

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060322\
 Data File : BF128680.D
 Acq On : 03 Jun 2022 15:17
 Operator : CG\JU
 Sample : N3143-04
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20220427-AMENDED-SB-8-(DISCRETE-COMP-G)

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-BF060222.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128680.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.057	462	471	474	rVB	1890150	3304471	100.00%	17.209%
2	5.481	540	543	549	rBV	426925	402538	12.18%	2.096%
3	6.357	687	692	700	rBV	27984	47997	1.45%	0.250%
4	6.486	710	714	724	rVB	1977567	1930775	58.43%	10.055%
5	6.563	724	727	730	rBV	63999	43081	1.30%	0.224%
6	6.822	767	771	774	rBV	682964	517691	15.67%	2.696%
7	7.386	861	867	870	rBV	1782973	1965429	59.48%	10.235%
8	7.539	889	893	896	rBV	266537	210671	6.38%	1.097%
9	8.104	985	989	992	rBV	771679	638272	19.32%	3.324%
10	8.175	997	1001	1011	rBV	33851	52857	1.60%	0.275%
11	9.186	1167	1173	1176	rBV	3788072	3168740	95.89%	16.502%
12	9.251	1181	1184	1189	rVV2	151624	150436	4.55%	0.783%
13	9.833	1278	1283	1285	rBV2	114395	166114	5.03%	0.865%
14	9.863	1285	1288	1291	rVB	786127	679081	20.55%	3.536%
15	10.374	1371	1375	1384	rVB	153203	155717	4.71%	0.811%
16	10.651	1406	1422	1429	rBV	504564	732286	22.16%	3.814%
17	10.774	1437	1443	1450	rVB	415223	379996	11.50%	1.979%
18	11.221	1514	1519	1528	rVB	359503	412031	12.47%	2.146%
19	11.345	1537	1540	1543	rBV	622002	574946	17.40%	2.994%
20	11.880	1627	1631	1636	rBV3	37687	42152	1.28%	0.220%
21	12.563	1744	1747	1751	rVB	42152	36337	1.10%	0.189%
22	12.792	1783	1786	1788	rVB	51219	37095	1.12%	0.193%
23	12.939	1807	1811	1814	rBV	2607044	2187210	66.19%	11.390%
24	13.992	1985	1990	1993	rBV	552286	516924	15.64%	2.692%
25	14.086	2001	2006	2012	rBV	230399	258423	7.82%	1.346%
26	15.027	2163	2166	2170	rBV2	29131	39663	1.20%	0.207%
27	15.327	2214	2217	2223	rVB2	30089	41845	1.27%	0.218%
28	15.386	2224	2227	2231	rBV	31563	37816	1.14%	0.197%
29	15.457	2234	2239	2243	rBV	387222	471762	14.28%	2.457%

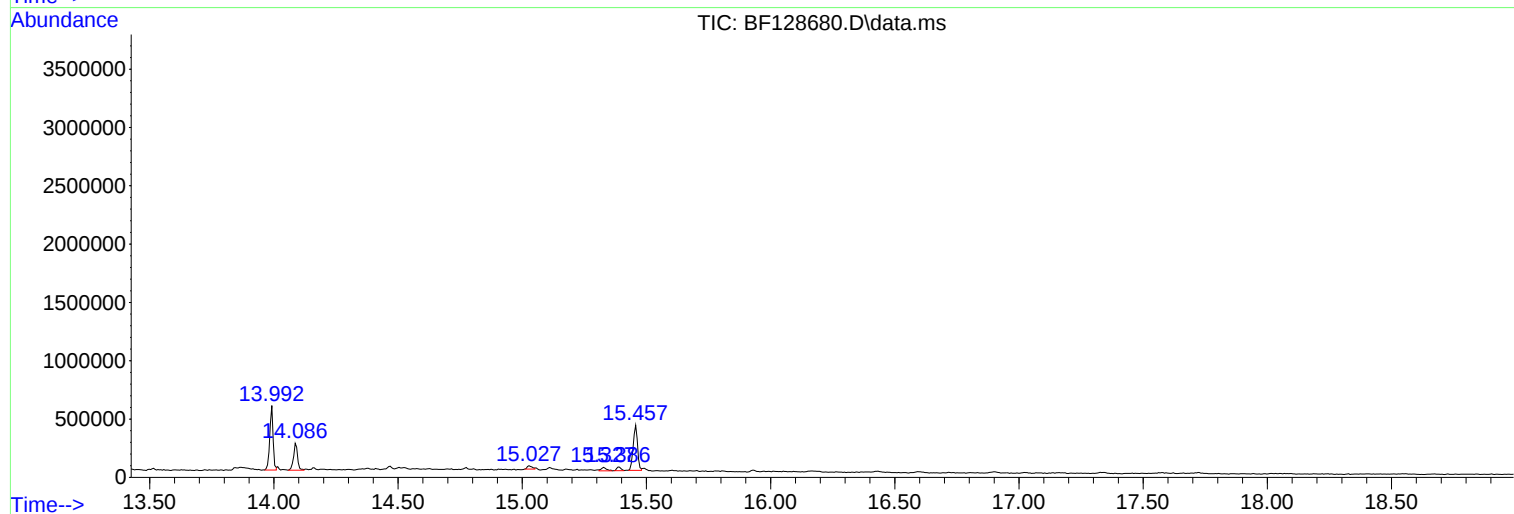
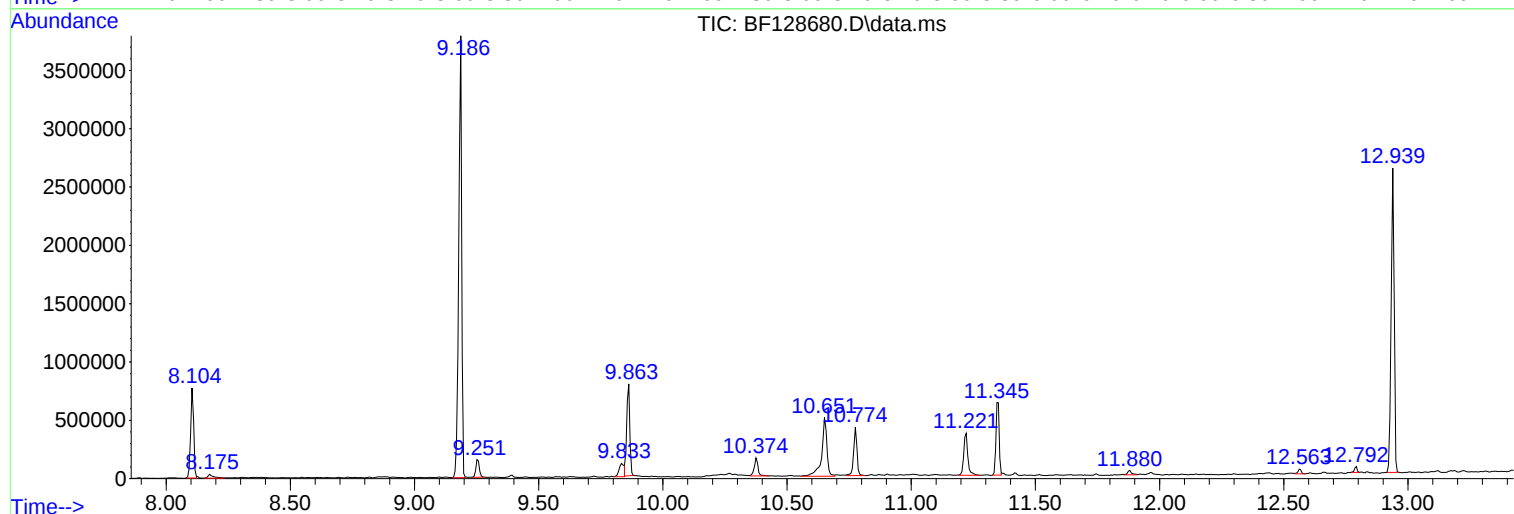
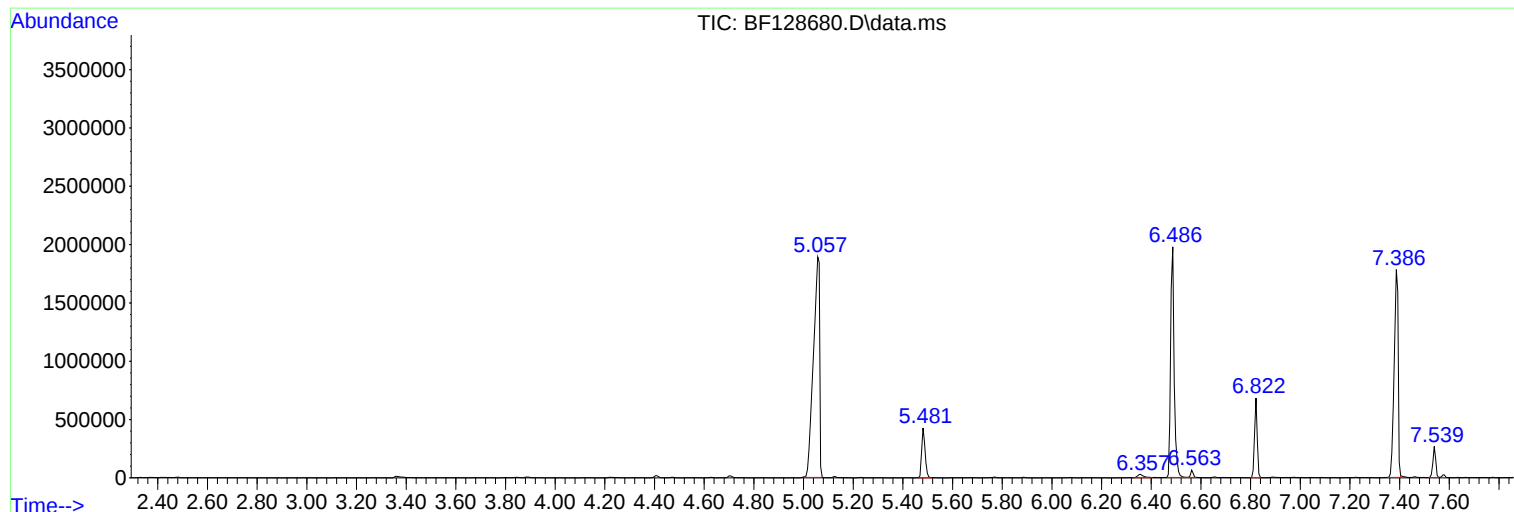
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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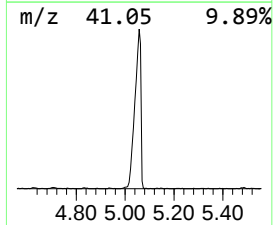
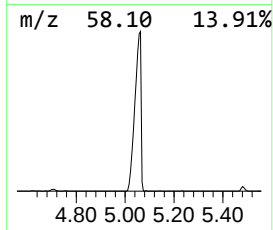
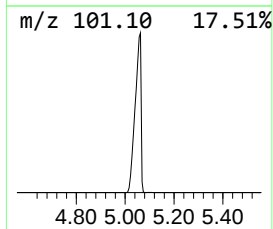
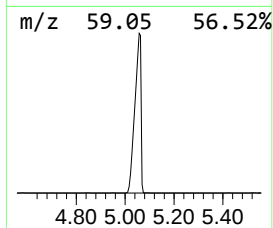
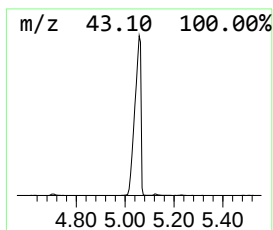
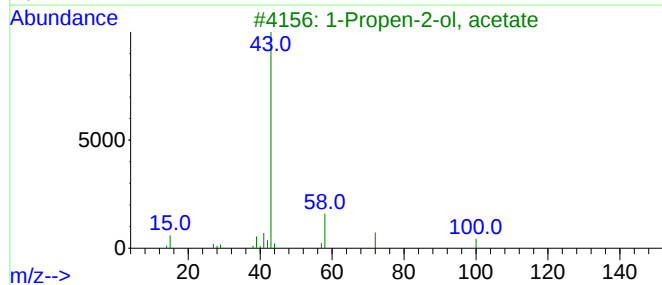
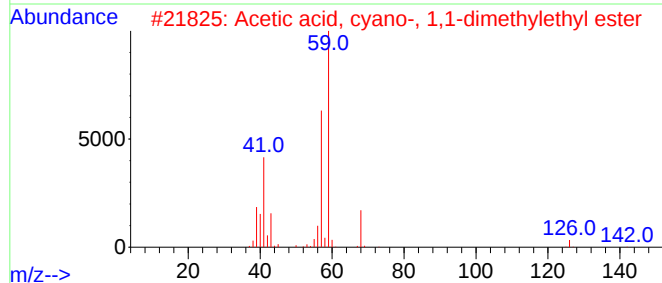
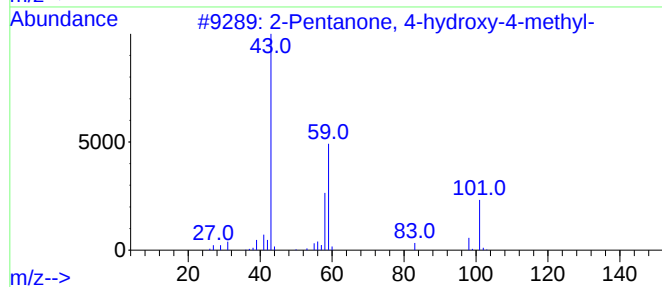
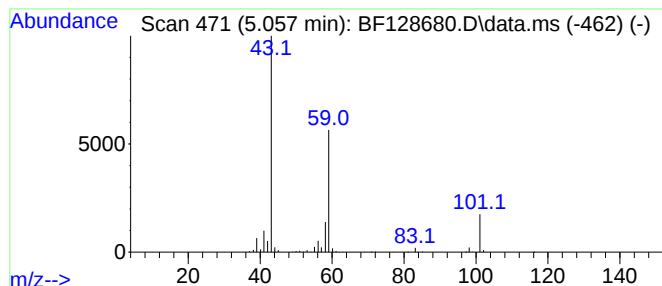
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.057	127.66 ng	3304470	1,4-Dichlorobenzene-d4	6.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
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	9		
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9		



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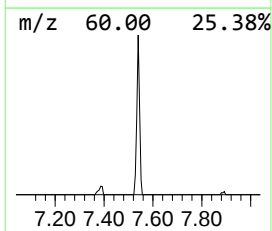
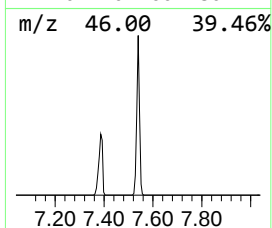
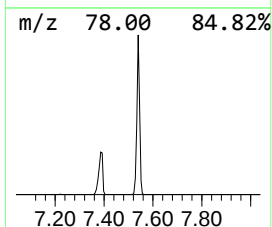
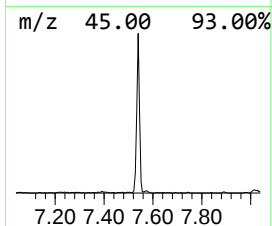
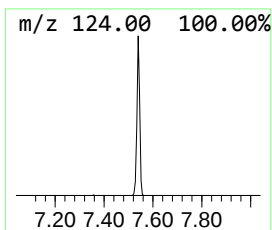
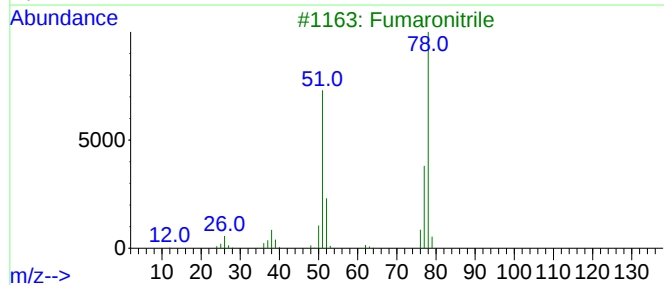
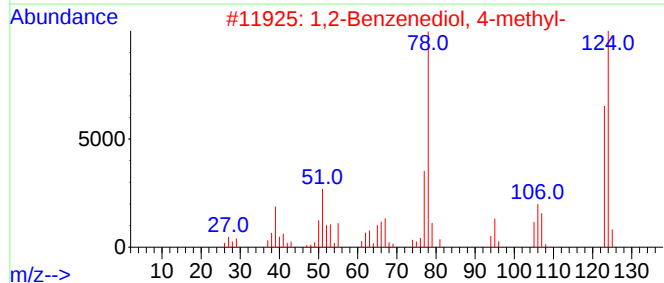
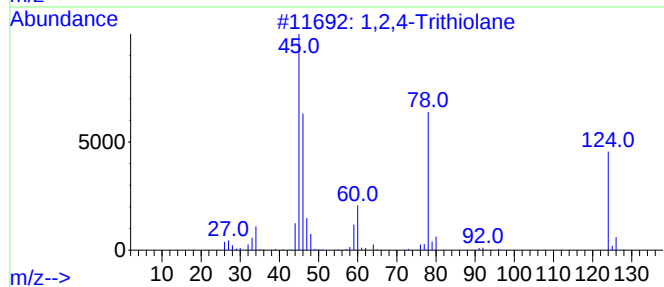
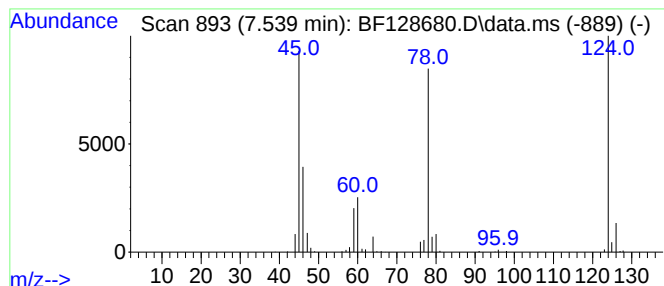
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Peak Number 2 1,2,4-Trithiolane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.539	6.60 ng	210671	Naphthalene-d8	8.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2,4-Trithiolane	124	C2H4S3	000289-16-7	83
2			1,2-Benzenediol, 4-methyl-	124	C7H8O2	000452-86-8	42
3			Fumaronitrile	78	C4H2N2	000764-42-1	9
4			1,3-Hexadien-5-yne	78	C6H6	010420-90-3	9
5			Benzene	78	C6H6	000071-43-2	9



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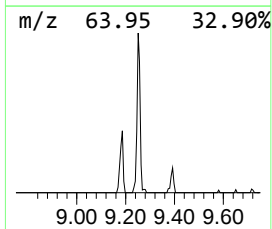
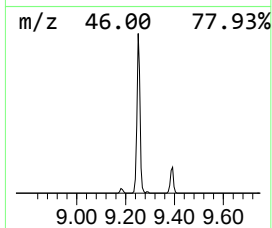
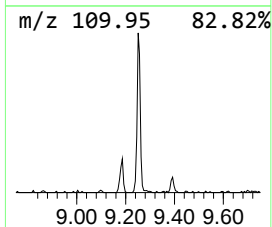
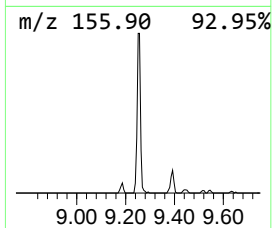
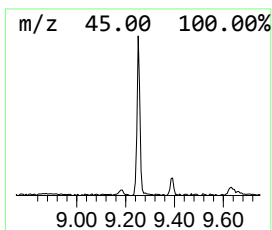
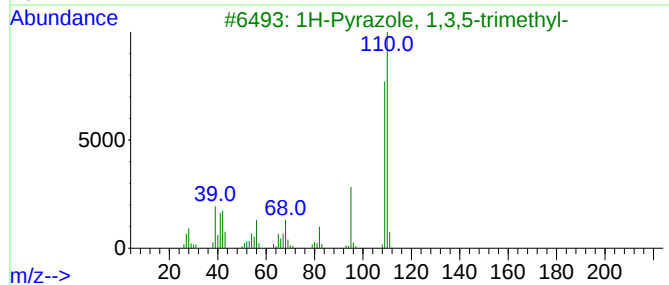
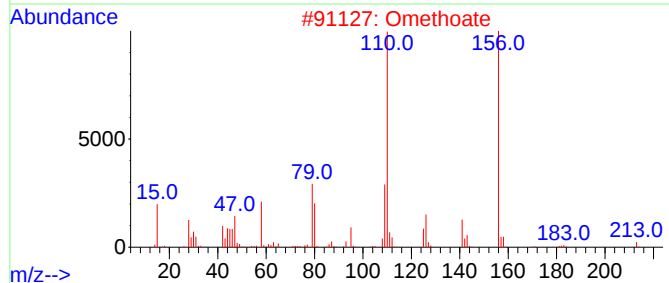
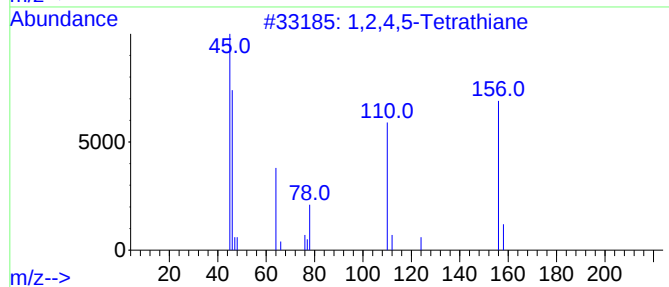
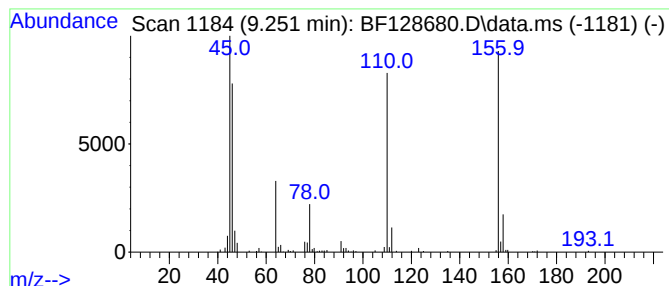
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 1,2,4,5-Tetrathiane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.251	4.43 ng	150436	Acenaphthene-d10	9.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4,5-Tetrathiane			156	C2H4S4	000291-22-5	53
2	Omethoate			213	C5H12NO4PS	001113-02-6	17
3	1H-Pyrazole, 1,3,5-trimethyl-			110	C6H10N2	001072-91-9	9
4	2,3'-Dipyridyl			156	C10H8N2	000581-50-0	9
5	Catechol			110	C6H6O2	000120-80-9	9



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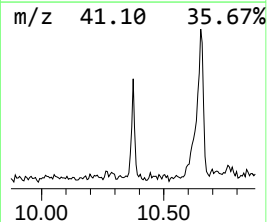
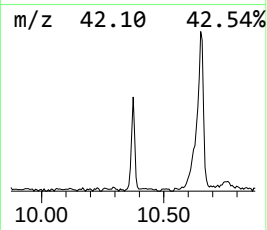
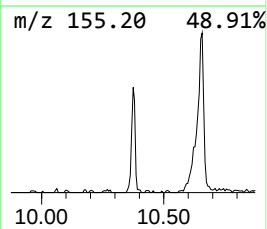
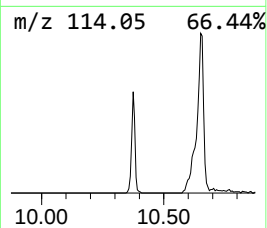
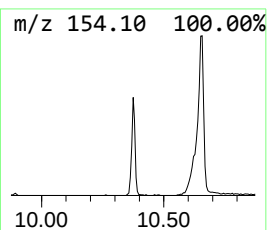
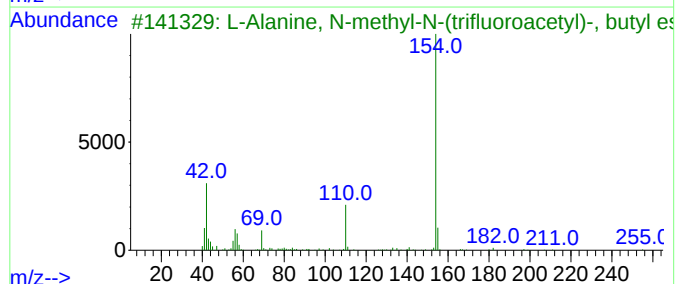
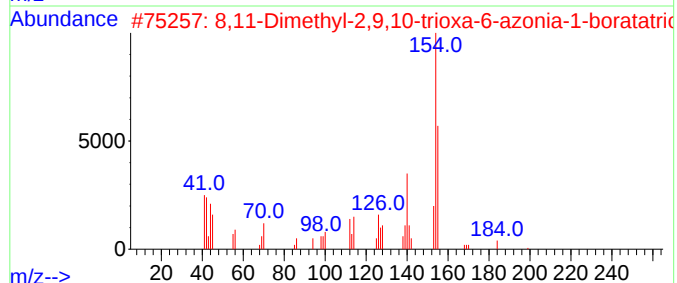
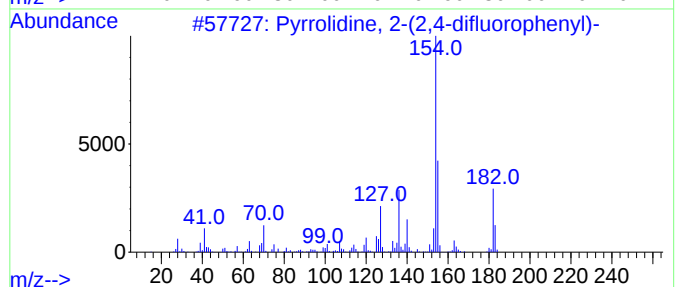
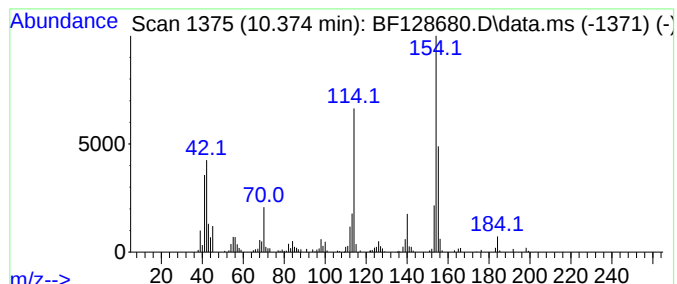
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 unknown10.374 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.374	4.59 ng	155717	Acenaphthene-d10	9.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrrolidine, 2-(2,4-difluorophen...	183	C10H11F2N	524674-05-3	37
2			8,11-Dimethyl-2,9,10-trioxa-6-az...	199	C9H18BN03	027664-58-0	36
3			L-Alanine, N-methyl-N-(trifluoro...	255	C10H16F3NO3	034815-08-2	32
4			Butanoic acid, 2-[(trifluoroacet...	283	C12H20F3NO3	057983-58-1	32
5			3-Fluoromethcathinone, N-trifluo...	277	C12H11F4NO2	1000448-09-3	25



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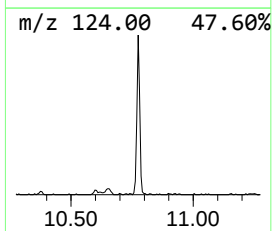
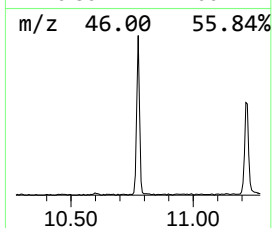
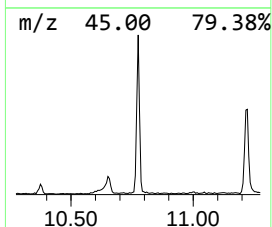
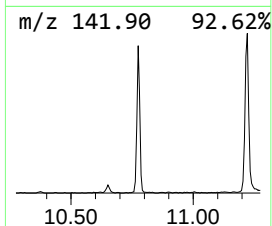
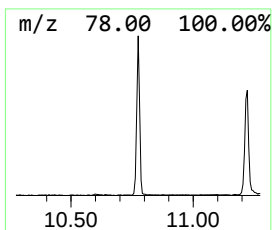
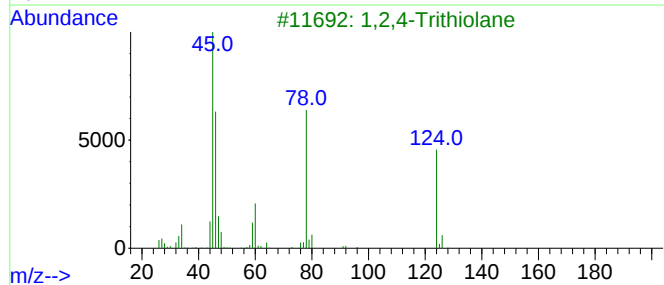
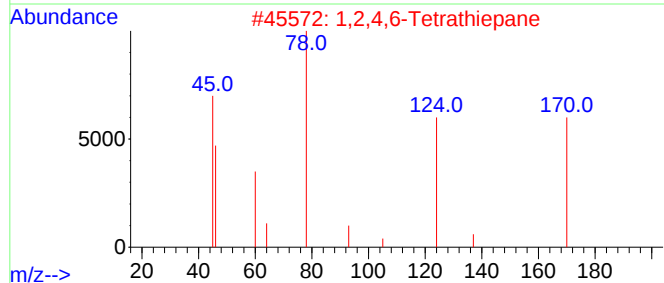
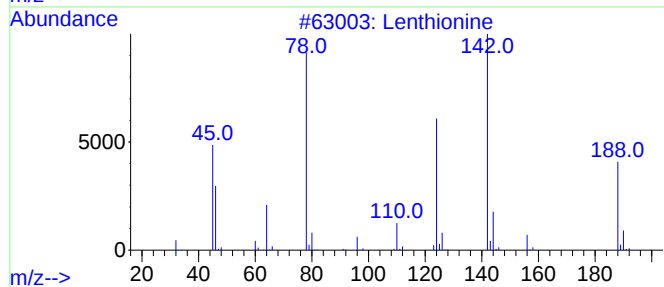
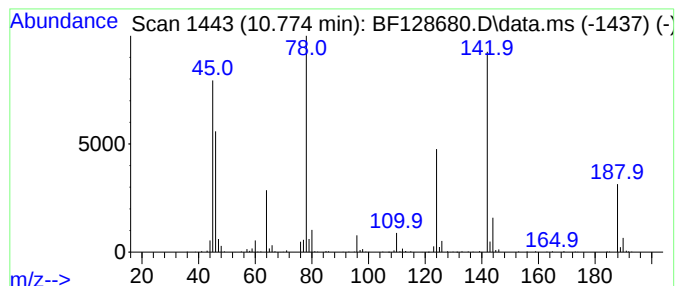
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Peak Number 5 Lenthionine Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.775	13.22 ng	379996	Phenanthrene-d10	11.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Lenthionine	188	C2H4S5	000292-46-6	95
2			1,2,4,6-Tetrathiepane	170	C3H6S4	000292-45-5	45
3			1,2,4-Trithiolane	124	C2H4S3	000289-16-7	14
4			Phenylphosphonous acid	142	C6H7O2P	001779-48-2	9
5			1,2-Benzenedithiol	142	C6H6S2	017534-15-5	9



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ClientSampleId :
20220427-AMENDED-SB-8-(DISCRETE-COMP-G)

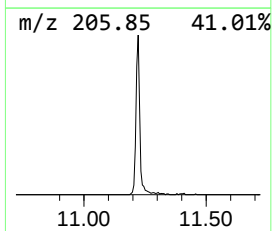
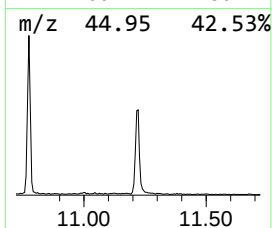
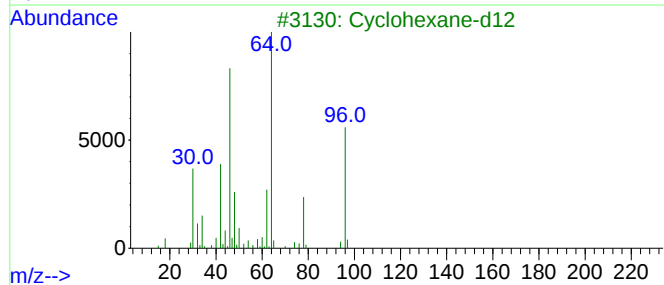
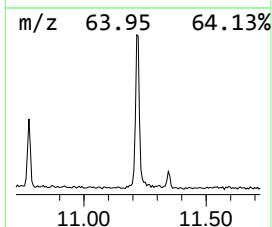
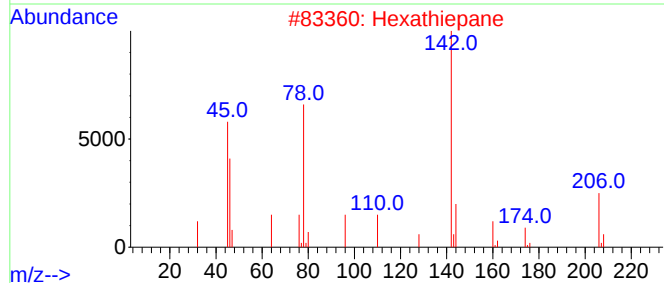
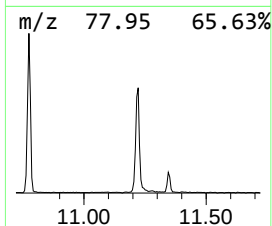
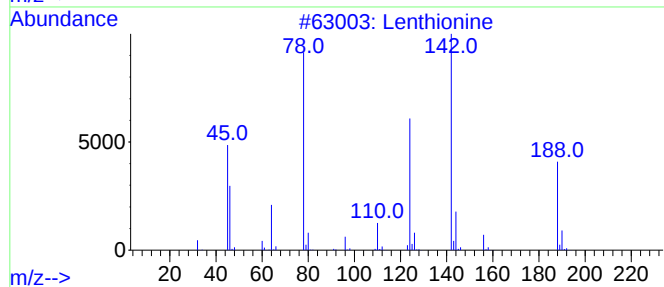
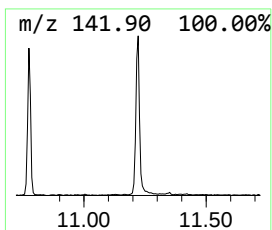
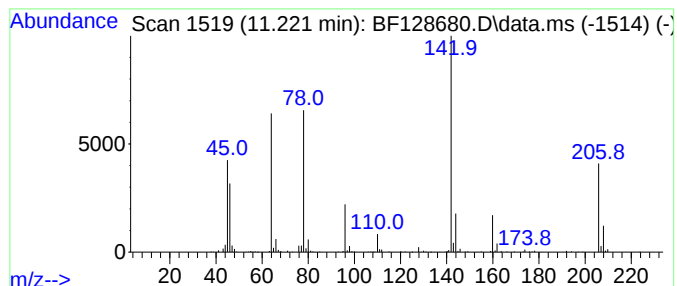
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown11.222 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.222	14.33 ng	412031	Phenanthrene-d10	11.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Lenthionine	188	C2H4S5	000292-46-6	22
2			Hexathiepane	206	CH2S6	017233-71-5	16
3			Cyclohexane-d12	96	C6D12	001735-17-7	9
4			Benzenesulfinic-acid-	142	C6H6O2S	000618-41-7	9
5			4(1H)-Pyrimidinone, 2-(methylthio)-	142	C5H6N2OS	005751-20-2	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060322\
Data File : BF128680.D
Acq On : 03 Jun 2022 15:17
Operator : CG\JU
Sample : N3143-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220427-AMENDED-SB-8-(DISCRETE-COMP-G)

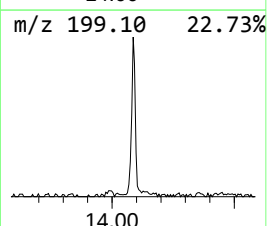
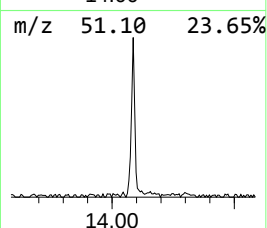
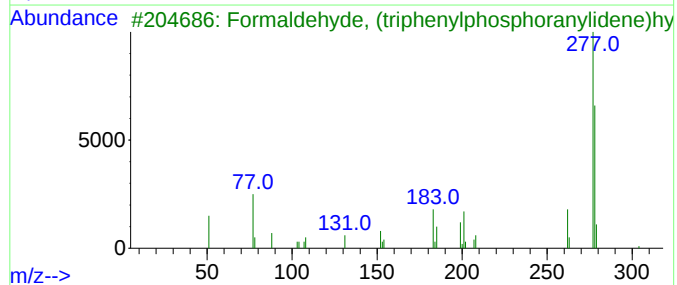
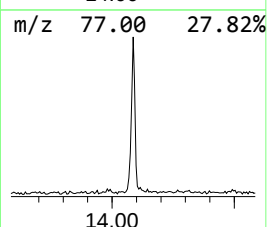
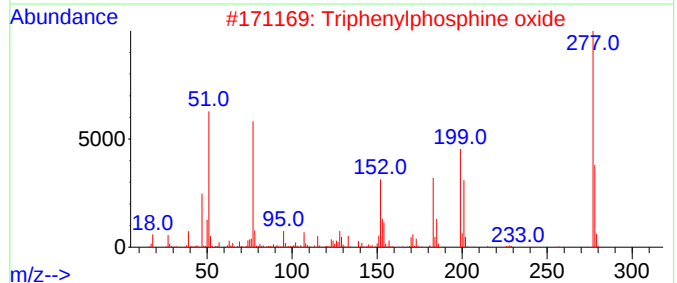
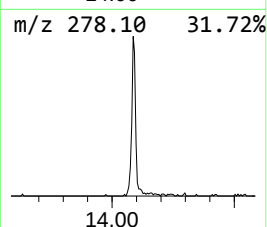
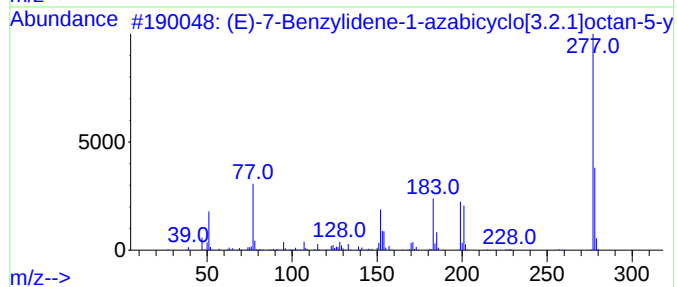
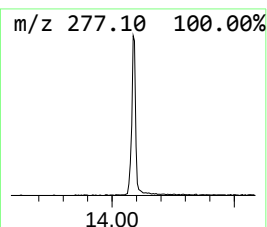
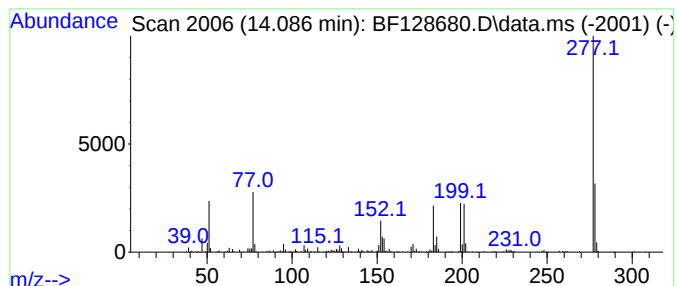
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 (E)-7-Benzylidene-1-azabicyclo... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.086	10.00 ng	258423	Chrysene-d12	13.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19N03S	1000483-83-4	93		
2	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	92		
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50		
4	Benzoic acid, 2-(diphenylphosphi...	306	C19H15O2P	017261-28-8	42		
5	Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15N02	299962-12-2	37		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060322\
Data File : BF128680.D
Acq On : 03 Jun 2022 15:17
Operator : CG\JU
Sample : N3143-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220427-AMENDED-SB-8-(DISCRETE-COMP-G)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.057	127.7	ng	3304470	1	6.822	517691	20.0
1,2,4-Trithiolane	7.539	6.6	ng	210671	2	8.104	638272	20.0
1,2,4,5-Tetrath...	9.251	4.4	ng	150436	3	9.863	679081	20.0
unknown10.374	10.374	4.6	ng	155717	3	9.863	679081	20.0
Lenthionine	10.775	13.2	ng	379996	4	11.351	574946	20.0
unknown11.222	11.222	14.3	ng	412031	4	11.351	574946	20.0
(E)-7-Benzylide...	14.086	10.0	ng	258423	5	13.992	516924	20.0