

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022624\
 Data File : BF137392.D
 Acq On : 26 Feb 2024 18:33
 Operator : CG\JU
 Sample : P1538-11
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20241104-AMENDED-COMPOSITE-35N-N-4-03

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: BF137392.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.063	491	506	509	rBV	7356927	20785728	100.00%	45.256%
2	5.410	562	565	581	rBV	894802	962434	4.63%	2.095%
3	6.416	732	736	750	rBV	2705323	2831955	13.62%	6.166%
4	6.781	795	798	805	rBV	1617283	1332423	6.41%	2.901%
5	7.339	889	893	909	rBV	2657051	2529986	12.17%	5.508%
6	7.498	916	920	925	rBV	1373368	1222216	5.88%	2.661%
7	8.057	1012	1015	1024	rBV	2017217	1773704	8.53%	3.862%
8	9.139	1194	1199	1202	rBV	4636087	4310811	20.74%	9.386%
9	9.816	1310	1314	1317	rVV	2117141	1901147	9.15%	4.139%
10	10.604	1445	1448	1455	rBV	223049	208071	1.00%	0.453%
11	10.728	1466	1469	1478	rVB2	387385	431802	2.08%	0.940%
12	11.175	1541	1545	1548	rBV	324365	343083	1.65%	0.747%
13	11.304	1564	1567	1570	rBV	1779494	1515103	7.29%	3.299%
14	12.904	1835	1839	1843	rBV	3701628	3094239	14.89%	6.737%
15	13.816	1991	1994	2001	rBV2	185024	230834	1.11%	0.503%
16	13.963	2015	2019	2022	rBV	1127450	1212713	5.83%	2.640%
17	15.439	2266	2270	2278	rBV	964153	1242827	5.98%	2.706%

Sum of corrected areas: 45929076

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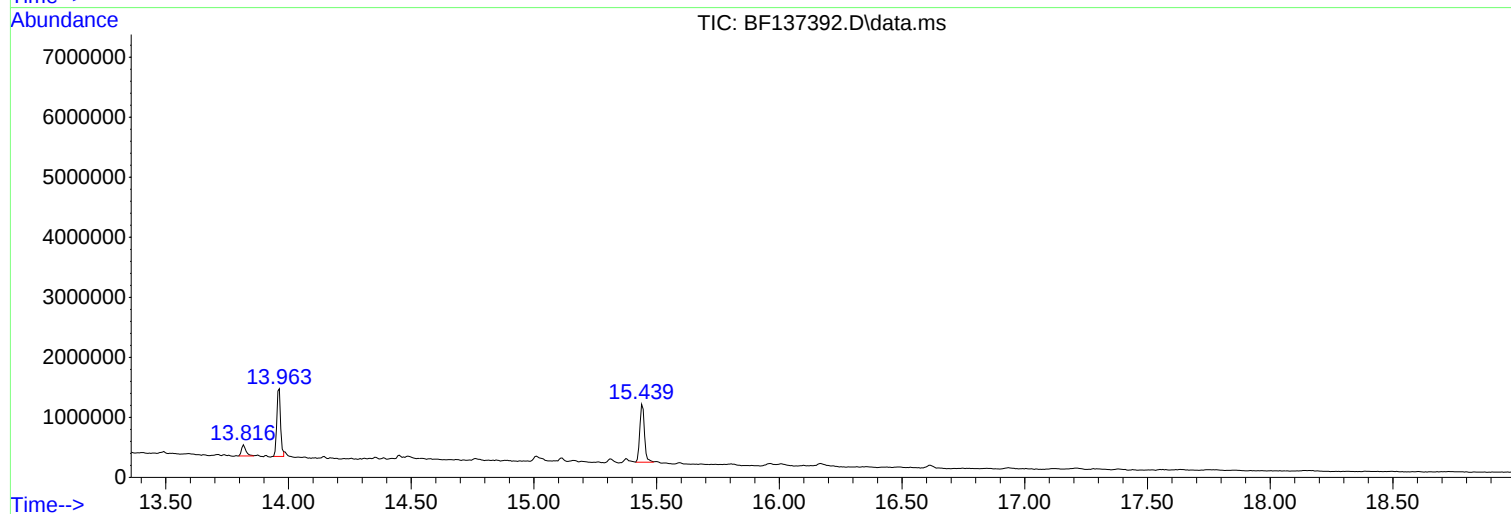
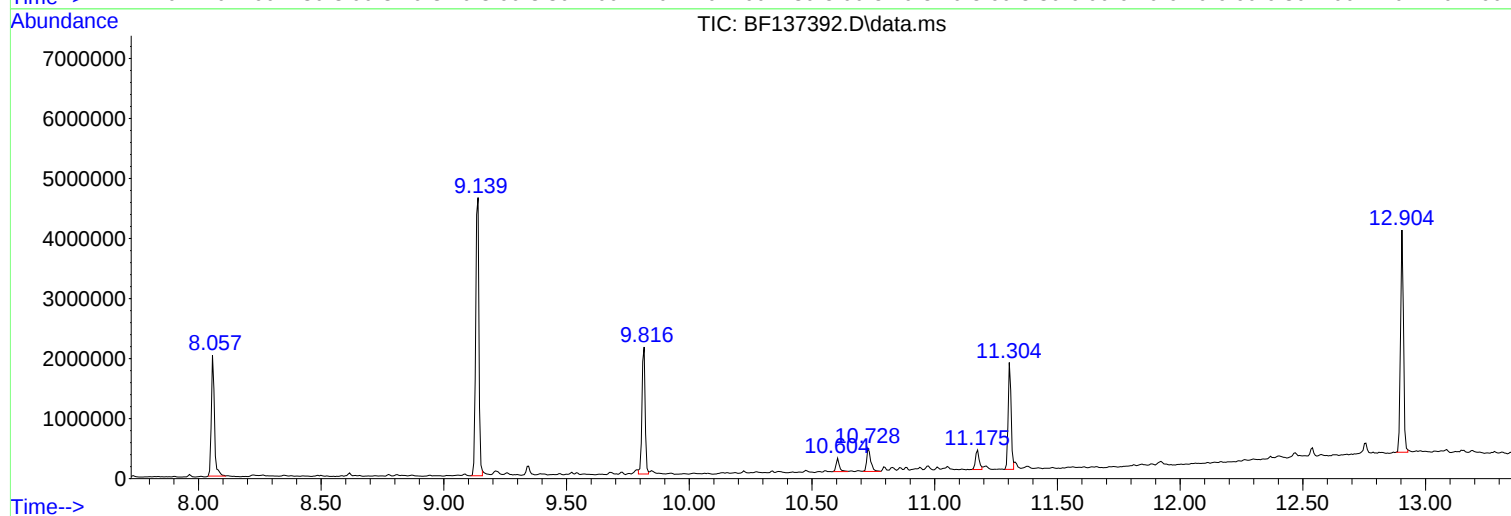
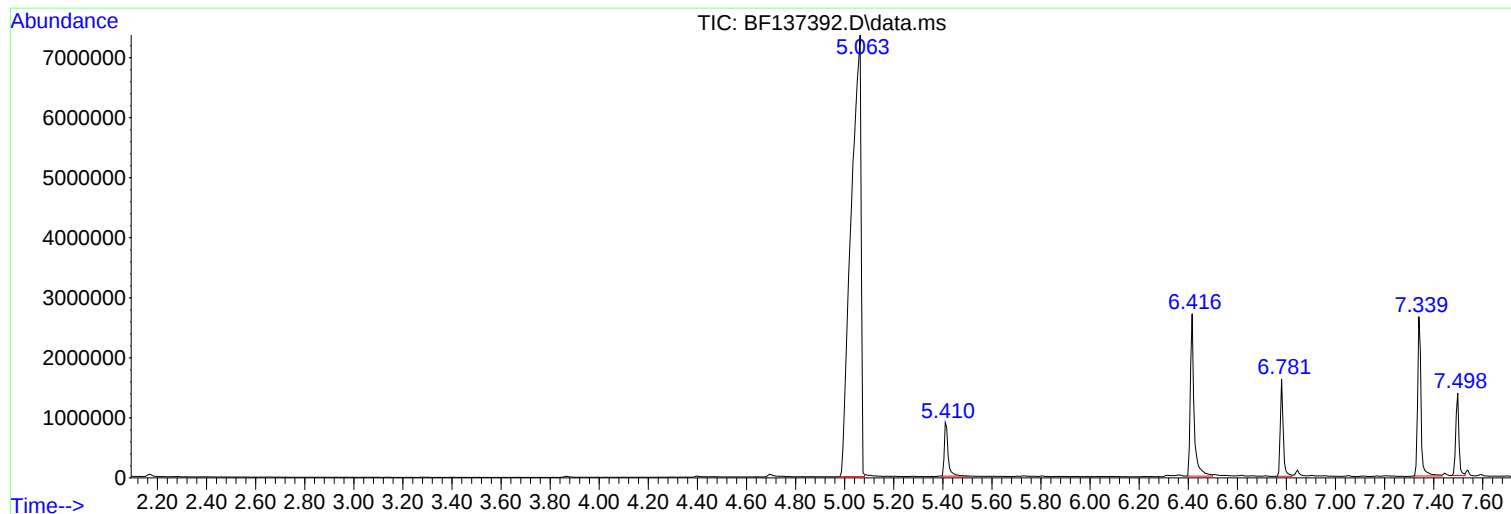
ClientSampleId :

20241104-AMENDED-COMPOSITE-35N-N-4-03

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

Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

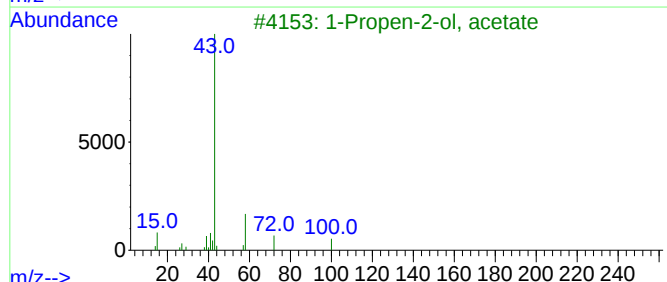
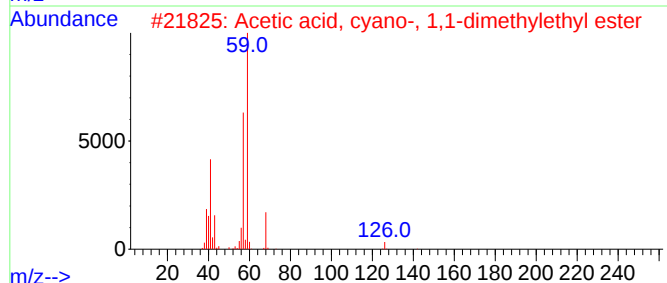
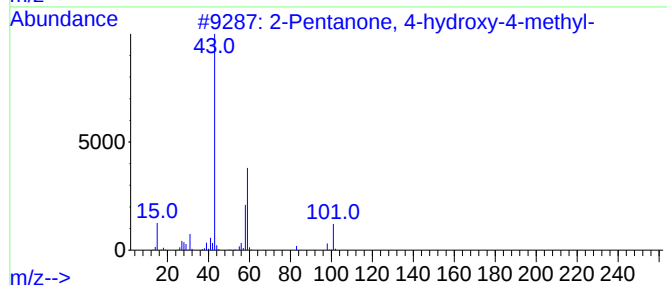
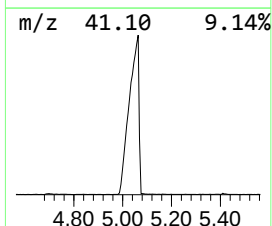
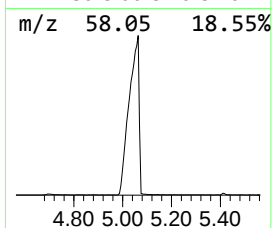
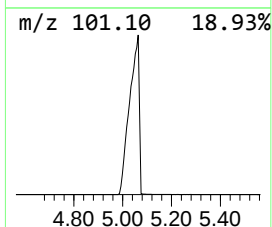
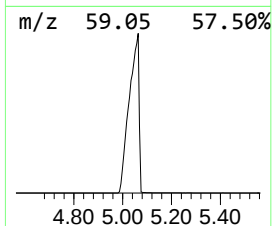
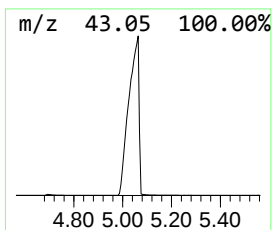
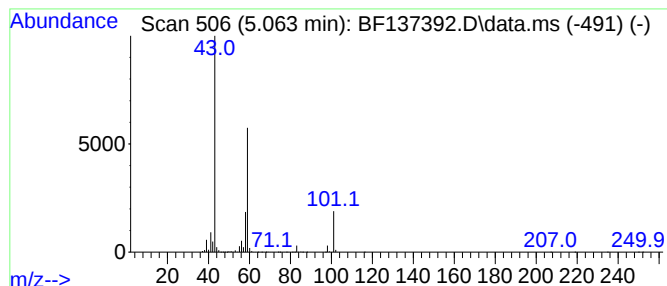
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.063	312.00 ng	20785700	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	32		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	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

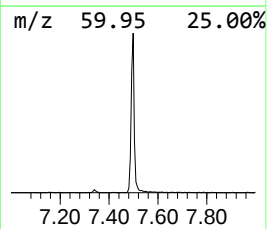
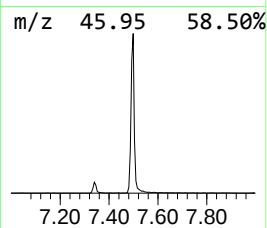
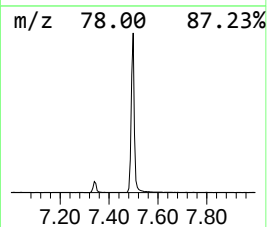
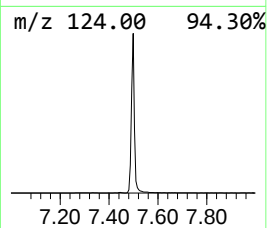
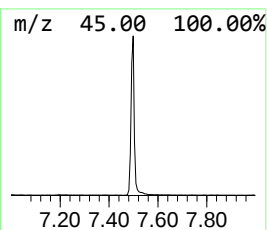
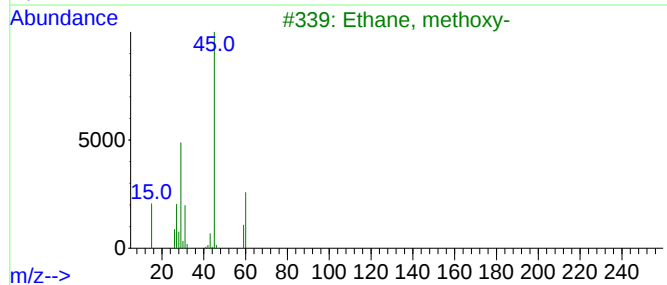
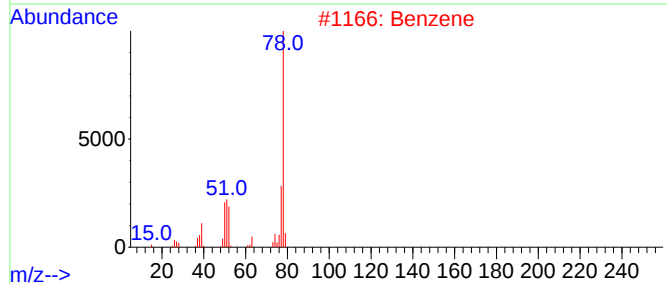
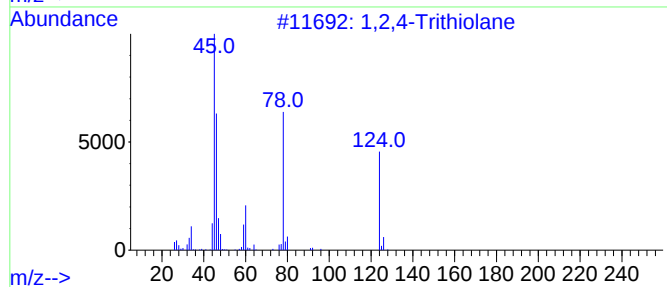
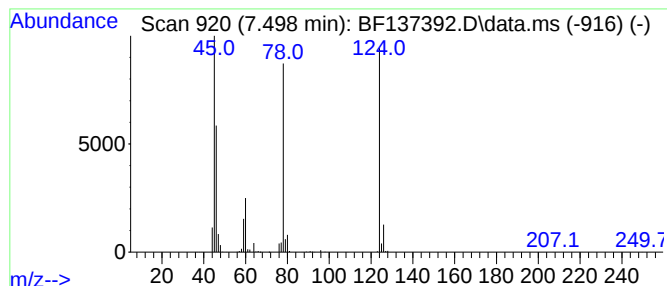
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 2 1,2,4-Trithiolane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.498	13.78 ng	1222220	Naphthalene-d8	8.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2,4-Trithiolane	124	C2H4S3	000289-16-7	94
2			Benzene	78	C6H6	000071-43-2	9
3			Ethane, methoxy-	60	C3H8O	000540-67-0	9
4			1,2-Benzenediol, 3-methyl-	124	C7H8O2	000488-17-5	9
5			Dimethyl ether	46	C2H6O	000115-10-6	9



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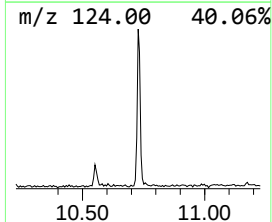
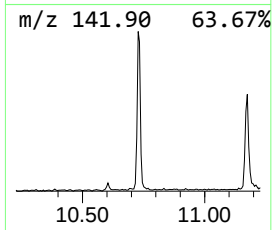
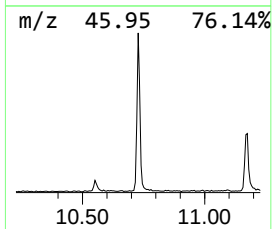
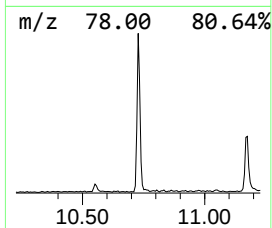
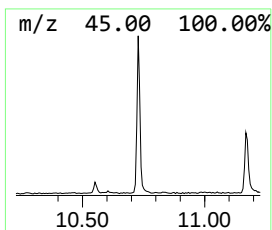
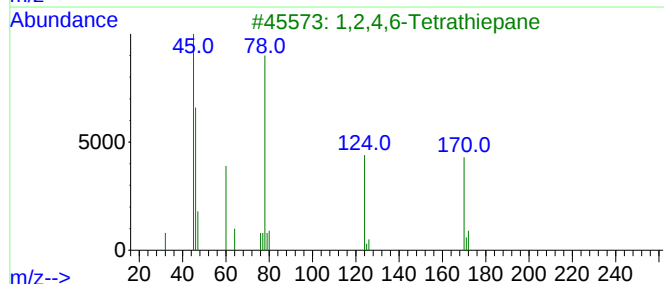
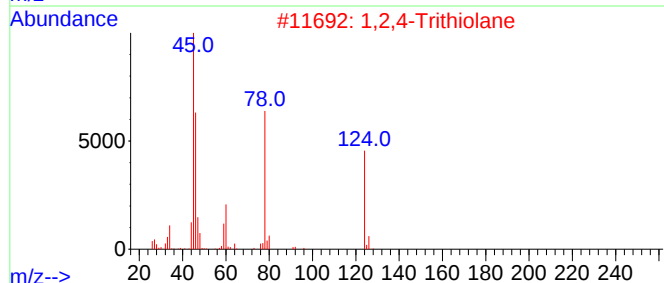
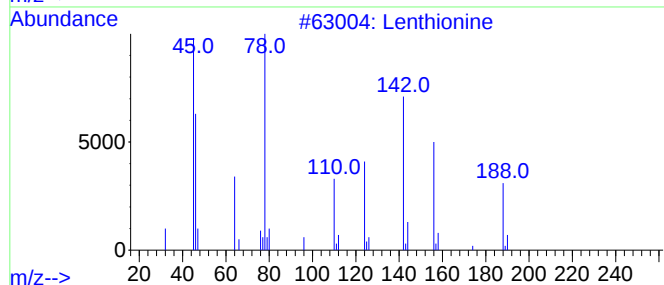
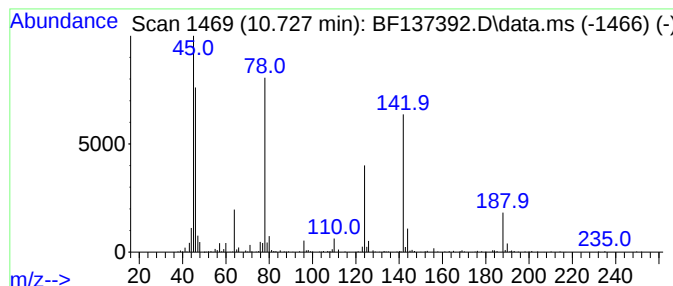
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	5.70 ng	431802	Phenanthrene-d10	11.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Lenthionine	188	C2H4S5	000292-46-6	81
2			1,2,4-Trithiolane	124	C2H4S3	000289-16-7	80
3			1,2,4,6-Tetrathiepane	170	C3H6S4	000292-45-5	50
4			Phosphoramidothioic acid, O,O-di...	141	C2H8N02PS	017321-47-0	33
5			1,2-Benzenedithiol	142	C6H6S2	017534-15-5	9



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Instrument :

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

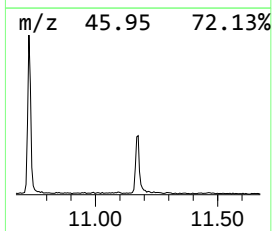
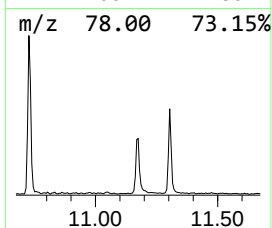
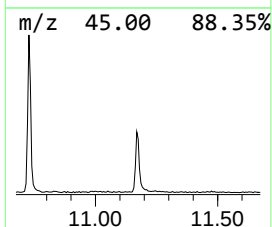
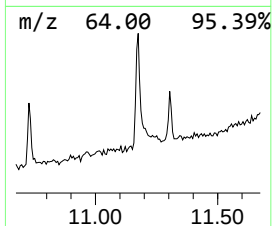
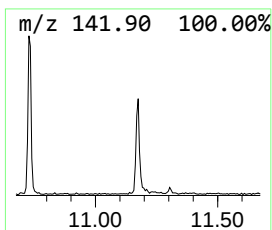
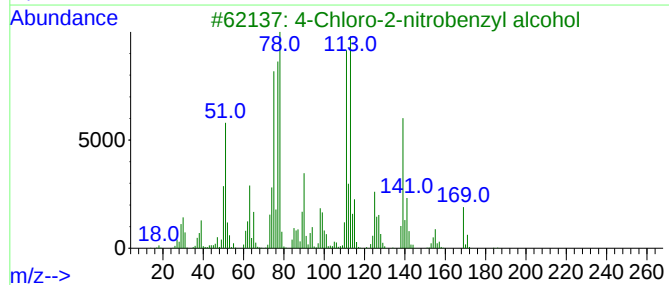
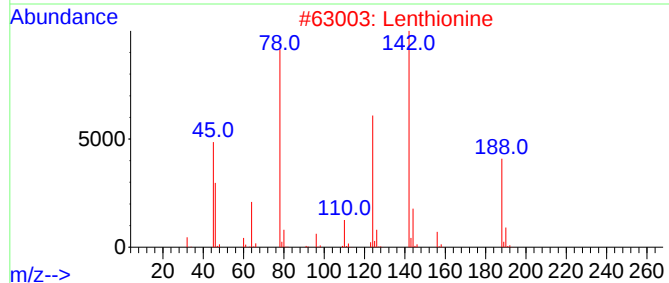
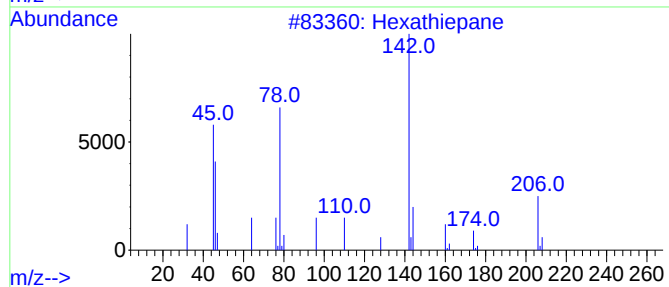
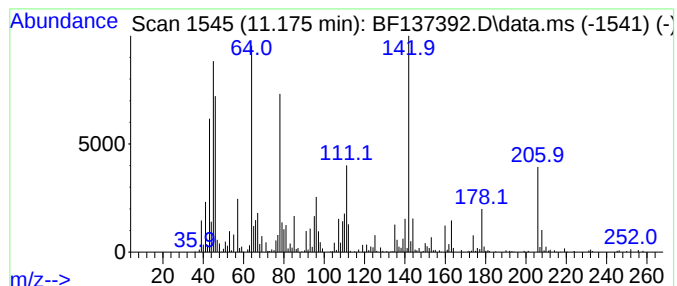
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TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexathiepane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.175	4.53 ng	343083	Phenanthrene-d10	11.304	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexathiepane	206	CH2S6	017233-71-5	78
2	Lenthionine	188	C2H4S5	000292-46-6	25
3	4-Chloro-2-nitrobenzyl alcohol	187	C7H6ClNO3	022996-18-5	22
4	1,2,4-Trithiolane	124	C2H4S3	000289-16-7	17
5	(S)-(-)-2-Chloropropionic acid	108	C3H5ClO2	029617-66-1	16



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

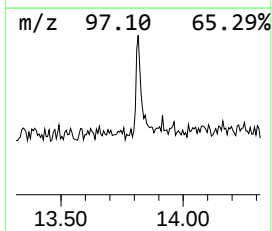
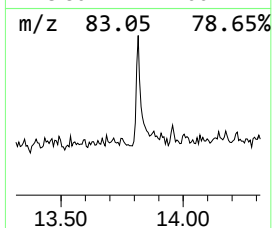
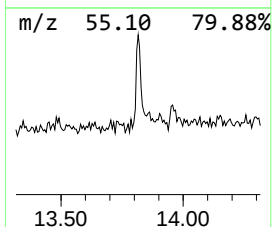
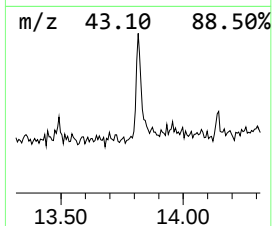
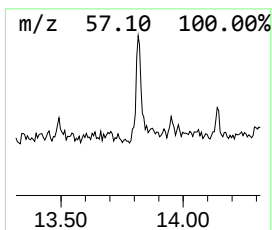
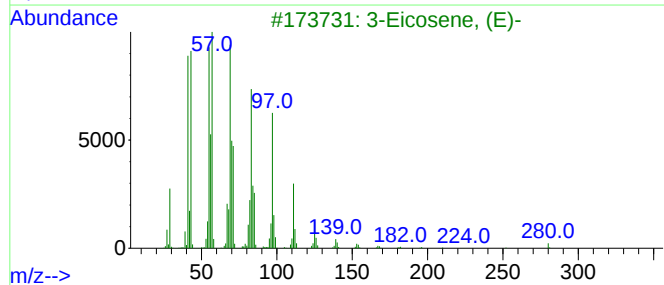
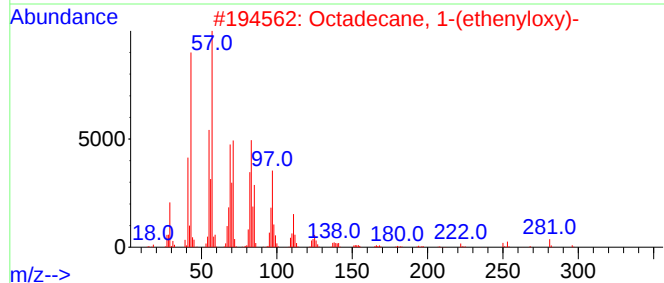
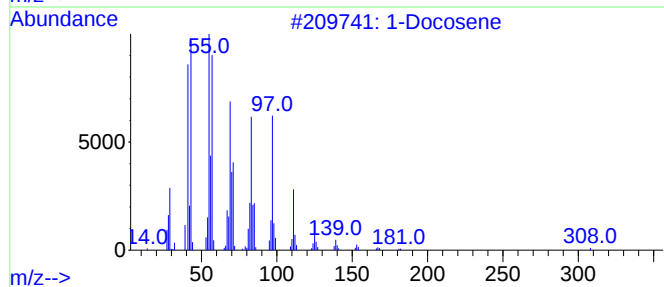
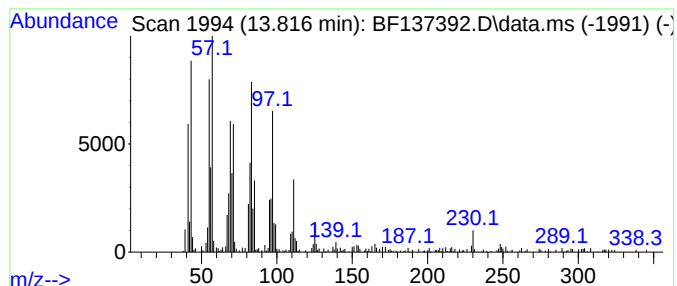
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.816	3.81 ng	230834	Chrysene-d12	13.963	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	93
2	Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	91
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	90
4	Behenic alcohol	326	C22H46O	000661-19-8	90
5	1-Heptacosanol	396	C27H56O	002004-39-9	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.063	312.0	ng	20785700	1	6.781	1332420	20.0
1,2,4-Trithiolane	7.498	13.8	ng	1222220	2	8.057	1773700	20.0
Lenthionine	10.727	5.7	ng	431802	4	11.304	1515100	20.0
Hexathiepane	11.175	4.5	ng	343083	4	11.304	1515100	20.0
1-Docosene	13.816	3.8	ng	230834	5	13.963	1212710	20.0