

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040722\
 Data File : BF127701.D
 Acq On : 07 Apr 2022 23:53
 Operator : CG\JU
 Sample : N2207-07
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20220351-AMENDED-096-21-03

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-BF040622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127701.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.316	3	5	12	rVB	311711	380899	4.72%	1.468%
2	5.240	489	502	504	rBV	3697726	8063602	100.00%	31.078%
3	5.575	555	559	563	rBV	499132	422218	5.24%	1.627%
4	6.569	724	728	731	rBV	1560075	1481924	18.38%	5.712%
5	6.604	731	734	741	rVB	195669	161327	2.00%	0.622%
6	6.963	791	795	798	rBV	988876	767527	9.52%	2.958%
7	7.522	885	890	894	rBV	1725912	1806217	22.40%	6.961%
8	7.687	913	918	924	rVB	1249878	1153936	14.31%	4.447%
9	8.245	1009	1013	1016	rBV	1186895	982329	12.18%	3.786%
10	9.322	1191	1196	1200	rBV	3236721	2998846	37.19%	11.558%
11	9.539	1229	1233	1237	rBV	269718	221248	2.74%	0.853%
12	10.004	1309	1312	1316	rVB	1203312	1133180	14.05%	4.367%
13	10.516	1395	1399	1404	rVB	120119	103338	1.28%	0.398%
14	10.792	1443	1446	1453	rVB2	277037	371354	4.61%	1.431%
15	10.928	1466	1469	1476	rVB	136091	134506	1.67%	0.518%
16	11.357	1538	1542	1544	rBV	78424	85121	1.06%	0.328%
17	11.498	1562	1566	1570	rBV	1356568	1175009	14.57%	4.529%
18	13.092	1832	1837	1840	rBV	2802819	2616727	32.45%	10.085%
19	13.980	1984	1988	1997	rBV	123286	145404	1.80%	0.560%
20	14.145	2010	2016	2020	rBV	913246	891591	11.06%	3.436%
21	15.674	2270	2276	2281	rBV	669549	849986	10.54%	3.276%

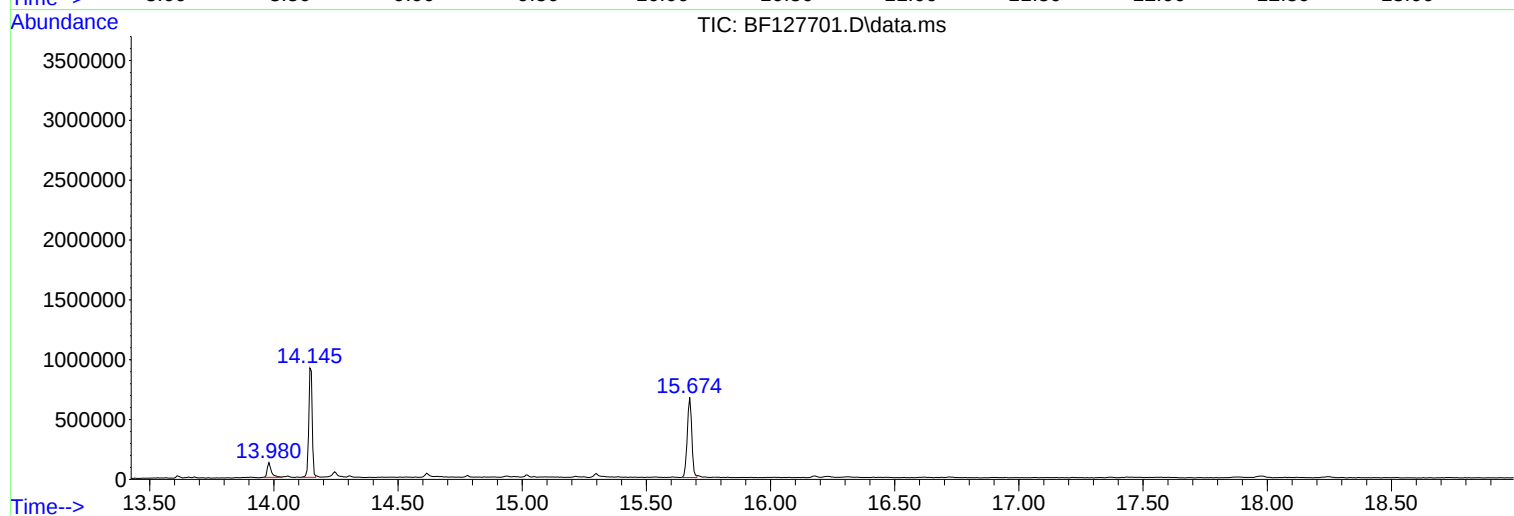
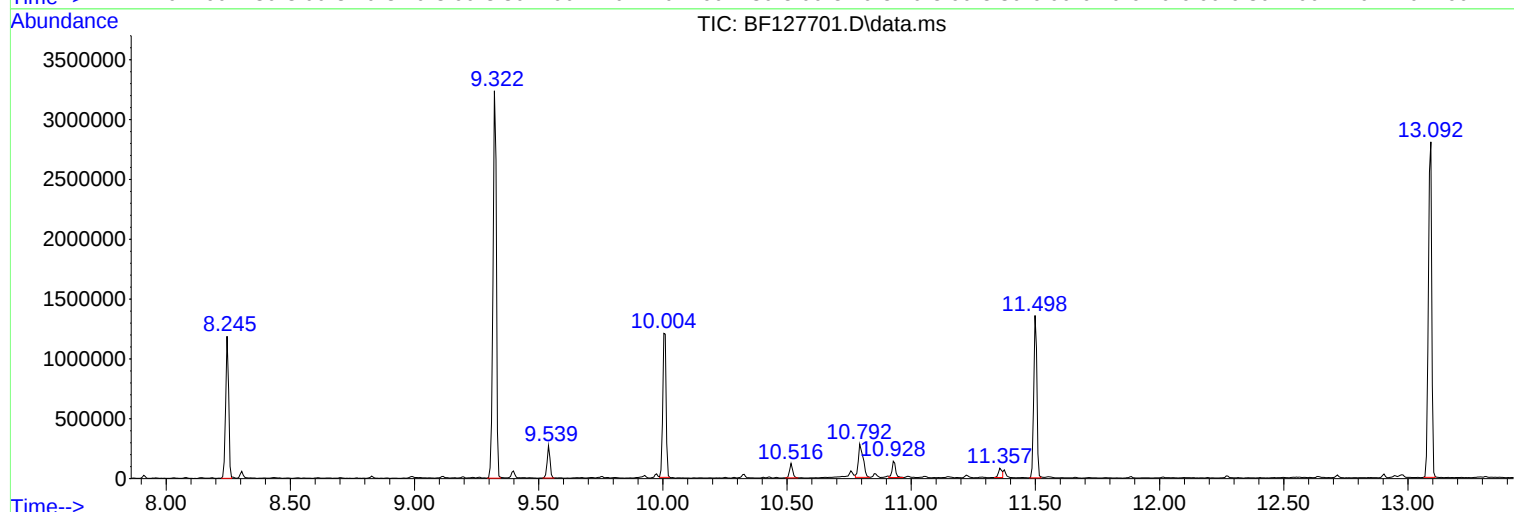
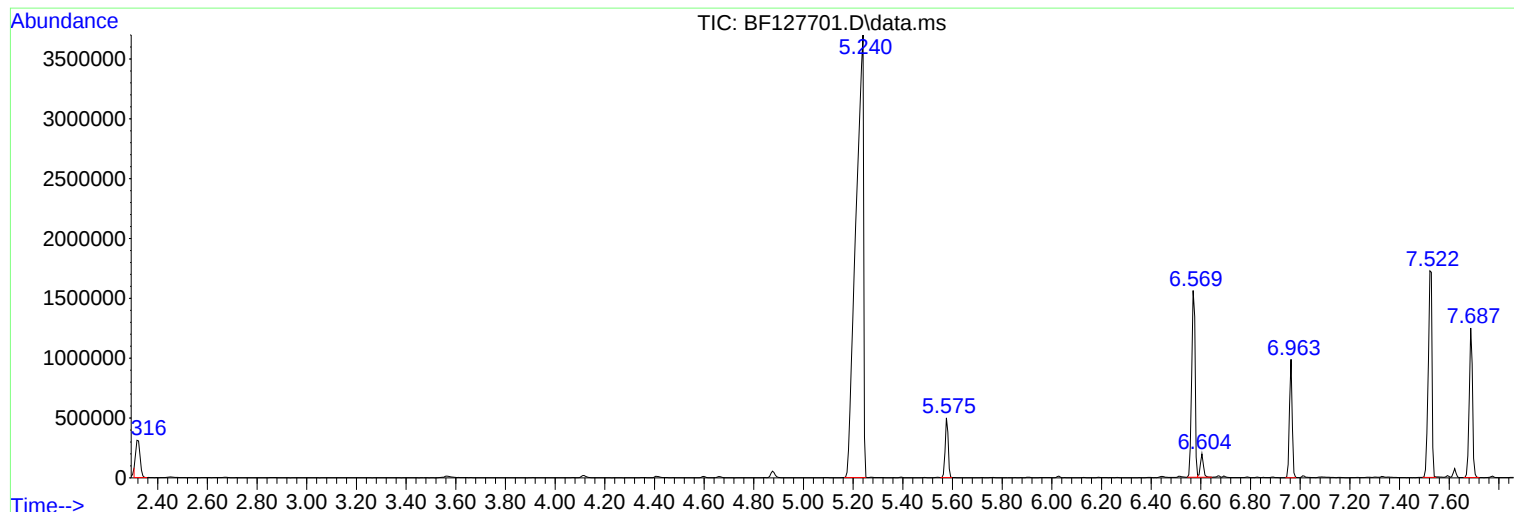
Sum of corrected areas: 25946289

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040722\
Data File : BF127701.D
Acq On : 07 Apr 2022 23:53
Operator : CG\JU
Sample : N2207-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220351-AMENDED-096-21-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040722\
Data File : BF127701.D
Acq On : 07 Apr 2022 23:53
Operator : CG\JU
Sample : N2207-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220351-AMENDED-096-21-03

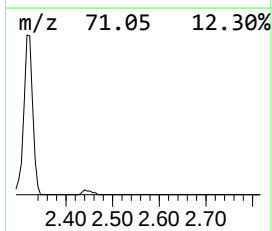
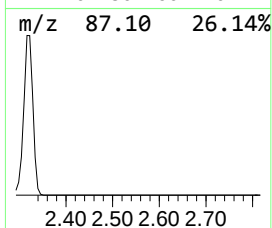
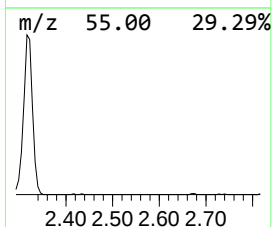
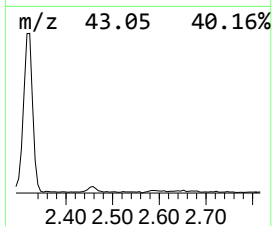
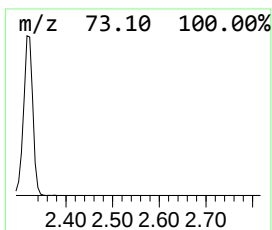
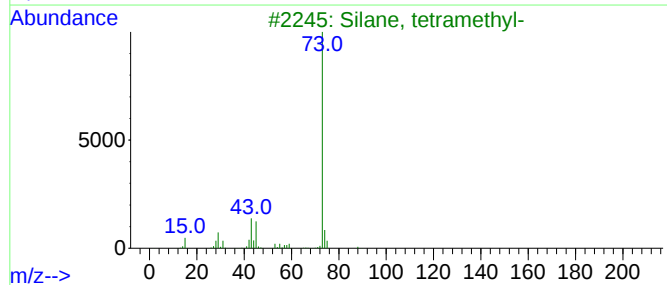
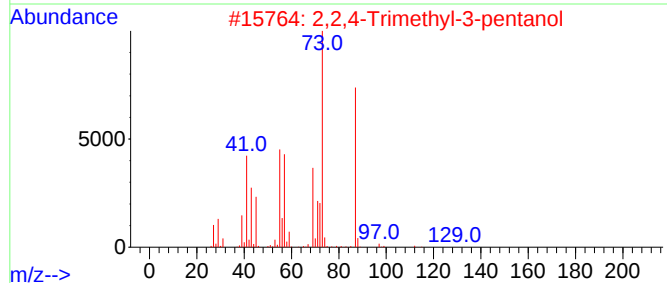
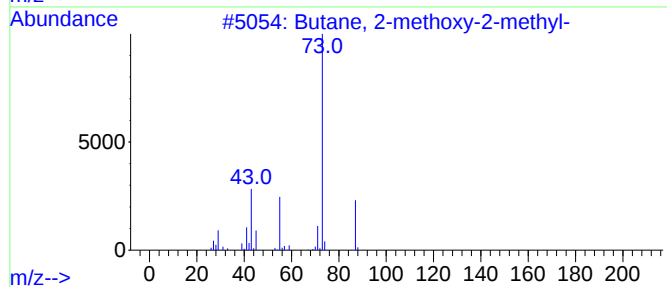
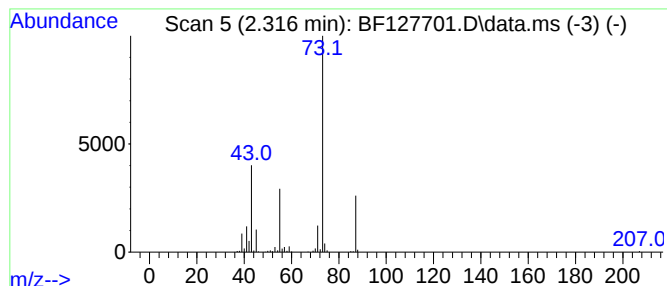
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.316	9.93 ng	380899	1,4-Dichlorobenzene-d4	6.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	32
5			Butanoic acid, 2-hydroxy-2-methy...	132	C6H12O3	032793-34-3	23



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040722\
Data File : BF127701.D
Acq On : 07 Apr 2022 23:53
Operator : CG\JU
Sample : N2207-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220351-AMENDED-096-21-03

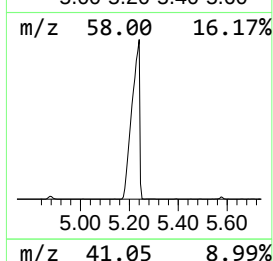
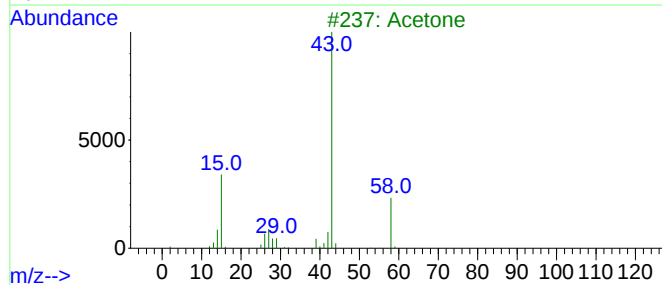
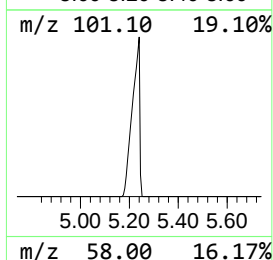
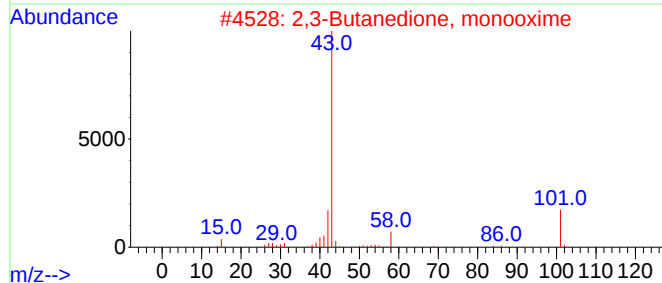
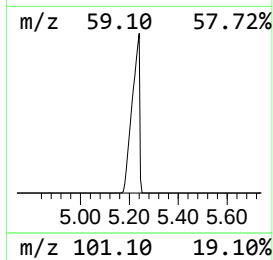
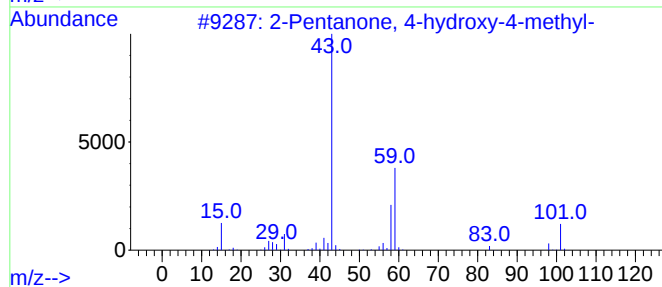
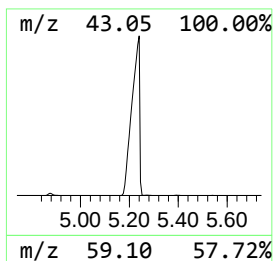
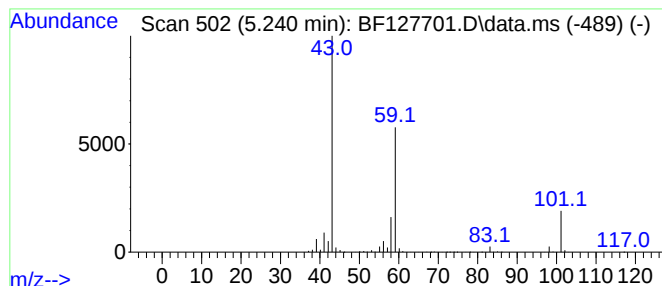
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.240	210.12 ng	8063600	1,4-Dichlorobenzene-d4	6.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
3	Acetone	58	C3H6O	000067-64-1	10		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040722\
Data File : BF127701.D
Acq On : 07 Apr 2022 23:53
Operator : CG\JU
Sample : N2207-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220351-AMENDED-096-21-03

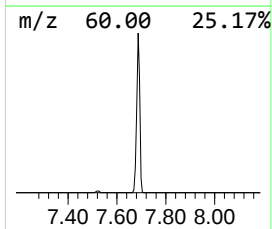
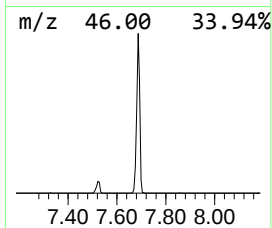
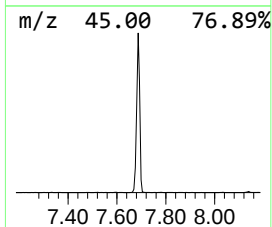
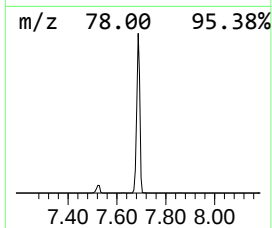
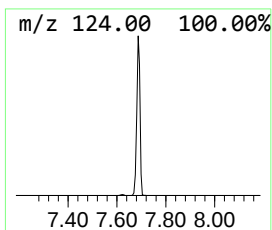
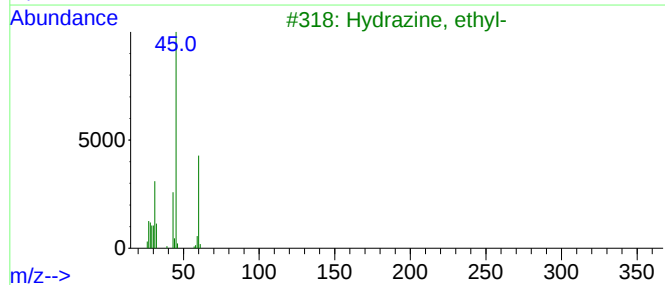
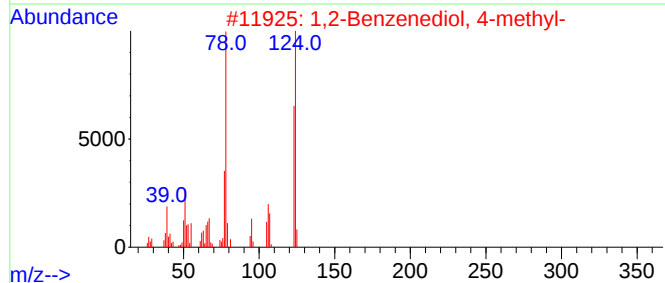
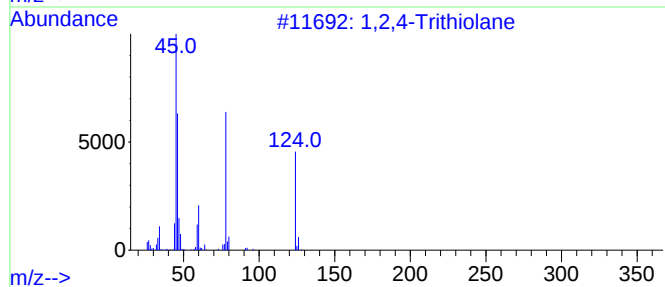
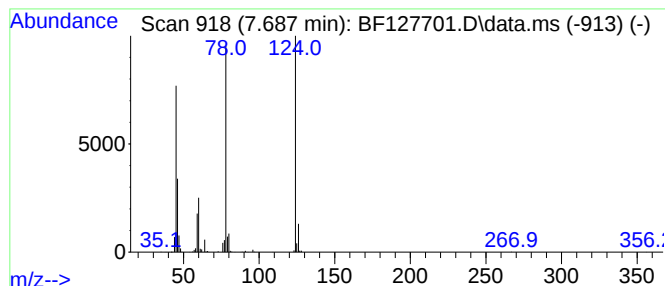
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 1,2,4-Trithiolane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.687	23.49 ng	1153940	Naphthalene-d8	8.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4-Trithiolane			124	C2H4S3	000289-16-7	90
2	1,2-Benzenediol, 4-methyl-			124	C7H8O2	000452-86-8	42
3	Hydrazine, ethyl-			60	C2H8N2	000624-80-6	10
4	1,2-Benzenediol, 3-methyl-			124	C7H8O2	000488-17-5	9
5	Ethane, methoxy-			60	C3H8O	000540-67-0	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040722\
Data File : BF127701.D
Acq On : 07 Apr 2022 23:53
Operator : CG\JU
Sample : N2207-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220351-AMENDED-096-21-03

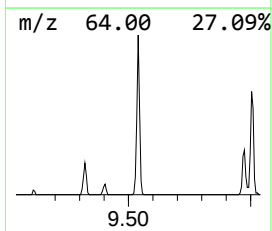
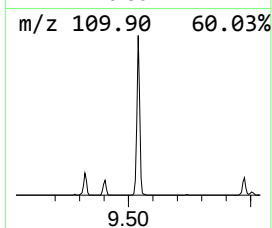
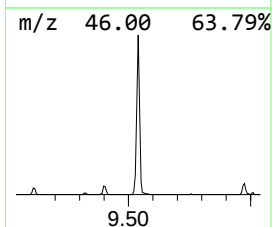
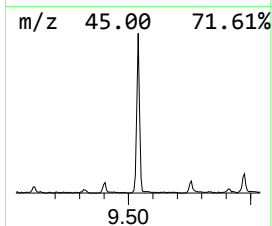
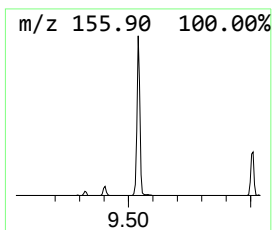
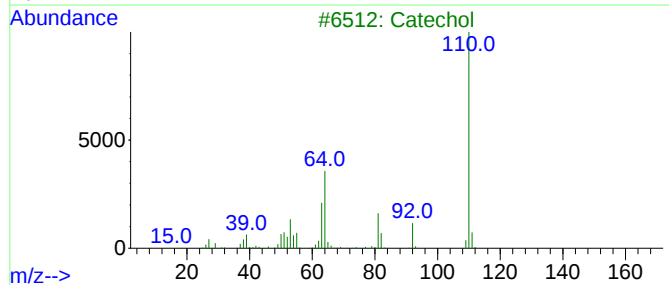
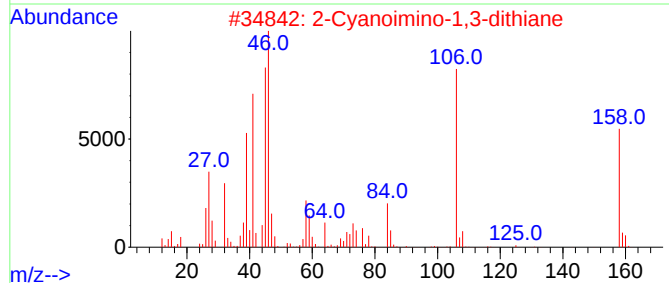
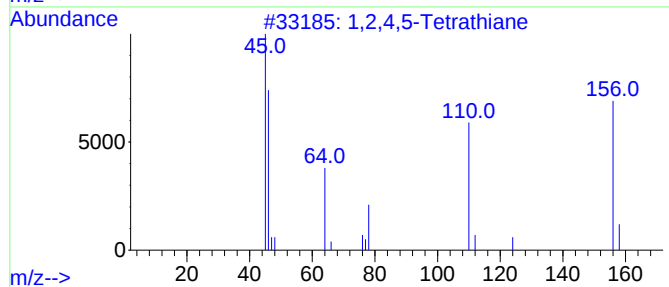
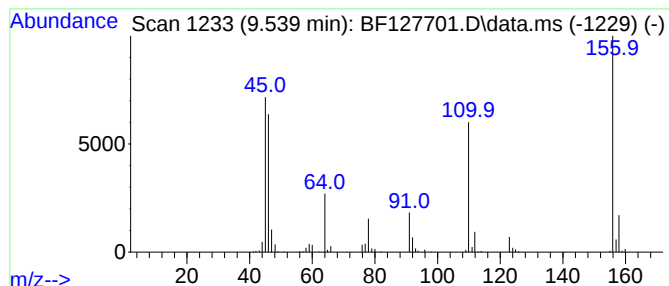
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.539	3.90 ng	221248	Acenaphthene-d10	10.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4,5-Tetrathiane			156	C2H4S4	000291-22-5	91
2	2-Cyanoimino-1,3-dithiane			158	C5H6N2S2	010191-73-8	27
3	Catechol			110	C6H6O2	000120-80-9	9
4	4H-1,2,4-triazole-3-carboxylic a...			156	C5H8N4O2	1000404-32-7	9
5	4,5-Diamino-6-methyl-2-thiopyrim...			156	C5H8N4S	006305-99-3	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040722\
Data File : BF127701.D
Acq On : 07 Apr 2022 23:53
Operator : CG\JU
Sample : N2207-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220351-AMENDED-096-21-03

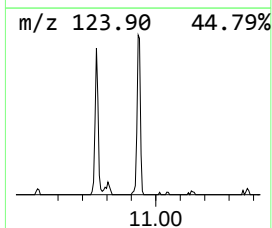
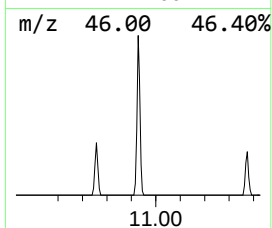
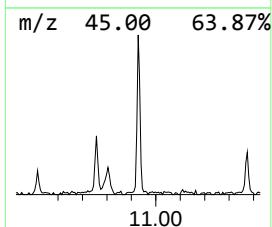
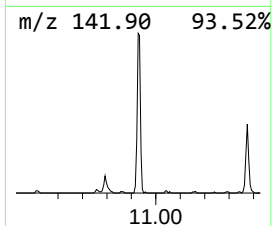
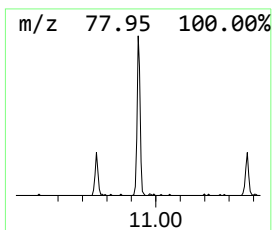
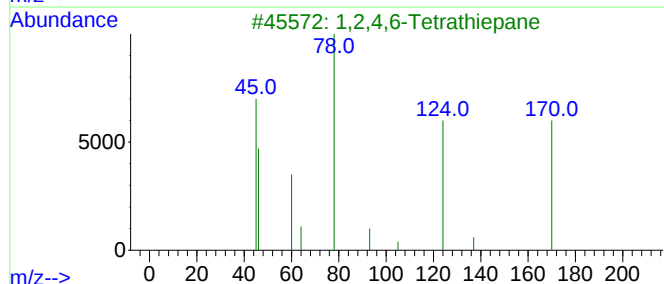
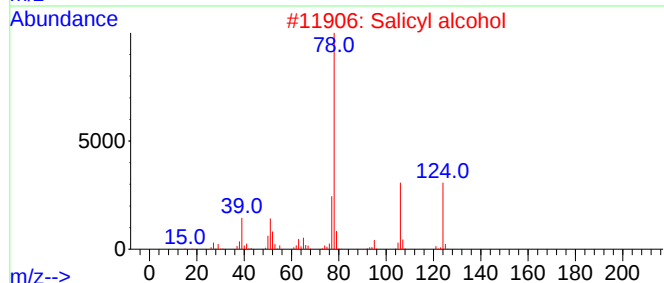
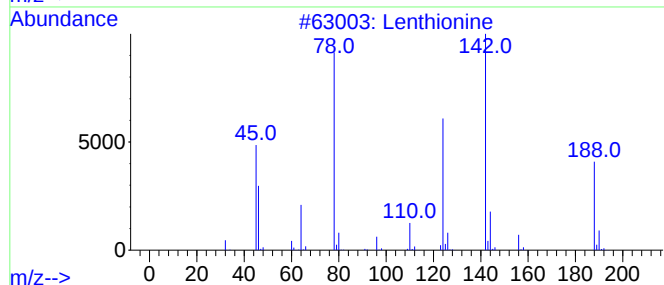
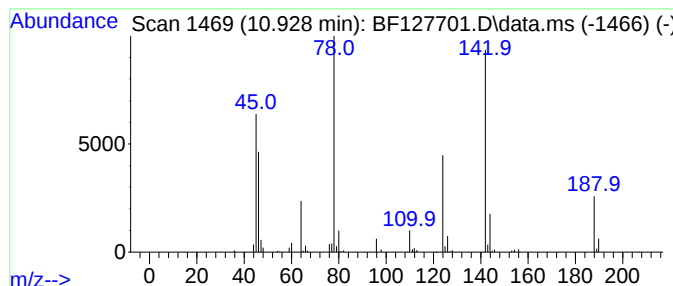
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Lenthionine Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.928	2.29 ng	134506	Phenanthrene-d10	11.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Lenthionine	188	C2H4S5	000292-46-6	95
2			Salicyl alcohol	124	C7H8O2	000090-01-7	49
3			1,2,4,6-Tetrathiepane	170	C3H6S4	000292-45-5	45
4			Ethylthiophosphonamide, o-methyl ...	139	C3H10NOPS	1000306-03-7	33
5			1,2-Benzenedithiol	142	C6H6S2	017534-15-5	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040722\
Data File : BF127701.D
Acq On : 07 Apr 2022 23:53
Operator : CG\JU
Sample : N2207-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220351-AMENDED-096-21-03

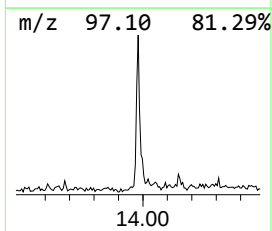
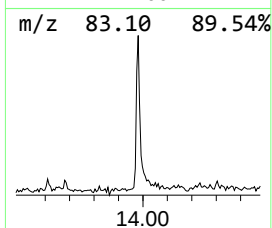
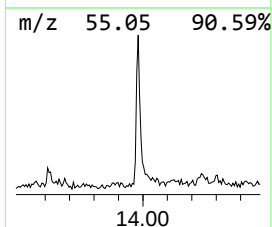
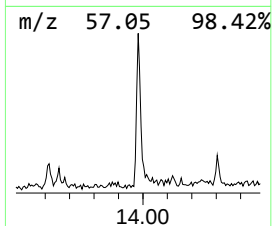
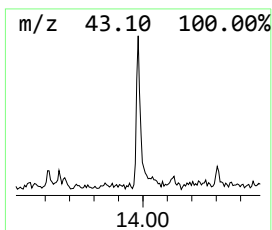
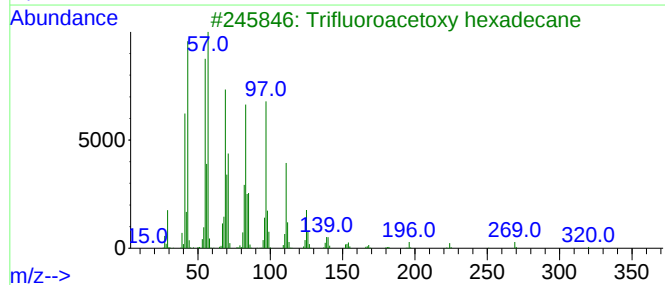
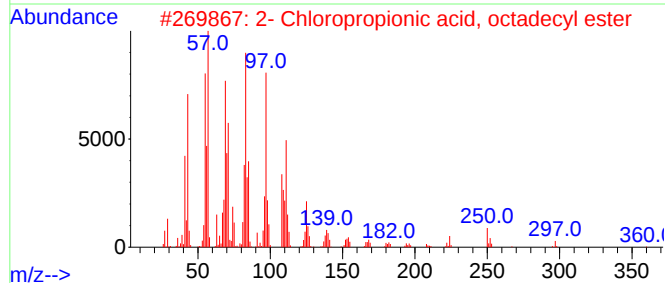
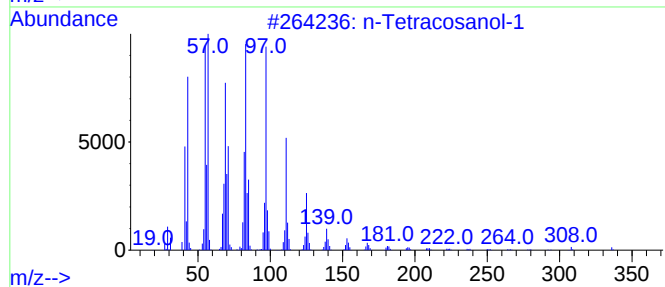
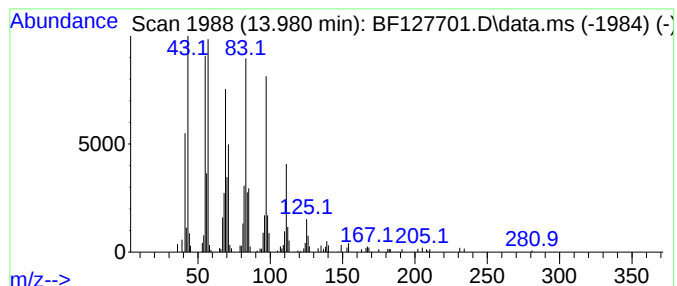
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Tetracosanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.980	3.26 ng	145404	Chrysene-d12	14.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2			2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
3			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4			Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	94
5			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040722\
Data File : BF127701.D
Acq On : 07 Apr 2022 23:53
Operator : CG\JU
Sample : N2207-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220351-AMENDED-096-21-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.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
Butane, 2-metho...	2.316	9.9	ng	380899	1	6.963	767527	20.0
2-Pentanone, 4-...	5.240	210.1	ng	8063600	1	6.963	767527	20.0
1,2,4-Trithiolane	7.687	23.5	ng	1153940	2	8.245	982329	20.0
1,2,4,5-Tetrath...	9.539	3.9	ng	221248	3	10.010	1133180	20.0
Lenthionine	10.928	2.3	ng	134506	4	11.498	1175010	20.0
n-Tetracosanol-1	13.980	3.3	ng	145404	5	14.151	891591	20.0