

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021022\
 Data File : BF126849.D
 Acq On : 10 Feb 2022 17:54
 Operator : CG\JU
 Sample : N1449-02
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20220042-AMENDED-NACOTE-2-COMP

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-BF020922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126849.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.169	349	354	361	rVB	171195	200497	7.46%	1.066%
2	5.557	415	420	423	rBV	2338776	2265190	84.32%	12.045%
3	6.557	584	590	593	rBV	2530289	2686482	100.00%	14.285%
4	6.581	593	594	601	rVB	70930	47472	1.77%	0.252%
5	6.939	651	655	658	rBV	935394	724228	26.96%	3.851%
6	7.498	745	750	753	rBV	1837864	1715389	63.85%	9.121%
7	7.663	774	778	783	rVB3	57413	65866	2.45%	0.350%
8	8.116	852	855	863	rBV	26527	36562	1.36%	0.194%
9	8.222	869	873	876	rBV	1203001	979142	36.45%	5.206%
10	9.292	1051	1055	1059	rBV	2760819	2566766	95.54%	13.648%
11	9.374	1065	1069	1071	rBV2	38844	42623	1.59%	0.227%
12	9.404	1071	1074	1078	rVB	121216	106405	3.96%	0.566%
13	9.951	1161	1167	1168	rBV2	50956	61839	2.30%	0.329%
14	9.980	1168	1172	1175	rVB	1187666	1094590	40.74%	5.820%
15	10.763	1302	1305	1309	rBV	1259529	1086592	40.45%	5.778%
16	10.898	1325	1328	1336	rVB	152242	142295	5.30%	0.757%
17	11.345	1400	1404	1411	rVB	175787	178006	6.63%	0.947%
18	11.468	1421	1425	1428	rBV	1347636	1081830	40.27%	5.752%
19	11.851	1486	1490	1493	rVB	37492	29985	1.12%	0.159%
20	12.557	1605	1610	1618	rVB	111382	113403	4.22%	0.603%
21	12.645	1622	1625	1629	rVB	50279	40744	1.52%	0.217%
22	13.057	1690	1695	1698	rBV	2559426	2259813	84.12%	12.016%
23	14.109	1871	1874	1878	rBV	791244	713605	26.56%	3.794%
24	15.621	2125	2131	2145	rBV	439278	566977	21.10%	3.015%

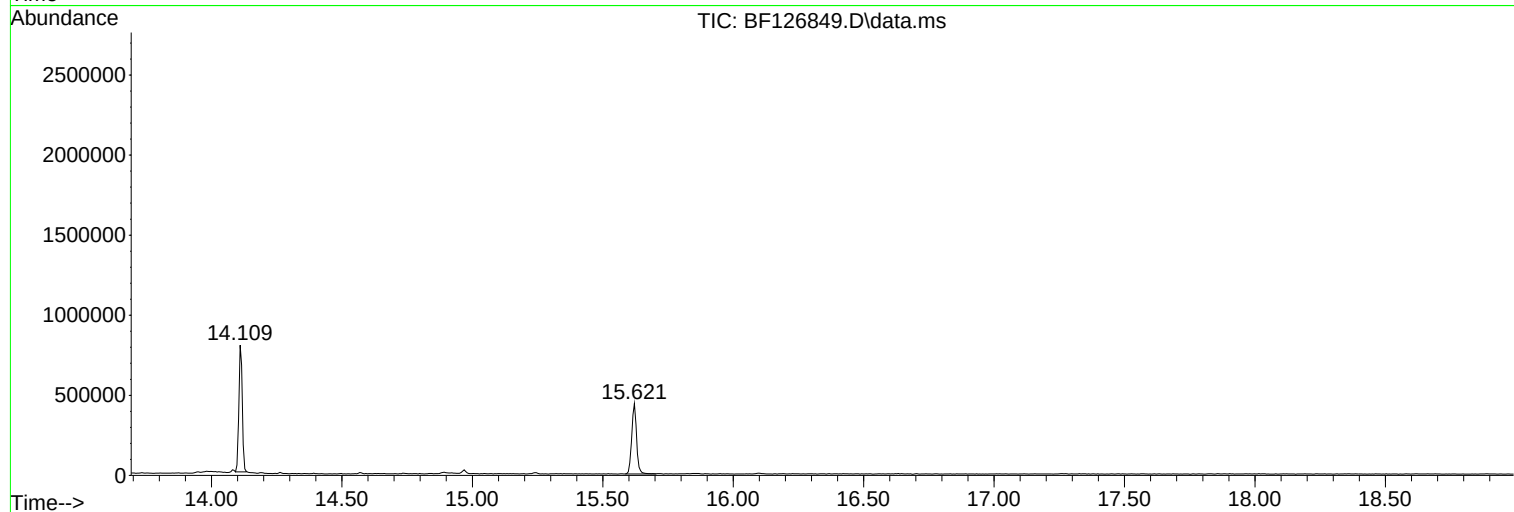
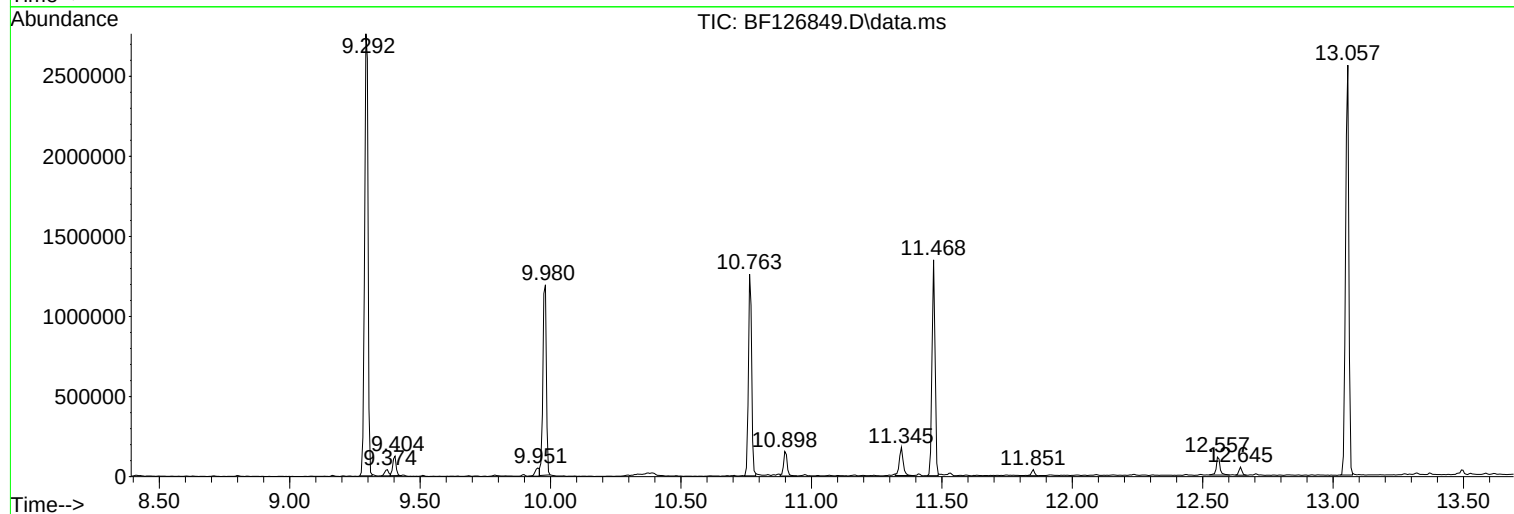
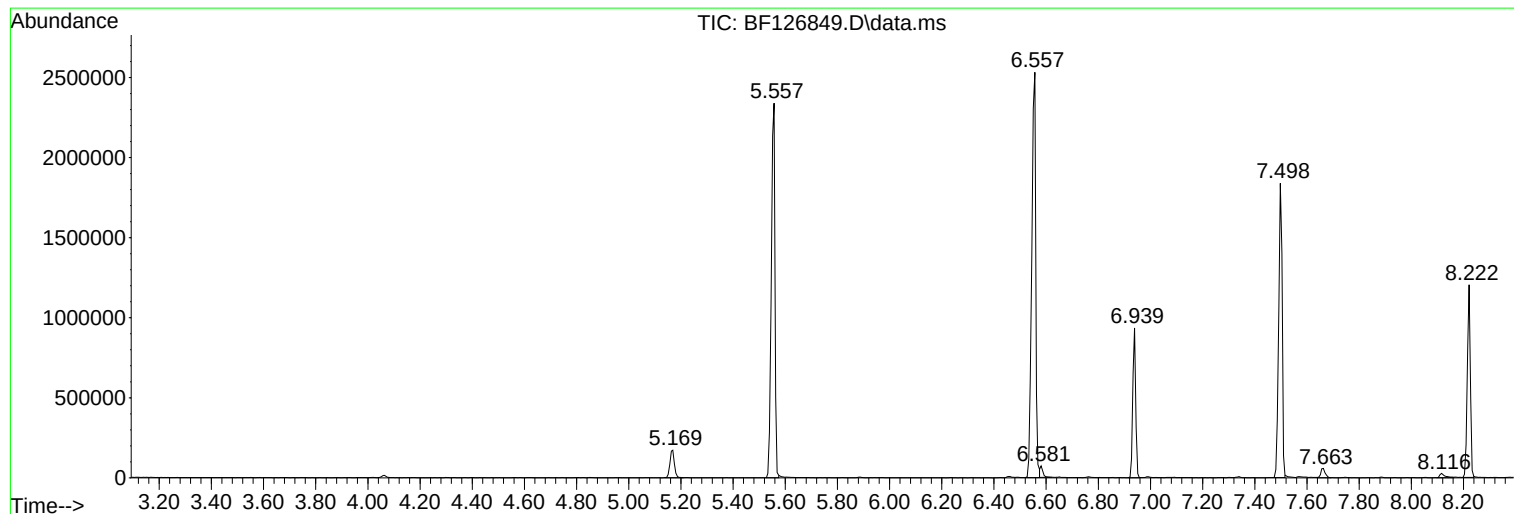
Sum of corrected areas: 18806301

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020922.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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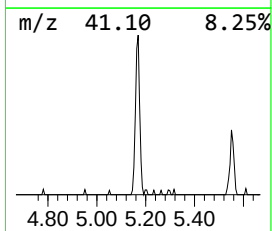
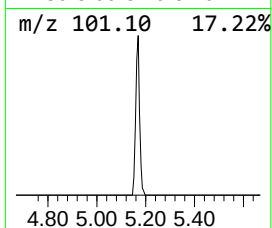
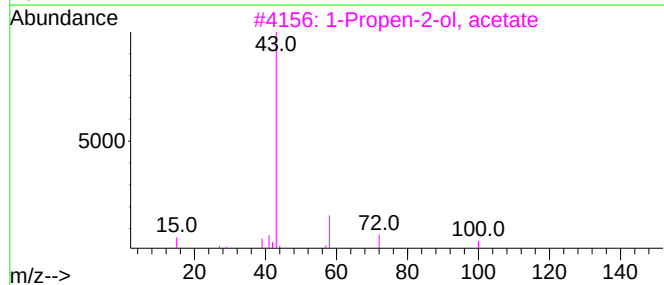
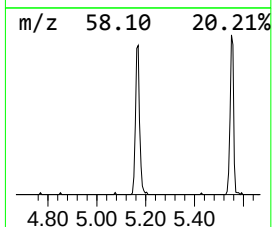
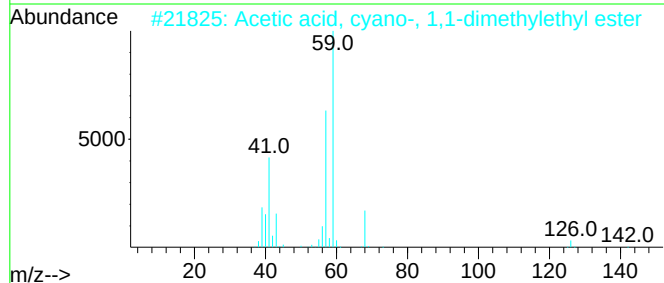
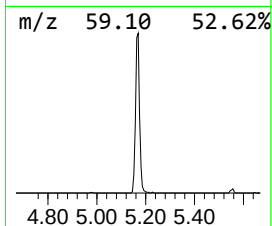
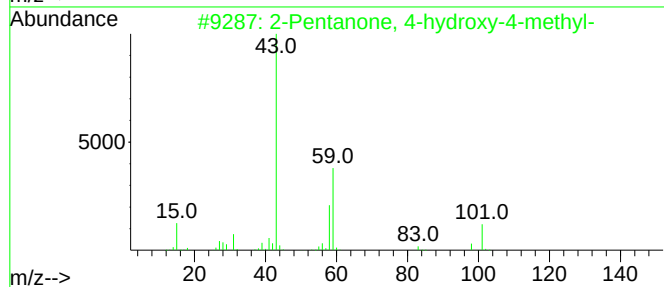
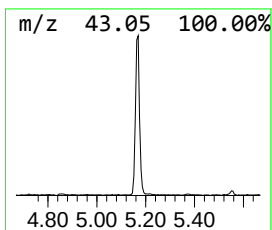
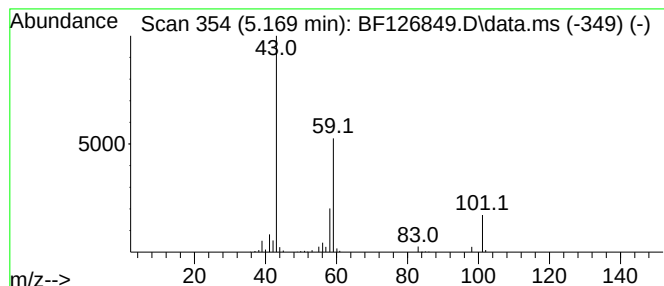
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.169	5.54 ng	200497	1,4-Dichlorobenzene-d4	6.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	78		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	16		
4	Acetone	58	C3H6O	000067-64-1	16		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12		



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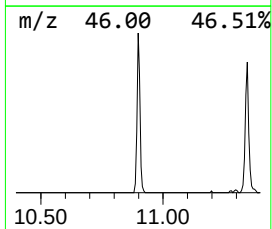
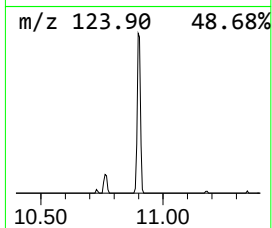
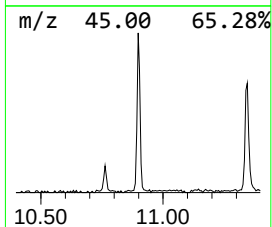
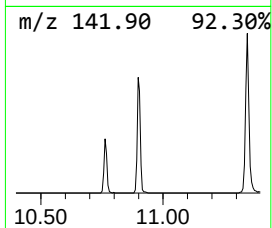
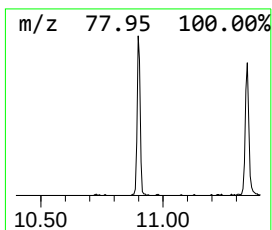
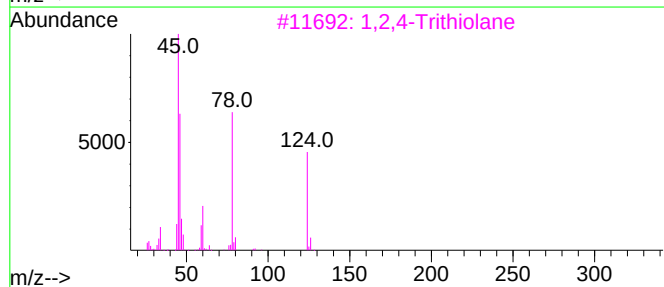
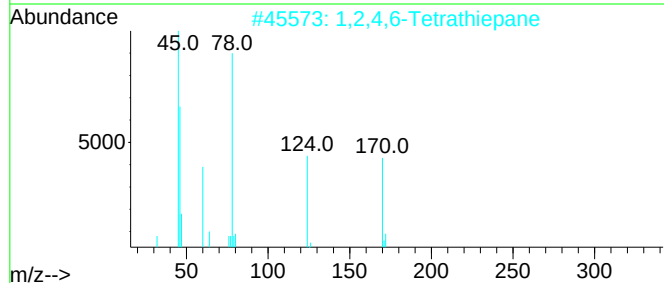
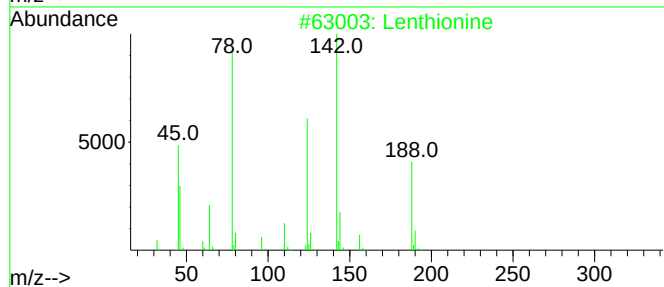
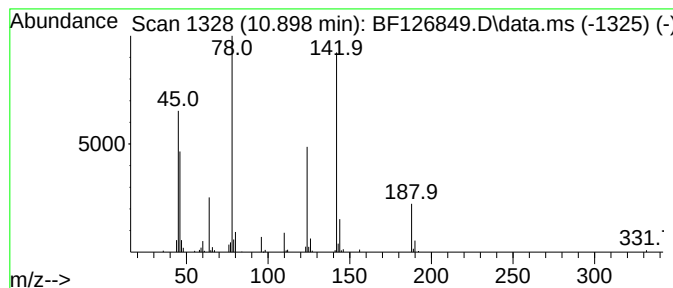
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Lenthionine Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.898	2.63 ng	142295	Phenanthrene-d10	11.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Lenthionine	188	C2H4S5	000292-46-6	94
2			1,2,4,6-Tetrathiepane	170	C3H6S4	000292-45-5	59
3			1,2,4-Trithiolane	124	C2H4S3	000289-16-7	59
4			Hexathiepane	206	CH2S6	017233-71-5	16
5			1,3-Benzenedithiol	142	C6H6S2	000626-04-0	9



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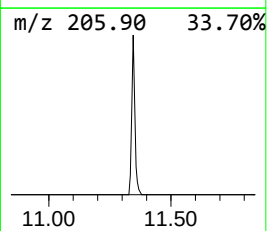
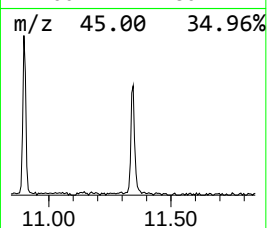
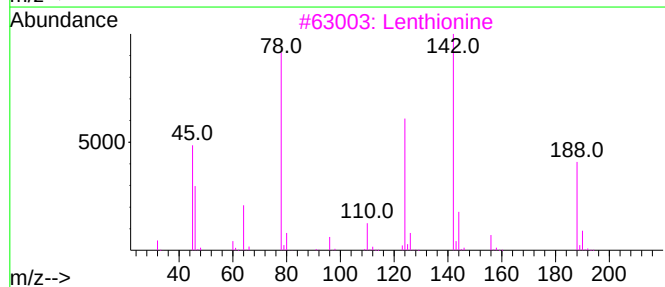
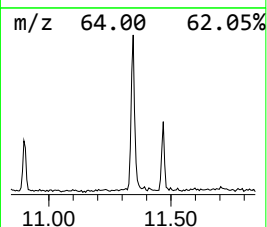
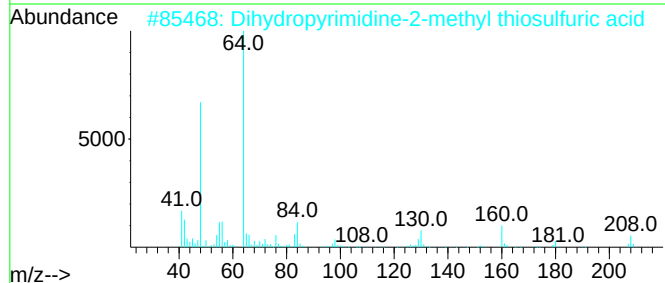
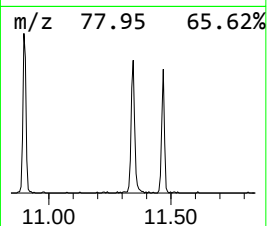
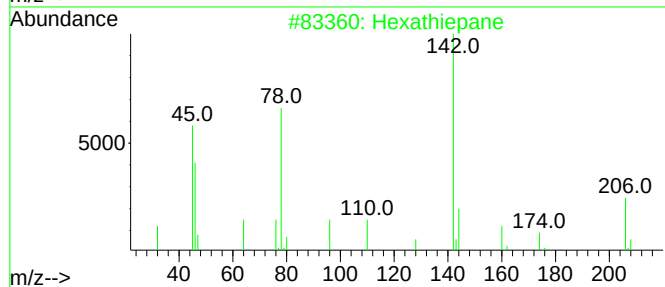
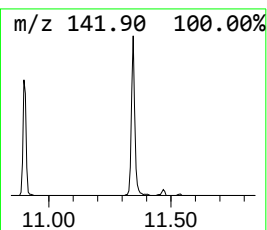
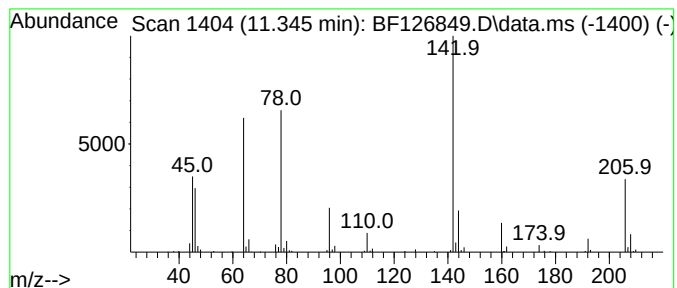
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Peak Number 3 unknown11.345 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.345	3.29 ng	178006	Phenanthrene-d10	11.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexathiepane	206	CH2S6	017233-71-5	38
2			Dihydropyrimidine-2-methyl thios...	208	C5H8N2O3S2	1000256-28-8	17
3			Lenthionine	188	C2H4S5	000292-46-6	14
4			1,3-Benzenedithiol	142	C6H6S2	000626-04-0	9
5			4(1H)-Pyrimidinone, 2-(methylthio)-	142	C5H6N2OS	005751-20-2	9



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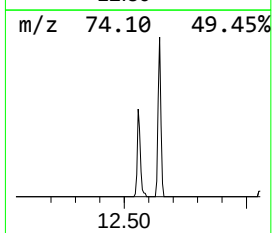
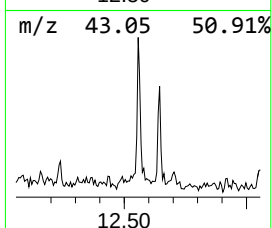
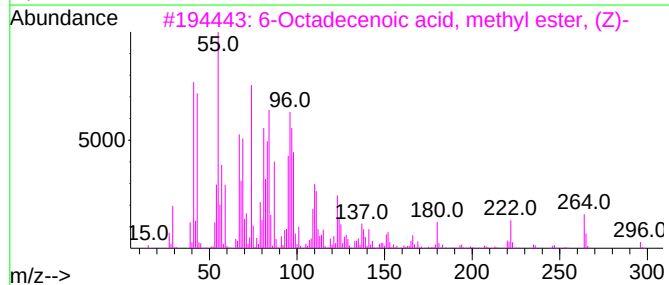
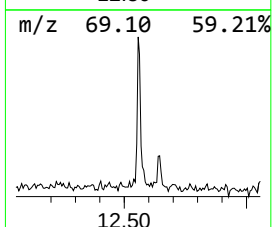
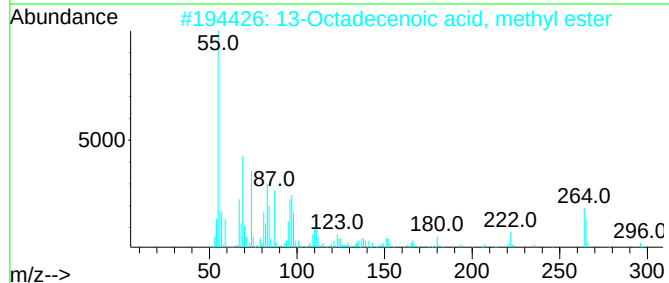
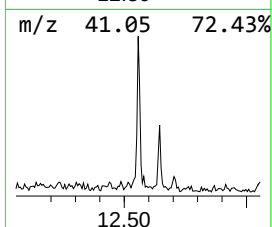
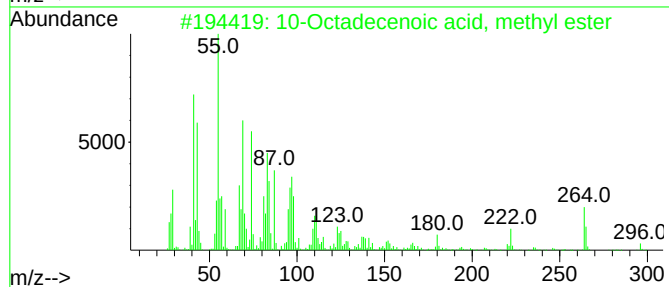
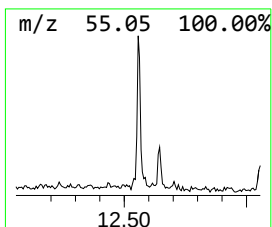
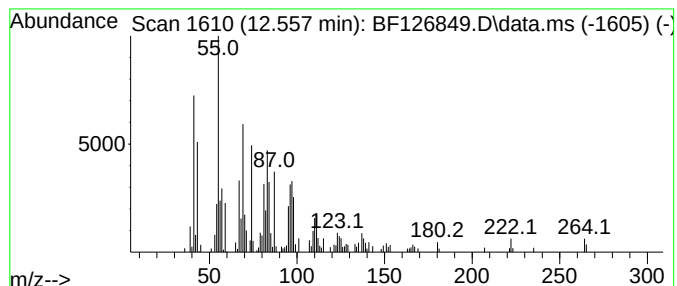
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Peak Number 4 10-Octadecenoic acid, methyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.557	2.10 ng	113403	Phenanthrene-d10	11.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	91
2			13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	90
3			6-Octadecenoic acid, methyl ester...	296	C19H36O2	002777-58-4	87
4			15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	86
5			14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	83



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.169	5.5	ng	200497	1	6.939	724228	20.0
Lenthionine	10.898	2.6	ng	142295	4	11.468	1081830	20.0
unknown11.345	11.345	3.3	ng	178006	4	11.468	1081830	20.0
10-Octadecenoic...	12.557	2.1	ng	113403	4	11.468	1081830	20.0