

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030321\
 Data File : BF123358.D
 Acq On : 3 Mar 2021 16:27
 Operator : JU/CG
 Sample : M1545-02
 Misc :
 ALS Vial : 7 Sample Multiplier: 4

Instrument :
 BNA_F
 ClientSampleId :
 MH-725

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-BF021921.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123358.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.840	123	128	132	rVB	5243929	6696130	29.51%	4.426%
2	5.557	584	590	593	rBV	5870574	6683959	29.45%	4.418%
3	6.504	744	751	766	rBV2	3096232	4735508	20.87%	3.130%
4	6.851	803	810	818	rBV	2677052	2785351	12.27%	1.841%
5	7.422	897	907	910	rBV	5174899	9763774	43.02%	6.454%
6	8.128	1019	1027	1031	rBV	2577081	3758840	16.56%	2.485%
7	8.704	1117	1125	1132	rBV2	150861	278932	1.23%	0.184%
8	9.210	1200	1211	1214	rVB	8146748	15450469	68.08%	10.214%
9	9.598	1270	1277	1280	rBV	265737	278047	1.23%	0.184%
10	9.886	1316	1326	1329	rBV	3089633	4375160	19.28%	2.892%
11	9.916	1329	1331	1335	rVB	342870	290558	1.28%	0.192%
12	10.292	1389	1395	1397	rBV	154153	240645	1.06%	0.159%
13	10.692	1450	1463	1466	rBV	6073016	10384904	45.76%	6.865%
14	11.380	1569	1580	1583	rBV	3676349	4243516	18.70%	2.805%
15	11.551	1600	1609	1610	rBV2	192666	437903	1.93%	0.289%
16	11.839	1654	1658	1659	rBV2	201689	245338	1.08%	0.162%
17	11.886	1659	1666	1668	rVV2	2428278	3775739	16.64%	2.496%
18	11.951	1668	1677	1680	rVB	5981472	11961827	52.71%	7.907%
19	12.198	1715	1719	1723	rVB	286363	338986	1.49%	0.224%
20	12.357	1742	1746	1749	rVB	1326410	1204013	5.31%	0.796%
21	12.410	1752	1755	1759	rVB	342604	317733	1.40%	0.210%
22	12.533	1773	1776	1779	rBV	403898	495458	2.18%	0.328%
23	12.569	1779	1782	1784	rVV	495133	494592	2.18%	0.327%
24	12.633	1784	1793	1795	rVV4	1061648	2304896	10.16%	1.524%
25	12.680	1795	1801	1803	rVV	4078030	6713624	29.58%	4.438%
26	12.757	1803	1814	1819	rVB	9210863	22694147	100.00%	15.002%
27	12.992	1841	1854	1857	rVB2	9044682	16174513	71.27%	10.692%
28	13.427	1925	1928	1936	rBV4	161457	251709	1.11%	0.166%
29	13.586	1943	1955	1958	rBV2	482988	1842814	8.12%	1.218%
30	13.874	2000	2004	2017	rVB	2112118	2909345	12.82%	1.923%
31	14.039	2027	2032	2035	rVB	3920143	3929049	17.31%	2.597%
32	14.516	2111	2113	2123	rVB2	216729	339724	1.50%	0.225%
33	15.515	2276	2283	2287	rBV	2819382	4171657	18.38%	2.758%
34	16.027	2365	2370	2383	rVV4	244658	705177	3.11%	0.466%

Sum of corrected areas: 151274037

Instrument :

BNA_F

ClientSampleId :

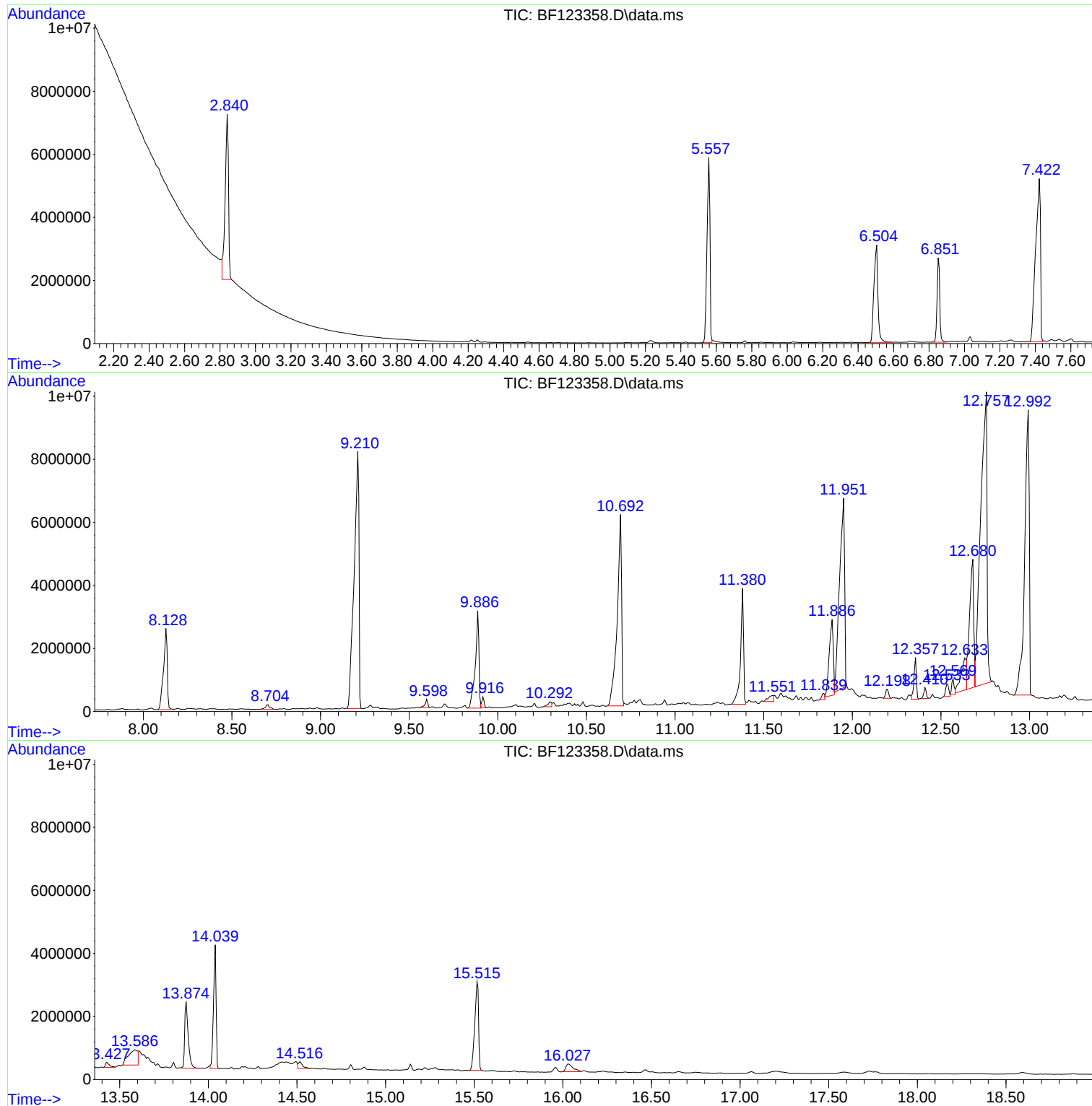
MH-725

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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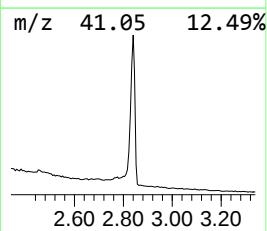
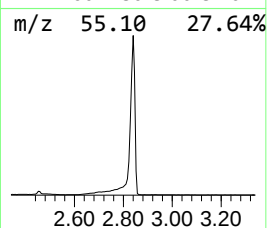
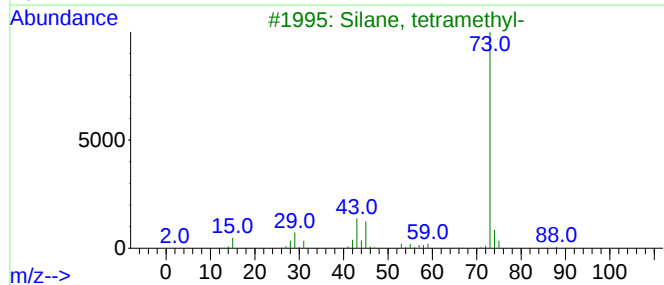
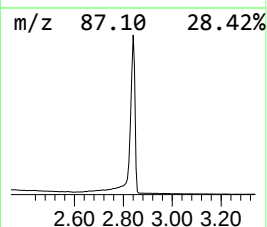
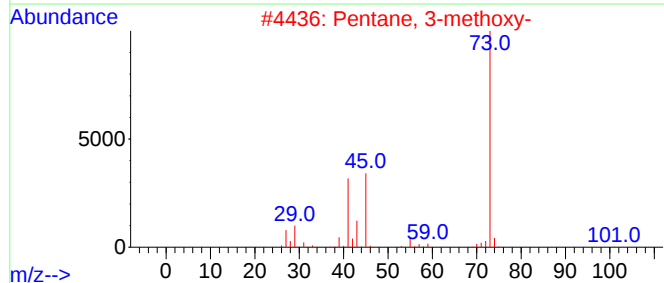
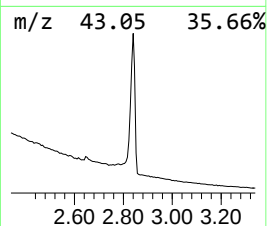
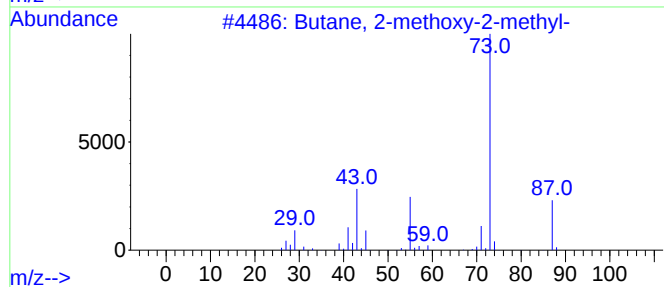
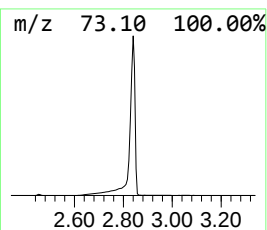
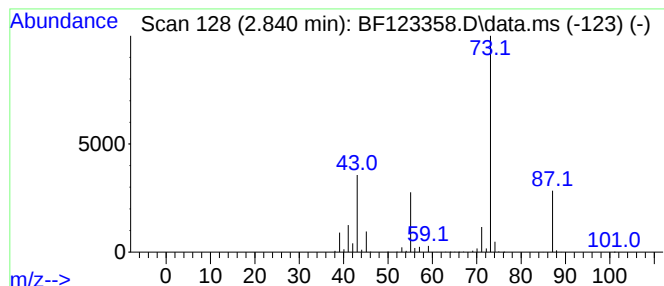
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.840	192.32 ng	6696130	1,4-Dichlorobenzene-d4	6.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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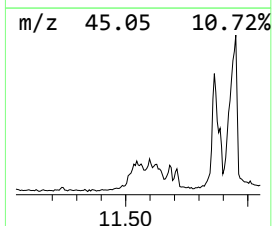
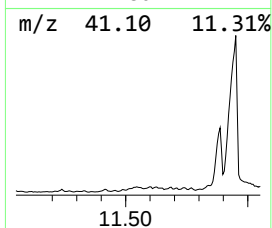
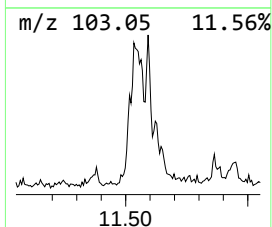
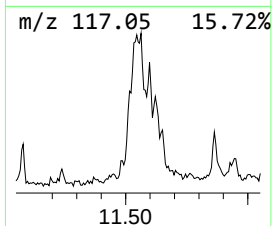
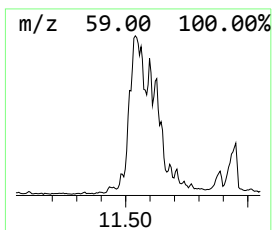
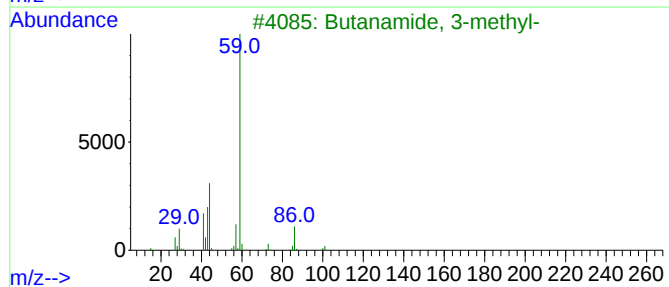
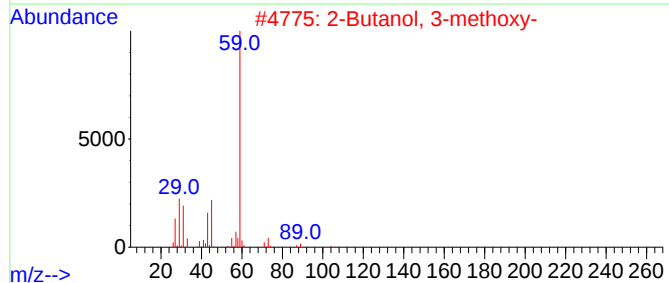
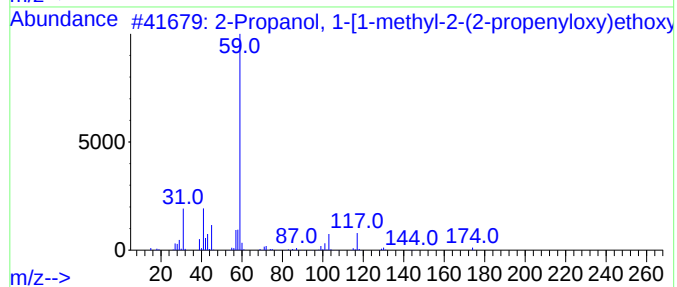
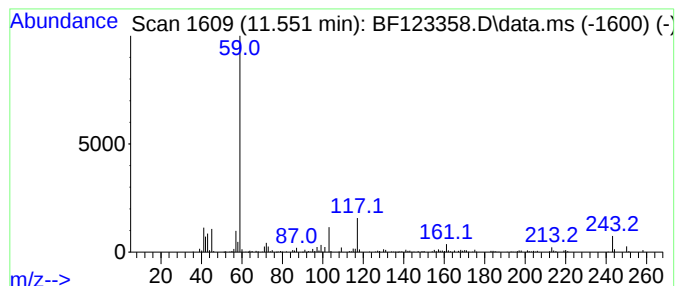
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Propanol, 1-[1-methyl-2-(... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.551	8.26 ng	437903	Phenanthrene-d10		11.381	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Propanol, 1-[1-methyl-2-(2-pro...		174	C9H18O3	055956-25-7	64
2	2-Butanol, 3-methoxy-		104	C5H12O2	053778-72-6	53
3	Butanamide, 3-methyl-		101	C5H11NO	000541-46-8	50
4	Tri(1,2-propyleneglycol), monome...		206	C10H22O4	1000262-26-6	45
5	2-Propanol, 1-[2-(2-methoxy-1-me...		206	C10H22O4	020324-33-8	45



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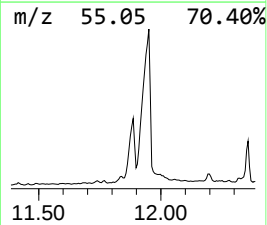
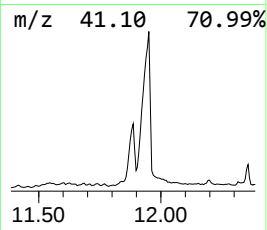
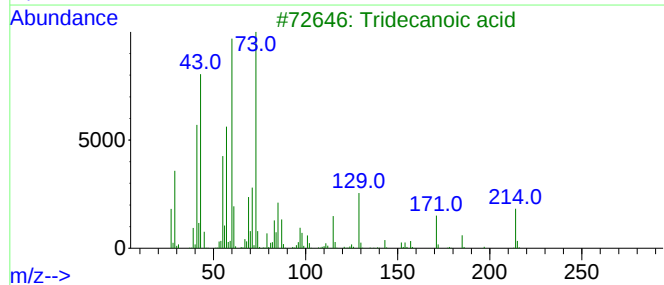
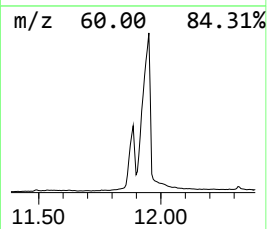
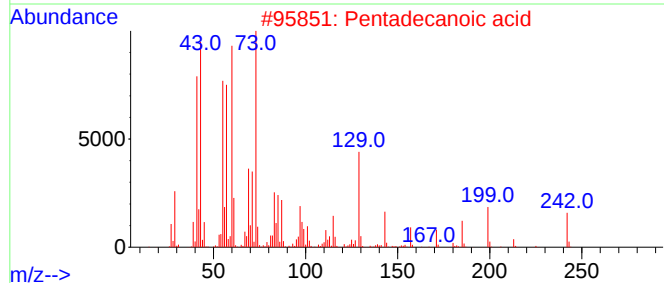
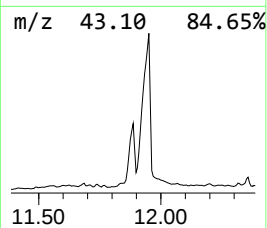
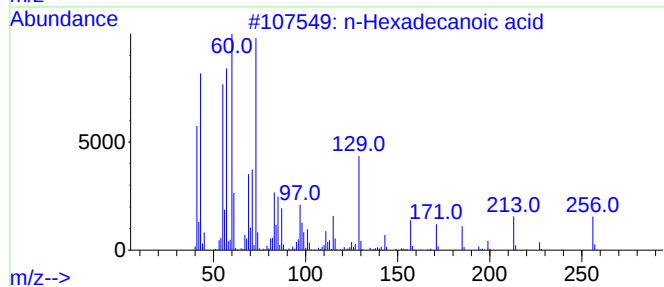
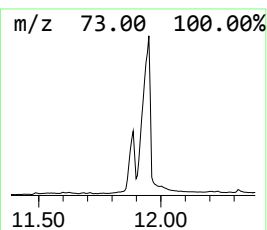
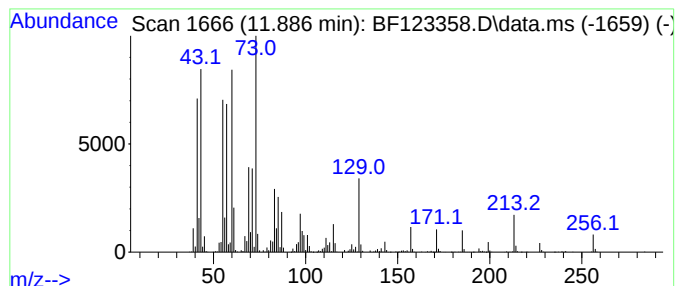
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	71.18 ng	3775740	Phenanthrene-d10	11.381

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tridecanoic acid	214	C13H26O2	000638-53-9	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Dodecanoic acid	200	C12H24O2	000143-07-7	72



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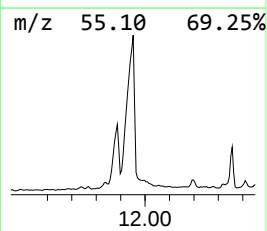
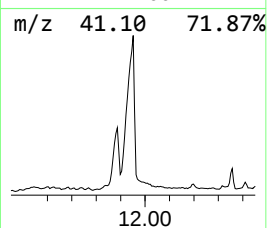
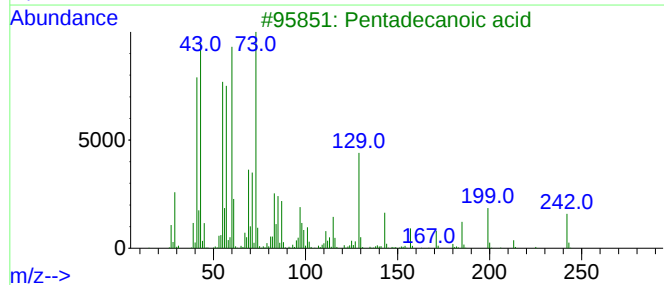
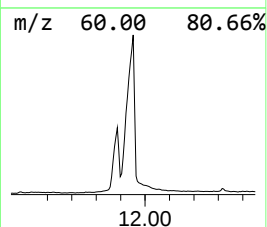
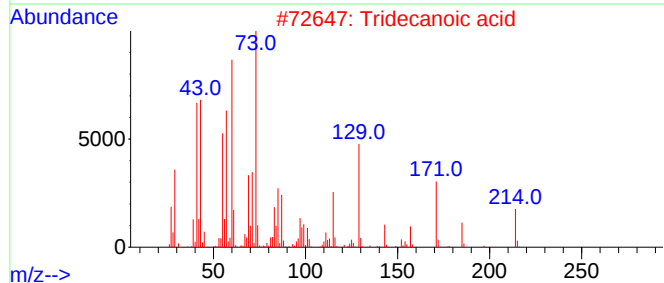
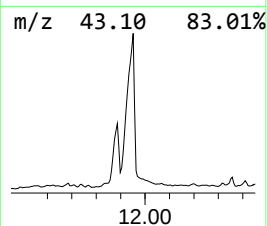
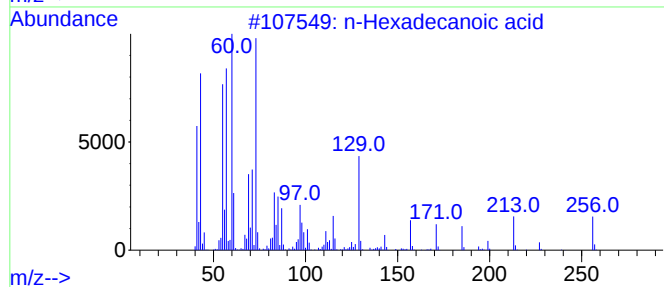
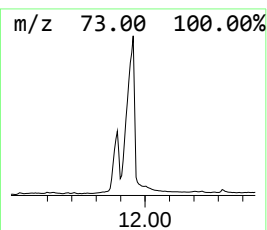
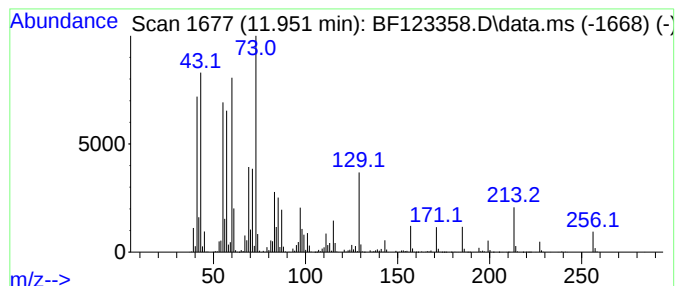
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Tridecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	225.51 ng	11961800	Phenanthrene-d10	11.381

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	92
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Estra-1,3,5(10)-trien-17.β-ol	256	C18H24O	002529-64-8	30



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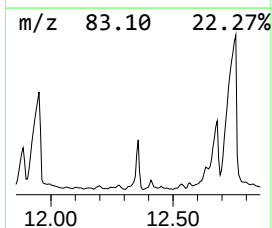
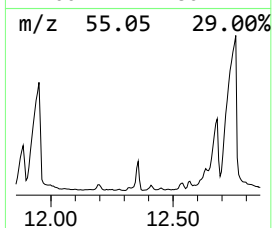
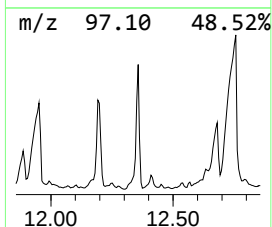
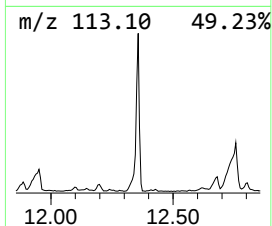
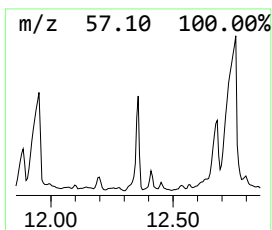
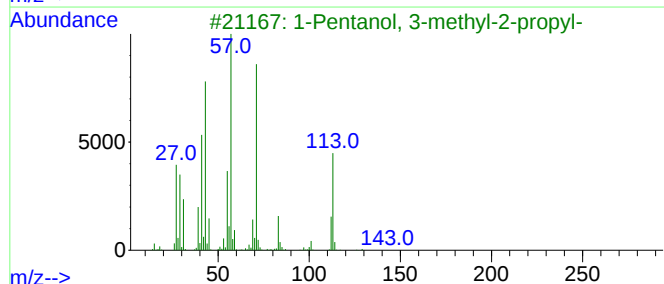
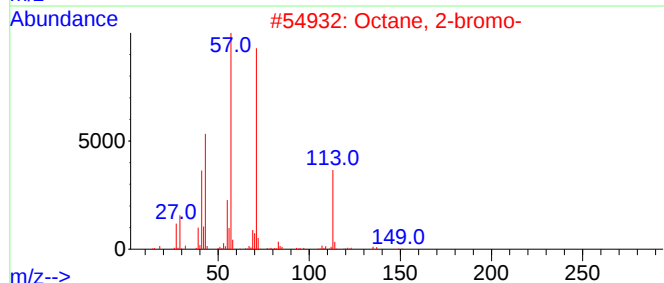
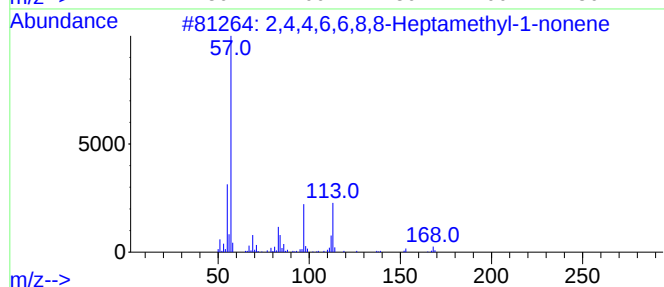
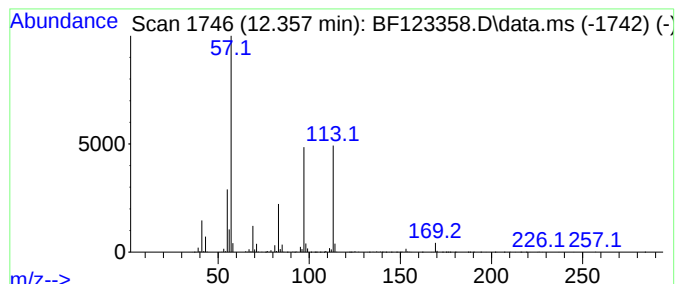
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.357	22.70 ng	1204010	Phenanthrene-d10	11.381

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	56		
2	Octane, 2-bromo-	192	C8H17Br	000557-35-7	37		
3	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	28		
4	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F502	1000365-51-0	27		
5	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F302	1000365-19-5	25		



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ALS Vial : 7 Sample Multiplier: 4

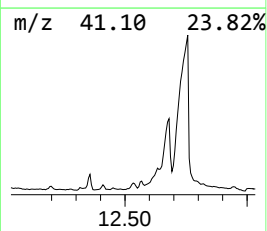
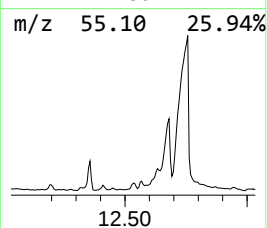
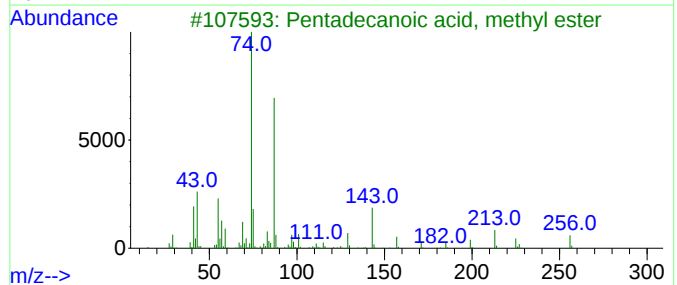
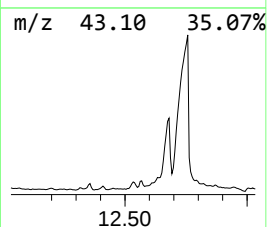
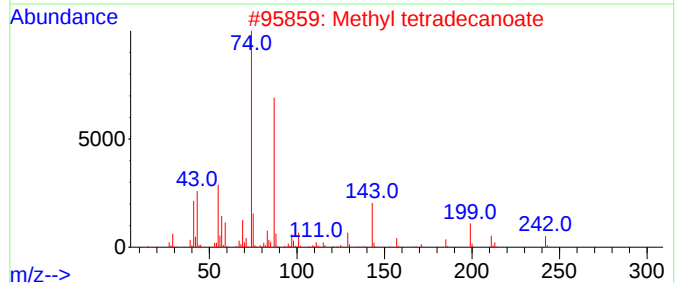
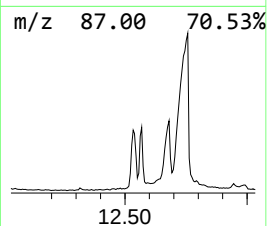
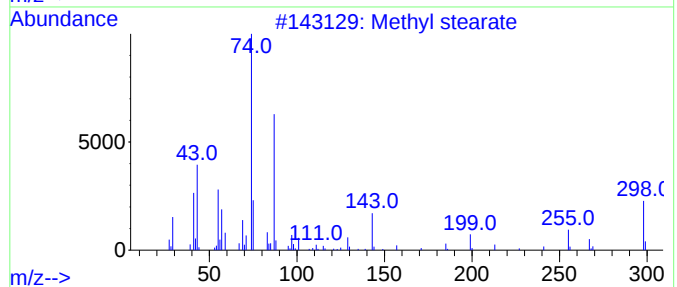
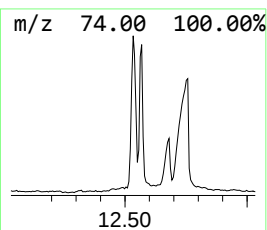
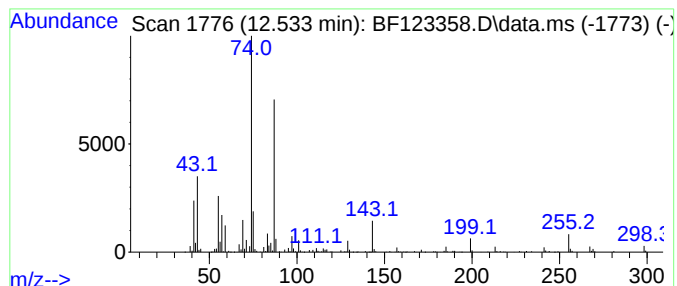
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ClientSampleId :
MH-725

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Methyl stearate Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.533	9.34 ng	495458	Phenanthrene-d10	11.381	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	97
2	Methyl tetradecanoate	242	C15H30O2	000124-10-7	94
3	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	94
4	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	93
5	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030321\
Data File : BF123358.D
Acq On : 3 Mar 2021 16:27
Operator : JU/CG
Sample : M1545-02
Misc :
ALS Vial : 7 Sample Multiplier: 4

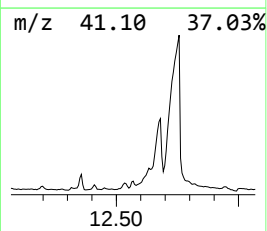
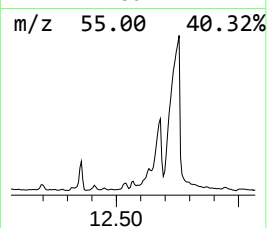
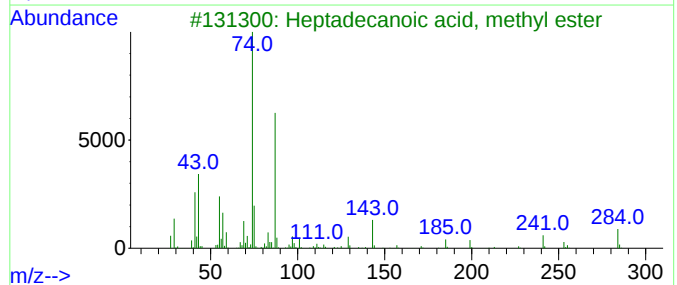
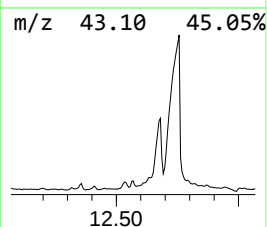
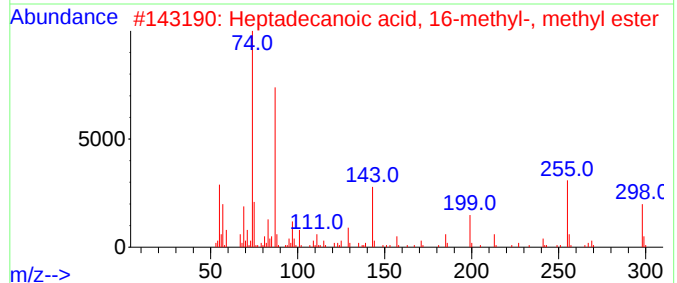
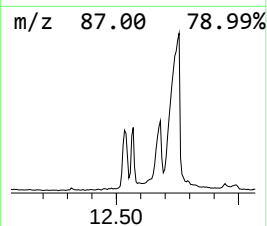
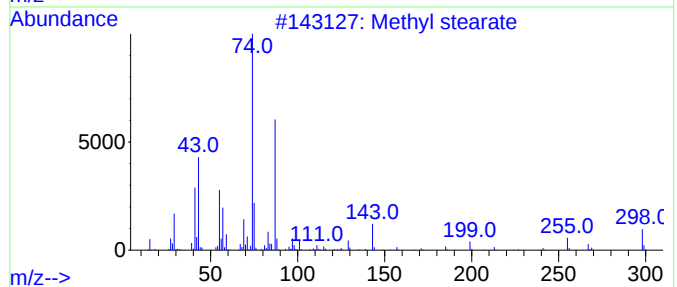
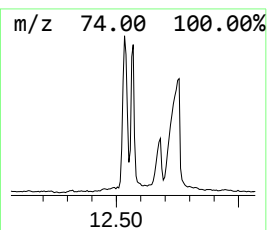
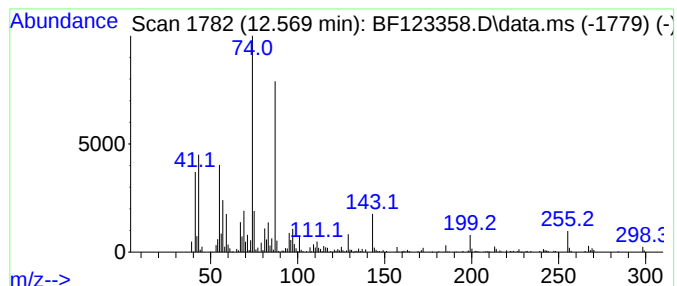
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Heptadecanoic acid, 16-meth... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.569	9.32 ng	494592	Phenanthrene-d10		11.381	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Methyl stearate		298	C19H38O2	000112-61-8	97
2	Heptadecanoic acid, 16-methyl-, ...		298	C19H38O2	005129-61-3	93
3	Heptadecanoic acid, methyl ester		284	C18H36O2	001731-92-6	90
4	Methyl tetradecanoate		242	C15H30O2	000124-10-7	87
5	Pentadecanoic acid, methyl ester		256	C16H32O2	007132-64-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030321\
Data File : BF123358.D
Acq On : 3 Mar 2021 16:27
Operator : JU/CG
Sample : M1545-02
Misc :
ALS Vial : 7 Sample Multiplier: 4

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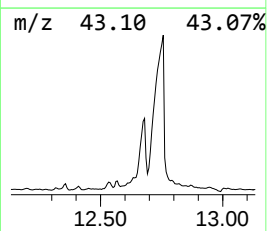
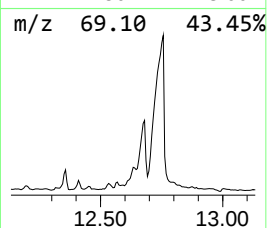
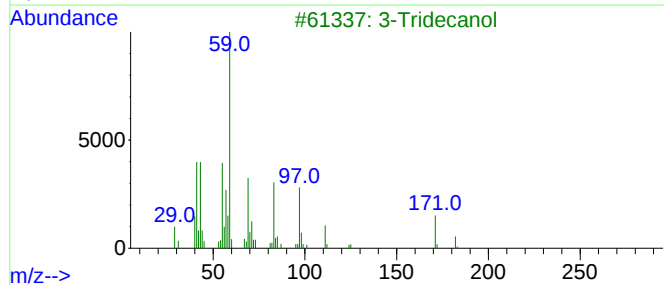
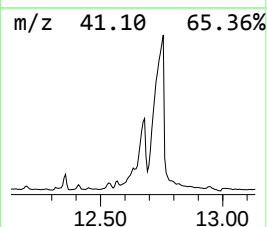
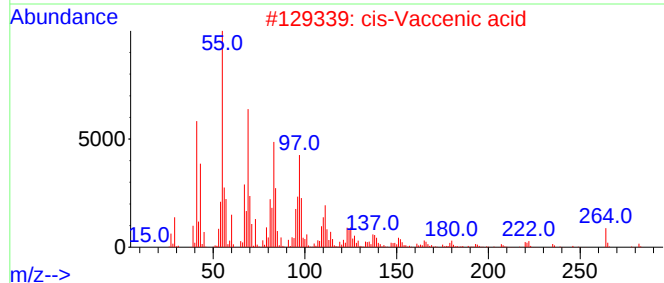
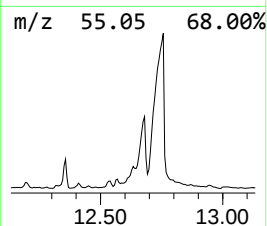
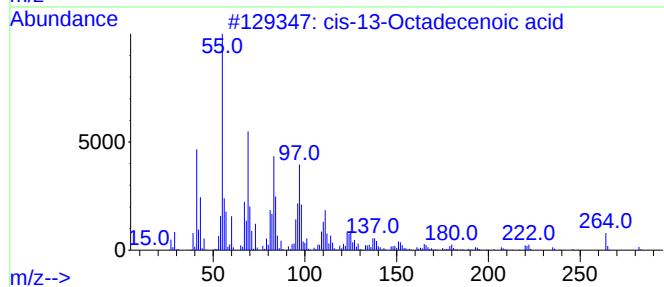
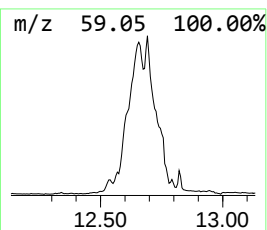
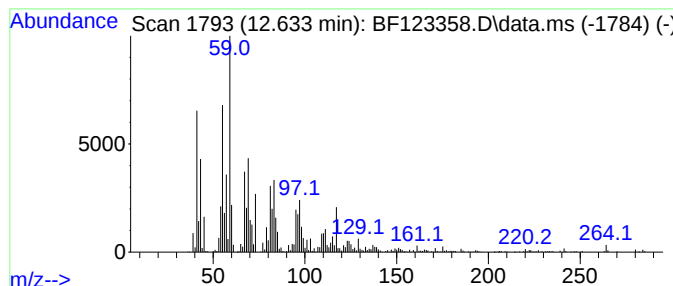
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 cis-13-Octadecenoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.633	43.45 ng	2304900	Phenanthrene-d10	11.381

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	91
2			cis-Vaccenic acid	282	C18H34O2	000506-17-2	60
3			3-Tridecanol	200	C13H28O	010289-68-6	47
4			3-Hydroxy-3-methyl-butyric acid,...	132	C5H12N2O2	1000193-80-2	43
5			Oleic Acid	282	C18H34O2	000112-80-1	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030321\
Data File : BF123358.D
Acq On : 3 Mar 2021 16:27
Operator : JU/CG
Sample : M1545-02
Misc :
ALS Vial : 7 Sample Multiplier: 4

Instrument :
BNA_F
ClientSampleId :
MH-725

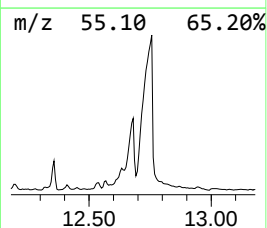
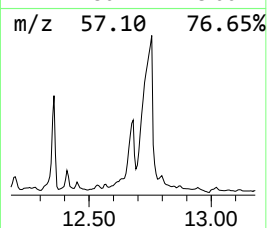
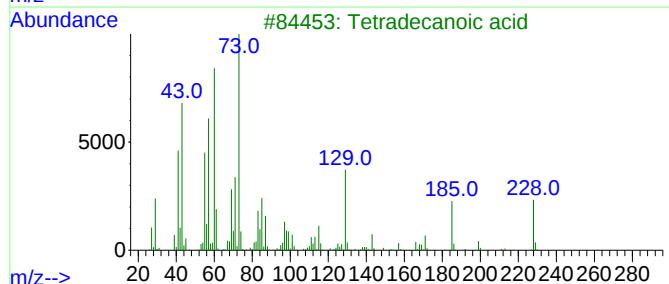
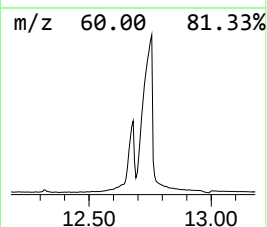
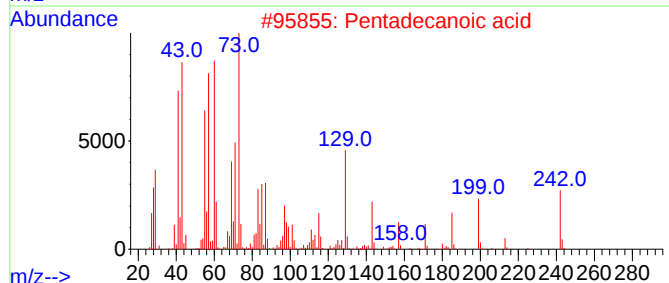
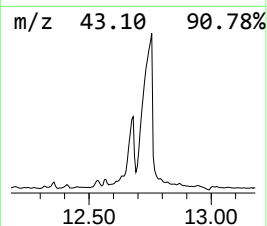
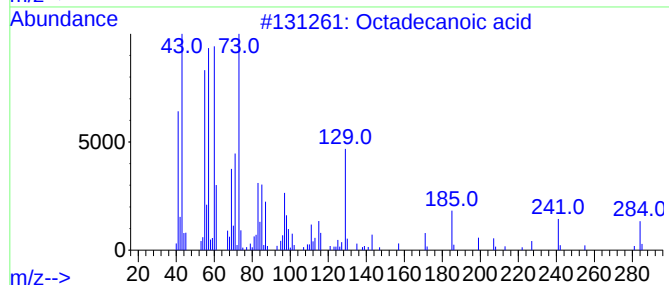
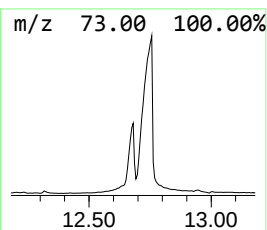
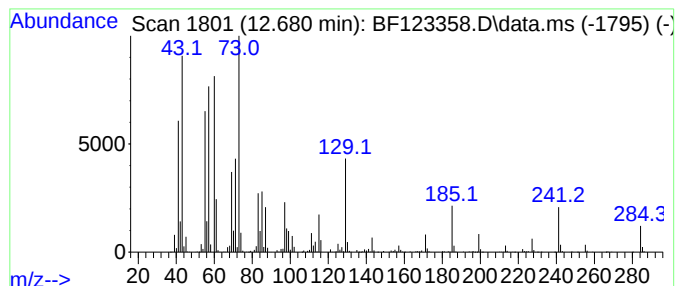
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.680	126.57 ng	6713620	Phenanthrene-d10	11.381

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	89
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			n-Decanoic acid	172	C10H20O2	000334-48-5	70
5			Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	20



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030321\
Data File : BF123358.D
Acq On : 3 Mar 2021 16:27
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Sample : M1545-02
Misc :
ALS Vial : 7 Sample Multiplier: 4

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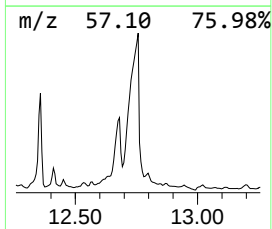
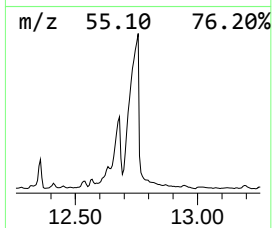
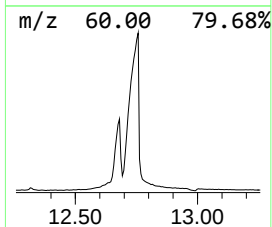
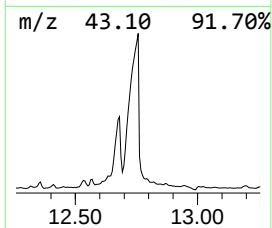
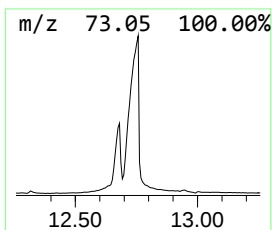
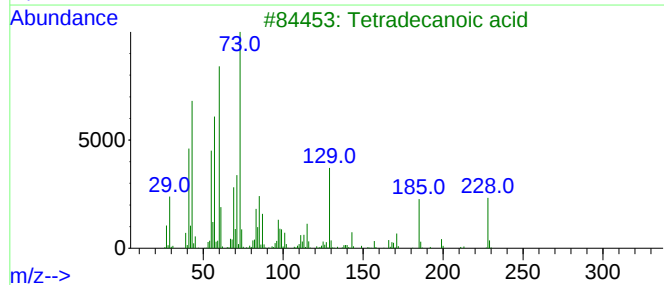
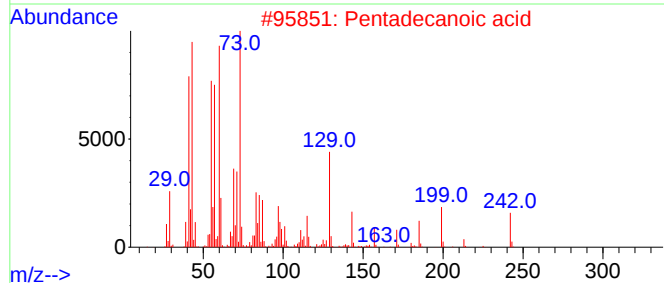
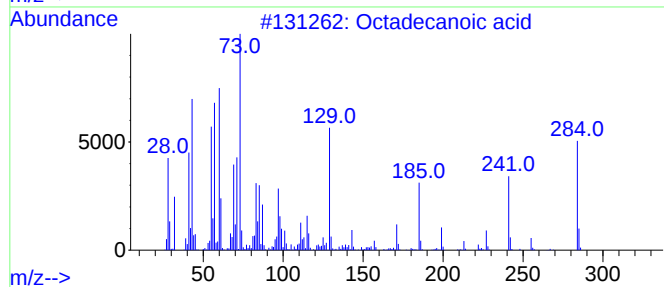
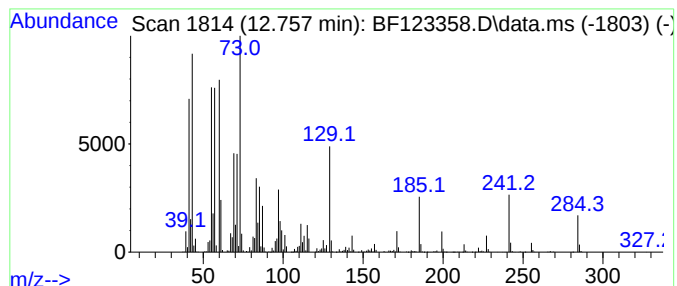
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Pentadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.757	462.08 ng	22694100	Chrysene-d12	14.039

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	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030321\
Data File : BF123358.D
Acq On : 3 Mar 2021 16:27
Operator : JU/CG
Sample : M1545-02
Misc :
ALS Vial : 7 Sample Multiplier: 4

Instrument :
BNA_F
ClientSampleId :
MH-725

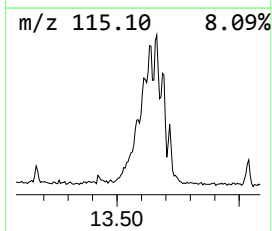
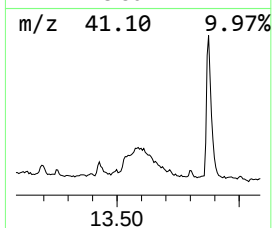
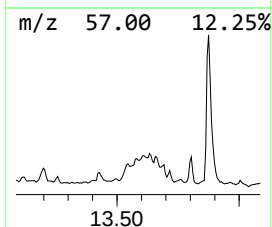
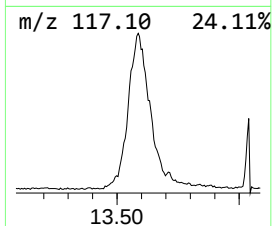
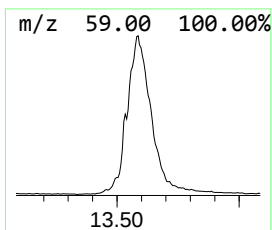
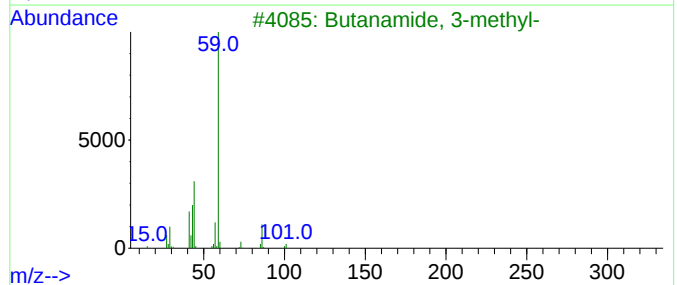
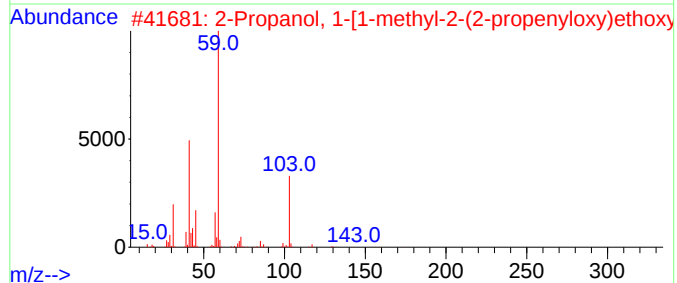
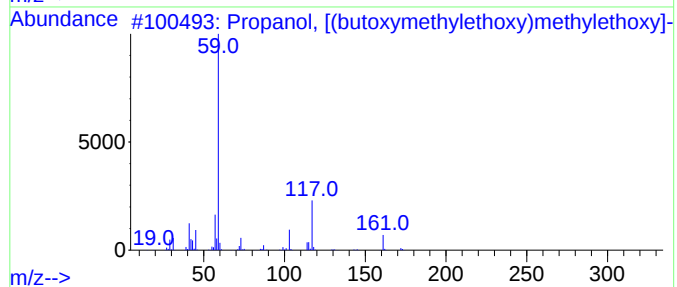
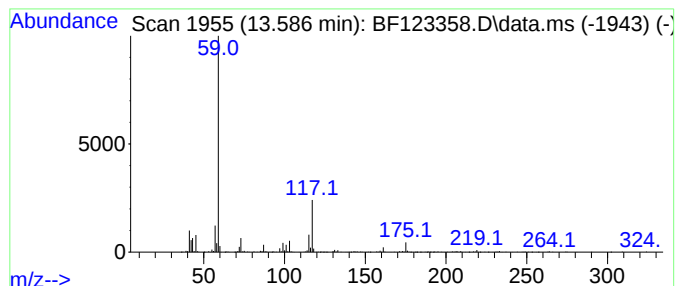
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Propanol, [(butoxymethyleth... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.586	37.52 ng	1842810	Chrysene-d12	14.039

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propanol, [(butoxymethylethoxy)m...	248	C13H28O4	055934-93-5	72
2		2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	53
3		Butanamide, 3-methyl-	101	C5H11NO	000541-46-8	50
4		2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3	013429-07-7	47
5		Pentane, 2-methoxy-	102	C6H14O	006795-88-6	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030321\
Data File : BF123358.D
Acq On : 3 Mar 2021 16:27
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Sample : M1545-02
Misc :
ALS Vial : 7 Sample Multiplier: 4

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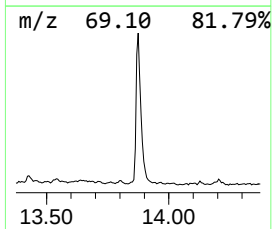
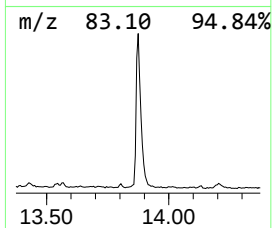
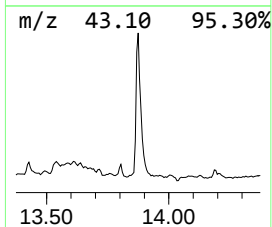
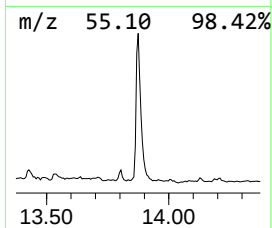
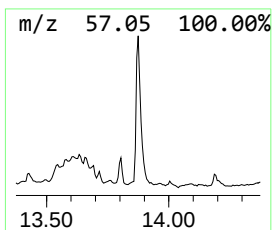
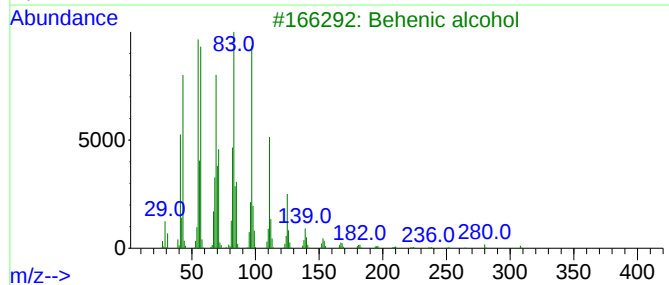
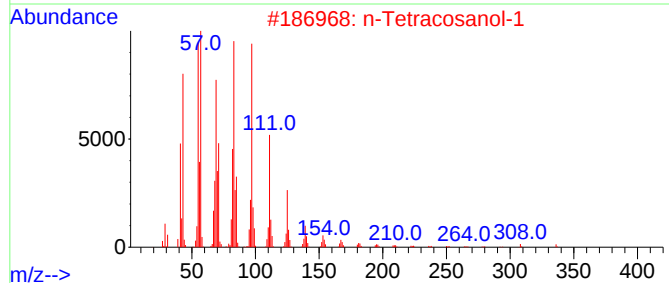
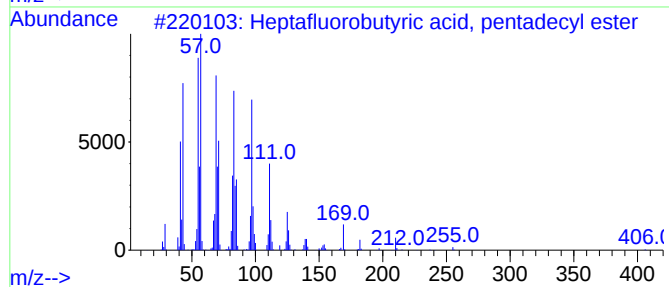
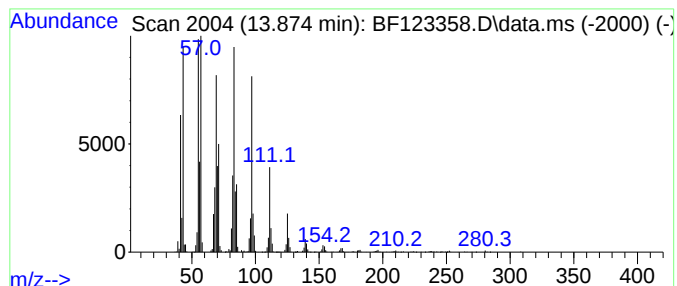
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Heptafluorobutyric acid, pe... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	59.24 ng	2909350	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3			Behenic alcohol	326	C22H46O	000661-19-8	94
4			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94



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Acq On : 3 Mar 2021 16:27
Operator : JU/CG
Sample : M1545-02
Misc :
ALS Vial : 7 Sample Multiplier: 4

Instrument :
BNA_F
ClientSampleId :
MH-725

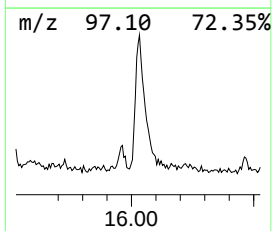
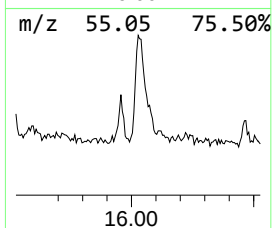
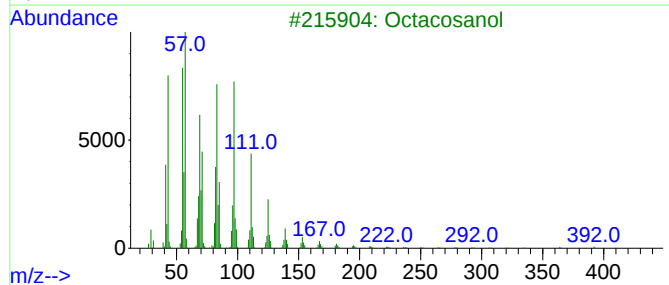
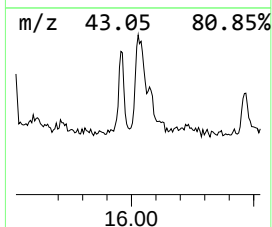
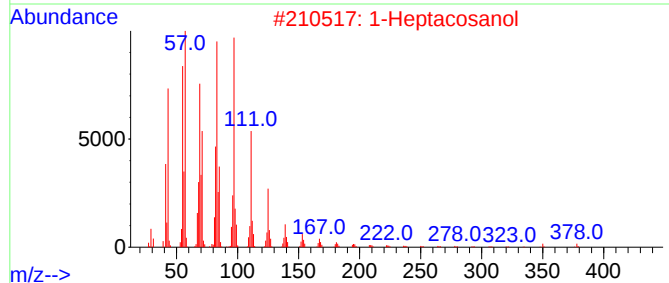
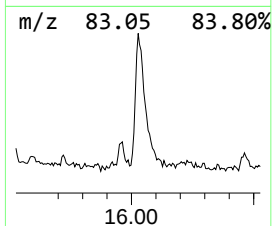
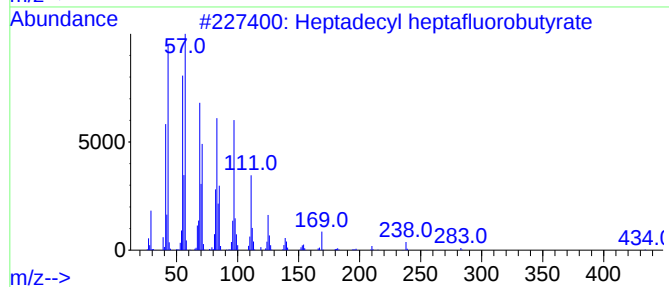
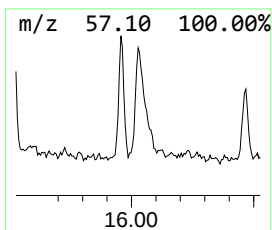
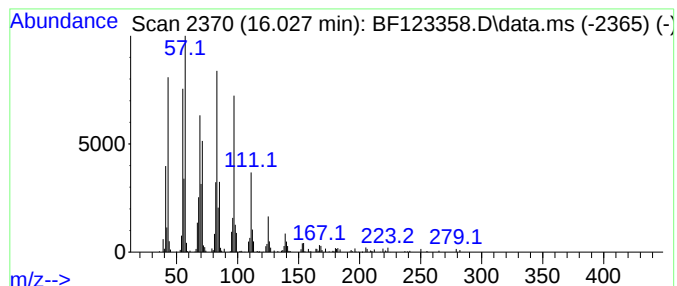
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Heptadecyl heptafluorobutyrate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.027	13.52 ng	705177	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2			1-Heptacosanol	396	C27H56O	002004-39-9	93
3			Octacosanol	410	C28H58O	000557-61-9	93
4			1-Heneicosanol	312	C21H44O	015594-90-8	93
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030321\
 Data File : BF123358.D
 Acq On : 3 Mar 2021 16:27
 Operator : JU/CG
 Sample : M1545-02
 Misc :
 ALS Vial : 7 Sample Multiplier: 4

Instrument :
 BNA_F
 ClientSampleId :
 MH-725

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.840	192.3	ng	6696130	1	6.851	2785350	20.0
2-Propanol, 1-...	11.551	8.3	ng	437903	4	11.381	4243520	20.0
n-Hexadecanoic ...	11.886	71.2	ng	3775740	4	11.381	4243520	20.0
Tridecanoic acid	11.951	225.5	ng	11961800	4	11.381	4243520	20.0
2,4,4,6,6,8,8-H...	12.357	22.7	ng	1204010	4	11.381	4243520	20.0
Methyl stearate	12.533	9.3	ng	495458	4	11.381	4243520	20.0
Heptadecanoic a...	12.569	9.3	ng	494592	4	11.381	4243520	20.0
cis-13-Octadece...	12.633	43.5	ng	2304900	4	11.381	4243520	20.0
Octadecanoic acid	12.680	126.6	ng	6713620	4	11.381	4243520	20.0
Pentadecanoic acid	12.757	462.1	ng	22694100	5	14.039	3929050	20.0
Propanol, [(but...	13.586	37.5	ng	1842810	5	14.039	3929050	20.0
Heptafluorobuty...	13.874	59.2	ng	2909350	5	14.039	3929050	20.0
Heptadecyl hept...	16.027	13.5	ng	705177	6	15.515	4171660	20.0