

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102020\
 Data File : BF122035.D
 Acq On : 20 Oct 2020 18:08
 Operator : JU/CG
 Sample : L4457-03
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NOTT-AVE-PR-2150

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-BF101220.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122035.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.345	551	554	572	rBV	963269	1118518	25.85%	4.039%
2	6.375	726	729	755	rVB	627845	828557	19.15%	2.992%
3	6.569	759	762	777	rBV	115840	151916	3.51%	0.549%
4	6.728	786	789	796	rBV	815041	684270	15.81%	2.471%
5	6.886	811	816	819	rBV	3064412	2836917	65.55%	10.245%
6	7.298	881	886	889	rBV	2368258	2480323	57.31%	8.957%
7	8.010	1003	1007	1017	rVB	972525	889691	20.56%	3.213%
8	8.739	1128	1131	1144	rBV	31907	56112	1.30%	0.203%
9	9.092	1185	1191	1194	rBV	4186603	4327582	100.00%	15.628%
10	9.210	1205	1211	1222	rVB	1344663	1363019	31.50%	4.922%
11	9.486	1254	1258	1262	rBV	409653	334552	7.73%	1.208%
12	9.763	1301	1305	1315	rVB	1188925	1016454	23.49%	3.671%
13	10.345	1401	1404	1422	rBV	463609	586992	13.56%	2.120%
14	10.557	1436	1440	1452	rBV	1911004	1724802	39.86%	6.229%
15	11.251	1554	1558	1565	rBV	1151240	997445	23.05%	3.602%
16	11.439	1583	1590	1596	rBV2	102391	162786	3.76%	0.588%
17	11.786	1645	1649	1664	rBV2	240465	300987	6.96%	1.087%
18	12.304	1733	1737	1751	rVB	203055	394391	9.11%	1.424%
19	12.492	1763	1769	1772	rBV	229629	218004	5.04%	0.787%
20	12.568	1779	1782	1786	rBV2	47051	49880	1.15%	0.180%
21	12.710	1802	1806	1808	rBV2	46826	47090	1.09%	0.170%
22	12.839	1823	1828	1831	rBV	4040989	4002123	92.48%	14.453%
23	13.062	1861	1866	1878	rBV	138609	252789	5.84%	0.913%
24	13.404	1920	1924	1927	rBV3	44511	58272	1.35%	0.210%
25	13.739	1977	1981	1994	rBV	476925	837773	19.36%	3.025%
26	13.892	2004	2007	2016	rVB	789530	723006	16.71%	2.611%
27	14.351	2082	2085	2088	rBV	51711	44671	1.03%	0.161%
28	14.380	2088	2090	2099	rVB6	27492	52027	1.20%	0.188%
29	14.651	2133	2136	2139	rVB	53880	53302	1.23%	0.192%
30	14.715	2144	2147	2152	rVB	59908	63523	1.47%	0.229%
31	14.968	2186	2190	2193	rVB	58983	63187	1.46%	0.228%
32	15.327	2246	2251	2260	rBV	570338	708801	16.38%	2.560%
33	15.733	2316	2320	2329	rBV	44072	59951	1.39%	0.217%
34	15.815	2329	2334	2346	rBV6	43386	140039	3.24%	0.506%
35	16.750	2489	2493	2500	rVB4	32181	61136	1.41%	0.221%

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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-BF101220.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

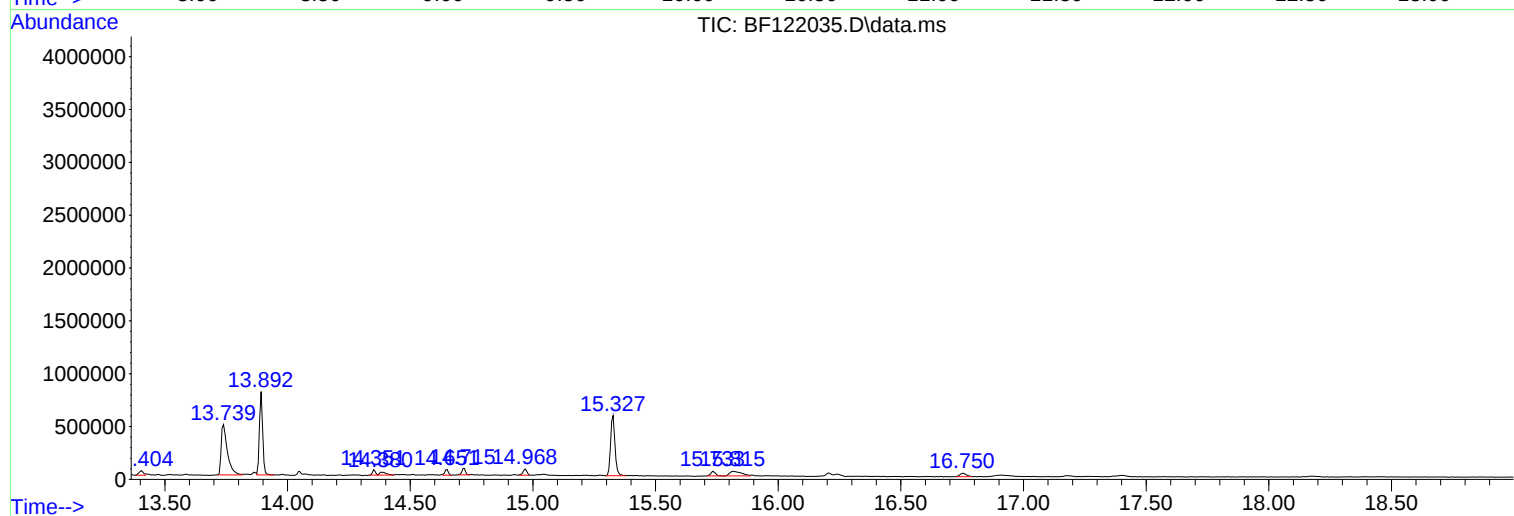
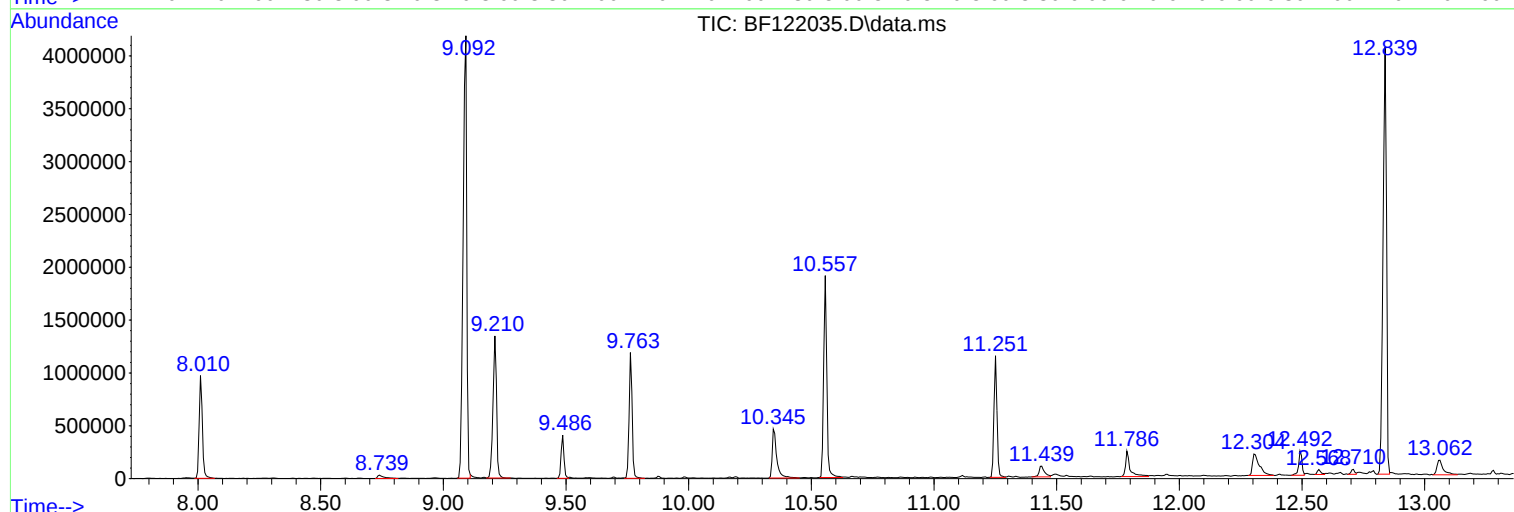
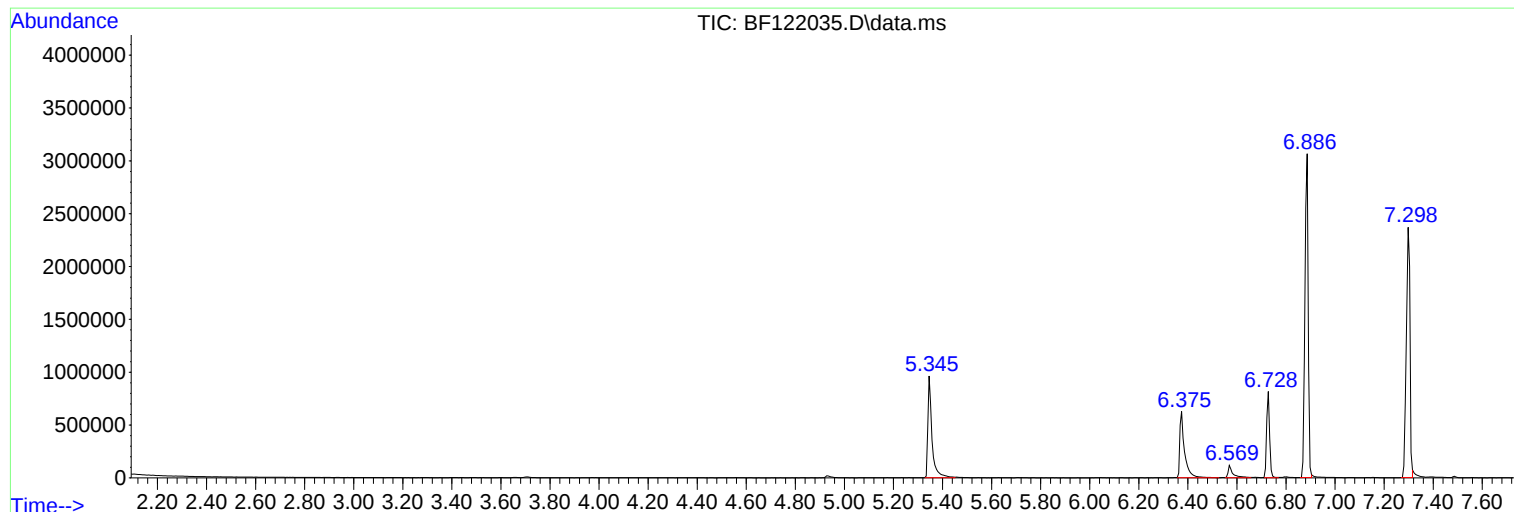
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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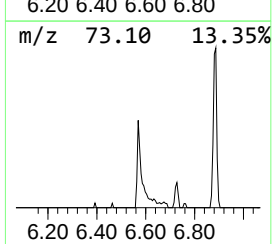
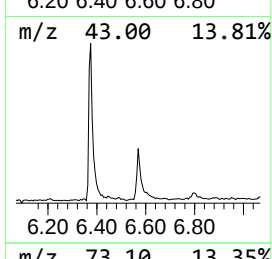
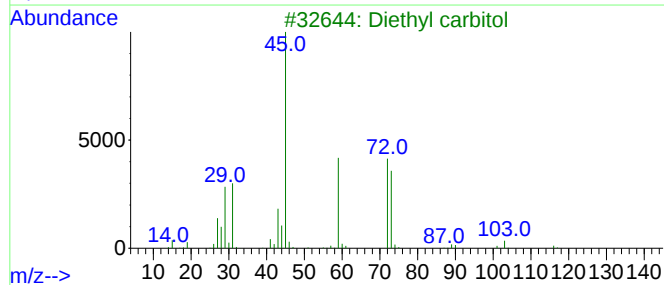
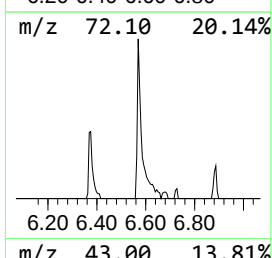
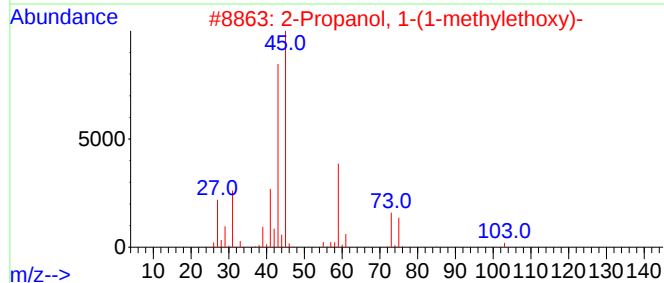
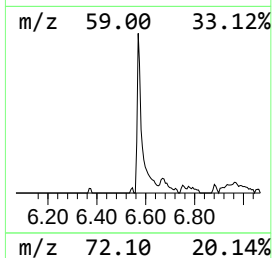
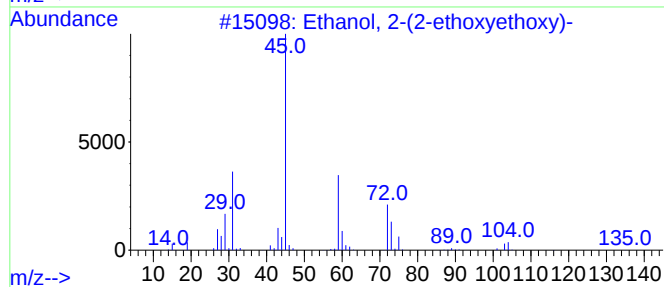
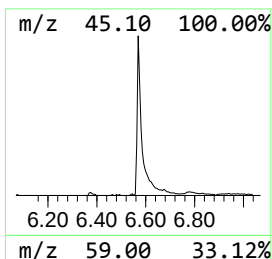
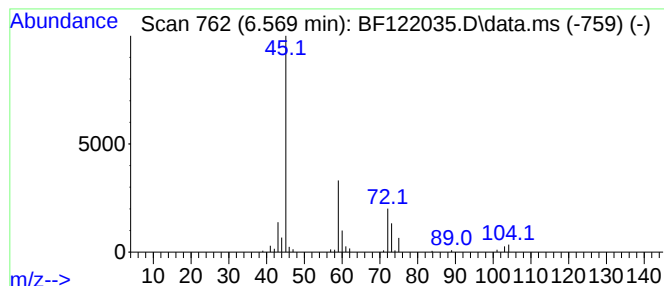
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.569	4.44 ng	151916	1,4-Dichlorobenzene-d4	6.728

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	38
3			Diethyl carbitol	162	C8H18O3	000112-36-7	38
4			Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	37
5			Ethanol, 2,2'-oxybis-	106	C4H10O3	000111-46-6	37



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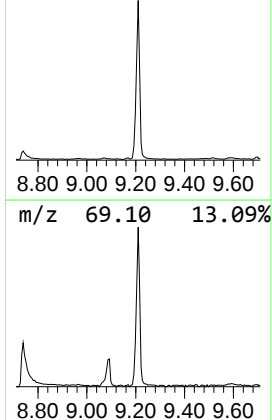
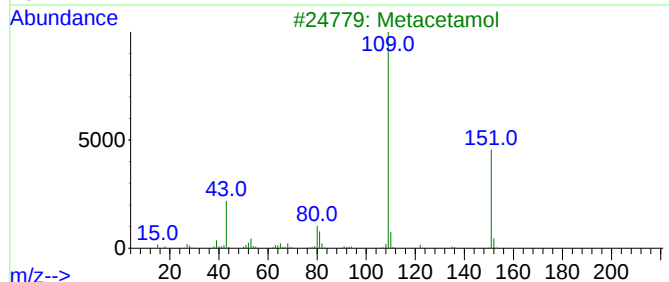
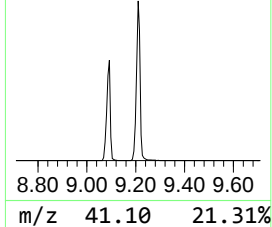
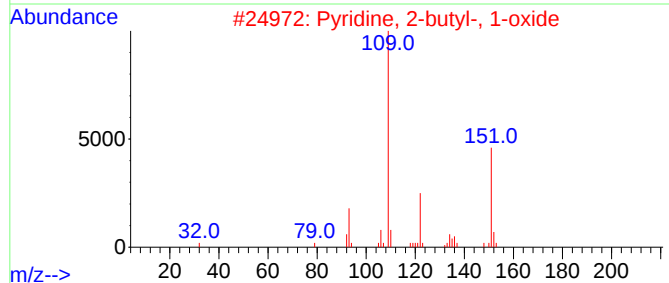
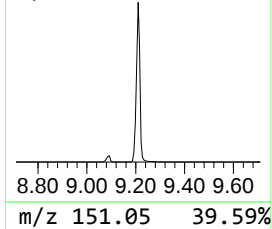
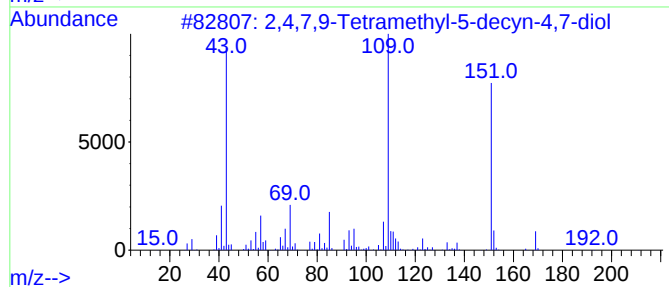
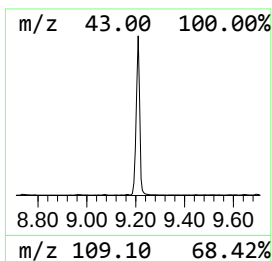
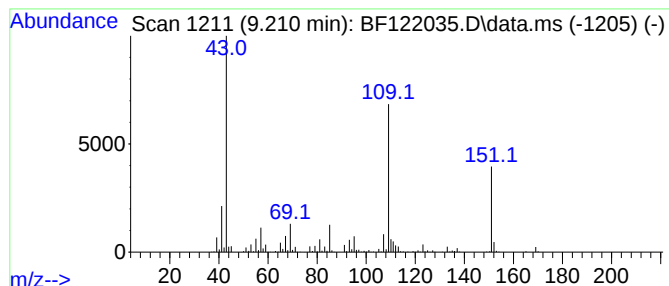
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.210	26.82 ng	1363020	Acenaphthene-d10	9.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	90	
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59	
3	Metacetamol	151	C8H9NO2	000621-42-1	58	
4	Acetaminophen	151	C8H9NO2	000103-90-2	53	
5	Butanamide, N-acetyl-N-(4-hydrox...	221	C12H15NO3	1000107-08-7	53	



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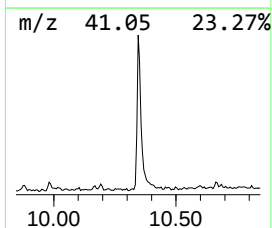
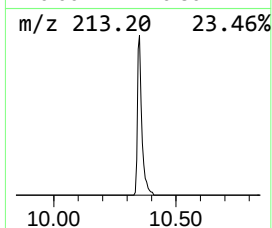
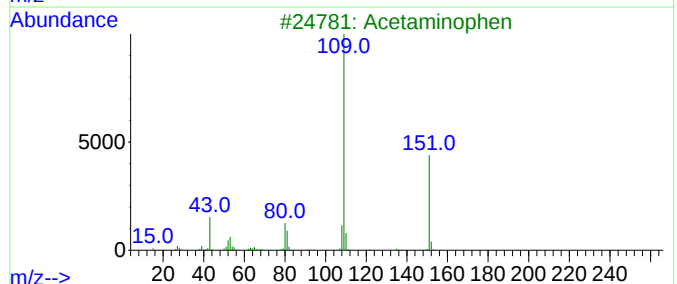
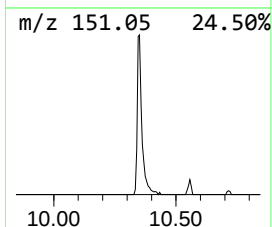
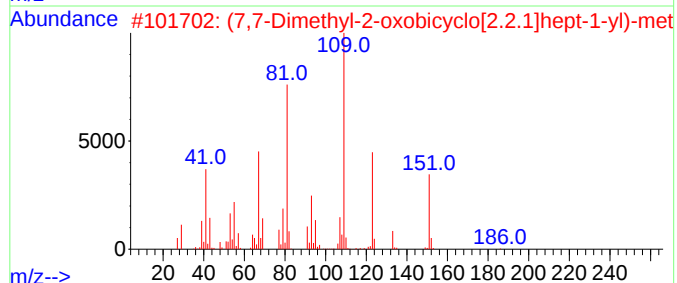
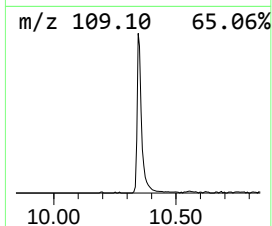
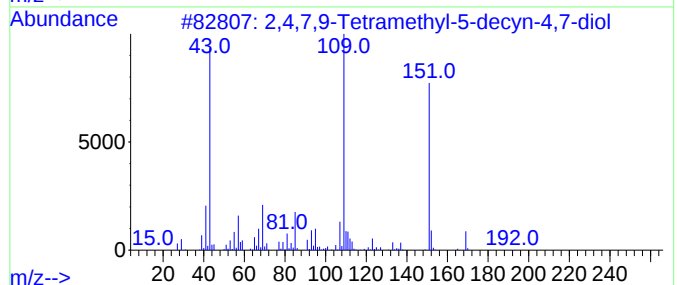
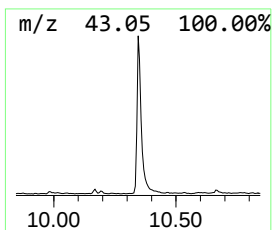
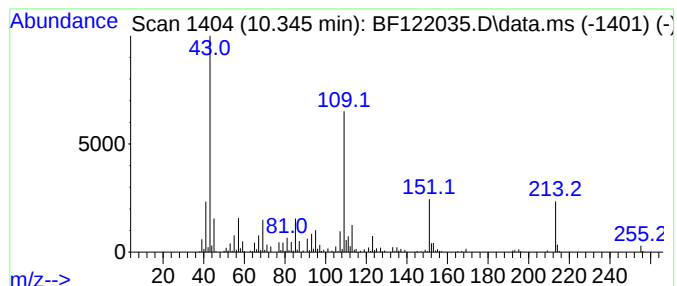
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 unknown10.345 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.345	11.55 ng	586992	Acenaphthene-d10	9.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	62		
2	(7,7-Dimethyl-2-oxobicyclo[2.2.1...]	250	C10H15ClO3S	1000194-76-1	38		
3	Acetaminophen	151	C8H9NO2	000103-90-2	35		
4	Metacetamol	151	C8H9NO2	000621-42-1	35		
5	4-Pyridinemethanol, acetate (ester)	151	C8H9NO2	001007-48-3	35		



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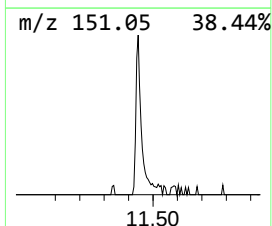
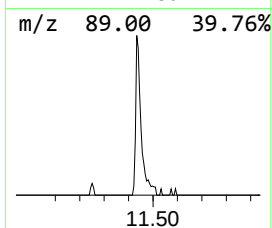
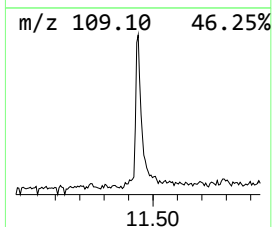
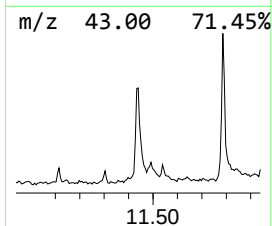
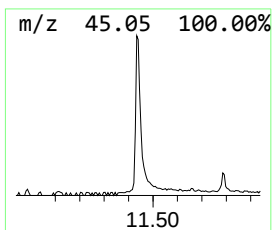
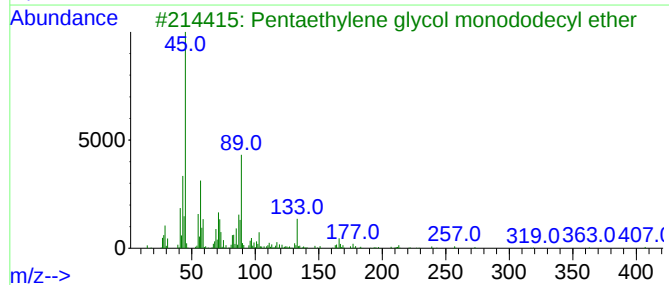
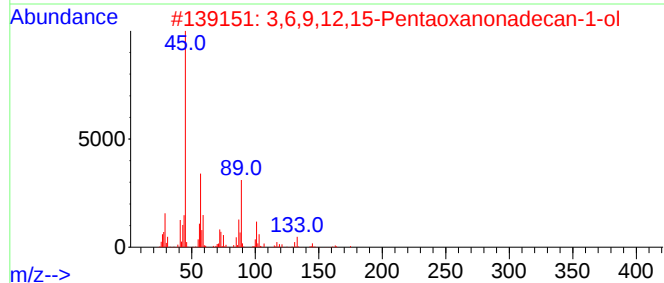
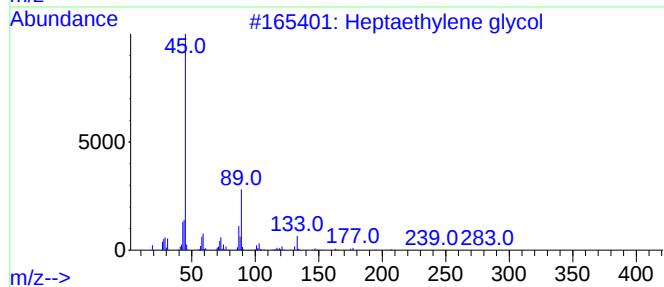
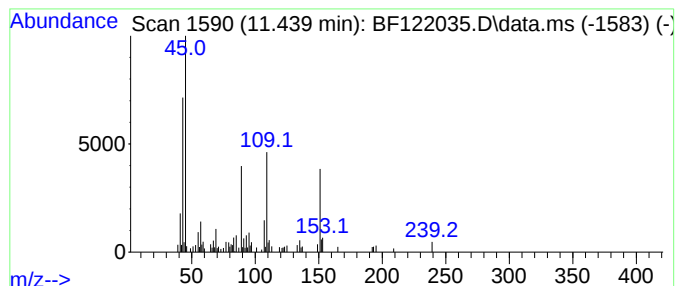
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown11.439 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.439	3.26 ng	162786	Phenanthrene-d10	11.251

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptaethylene glycol	326	C14H30O8	005617-32-3	32
2			3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	23
3			Pentaethylene glycol monododecyl...	406	C22H46O6	003055-95-6	23
4			3-Methoxymethoxy-2-methyl-non-1-ene	200	C12H24O2	1000192-54-6	22
5			Butane, 1-chloro-4-methoxy-	122	C5H11ClO	017913-18-7	22



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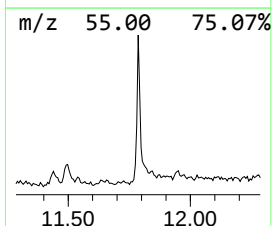
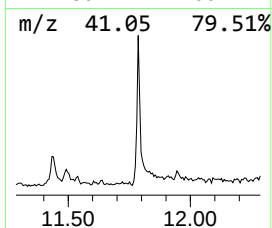
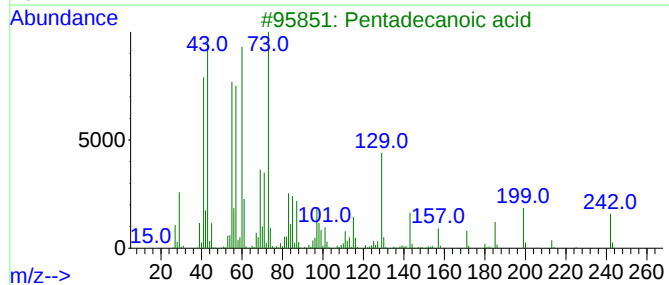
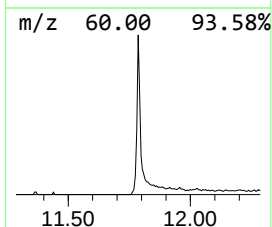
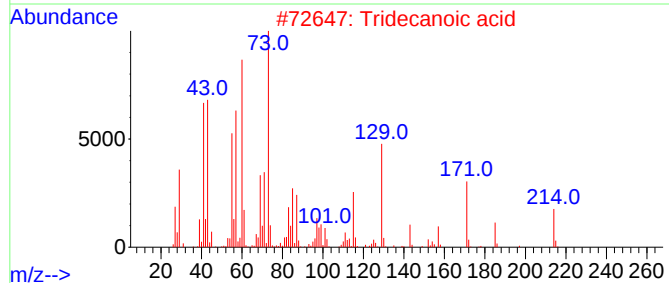
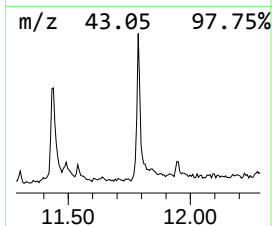
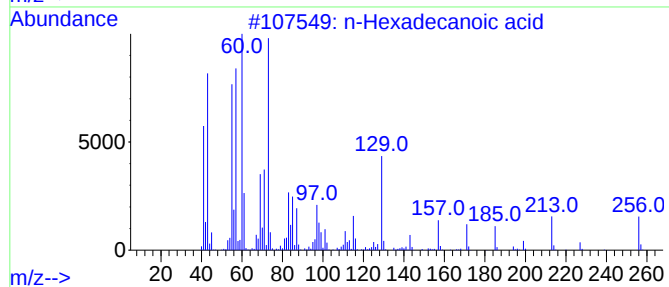
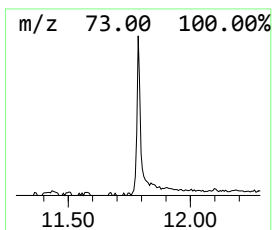
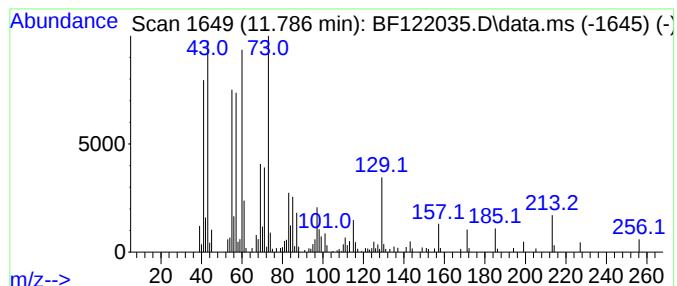
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.786	6.04 ng	300987	Phenanthrene-d10	11.251

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	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			n-Decanoic acid	172	C10H20O2	000334-48-5	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102020\
Data File : BF122035.D
Acq On : 20 Oct 2020 18:08
Operator : JU/CG
Sample : L4457-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NOTT-AVE-PR-2150

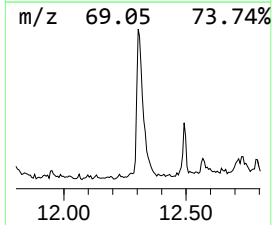
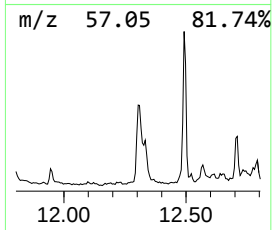
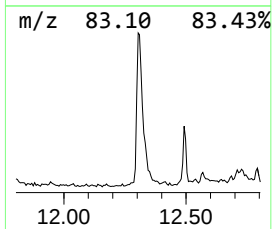
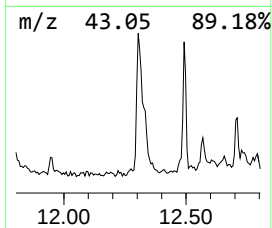
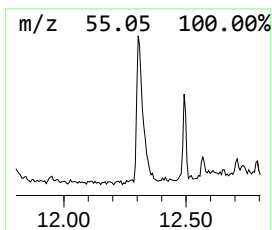
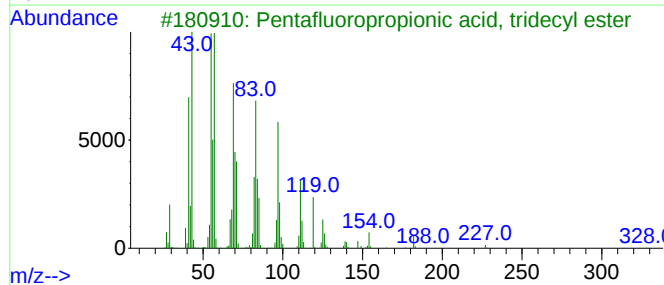
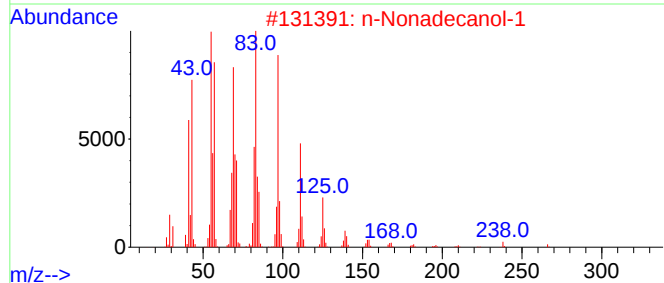
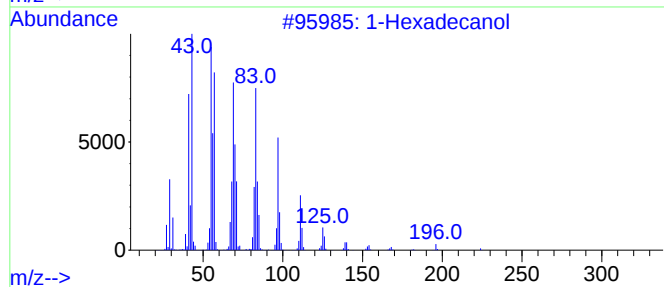
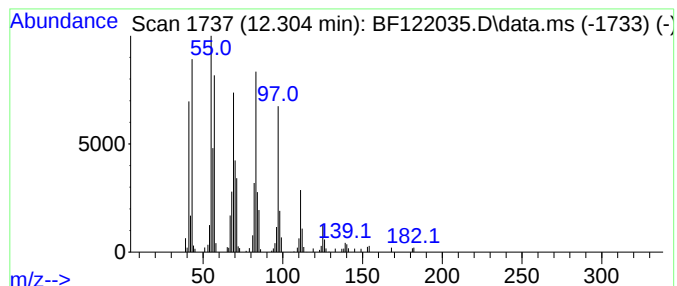
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Hexadecanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.304	7.91 ng	394391	Phenanthrene-d10	11.251

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexadecanol	242	C16H34O	036653-82-4	95
2			n-Nonadecanol-1	284	C19H40O	001454-84-8	94
3			Pentafluoropropionic acid, tridecyl ester	346	C16H27F5O2	959261-22-4	94
4			n-Heptadecanol-1	256	C17H36O	001454-85-9	91
5			1-Nonadecene	266	C19H38	018435-45-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102020\
Data File : BF122035.D
Acq On : 20 Oct 2020 18:08
Operator : JU/CG
Sample : L4457-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NOTT-AVE-PR-2150

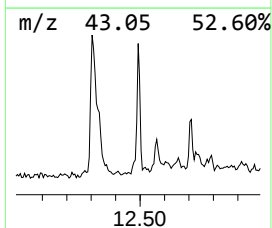
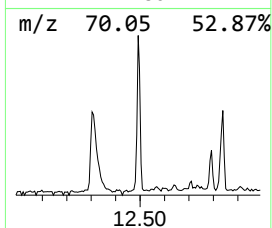
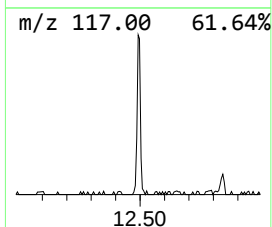
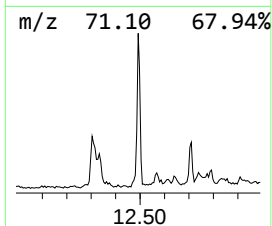
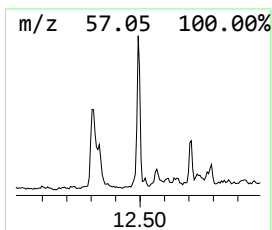
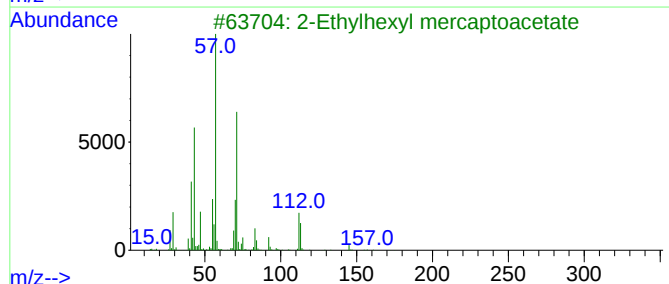
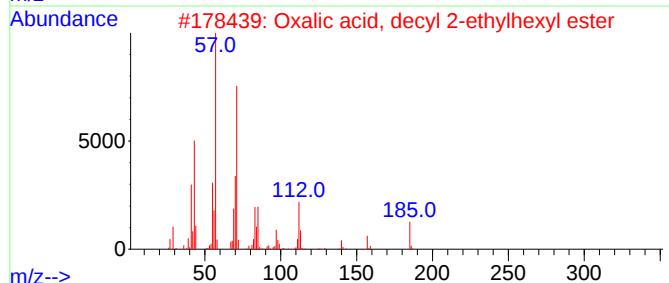
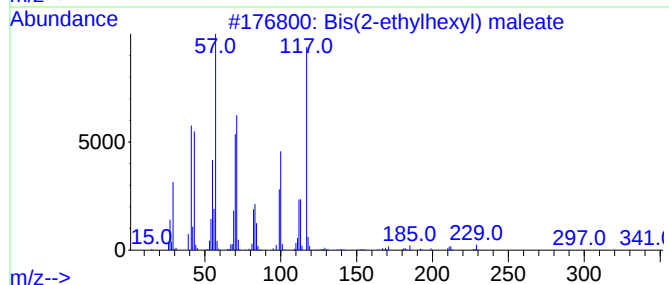
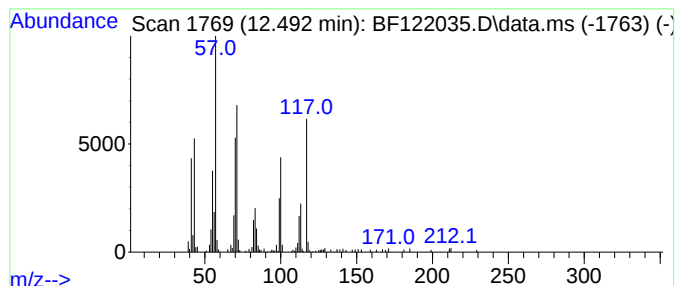
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Bis(2-ethylhexyl) maleate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.492	4.37 ng	218004	Phenanthrene-d10	11.251

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bis(2-ethylhexyl) maleate	340	C20H36O4	000142-16-5	87
2			Oxalic acid, decyl 2-ethylhexyl ...	342	C20H38O4	1000309-39-3	38
3			2-Ethylhexyl mercaptoacetate	204	C10H20O2S	007659-86-1	35
4			Sulfurous acid, 2-ethylhexyl pen...	404	C23H48O3S	1000309-19-8	35
5			Oxalic acid, 2-ethylhexyl octyl ...	314	C18H34O4	1000309-39-1	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102020\
Data File : BF122035.D
Acq On : 20 Oct 2020 18:08
Operator : JU/CG
Sample : L4457-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

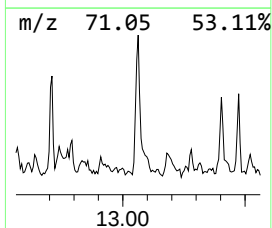
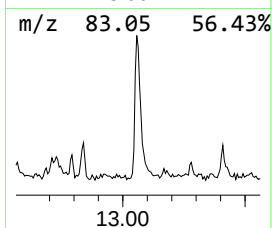
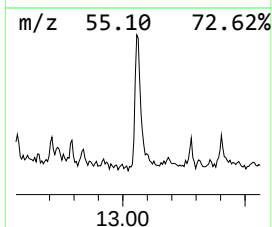
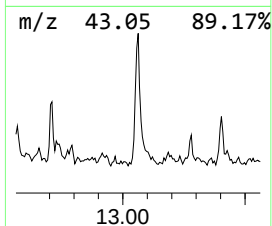
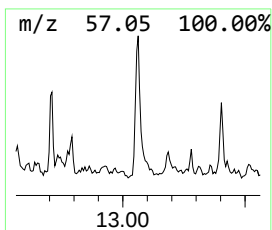
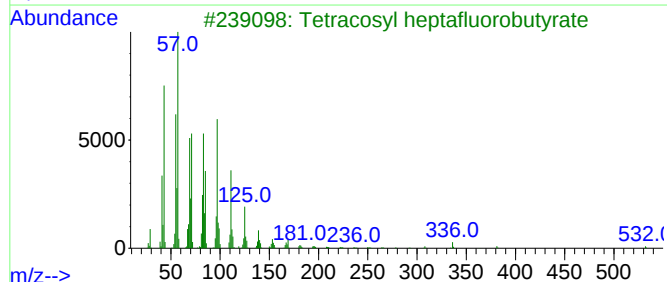
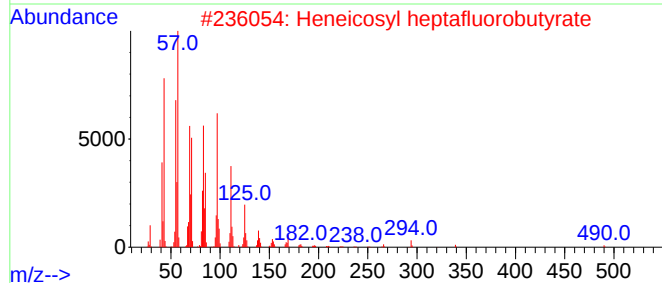
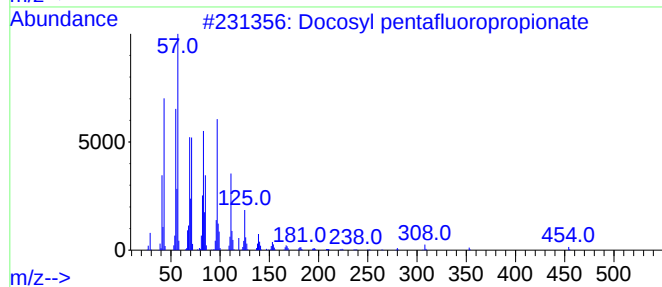
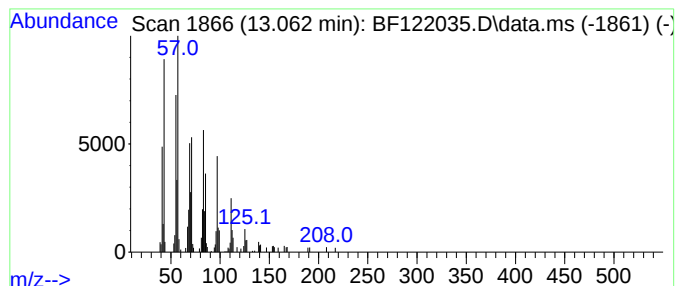
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ClientSampleId :
NOTT-AVE-PR-2150

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Docosyl pentafluoropropionate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.063	6.99 ng	252789	Chrysene-d12	13.892	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
2	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
3	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	91
4	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102020\
Data File : BF122035.D
Acq On : 20 Oct 2020 18:08
Operator : JU/CG
Sample : L4457-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NOTT-AVE-PR-2150

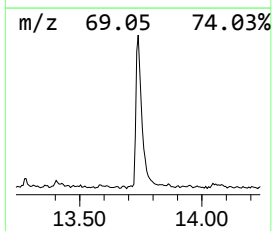
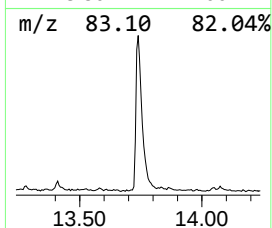
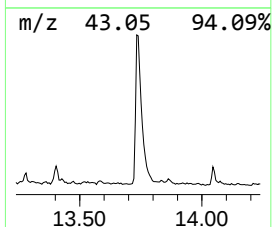
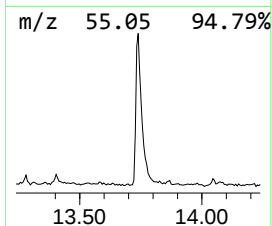
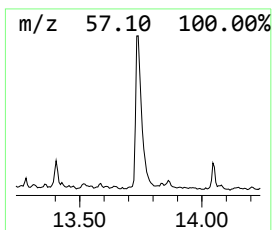
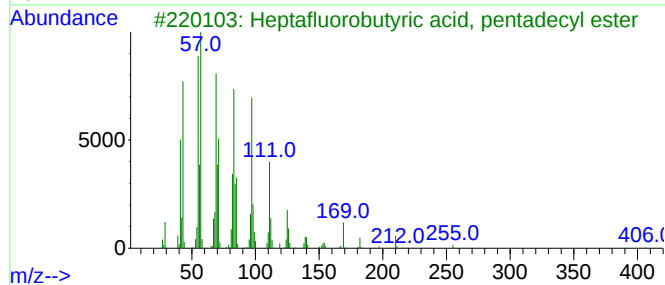
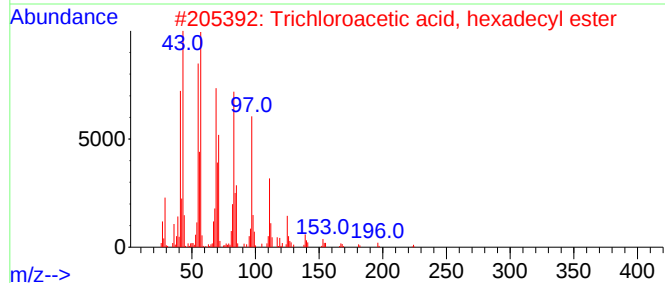
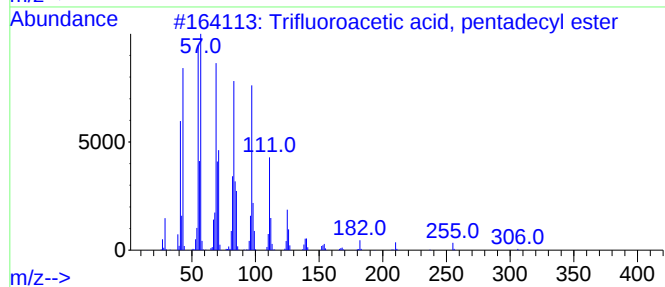
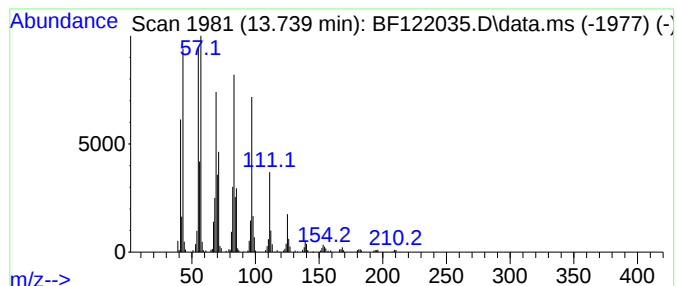
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Trifluoroacetic acid, penta... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.739	23.17 ng	837773	Chrysene-d12	13.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5			1-Heneicosanol	312	C21H44O	015594-90-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102020\
Data File : BF122035.D
Acq On : 20 Oct 2020 18:08
Operator : JU/CG
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Misc :
ALS Vial : 13 Sample Multiplier: 1

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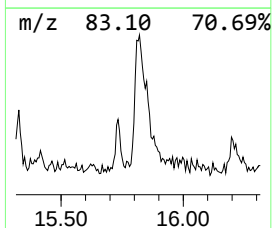
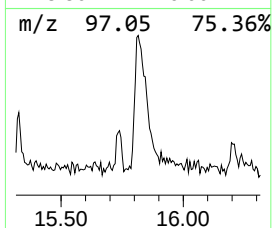
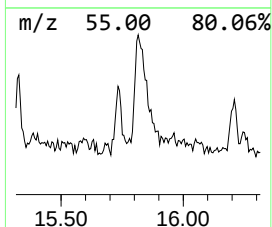
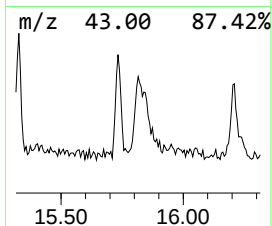
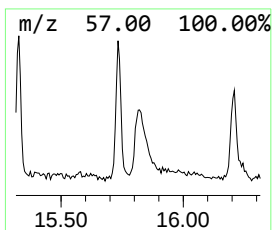
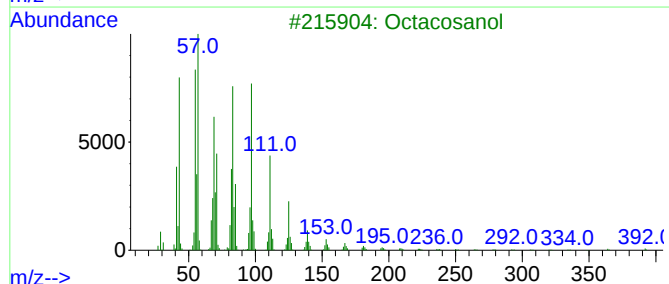
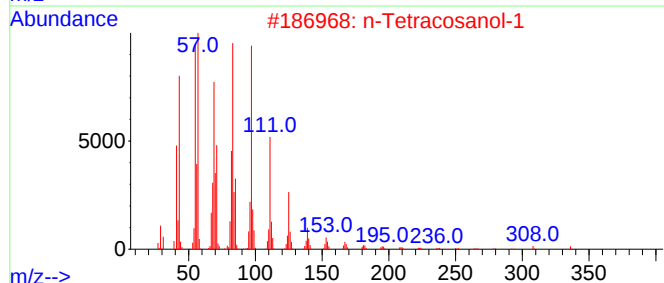
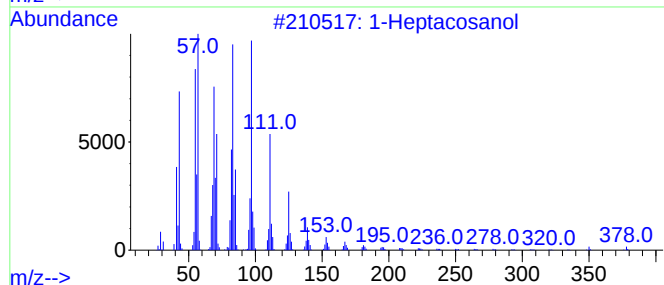
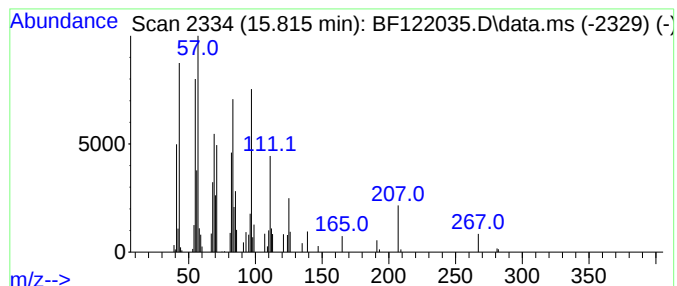
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Heptacosanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.815	3.95 ng	140039	Perylene-d12	15.327

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heptacosanol	396	C27H56O	002004-39-9	93
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	93
3		Octacosanol	410	C28H58O	000557-61-9	93
4		Octacosyl acetate	452	C30H60O2	018206-97-8	93
5		Heptacosyl acetate	438	C29H58O2	1000351-78-2	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102020\
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Acq On : 20 Oct 2020 18:08
Operator : JU/CG
Sample : L4457-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NOTT-AVE-PR-2150

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.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
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2,4,7,9-Tetrame...	9.210	26.8	ng	1363020	3	9.763	1016450	20.0
unknown10.345	10.345	11.6	ng	586992	3	9.763	1016450	20.0
unknown11.439	11.439	3.3	ng	162786	4	11.251	997445	20.0
n-Hexadecanoic ...	11.786	6.0	ng	300987	4	11.251	997445	20.0
1-Hexadecanol	12.304	7.9	ng	394391	4	11.251	997445	20.0
Bis(2-ethylhexy...	12.492	4.4	ng	218004	4	11.251	997445	20.0
Docosyl pentafl...	13.063	7.0	ng	252789	5	13.892	723006	20.0
Trifluoroacetic...	13.739	23.2	ng	837773	5	13.892	723006	20.0
1-Heptacosanol	15.815	4.0	ng	140039	6	15.327	708801	20.0