

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022624\
Data File : BF137390.D
Acq On : 26 Feb 2024 17:35
Operator : CG\JU
Sample : P1538-09
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20241102-AMENDED-COMPOSITE-35N-N-4-01

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: BF137390.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.034	491	501	504	rBV	5001668	8675415	100.00%	22.882%
2	5.410	562	565	582	rBV	2507153	2554879	29.45%	6.739%
3	6.416	732	736	750	rBV	3320064	3445651	39.72%	9.088%
4	6.781	795	798	806	rBV	1393843	1202709	13.86%	3.172%
5	7.340	889	893	909	rBV	2388245	2275755	26.23%	6.002%
6	7.498	916	920	925	rBV	1335493	1275380	14.70%	3.364%
7	8.057	1012	1015	1036	rVB	1794526	1689076	19.47%	4.455%
8	9.139	1195	1199	1202	rBV	4600565	4145423	47.78%	10.934%
9	9.345	1230	1234	1239	rBV2	104505	111418	1.28%	0.294%
10	9.781	1305	1308	1310	rBV	79314	101399	1.17%	0.267%
11	9.816	1310	1314	1317	rVV	2095284	1820631	20.99%	4.802%
12	9.845	1317	1319	1329	rVB	74867	91677	1.06%	0.242%
13	10.604	1444	1448	1455	rBV	1129653	1024600	11.81%	2.702%
14	10.728	1466	1469	1476	rVB	382862	387736	4.47%	1.023%
15	11.175	1541	1545	1549	rBV	360965	386666	4.46%	1.020%
16	11.304	1564	1567	1570	rBV	1677886	1518369	17.50%	4.005%
17	11.328	1570	1571	1576	rVV	408621	322739	3.72%	0.851%
18	11.380	1577	1580	1584	rVB	110727	118312	1.36%	0.312%
19	11.845	1656	1659	1664	rVB2	112611	127432	1.47%	0.336%
20	11.922	1669	1672	1675	rBV2	111968	120656	1.39%	0.318%
21	12.527	1773	1775	1779	rBV	304478	264782	3.05%	0.698%
22	12.751	1809	1813	1817	rBV	341381	351141	4.05%	0.926%
23	12.904	1835	1839	1847	rBV	3500378	3052992	35.19%	8.052%
24	13.821	1991	1995	2002	rBV2	127808	188549	2.17%	0.497%
25	13.963	2014	2019	2022	rBV2	1001709	1141194	13.15%	3.010%
26	15.010	2193	2197	2206	rVB2	104664	209463	2.41%	0.552%
27	15.310	2246	2248	2255	rVB	72982	89222	1.03%	0.235%
28	15.374	2256	2259	2265	rBV	93998	126025	1.45%	0.332%
29	15.439	2266	2270	2279	rVV	871280	1095206	12.62%	2.889%

Sum of corrected areas: 37914497

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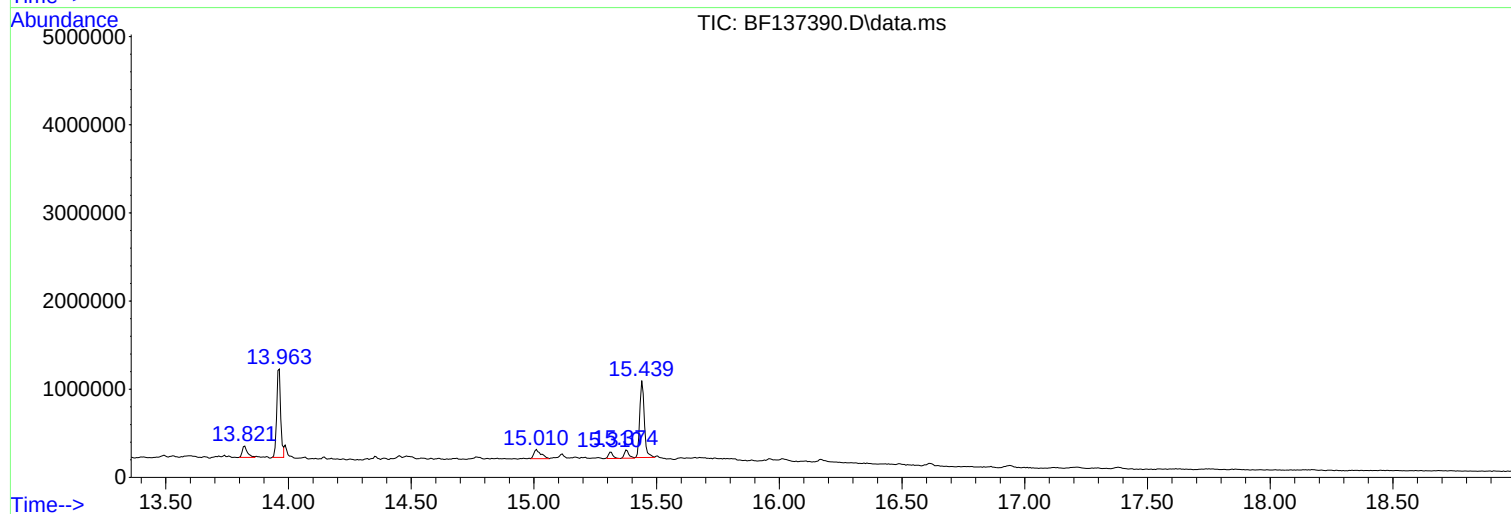
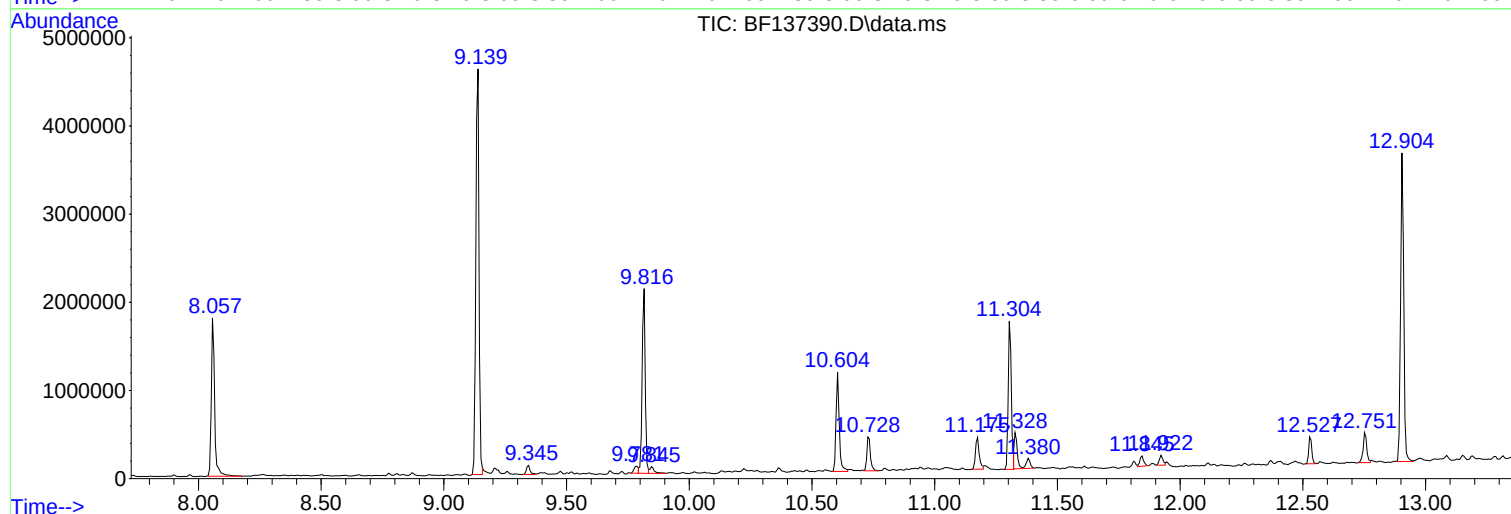
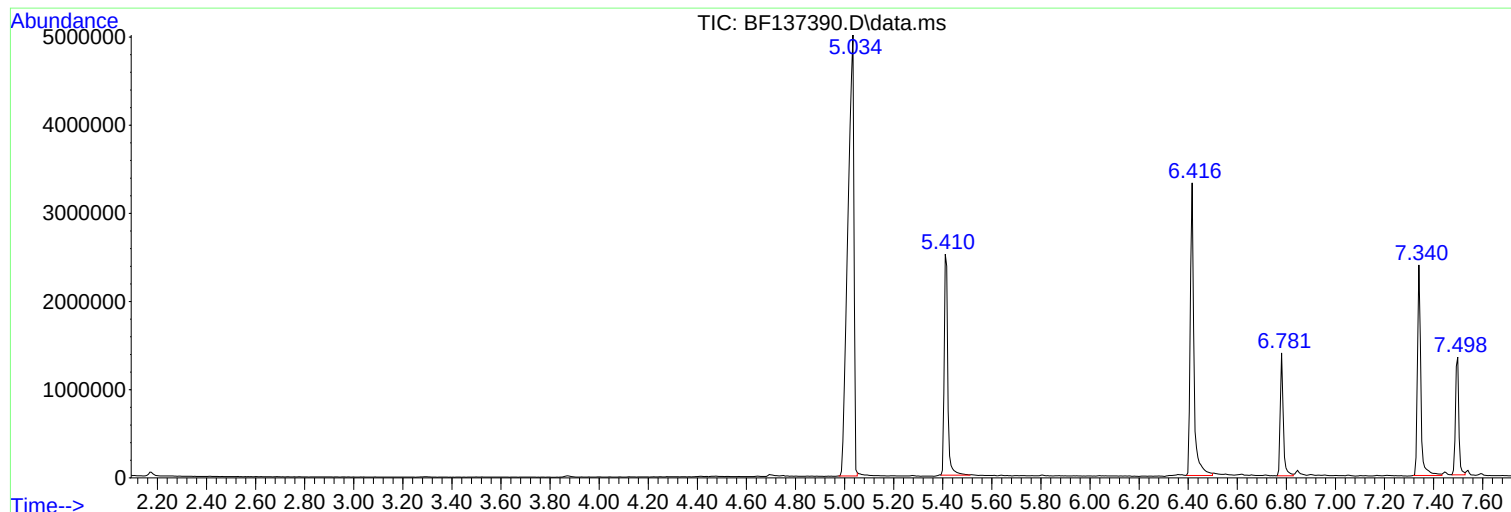
ClientSampleId :

20241102-AMENDED-COMPOSITE-35N-N-4-01

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

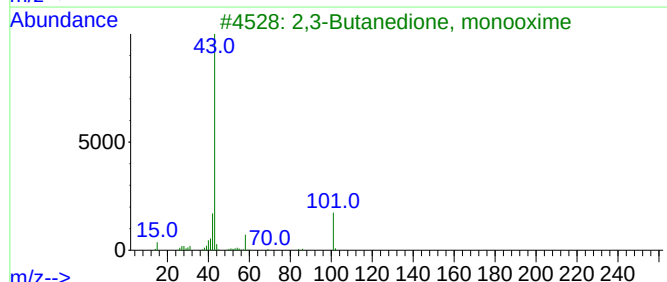
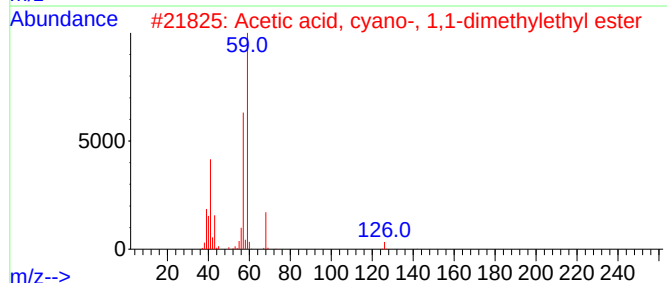
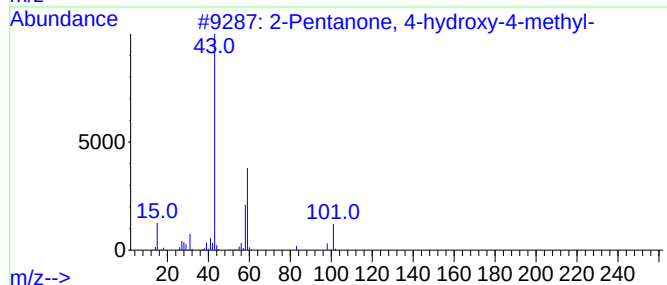
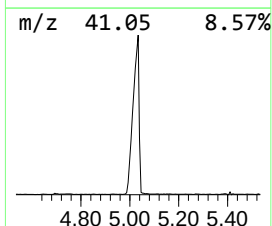
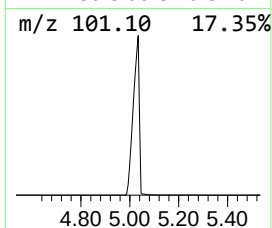
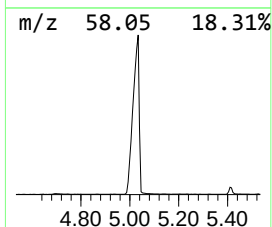
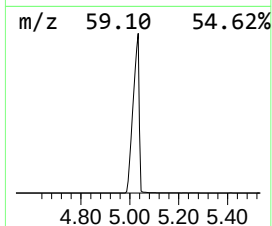
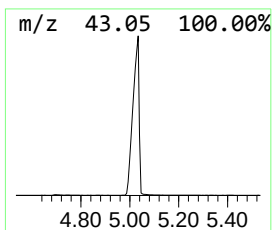
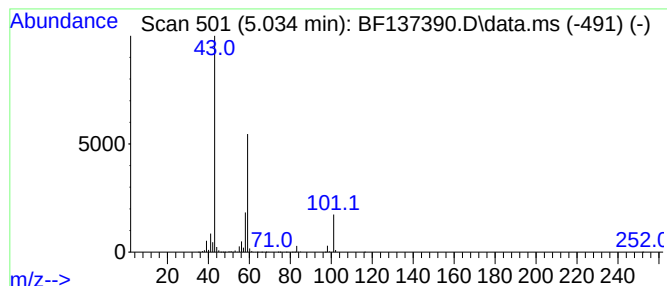
TIC Library : C:\Database\NIST20.L

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.
5.034	144.26 ng	8675420	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	25
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			5-Hexen-2-one	98	C6H10O	000109-49-9	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

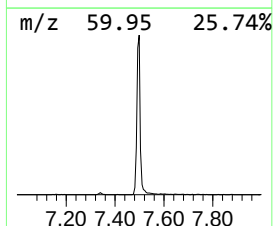
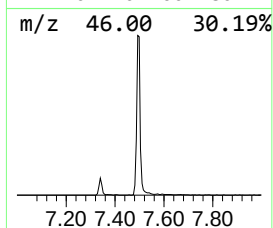
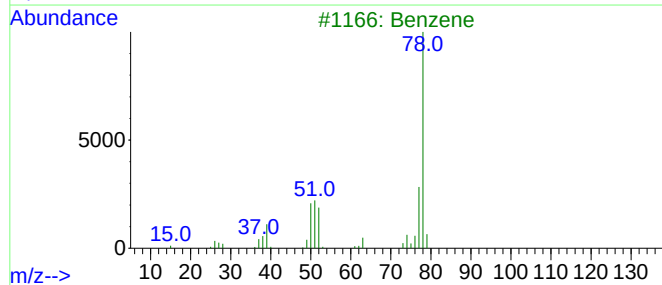
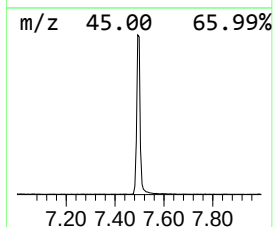
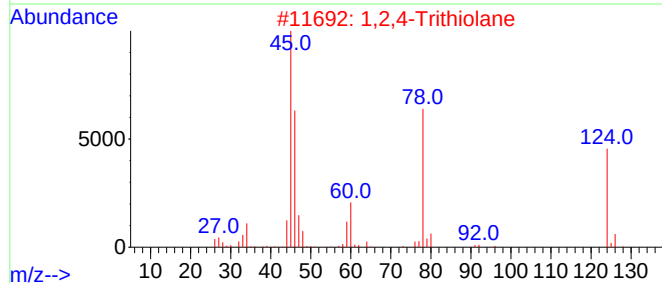
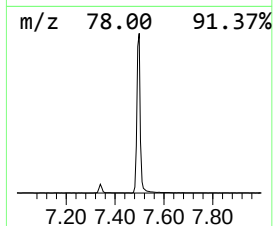
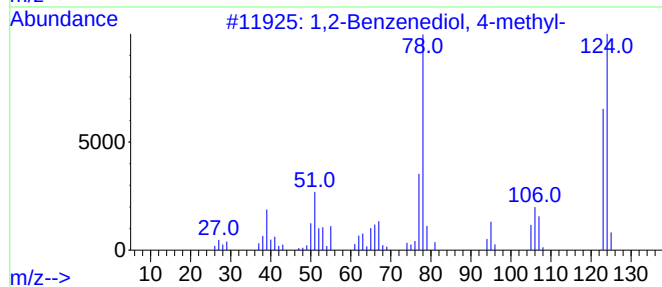
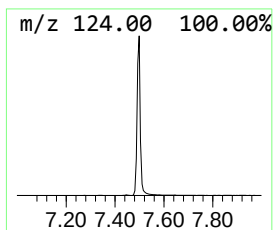
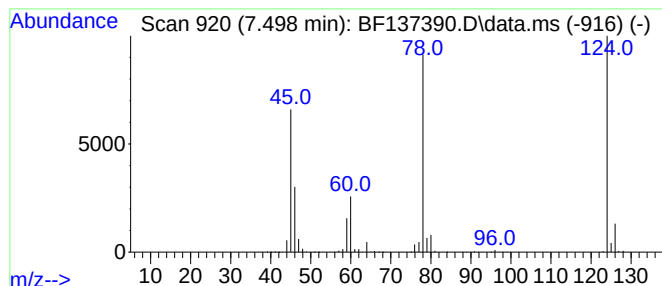
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.498

Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.498	15.10 ng	1275380	Naphthalene-d8	8.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Benzenediol, 4-methyl-	124	C7H8O2	000452-86-8	45
2			1,2,4-Trithiolane	124	C2H4S3	000289-16-7	39
3			Benzene	78	C6H6	000071-43-2	9
4			Fumaronitrile	78	C4H2N2	000764-42-1	9
5			Propanedinitrile, methylene-	78	C4H2N2	000922-64-5	7



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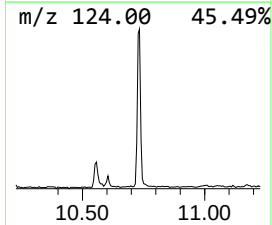
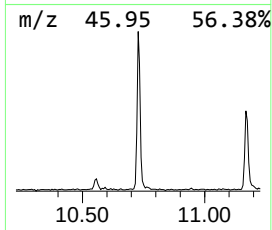
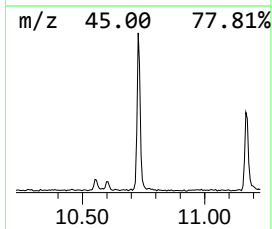
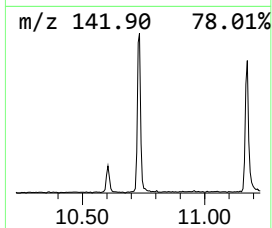
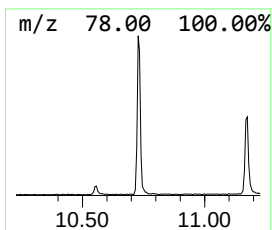
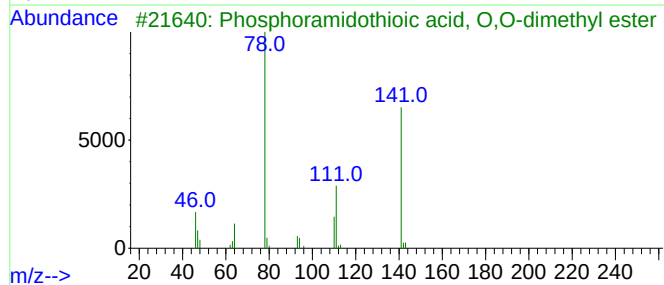
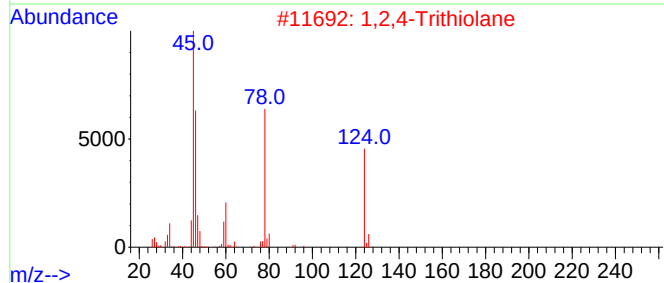
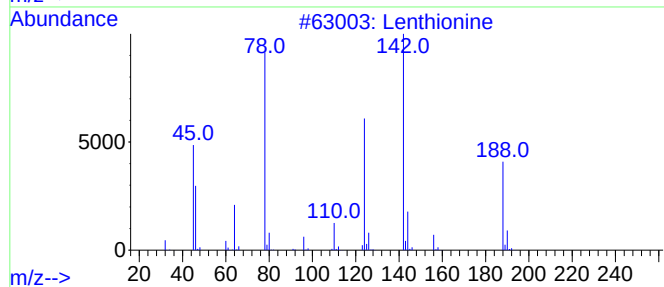
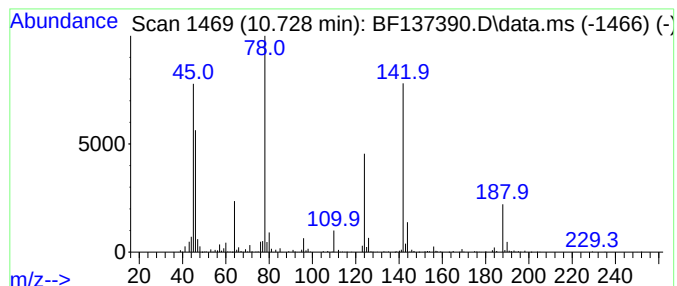
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 3 Lenthionine Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.728	5.11 ng	387736	Phenanthrene-d10	11.304	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Lenthionine	188	C2H4S5	000292-46-6	94
2	1,2,4-Trithiolane	124	C2H4S3	000289-16-7	59
3	Phosphoramidothioic acid, O,O-di...	141	C2H8N02PS	017321-47-0	38
4	Phenylphosphonous acid	142	C6H7O2P	001779-48-2	28
5	4-Chloro-2-nitrobenzyl alcohol	187	C7H6ClNO3	022996-18-5	23



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

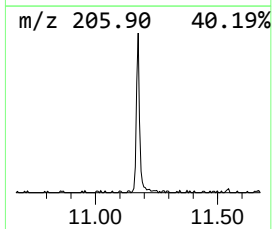
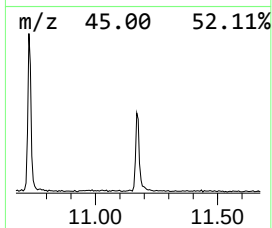
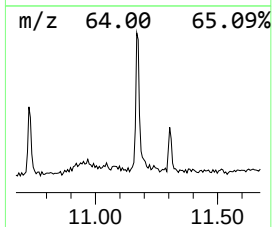
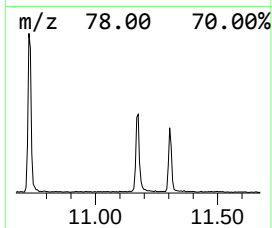
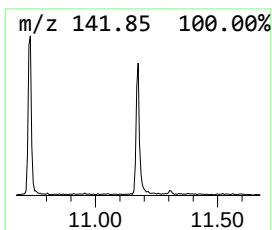
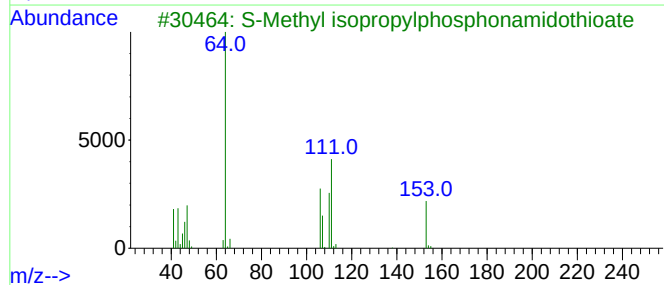
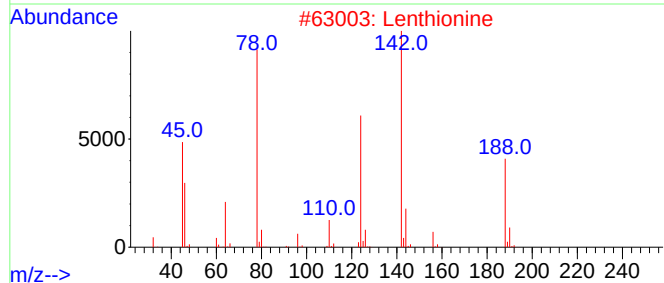
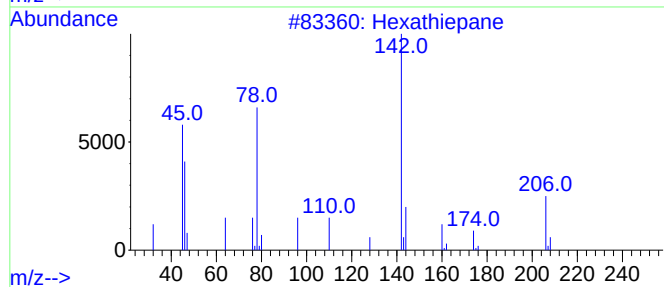
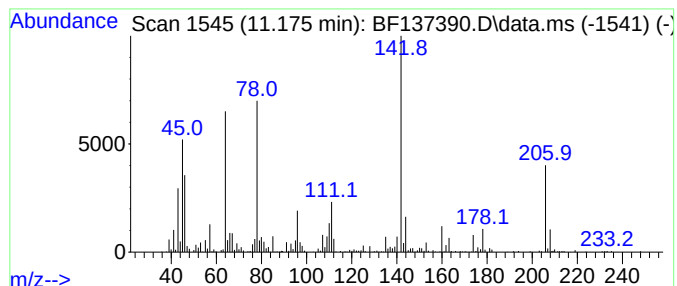
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown11.175 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.175	5.09 ng	386666	Phenanthrene-d10	11.304	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexathiepane	206	CH2S6	017233-71-5	43
2	Lenthionine	188	C2H4S5	000292-46-6	22
3	S-Methyl isopropylphosphonamidot...	153	C4H12NOPS	1000306-04-4	12
4	Dihydropyrimidine-2-methyl thios...	208	C5H8N2O3S2	1000256-28-8	12
5	N-[2,3-Difluoro-2,3-di-(difluoro...	277	C3F9N5	1000305-83-6	12



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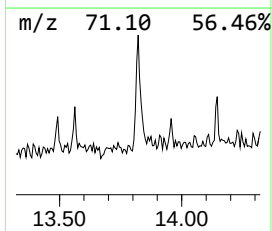
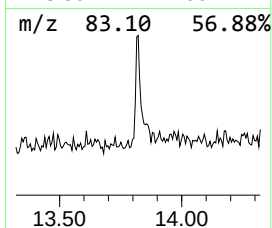
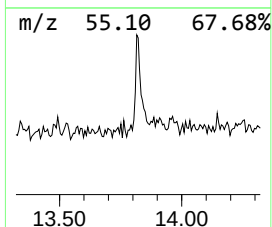
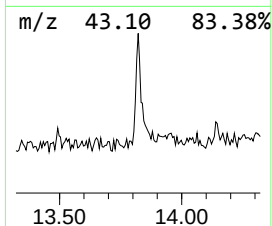
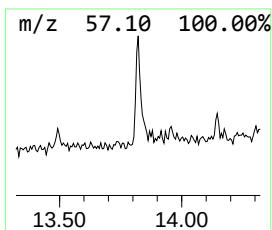
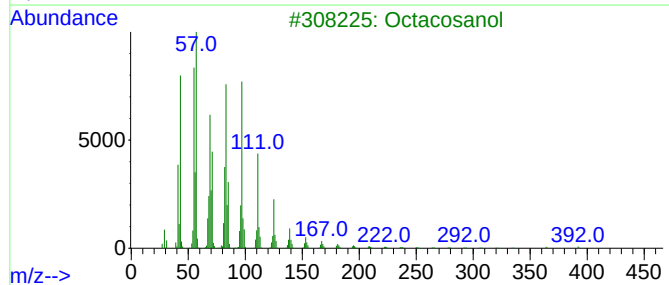
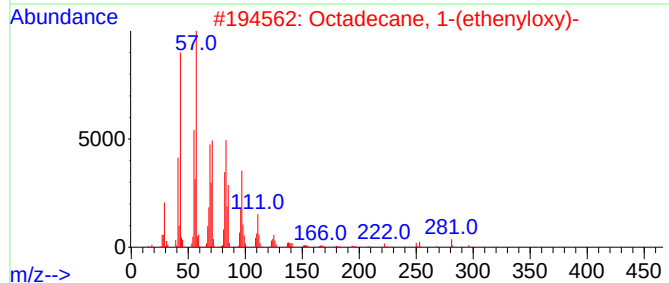
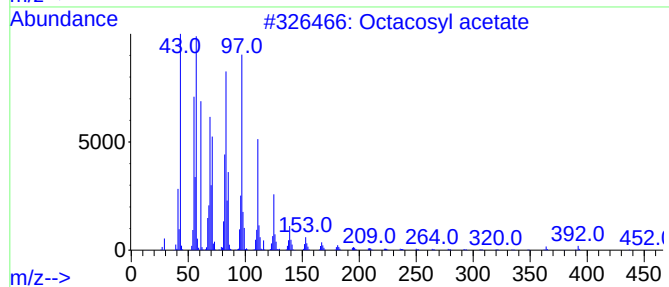
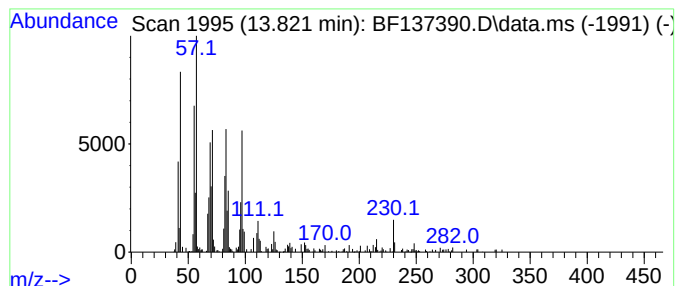
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 5 Octacosyl acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.822	3.30 ng	188549	Chrysene-d12	13.963	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl acetate	452	C30H60O2	018206-97-8	81
2	Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	74
3	Octacosanol	410	C28H58O	000557-61-9	68
4	1-Hexacosanol	382	C26H54O	000506-52-5	68
5	Behenic alcohol	326	C22H46O	000661-19-8	62



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.034	144.3	ng	8675420	1	6.781	1202710	20.0
unknown7.498	7.498	15.1	ng	1275380	2	8.057	1689080	20.0
Lenthionine	10.728	5.1	ng	387736	4	11.304	1518370	20.0
unknown11.175	11.175	5.1	ng	386666	4	11.304	1518370	20.0
Octacosyl acetate	13.822	3.3	ng	188549	5	13.963	1141190	20.0