

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040722\
 Data File : BF127700.D
 Acq On : 07 Apr 2022 23:24
 Operator : CG\JU
 Sample : N2207-06
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20220350-AMENDED-096-21-02

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: BF127700.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.322	3	6	12	rVB	304804	371908	4.64%	1.456%
2	5.240	489	502	504	rBV	3647787	8015714	100.00%	31.381%
3	5.575	555	559	563	rBV	309134	250149	3.12%	0.979%
4	6.569	724	728	731	rBV	1381867	1205904	15.04%	4.721%
5	6.604	731	734	741	rVB	116958	102111	1.27%	0.400%
6	6.963	791	795	798	rBV	969757	775774	9.68%	3.037%
7	7.528	885	891	894	rBV	1812973	1880123	23.46%	7.361%
8	7.686	914	918	923	rVB	938308	824059	10.28%	3.226%
9	8.245	1009	1013	1017	rBV	1150349	989031	12.34%	3.872%
10	9.322	1191	1196	1200	rBV	3269067	3171410	39.56%	12.416%
11	9.398	1204	1209	1214	rVB4	77651	98355	1.23%	0.385%
12	9.539	1230	1233	1237	rVB	132682	107423	1.34%	0.421%
13	10.010	1308	1313	1316	rBV	1317859	1125905	14.05%	4.408%
14	10.516	1395	1399	1409	rVB	84865	81602	1.02%	0.319%
15	10.810	1443	1449	1454	rVB2	190441	255517	3.19%	1.000%
16	10.933	1466	1470	1477	rVB	205242	206829	2.58%	0.810%
17	11.498	1562	1566	1570	rBV	1313416	1138041	14.20%	4.455%
18	11.886	1628	1632	1635	rVB	141936	108521	1.35%	0.425%
19	13.092	1832	1837	1840	rBV	2902848	2651319	33.08%	10.380%
20	13.980	1984	1988	1996	rBV	157504	197516	2.46%	0.773%
21	14.145	2010	2016	2020	rBV	929809	848882	10.59%	3.323%
22	14.615	2092	2096	2102	rBV3	51433	85241	1.06%	0.334%
23	15.674	2270	2276	2285	rBV	686070	860166	10.73%	3.367%
24	17.974	2661	2667	2676	rVB7	47116	110284	1.38%	0.432%
25	18.245	2707	2713	2720	rBV8	34287	81585	1.02%	0.319%

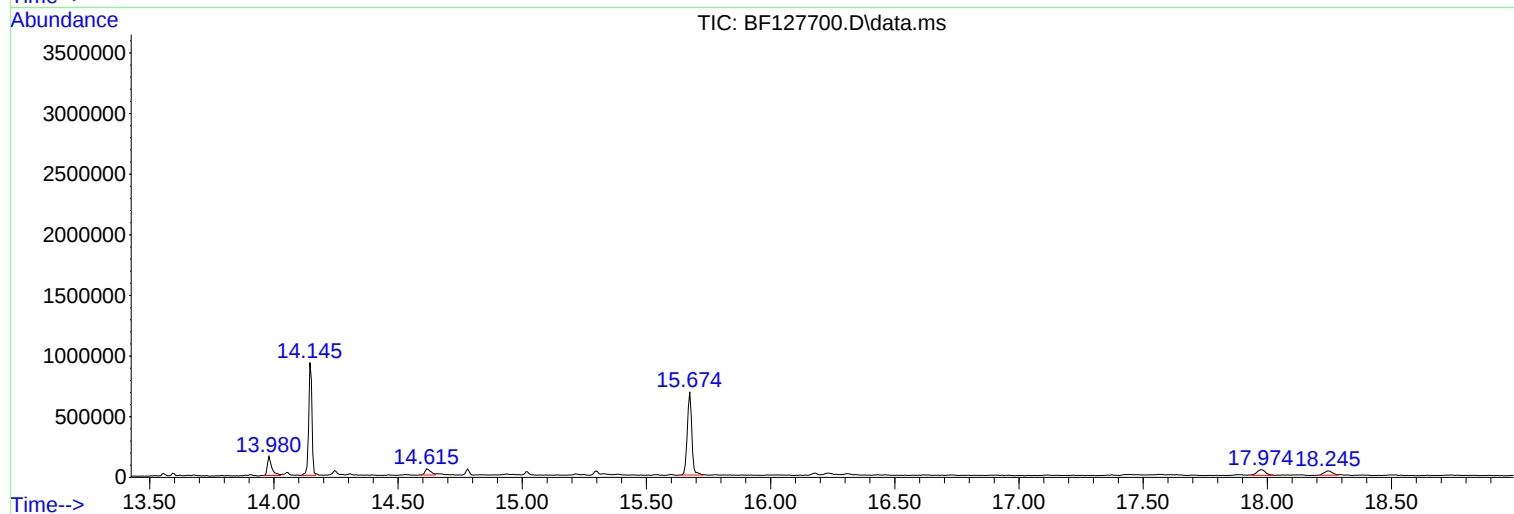
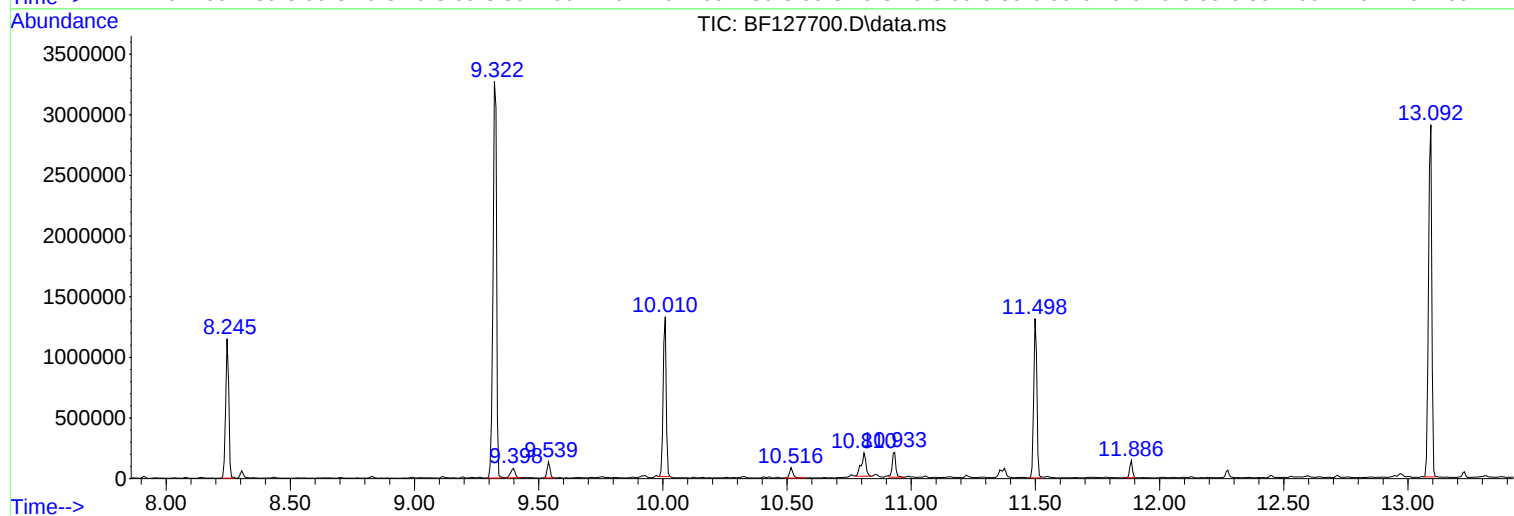
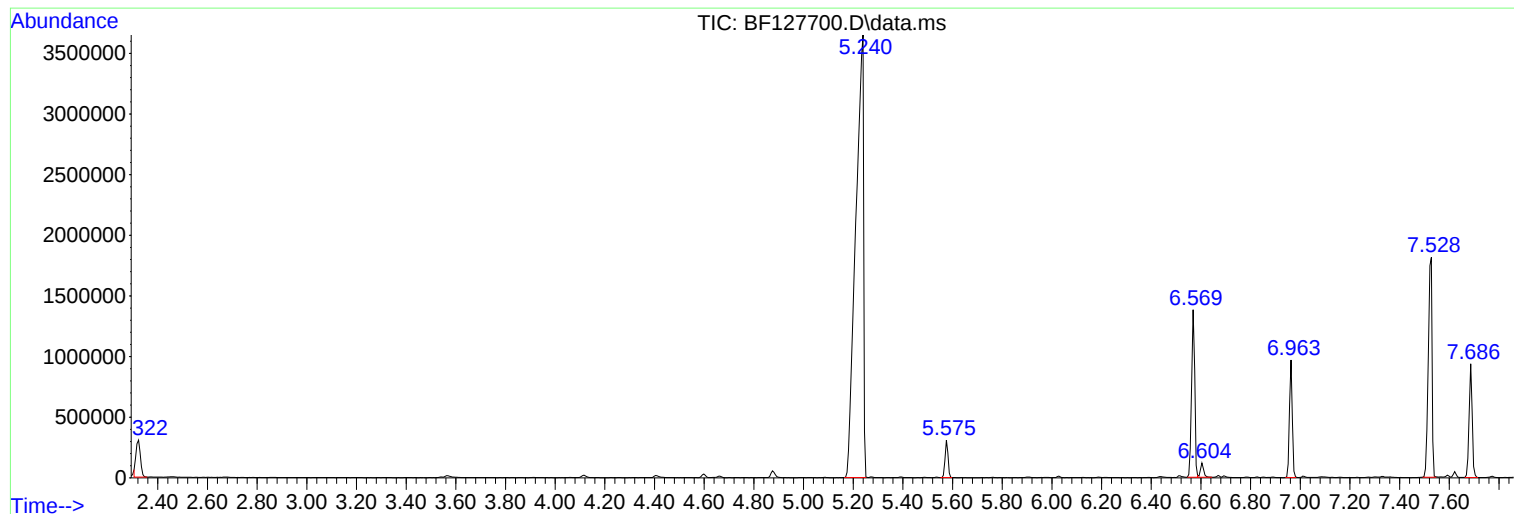
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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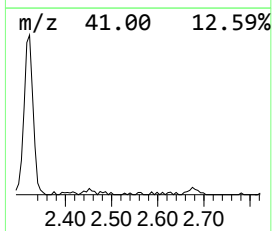
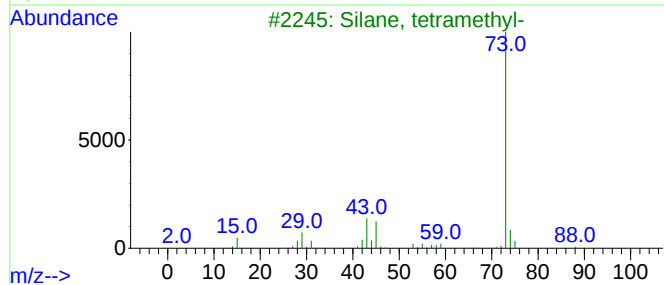
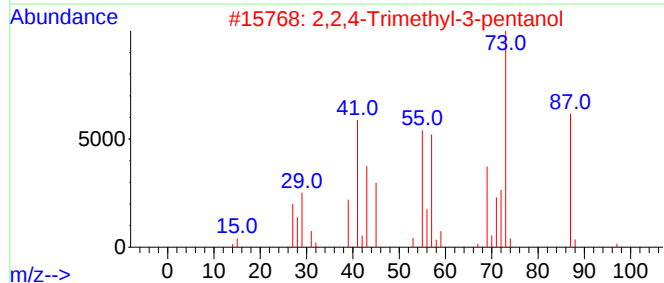
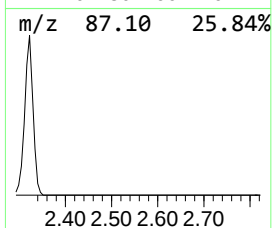
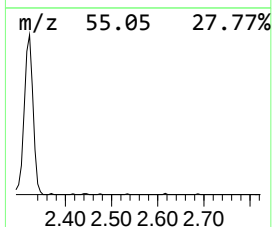
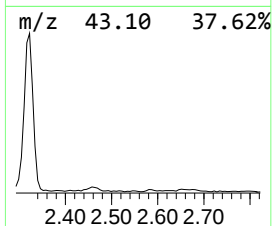
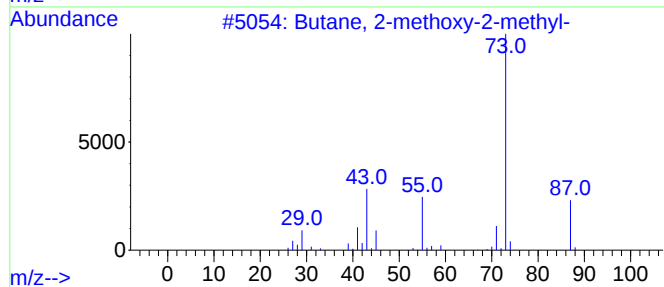
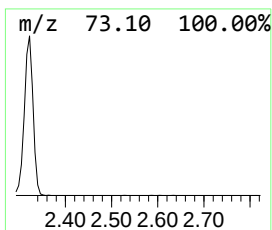
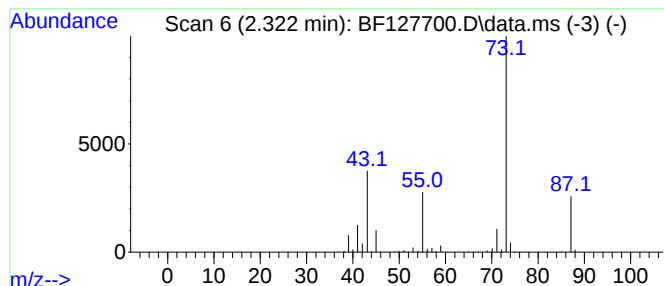
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.322	9.59 ng	371908	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			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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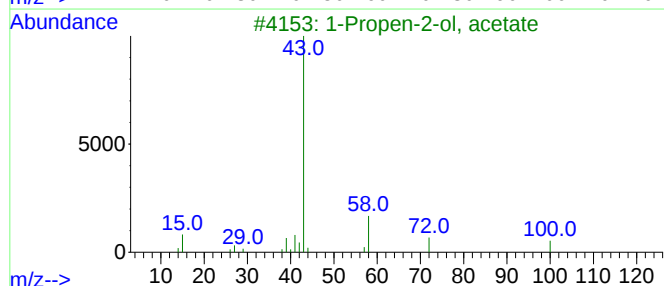
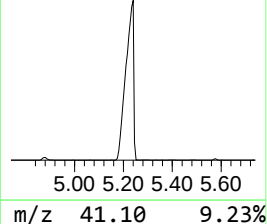
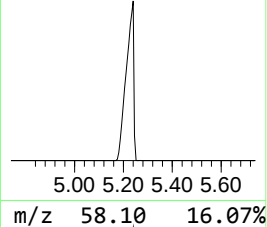
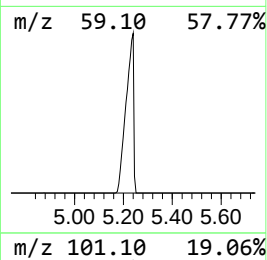
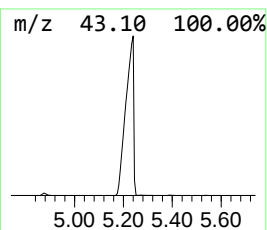
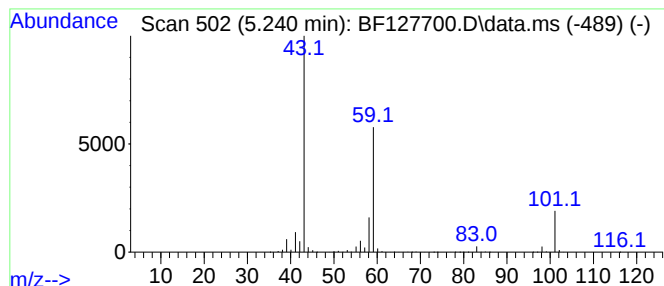
Instrument :
BNA_F
ClientSampleId :
20220350-AMENDED-096-21-02

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	206.65 ng	8015710	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	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	10
4	Acetone		58	C3H6O	000067-64-1	10
5	5-Hexen-2-one		98	C6H10O	000109-49-9	9



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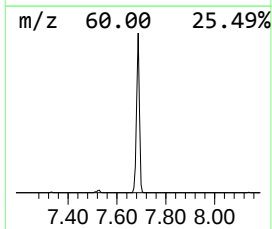
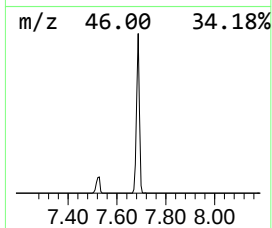
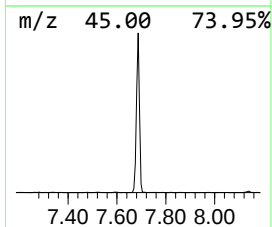
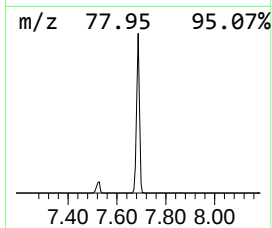
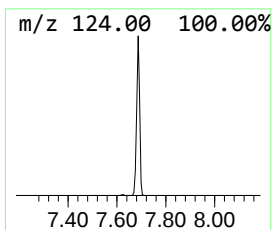
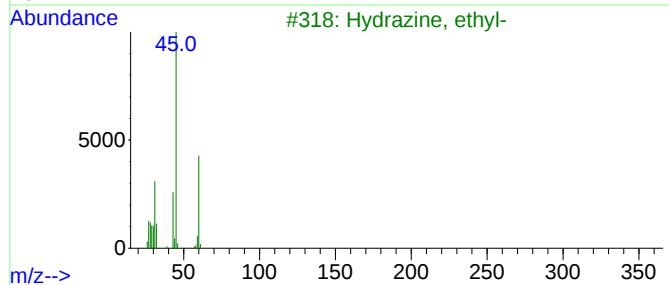
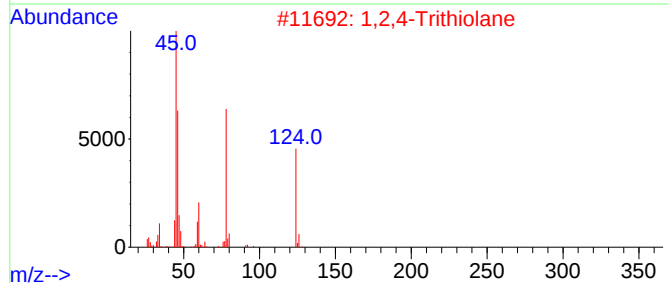
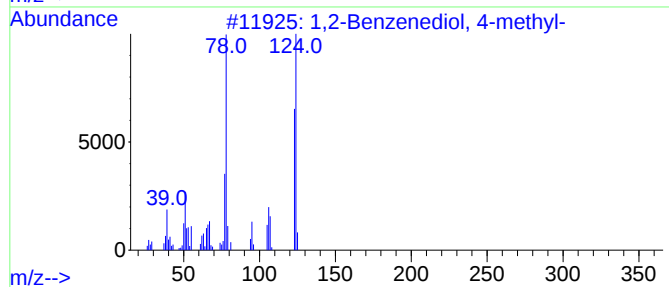
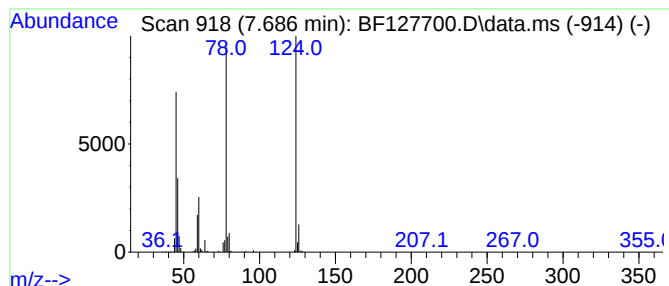
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown7.686 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.686	16.66 ng	824059	Naphthalene-d8	8.245

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,2-Benzenediol, 4-methyl-	124	C7H8O2	000452-86-8	42
2		1,2,4-Trithiolane	124	C2H4S3	000289-16-7	34
3		Hydrazine, ethyl-	60	C2H8N2	000624-80-6	10
4		Ethane, methoxy-	60	C3H8O	000540-67-0	9
5		Benzene	78	C6H6	000071-43-2	9



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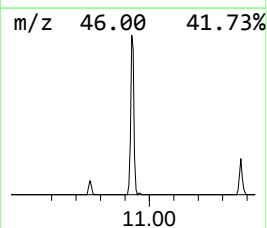
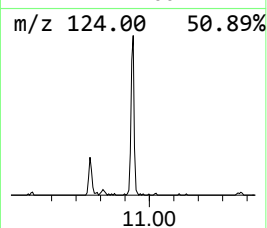
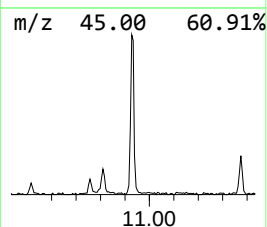
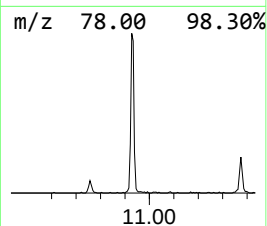
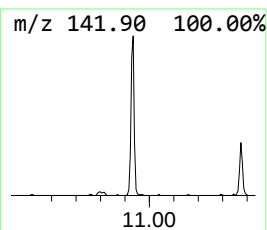
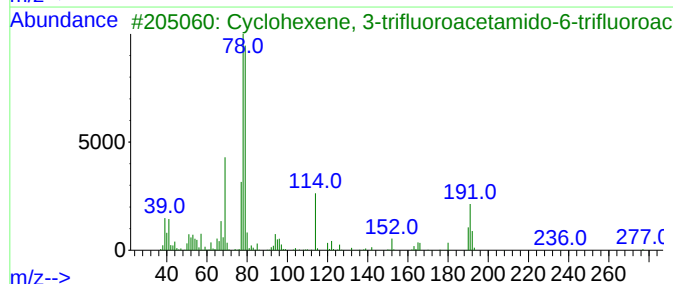
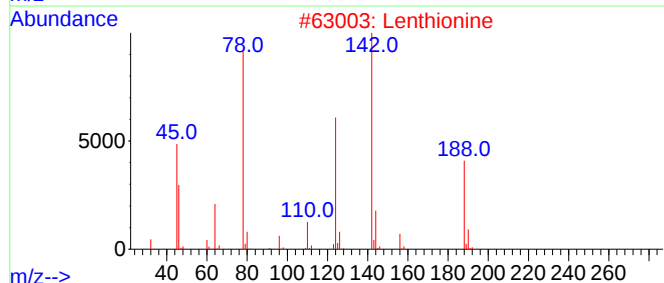
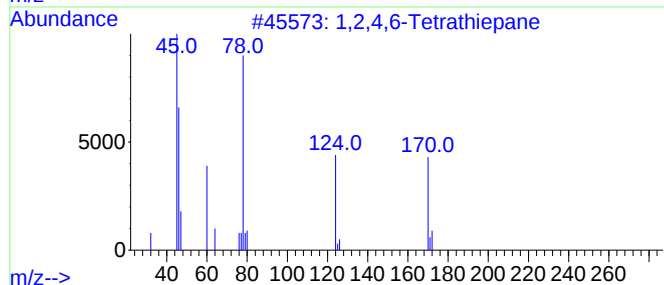
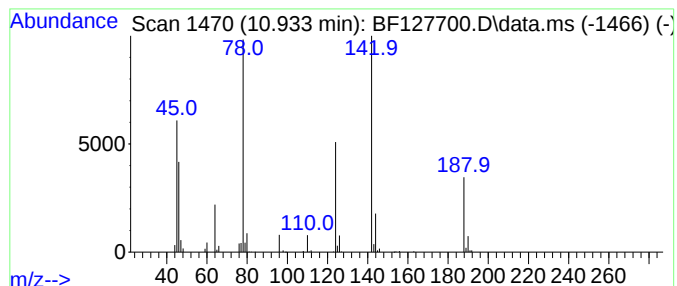
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 unknown10.933 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.933	3.63 ng	206829	Phenanthrene-d10	11.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2,4,6-Tetrathiepane	170	C3H6S4	000292-45-5	45
2			Lenthionine	188	C2H4S5	000292-46-6	35
3			Cyclohexene, 3-trifluoroacetamid...	305	C10H9F6NO3	1000153-70-3	9
4			Ethyl phenyl sulfoxide	154	C8H10OS	1000343-40-9	9
5			1,2,4,5,7,8-Hexathiocyclononane	234	C3H6S6	081531-38-6	9



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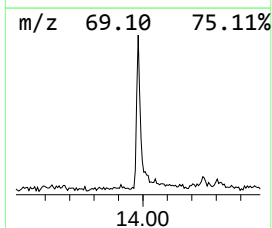
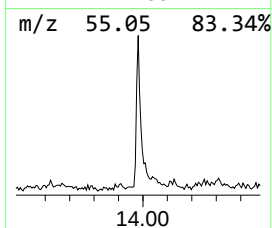
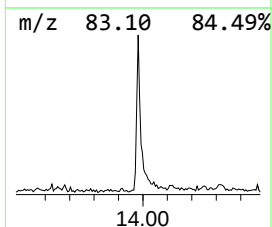
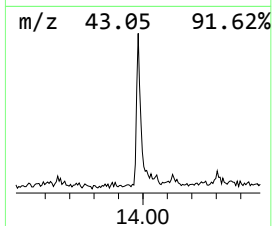
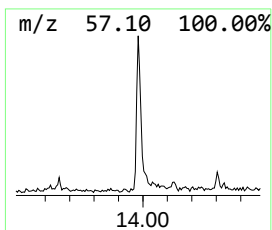
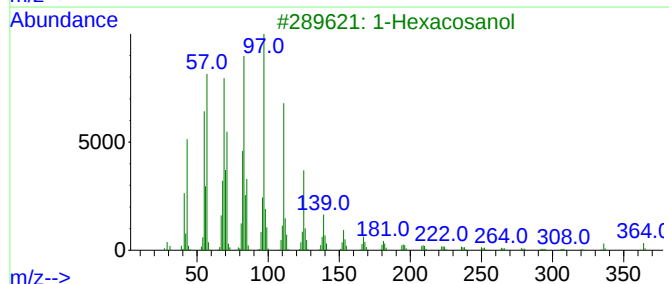
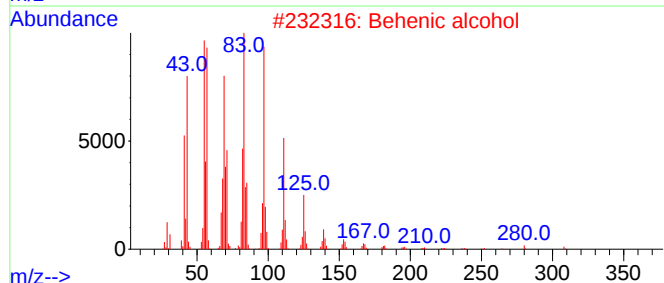
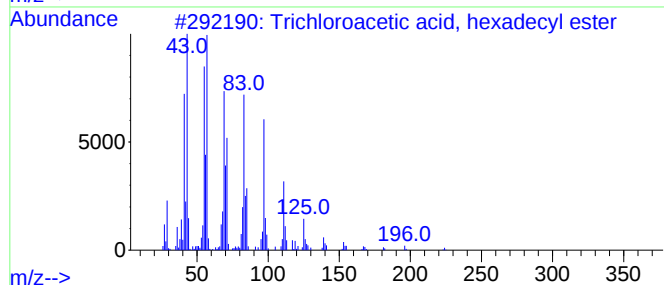
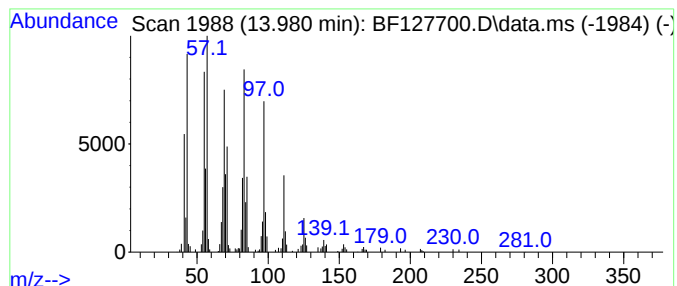
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.980	4.65 ng	197516	Chrysene-d12	14.145

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2			Behenic alcohol	326	C22H46O	000661-19-8	94
3			1-Hexacosanol	382	C26H54O	000506-52-5	91
4			1-Heneicosanol	312	C21H44O	015594-90-8	91
5			1-Nonadecene	266	C19H38	018435-45-5	91



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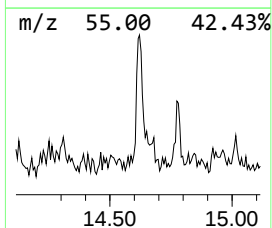
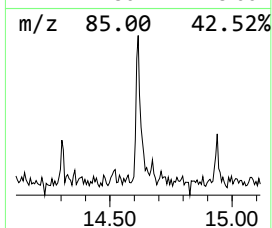
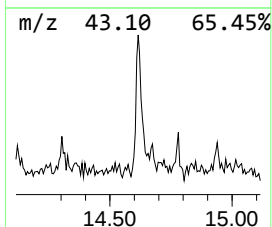
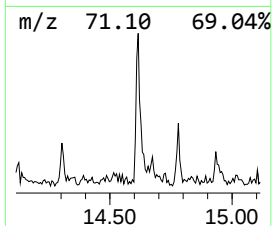
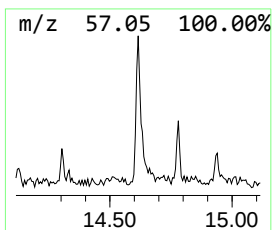
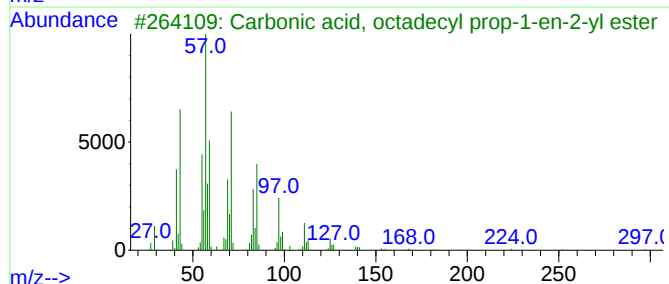
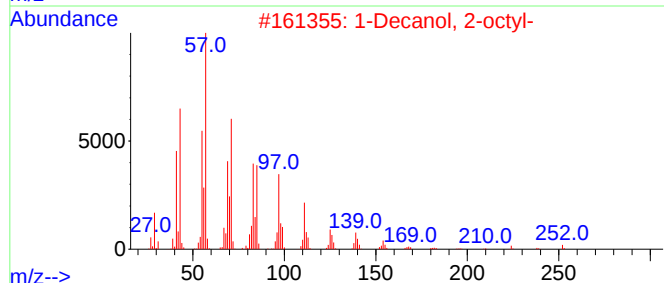
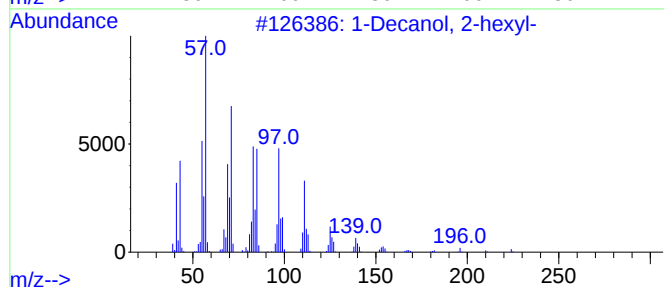
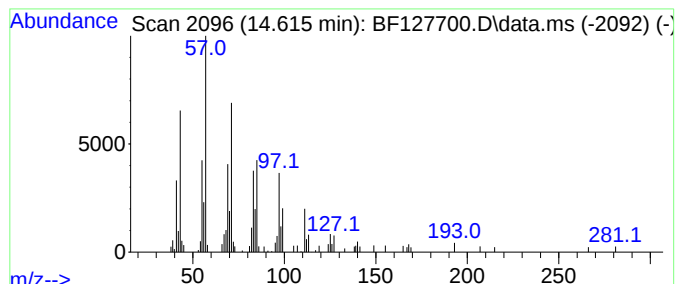
Instrument :
BNA_F
ClientSampleId :
20220350-AMENDED-096-21-02

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 1-Decanol, 2-hexyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.615	2.01 ng	85241	Chrysene-d12		14.145	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-Decanol, 2-hexyl-		242	C16H34O	002425-77-6	86
2	1-Decanol, 2-octyl-		270	C18H38O	045235-48-1	86
3	Carbonic acid, octadecyl prop-1-...		354	C22H42O3	1000383-11-5	83
4	Carbonic acid, hexadecyl prop-1-...		326	C20H38O3	1000382-90-3	80
5	Eicosyl isobutyl ether		354	C24H50O	1000406-33-0	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040722\
Data File : BF127700.D
Acq On : 07 Apr 2022 23:24
Operator : CG\JU
Sample : N2207-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220350-AMENDED-096-21-02

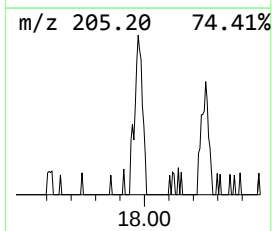
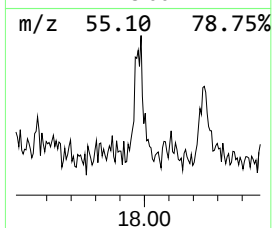
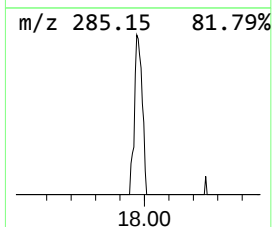
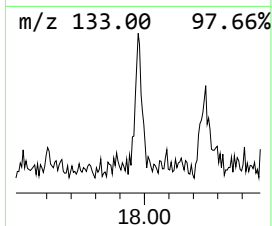
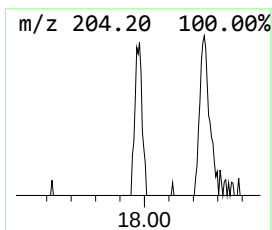
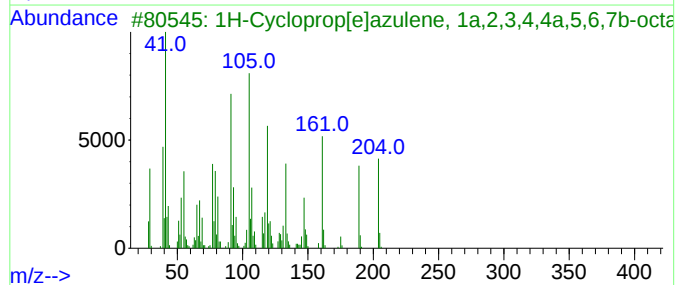
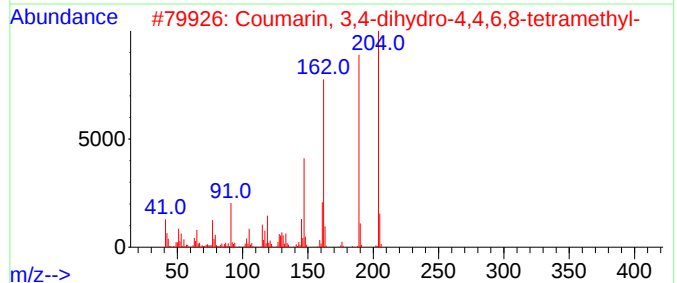
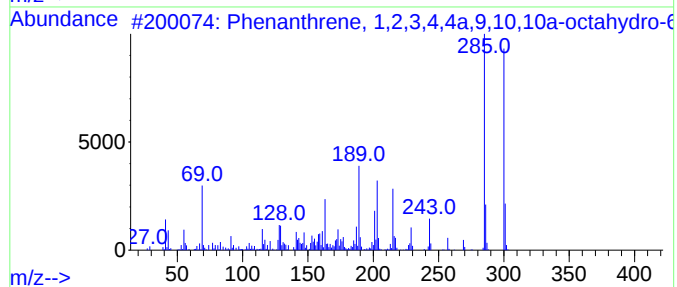
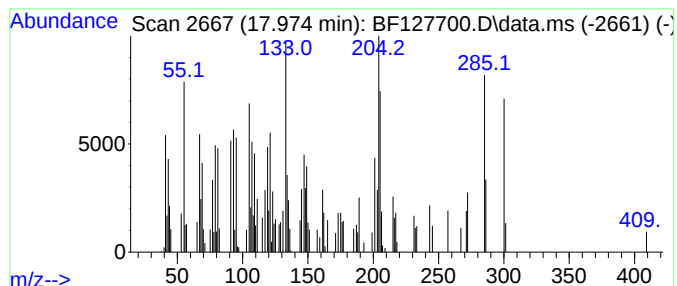
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown17.974 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.974	2.56 ng	110284	Perylene-d12	15.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 1,2,3,4,4a,9,10,10...	300	C21H32O	010064-26-3	44
2			Coumarin, 3,4-dihydro-4,4,6,8-te...	204	C13H16O2	249629-60-5	25
3			1H-Cycloprop[e]azulene, 1a,2,3,4...	204	C15H24	000489-40-7	20
4			cis-(-)-2,4a,5,6,9a-Hexahydro-3,...	204	C15H24	1000104-20-1	20
5			Quinoline, 2-phenyl-	205	C15H11N	000612-96-4	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040722\
Data File : BF127700.D
Acq On : 07 Apr 2022 23:24
Operator : CG\JU
Sample : N2207-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220350-AMENDED-096-21-02

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...	2.322	9.6	ng	371908	1	6.963	775774	20.0
2-Pentanone, 4-...	5.240	206.7	ng	8015710	1	6.963	775774	20.0
unknown7.686	7.686	16.7	ng	824059	2	8.245	989031	20.0
unknown10.933	10.933	3.6	ng	206829	4	11.498	1138040	20.0
Trichloroacetic...	13.980	4.7	ng	197516	5	14.145	848882	20.0
1-Decanol, 2-he...	14.615	2.0	ng	85241	5	14.145	848882	20.0
unknown17.974	17.974	2.6	ng	110284	6	15.674	860166	20.0