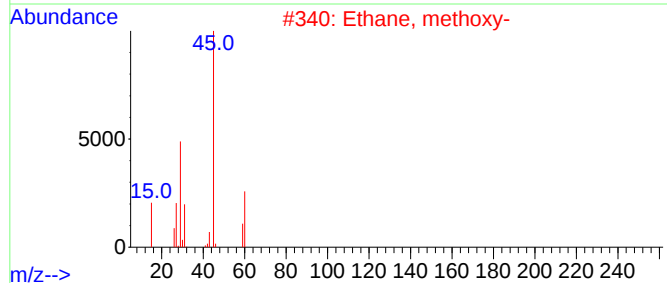
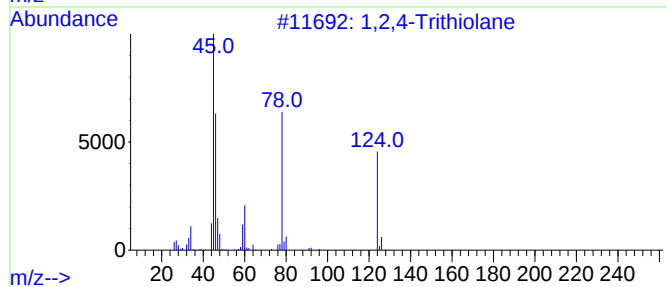
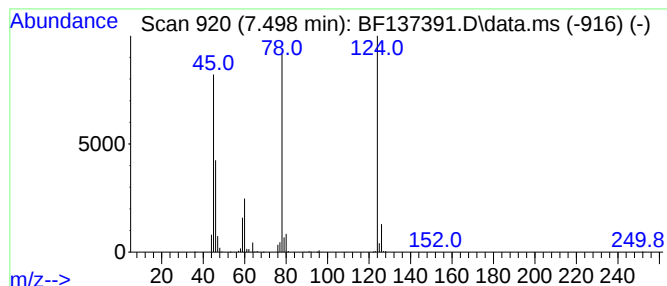
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.498

Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.498	12.11 ng	1071460	Naphthalene-d8	8.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2,4-Trithiolane	124	C2H4S3	000289-16-7	36
2			Ethane, methoxy-	60	C3H8O	000540-67-0	9
3			1,2-Benzenediol, 4-methyl-	124	C7H8O2	000452-86-8	9
4			Fumaronitrile	78	C4H2N2	000764-42-1	9
5			Dimethyl ether	46	C2H6O	000115-10-6	9



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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022324.M

Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

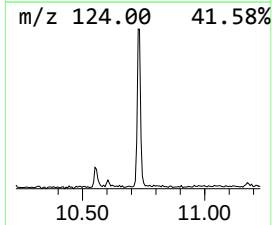
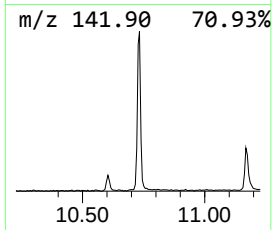
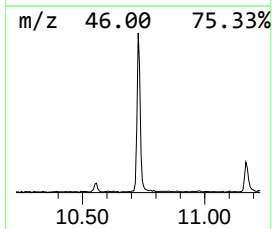
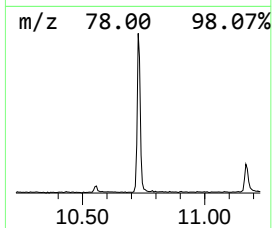
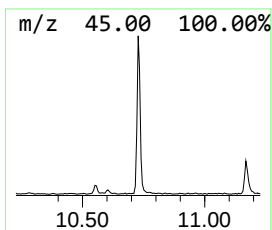
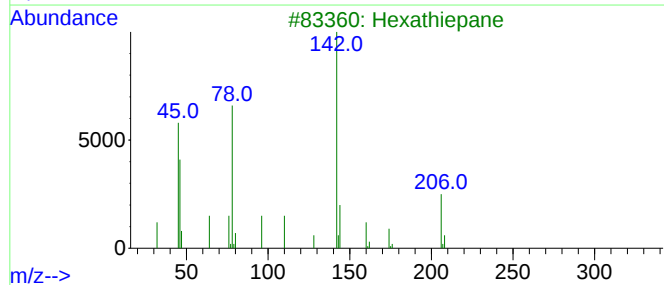
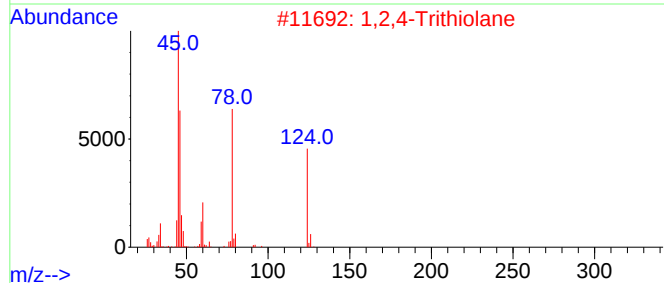
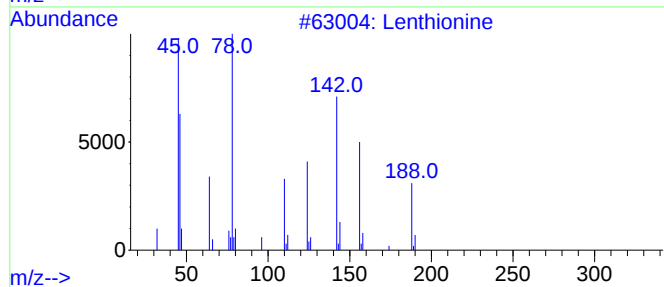
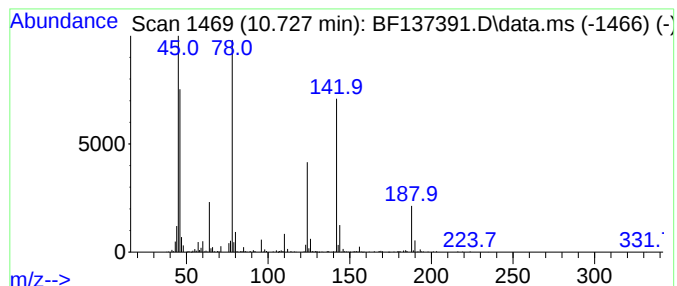
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 3 Lenthionine Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.727	4.82 ng	359711	Phenanthrene-d10	11.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Lenthionine	188	C2H4S5	000292-46-6	93
2			1,2,4-Trithiolane	124	C2H4S3	000289-16-7	72
3			Hexathiepane	206	CH2S6	017233-71-5	39
4			Formic acid	46	CH2O2	000064-18-6	9
5			Fumaronitrile	78	C4H2N2	000764-42-1	9



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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022324.M

Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

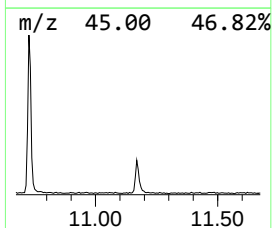
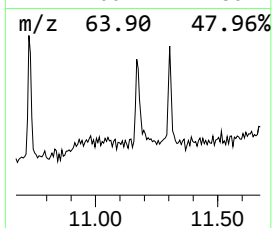
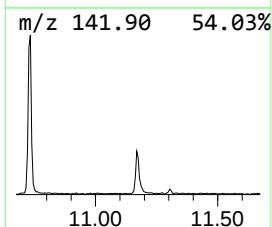
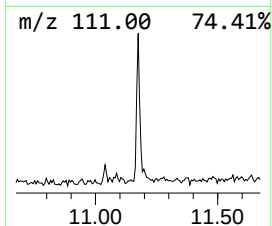
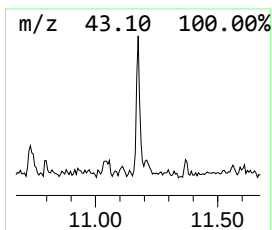
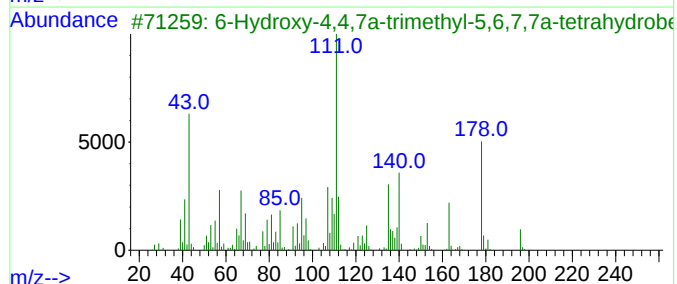
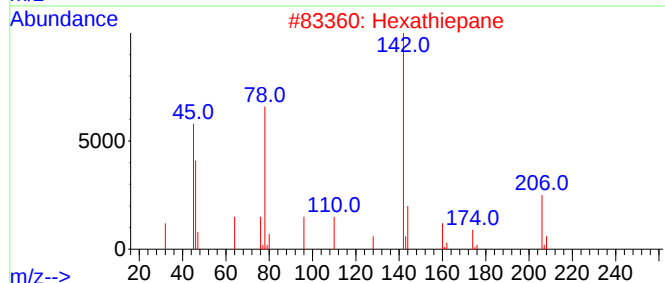
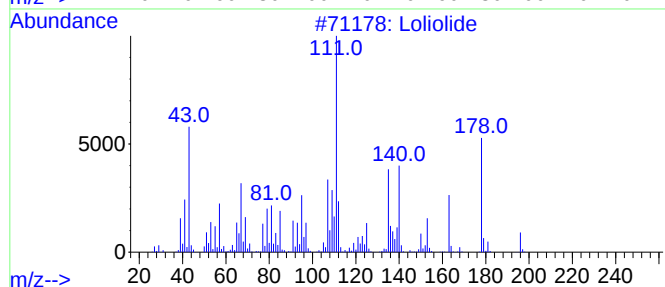
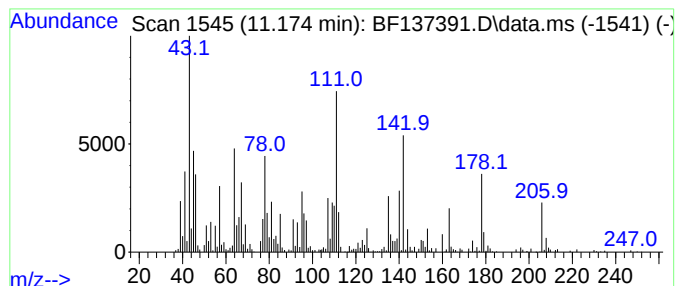
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown11.174 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.174	3.65 ng	272151	Phenanthrene-d10	11.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Loliolide	196	C11H16O3	005989-02-6	42
2			Hexathiepane	206	CH2S6	017233-71-5	41
3			6-Hydroxy-4,4,7a-trimethyl-5,6,7...	196	C11H16O3	073410-02-3	25
4			2-Pentenoic acid, 3-ethyl-, meth...	142	C8H14O2	013979-17-4	14
5			5-Amino-3H-[1,2,3]triazole-4-car...	142	C3H6N6O	1000318-26-9	14



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.069	382.6	ng	24613200	1	6.781	1286480	20.0
unknown7.498	7.498	12.1	ng	1071460	2	8.057	1770060	20.0
Lenthionine	10.727	4.8	ng	359711	4	11.304	1492720	20.0
unknown11.174	11.174	3.6	ng	272151	4	11.304	1492720	20.0