

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010224\
 Data File : BF136881.D
 Acq On : 02 Jan 2024 20:26
 Operator : CG\JU
 Sample : 05898-08
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GHL-SS-72a

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-BF122023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136881.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.428	564	568	583	rBV	1521520	1471290	30.70%	6.376%
2	6.428	734	738	756	rBV	1472984	1586849	33.12%	6.877%
3	6.781	794	798	801	rBV	534963	421440	8.79%	1.826%
4	7.345	889	894	897	rBV	1140704	1034801	21.59%	4.485%
5	8.057	1011	1015	1017	rBV	669880	541973	11.31%	2.349%
6	8.075	1017	1018	1023	rVB	79917	57784	1.21%	0.250%
7	8.769	1133	1136	1139	rBV	100267	76494	1.60%	0.332%
8	9.133	1193	1198	1201	rBV	2266944	1839063	38.38%	7.970%
9	9.810	1310	1313	1316	rBV	651803	564954	11.79%	2.448%
10	9.845	1316	1319	1324	rVB	77166	67330	1.41%	0.292%
11	10.016	1345	1348	1353	rBV	149901	133414	2.78%	0.578%
12	10.363	1403	1407	1413	rBV	335352	291030	6.07%	1.261%
13	10.604	1442	1448	1460	rBV	1008665	960176	20.04%	4.161%
14	10.974	1508	1511	1518	rBV	93079	87740	1.83%	0.380%
15	11.304	1562	1567	1569	rBV	679428	601088	12.54%	2.605%
16	11.327	1569	1571	1574	rVV	679529	542745	11.33%	2.352%
17	11.386	1576	1581	1583	rVV	2050126	1740750	36.33%	7.544%
18	11.410	1583	1585	1589	rVB3	228939	217652	4.54%	0.943%
19	11.539	1604	1607	1610	rBV	601468	517031	10.79%	2.241%
20	11.769	1642	1646	1649	rBV2	42270	64029	1.34%	0.277%
21	11.874	1655	1664	1670	rBV	2831684	4791888	100.00%	20.768%
22	12.010	1680	1687	1692	rBV4	79076	136103	2.84%	0.590%
23	12.080	1696	1699	1702	rVV	133447	138270	2.89%	0.599%
24	12.139	1706	1709	1713	rBV2	573081	521292	10.88%	2.259%
25	12.174	1713	1715	1720	rVV4	50106	59912	1.25%	0.260%
26	12.227	1721	1724	1725	rVV	50925	50046	1.04%	0.217%
27	12.245	1725	1727	1731	rVV4	94463	107465	2.24%	0.466%
28	12.521	1768	1774	1776	rBV	169060	199589	4.17%	0.865%
29	12.557	1776	1780	1788	rVV	873531	1120336	23.38%	4.855%
30	12.633	1790	1793	1799	rVB	147932	152850	3.19%	0.662%
31	12.751	1806	1813	1816	rBV	104990	143254	2.99%	0.621%
32	12.904	1832	1839	1842	rBV	1509946	1442545	30.10%	6.252%
33	13.010	1854	1857	1860	rBV	336753	287308	6.00%	1.245%
34	13.474	1933	1936	1943	rVB	49014	60514	1.26%	0.262%
35	13.851	1996	2000	2010	rVB6	44077	106132	2.21%	0.460%
36	13.963	2012	2019	2021	rBV2	377793	469214	9.79%	2.034%

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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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.986	2021	2023	2026	rVB	69821	57308	1.20%	0.248%
38	15.439	2265	2270	2274	rBV	319452	412092	8.60%	1.786%

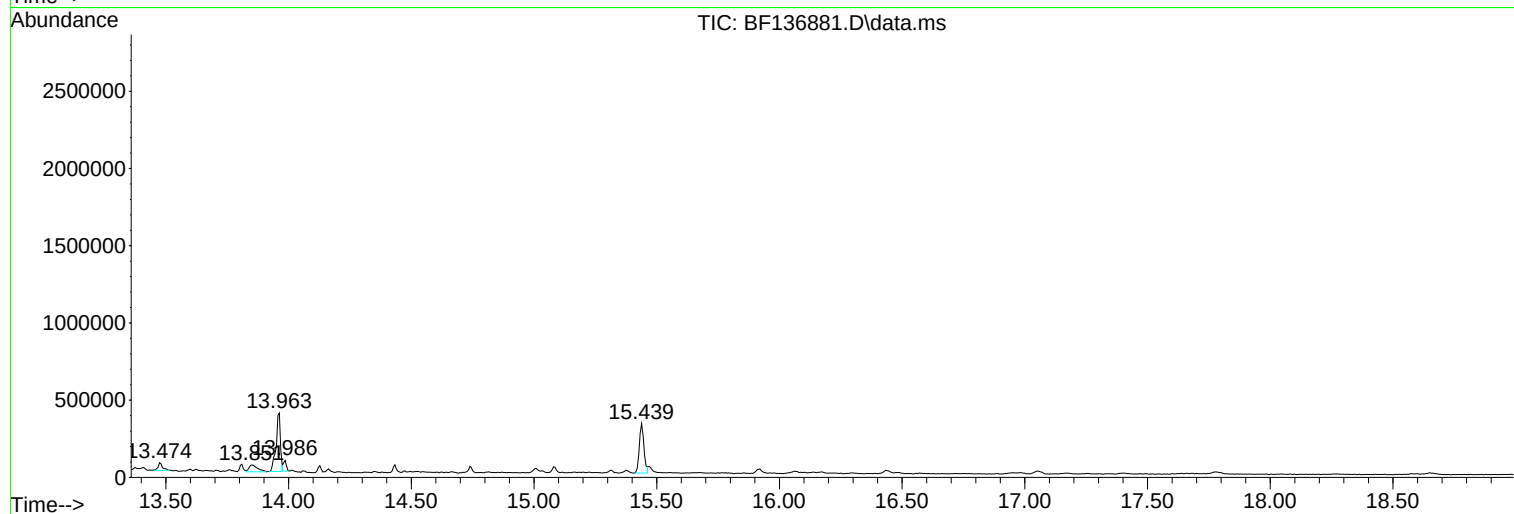
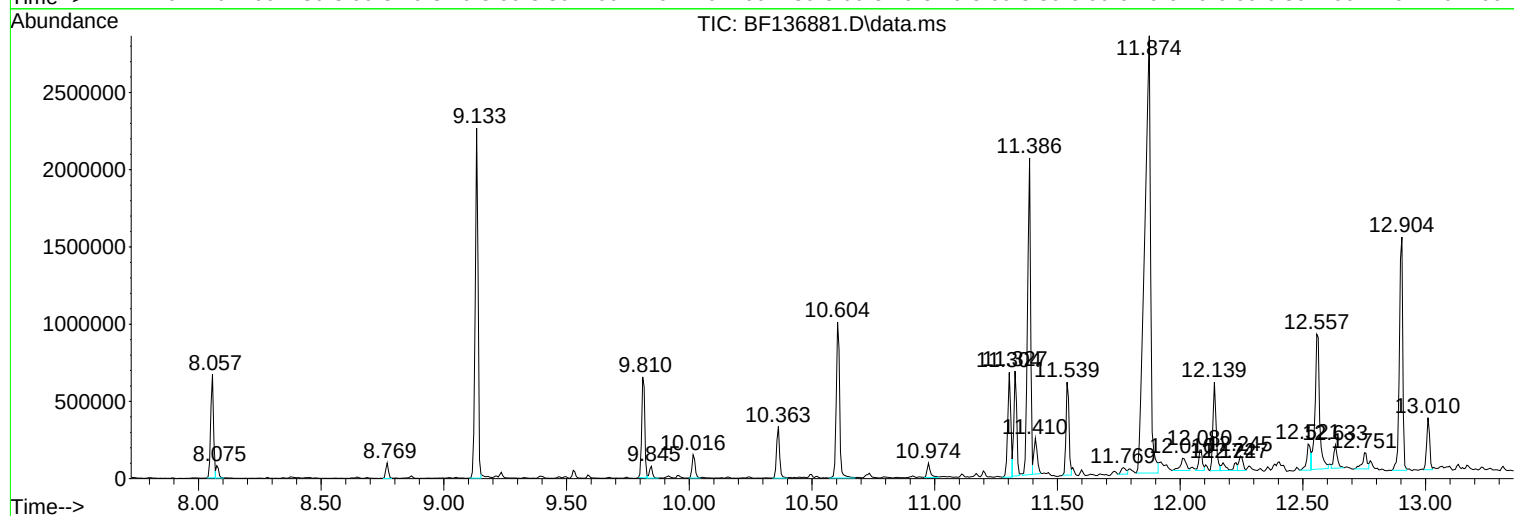
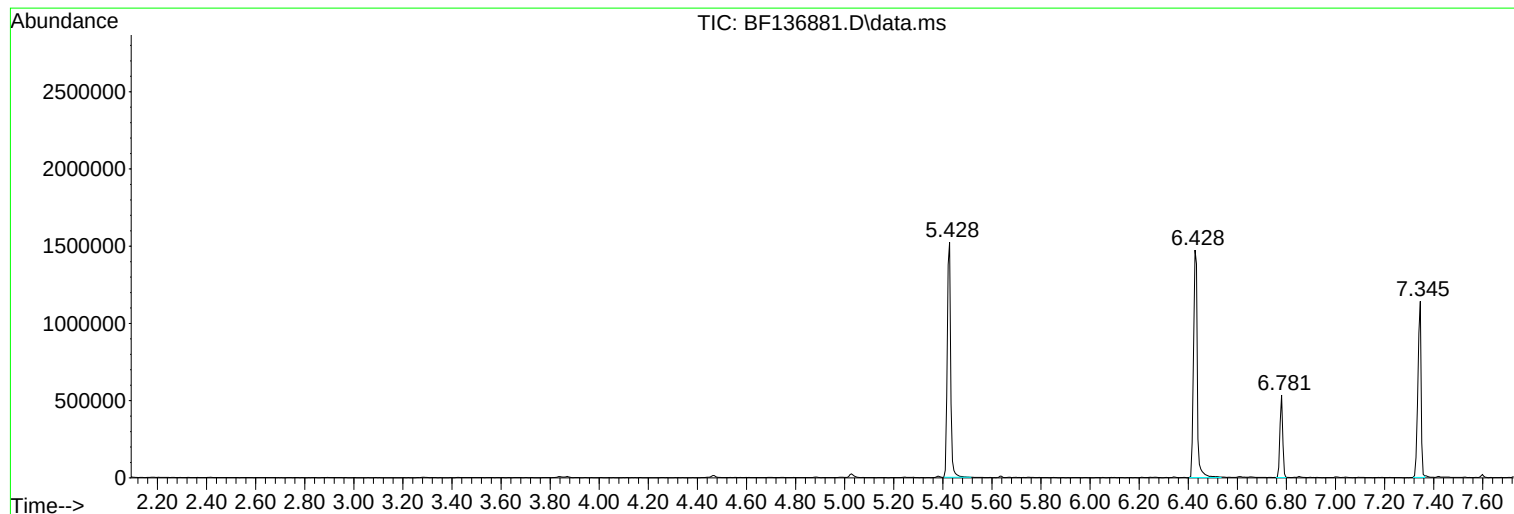
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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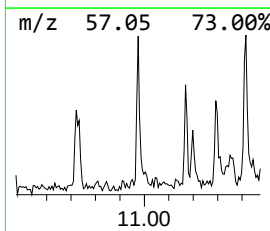
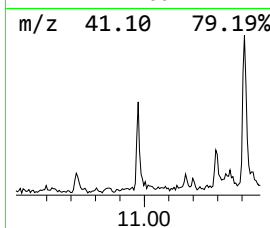
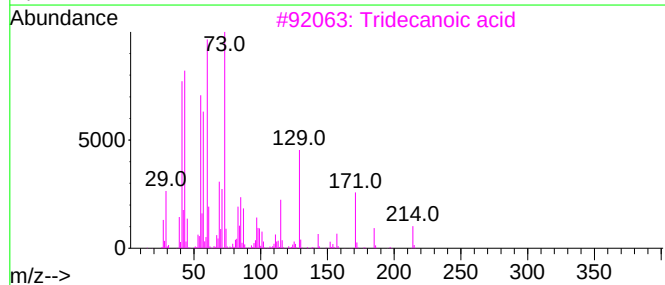
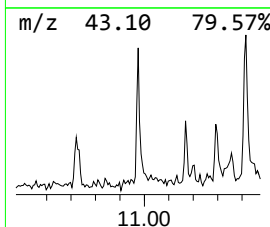
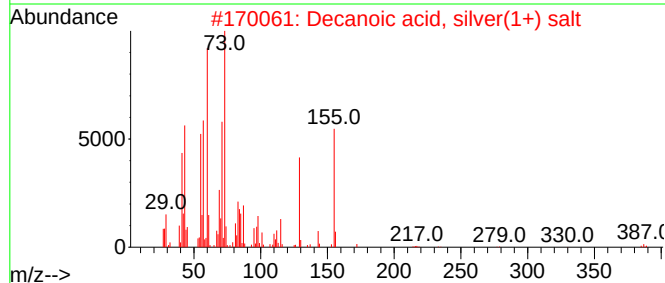
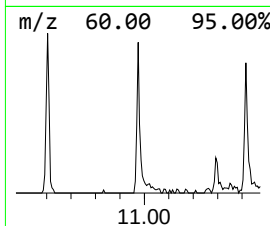
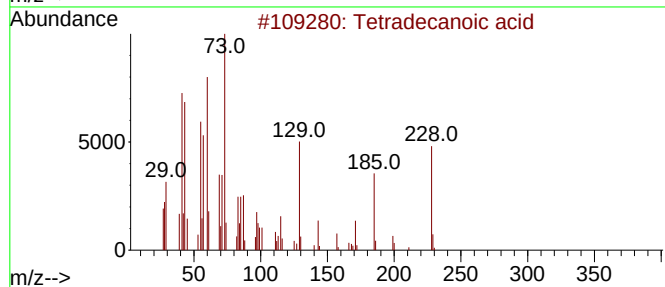
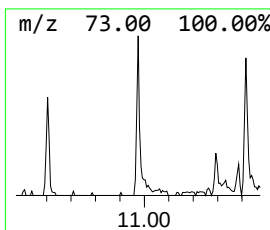
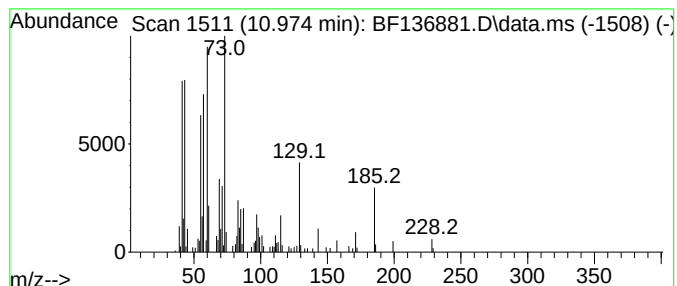
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Tetradecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.975	2.92 ng	87740	Phenanthrene-d10	11.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid	228	C14H28O2	000544-63-8	95
2			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	80
3			Tridecanoic acid	214	C13H26O2	000638-53-9	74
4			n-Decanoic acid	172	C10H20O2	000334-48-5	70
5			Dodecanoic acid	200	C12H24O2	000143-07-7	64



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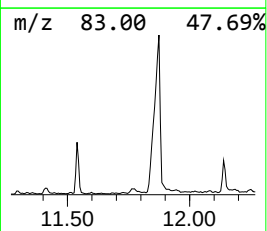
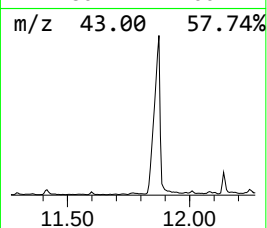
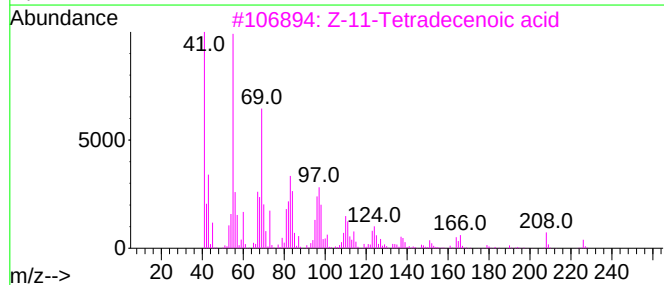
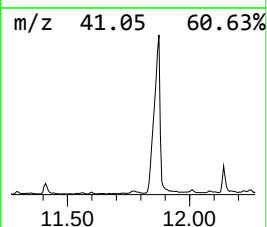
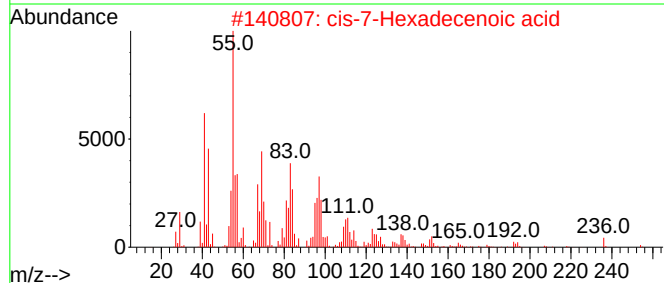
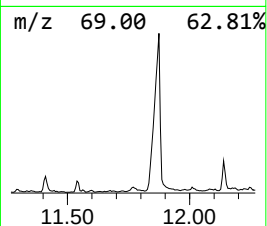
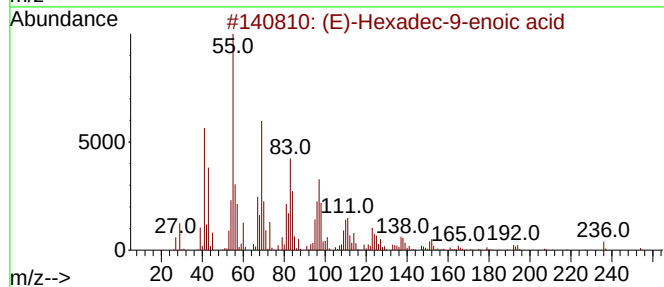
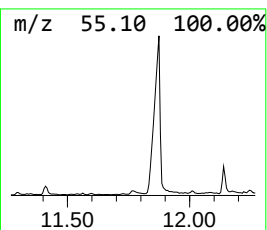
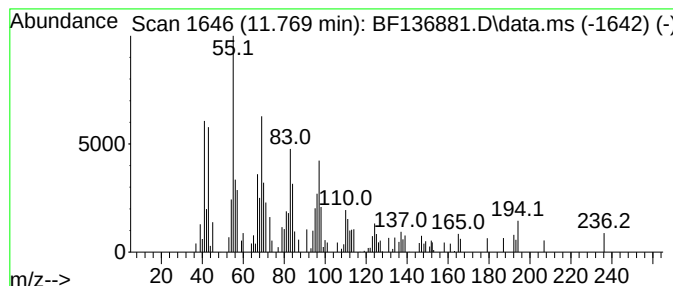
Instrument :
BNA_F
ClientSampleId :
GHL-SS-72a

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 (E)-Hexadec-9-enoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.769	2.13 ng	64029	Phenanthrene-d10		11.304	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	(E)-Hexadec-9-enoic acid		254	C16H30O2	010030-73-6	91
2	cis-7-Hexadecenoic acid		254	C16H30O2	002416-19-5	90
3	Z-11-Tetradecenoic acid		226	C14H26O2	1000130-83-3	86
4	Hexadecenoic acid, Z-11-		254	C16H30O2	002416-20-8	80
5	Myristoleic acid		226	C14H26O2	000544-64-9	74



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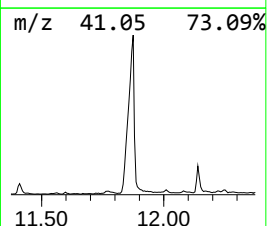
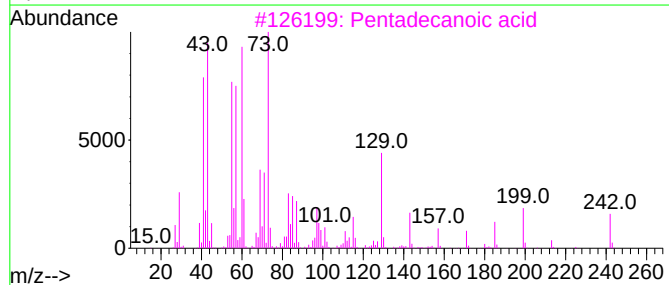
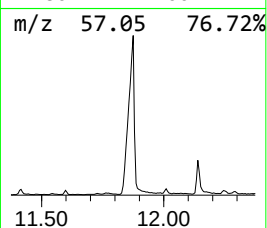
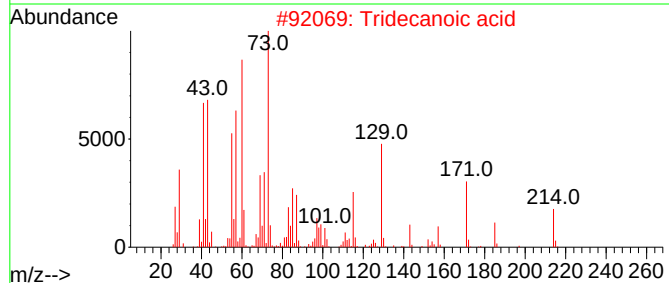
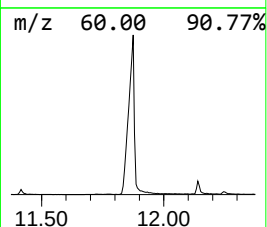
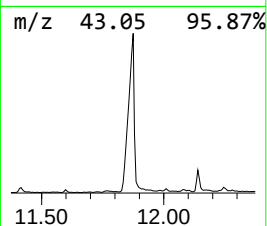
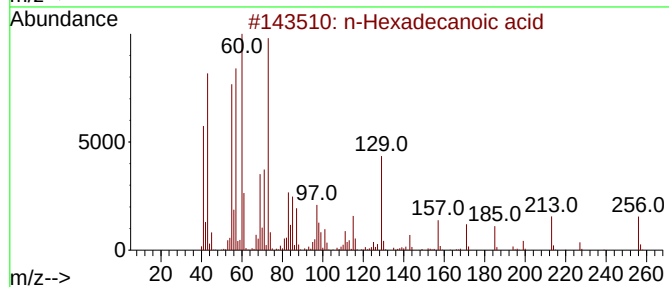
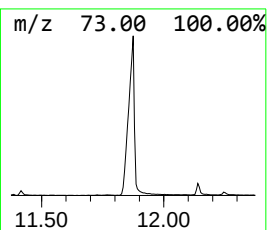
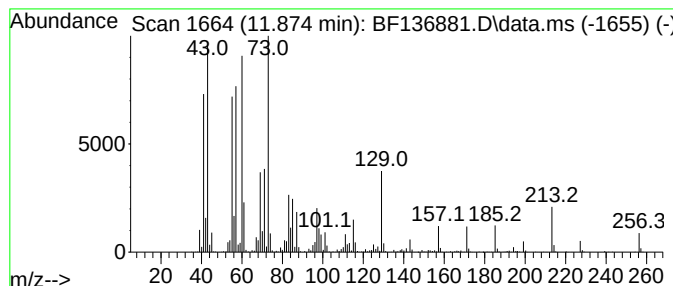
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.874	159.44 ng	4791890	Phenanthrene-d10	11.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	95
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5			Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	25



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GHL-SS-72a

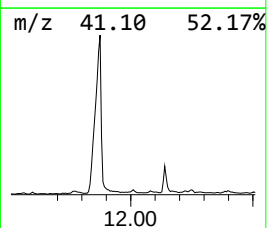
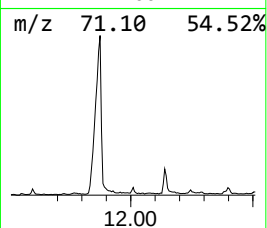
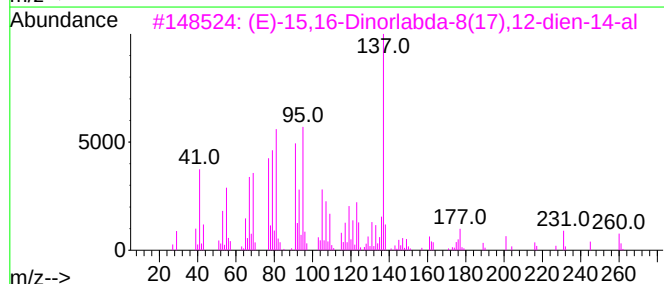
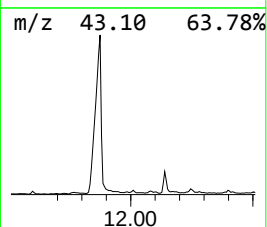
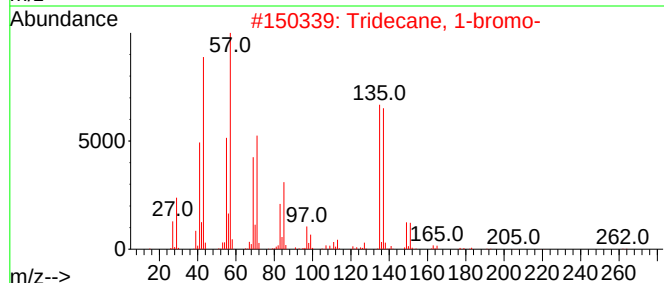
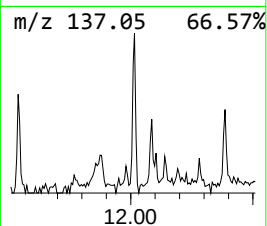
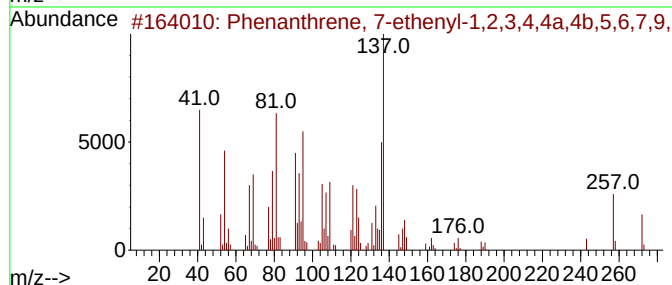
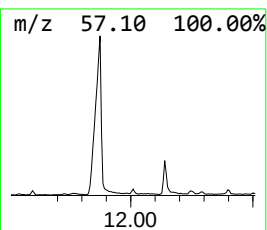
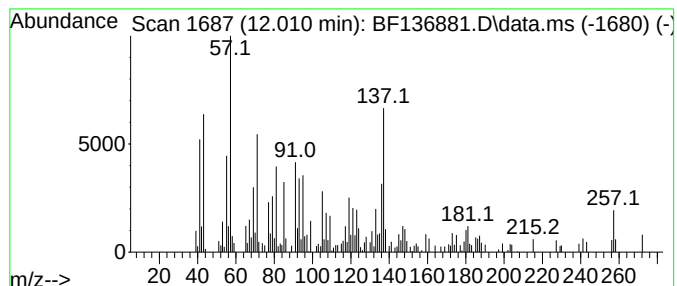
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Phenanthrene, 7-ethenyl-1,2... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.010	4.53 ng	136103	Phenanthrene-d10	11.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 7-ethenyl-1,2,3,4,...	272	C20H32	001686-56-2	95
2			Tridecane, 1-bromo-	262	C13H27Br	000765-09-3	38
3			(E)-15,16-Dinorlabda-8(17),12-di...	260	C18H28O	167817-63-2	27
4			Benzamide, 2-hydroxy-N-(4-methox...	257	C15H15NO3	1000337-81-8	18
5			Phosphonic acid, bicyclo[2.2.1]h...	204	C9H17O3P	031061-88-8	15



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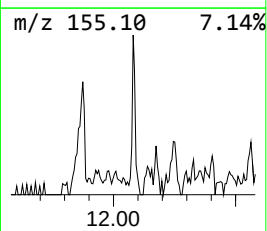
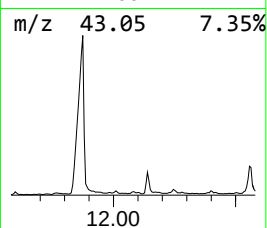
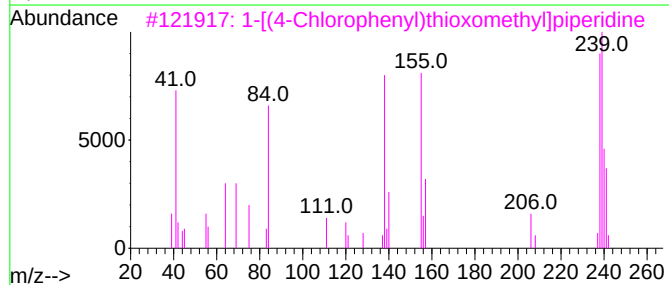
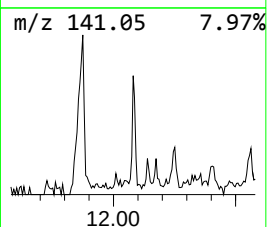
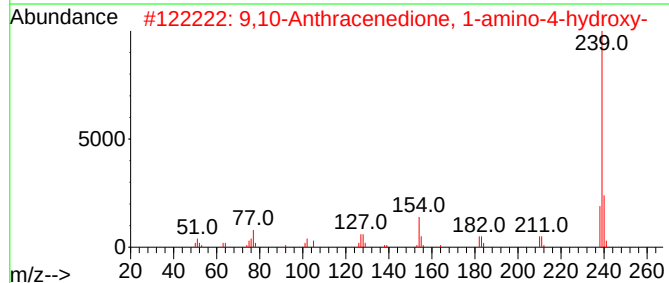
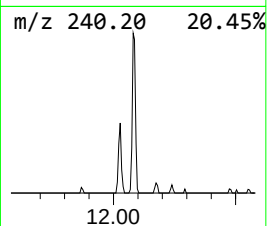
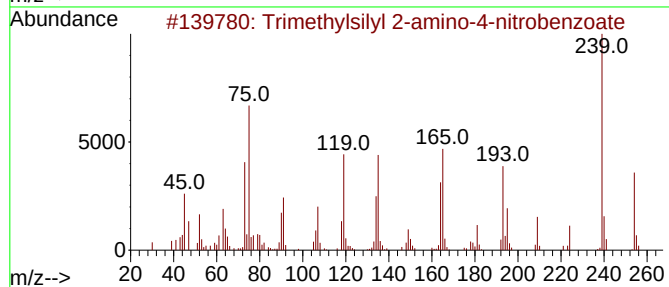
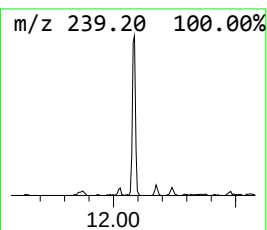
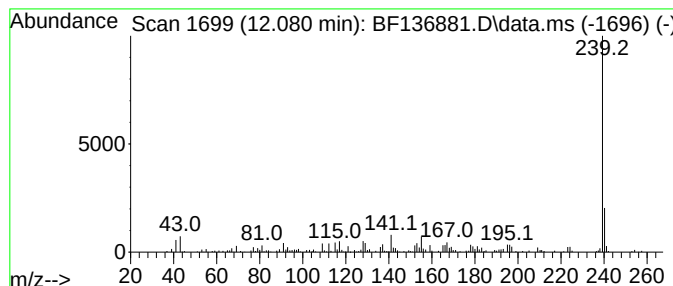
Instrument :
BNA_F
ClientSampleId :
GHL-SS-72a

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Trimethylsilyl 2-amino-4-ni... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD			R.T.
12.080	4.60 ng	138270	Phenanthrene-d10			11.304
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Trimethylsilyl 2-amino-4-nitrobenzoate		254	C10H14N2O4Si	1000473-63-5	74
2	9,10-Anthracenedione, 1-amino-4-hydroxy-		239	C14H9NO3	000116-85-8	64
3	1-[(4-Chlorophenyl)thioxomethyl]piperidine		239	C12H14ClNS	003335-29-3	64
4	4-(4-Oxo-1,2,3,4,6,7,12,12b-octalindol-5-yl)-2-methyl-1H-imidazole		326	C19H22N2O3	1000137-91-1	56
5	Benzaldehyde, 3-[4-(1,1-dimethyl-2-oxo-1,2,3,4-tetrahydropyridin-5-yl)-2-methyl-1H-imidazol-5-yl]-		254	C17H18O2	069770-23-6	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010224\
Data File : BF136881.D
Acq On : 02 Jan 2024 20:26
Operator : CG\JU
Sample : 05898-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
GHL-SS-72a

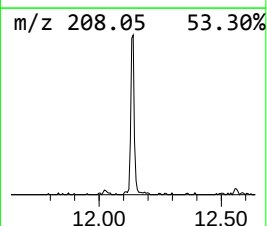
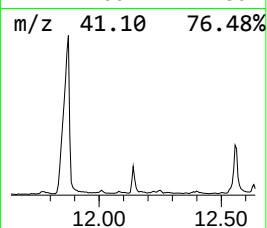
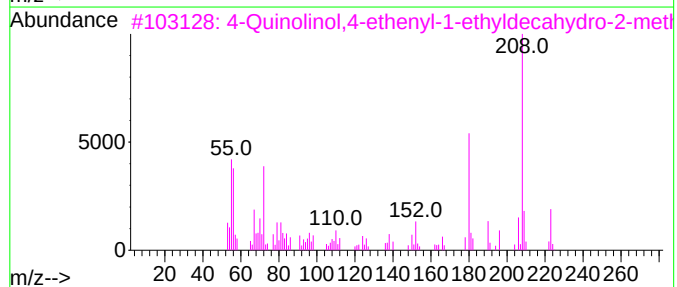
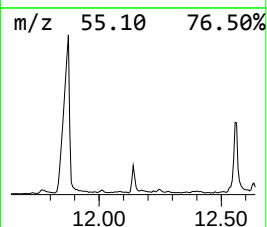
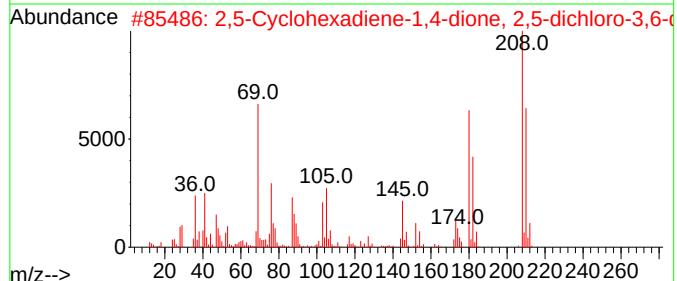
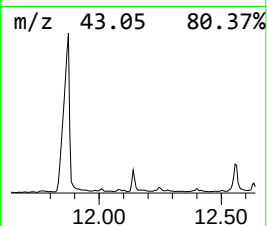
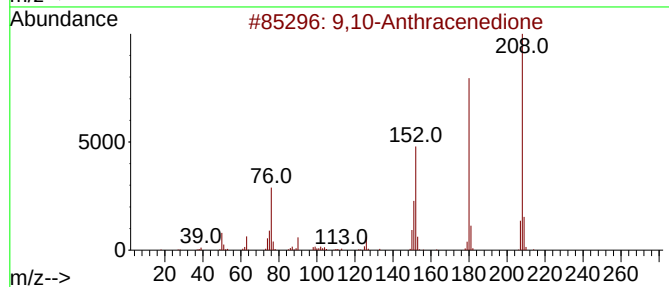
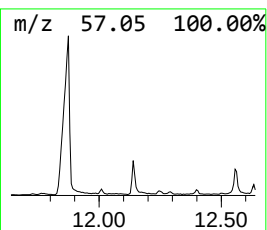
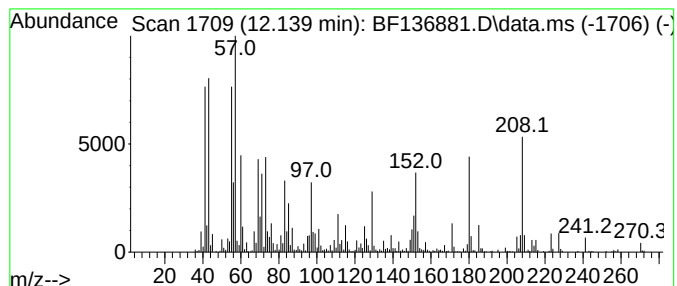
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown12.139 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.139	17.34 ng	521292	Phenanthrene-d10	11.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Anthracenedione		208	C14H8O2	000084-65-1	46	
2	2,5-Cyclohexadiene-1,4-dione, 2,...		208	C6H2C12O4	000087-88-7	22	
3	4-Quinolinol,4-ethenyl-1-ethylde...		223	C14H25NO	038463-59-1	16	
4	2-(Dicyanomethylene)indene-1,3-d...		208	C12H4N2O2	016954-74-8	14	
5	1,4-Anthracenedione		208	C14H8O2	000635-12-1	14	



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Data File : BF136881.D
Acq On : 02 Jan 2024 20:26
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Sample : 05898-08
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ALS Vial : 7 Sample Multiplier: 1

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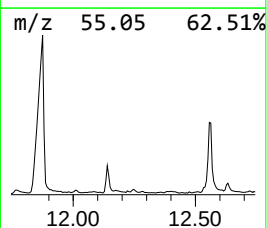
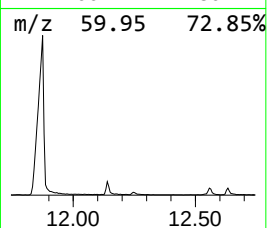
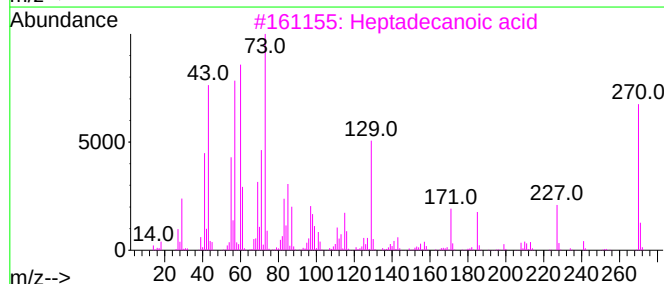
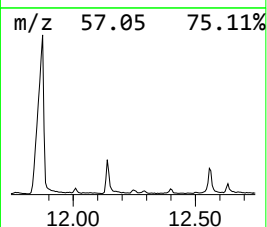
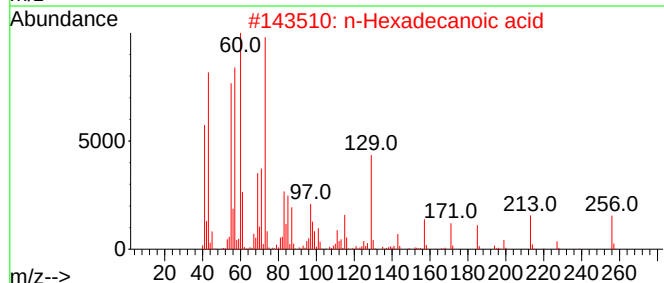
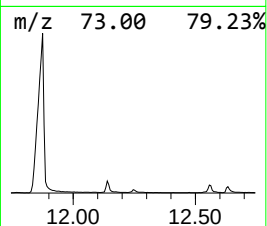
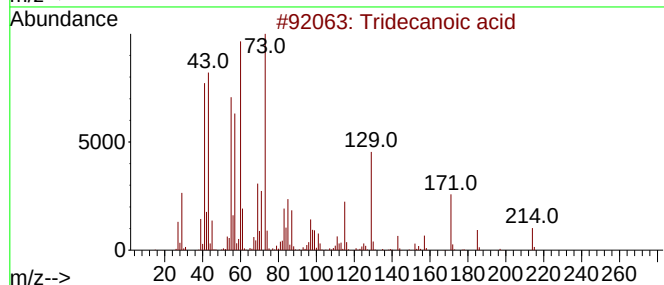
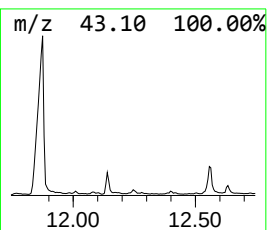
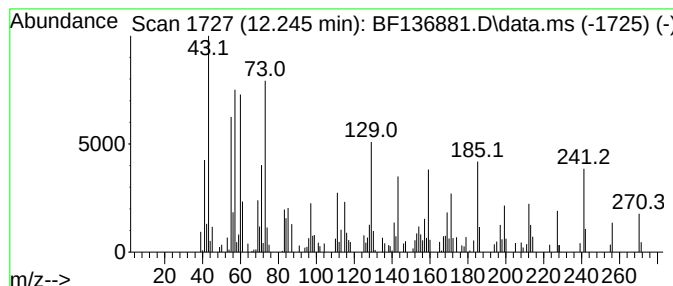
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tridecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.245	3.58 ng	107465	Phenanthrene-d10	11.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	53
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	41
3			Heptadecanoic acid	270	C17H34O2	000506-12-7	38
4			Carbanilic acid, m-chloro-, 1-me...	241	C12H16ClNO2	005513-20-2	25
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010224\
Data File : BF136881.D
Acq On : 02 Jan 2024 20:26
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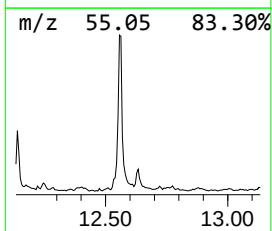
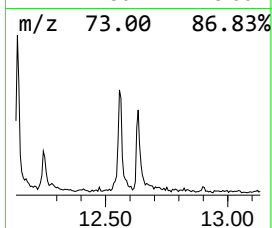
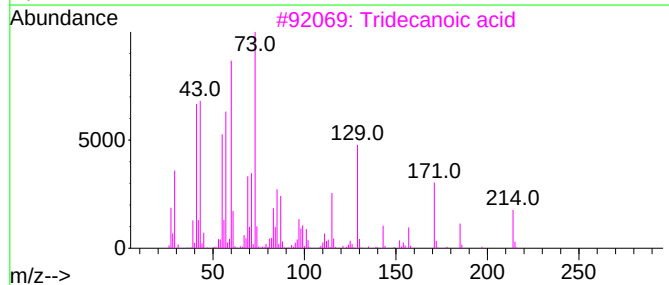
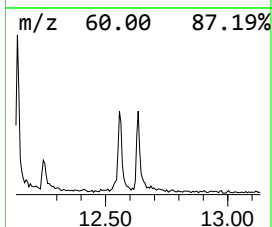
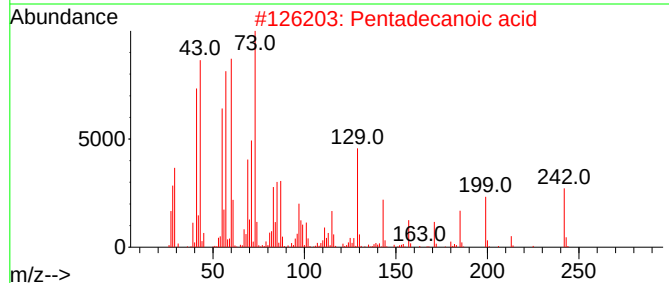
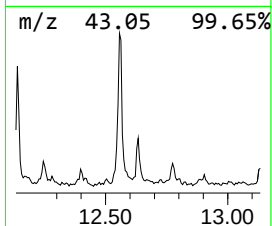
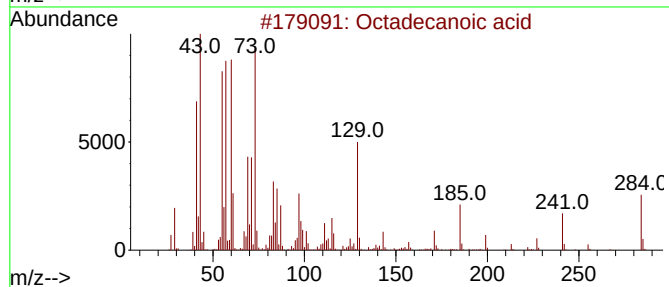
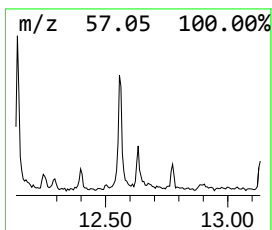
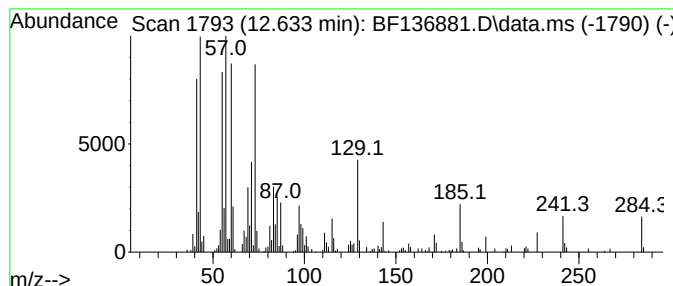
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.633	5.09 ng	152850	Phenanthrene-d10	11.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Tridecanoic acid	214	C13H26O2	000638-53-9	86
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010224\
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Sample : 05898-08
Misc :
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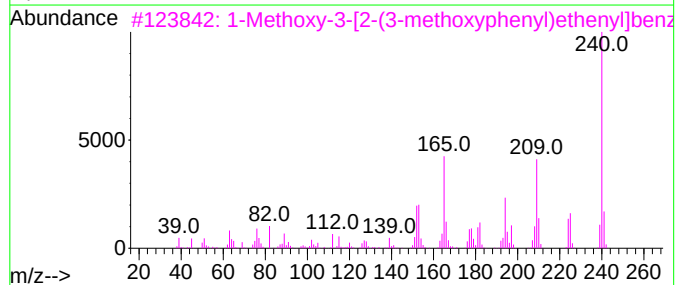
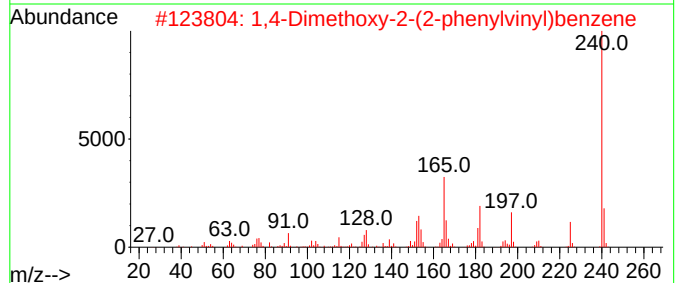
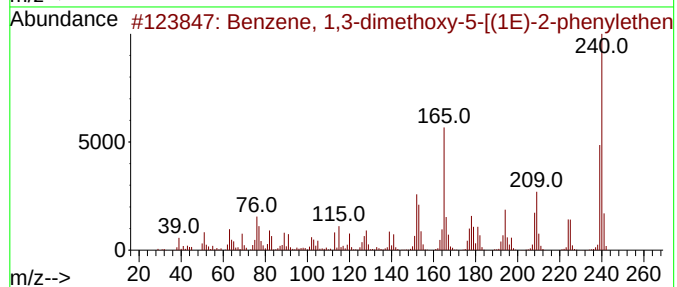
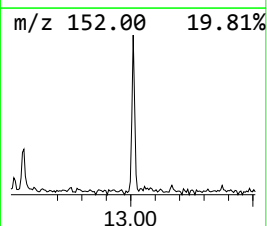
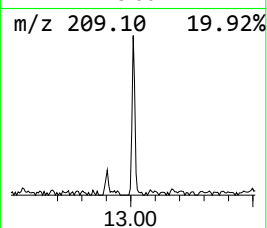
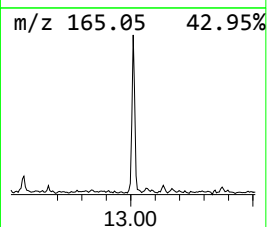
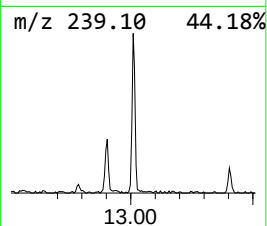
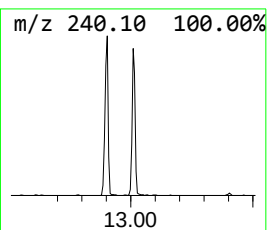
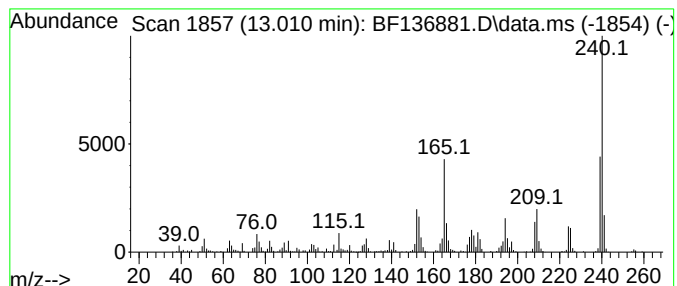
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzene, 1,3-dimethoxy-5-[(... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.010	12.25 ng	287308	Chrysene-d12	13.963	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3-dimethoxy-5-[(1E)-2...	240	C16H16O2	021956-56-9	99
2	1,4-Dimethoxy-2-(2-phenylvinyl)b...	240	C16H16O2	021889-09-8	78
3	1-Methoxy-3-[2-(3-methoxyphenyl)...	240	C16H16O2	006325-63-9	70
4	Cyclohexane, hexaethylidene-	240	C18H24	001482-93-5	55
5	[1,1'-Biphenyl]-4,4'-diamine, 3,...	240	C16H20N2	054827-17-7	55



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010224\
Data File : BF136881.D
Acq On : 02 Jan 2024 20:26
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Sample : 05898-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

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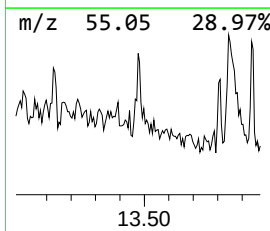
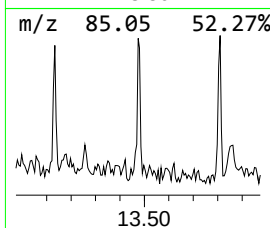
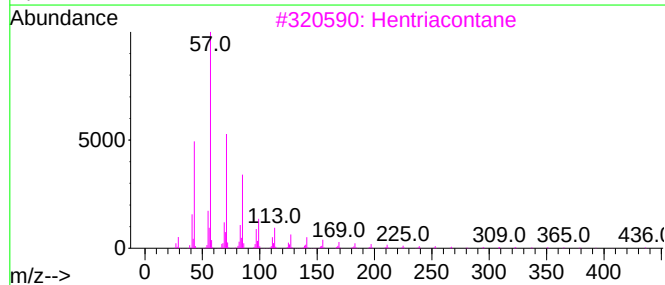
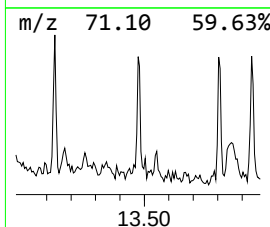
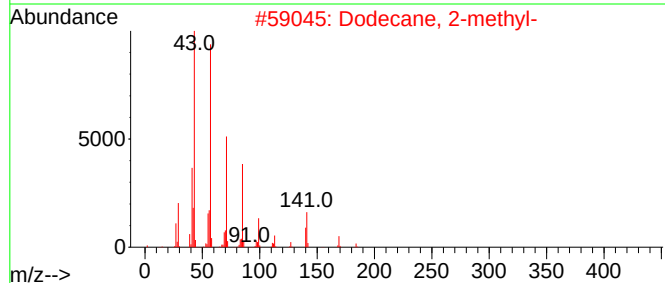
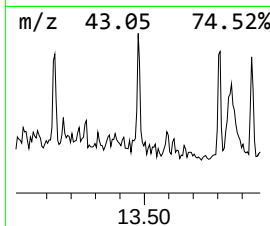
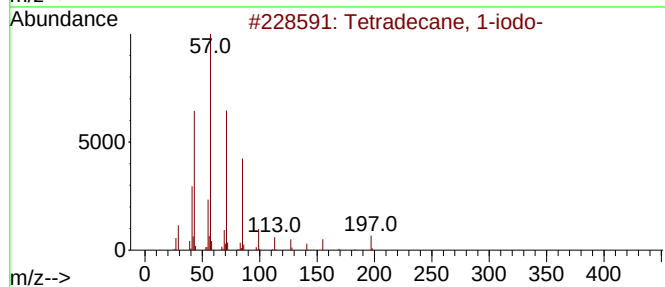
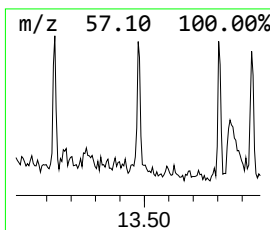
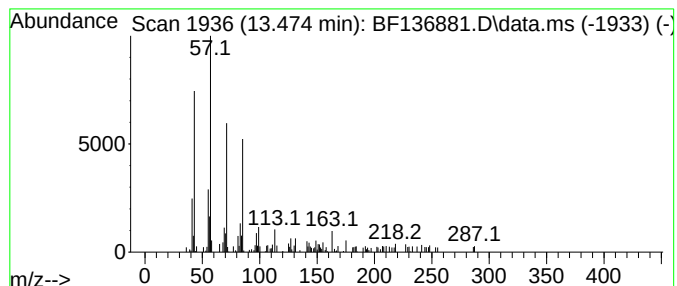
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tetradecane, 1-iodo- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.474	2.58 ng	60514	Chrysene-d12	13.963

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	80
2		Dodecane, 2-methyl-	184	C13H28	001560-97-0	64
3		Hentriacontane	437	C31H64	000630-04-6	62
4		Octadecane	254	C18H38	000593-45-3	58
5		Eicosane	282	C20H42	000112-95-8	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010224\
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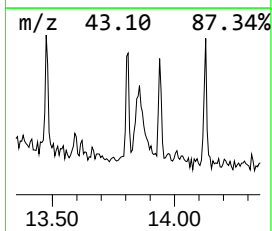
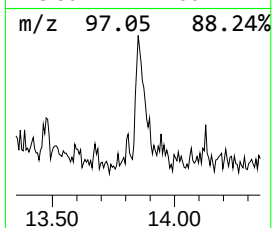
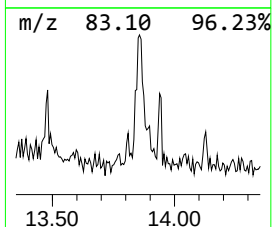
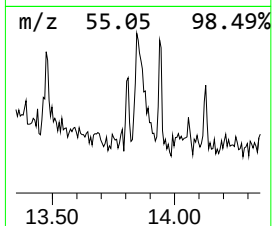
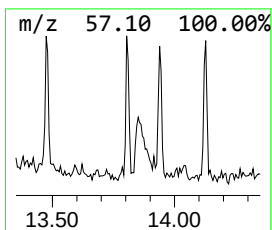
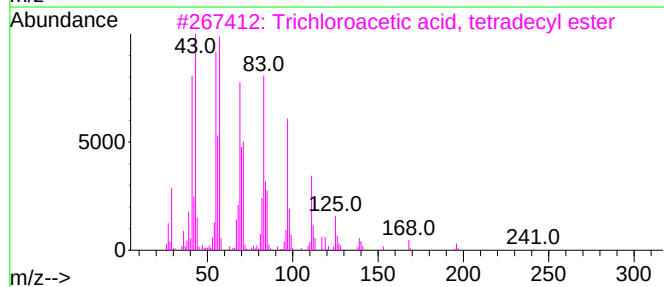
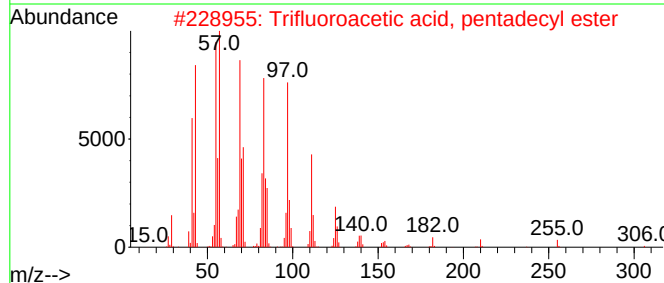
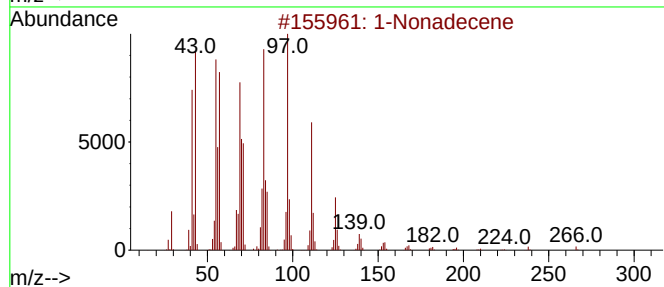
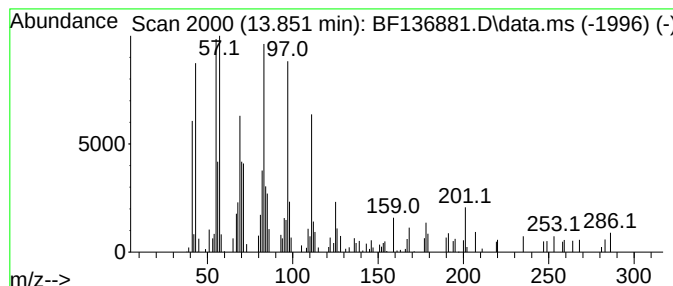
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Nonadecene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.851	4.52 ng	106132	Chrysene-d12		13.963	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-Nonadecene		266	C19H38	018435-45-5	94
2	Trifluoroacetic acid, pentadecyl...		324	C17H31F3O2	959010-23-2	91
3	Trichloroacetic acid, tetradecyl...		358	C16H29Cl3O2	074339-52-9	91
4	Bacteriochlorophyll-c-stearyl		841	C52H72MgN4O4	1010164-49-7	91
5	11-Tricosene		322	C23H46	052078-56-5	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010224\
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Misc :
ALS Vial : 7 Sample Multiplier: 1

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

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

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					#	RT	Resp	Conc
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(E)-Hexadec-9-e...	11.769	2.1	ng	64029	4	11.304	601088	20.0
n-Hexadecanoic ...	11.874	159.4	ng	4791890	4	11.304	601088	20.0
Phenanthrene, 7...	12.010	4.5	ng	136103	4	11.304	601088	20.0
Trimethylsilyl ...	12.080	4.6	ng	138270	4	11.304	601088	20.0
unknown12.139	12.139	17.3	ng	521292	4	11.304	601088	20.0
Tridecanoic acid	12.245	3.6	ng	107465	4	11.304	601088	20.0
Octadecanoic acid	12.633	5.1	ng	152850	4	11.304	601088	20.0
Benzene, 1,3-di...	13.010	12.3	ng	287308	5	13.963	469214	20.0
Tetradecane, 1-...	13.474	2.6	ng	60514	5	13.963	469214	20.0
1-Nonadecene	13.851	4.5	ng	106132	5	13.963	469214	20.0