

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011821\
 Data File : BF123008.D
 Acq On : 19 Jan 2021 2:19
 Operator : JU/CG
 Sample : M1157-02
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-2

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-BF011621.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123008.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	18	24	30	rVB	1809633	2246616	65.32%	8.599%
2	5.116	509	515	522	rVB	49895	57383	1.67%	0.220%
3	5.510	577	582	585	rBV	2615996	2330519	67.76%	8.920%
4	6.504	747	751	757	rVB2	1224699	1474896	42.88%	5.645%
5	6.716	784	787	794	rBV	178356	153685	4.47%	0.588%
6	6.892	813	817	821	rBV	753825	636790	18.51%	2.437%
7	7.457	906	913	916	rBV	1907702	2154358	62.63%	8.246%
8	7.534	921	926	933	rVB2	26488	42002	1.22%	0.161%
9	8.175	1030	1035	1038	rBV	1032988	992012	28.84%	3.797%
10	8.198	1038	1039	1042	rVB	163509	82960	2.41%	0.318%
11	8.722	1123	1128	1132	rVB2	67441	63254	1.84%	0.242%
12	8.845	1145	1149	1152	rBV	51565	44189	1.28%	0.169%
13	8.886	1152	1156	1159	rVB	42585	36632	1.07%	0.140%
14	9.251	1213	1218	1222	rBV	2539144	2591853	75.35%	9.920%
15	9.369	1234	1238	1241	rVB	303021	264235	7.68%	1.011%
16	9.645	1281	1285	1288	rBV	261452	210876	6.13%	0.807%
17	9.933	1327	1334	1338	rBV	858801	877072	25.50%	3.357%
18	10.722	1462	1468	1471	rBV	3062174	2779913	80.82%	10.640%
19	11.280	1558	1563	1569	rBV7	21501	38531	1.12%	0.147%
20	11.422	1582	1587	1590	rBV	835413	701581	20.40%	2.685%
21	11.951	1670	1677	1681	rBV	608259	613765	17.84%	2.349%
22	12.404	1750	1754	1757	rBV	47898	53237	1.55%	0.204%
23	12.657	1795	1797	1803	rVB3	31082	41099	1.19%	0.157%
24	12.733	1806	1810	1819	rBV	335204	379913	11.05%	1.454%
25	12.886	1834	1836	1838	rBV	84415	66887	1.94%	0.256%
26	13.016	1852	1858	1861	rBV	3530868	3439553	100.00%	13.165%
27	13.227	1890	1894	1895	rBV2	34398	36887	1.07%	0.141%
28	13.245	1895	1897	1901	rVB	72112	58581	1.70%	0.224%
29	13.586	1950	1955	1958	rBV2	67629	76291	2.22%	0.292%
30	13.910	2007	2010	2019	rBV	807893	868889	25.26%	3.326%
31	14.063	2032	2036	2040	rBV	1097997	1023808	29.77%	3.919%
32	14.233	2062	2065	2072	rBV	82742	85271	2.48%	0.326%
33	14.539	2114	2117	2122	rVB2	80985	112336	3.27%	0.430%
34	14.851	2166	2170	2175	rBV	63541	75044	2.18%	0.287%
35	15.192	2225	2228	2232	rBV	54257	65114	1.89%	0.249%
36	15.409	2262	2265	2267	rBV3	24590	34584	1.01%	0.132%

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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-BF011621.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.545	2282	2288	2292	rBV	729276	887962	25.82%	3.399%
38	15.586	2292	2295	2302	rVB	70937	121203	3.52%	0.464%
39	16.027	2363	2370	2375	rBV2	52122	86422	2.51%	0.331%
40	16.086	2375	2380	2387	rVV3	68596	134236	3.90%	0.514%
41	16.551	2454	2459	2462	rBV3	28579	47184	1.37%	0.181%
42	17.156	2554	2562	2566	rBV6	16895	39318	1.14%	0.150%

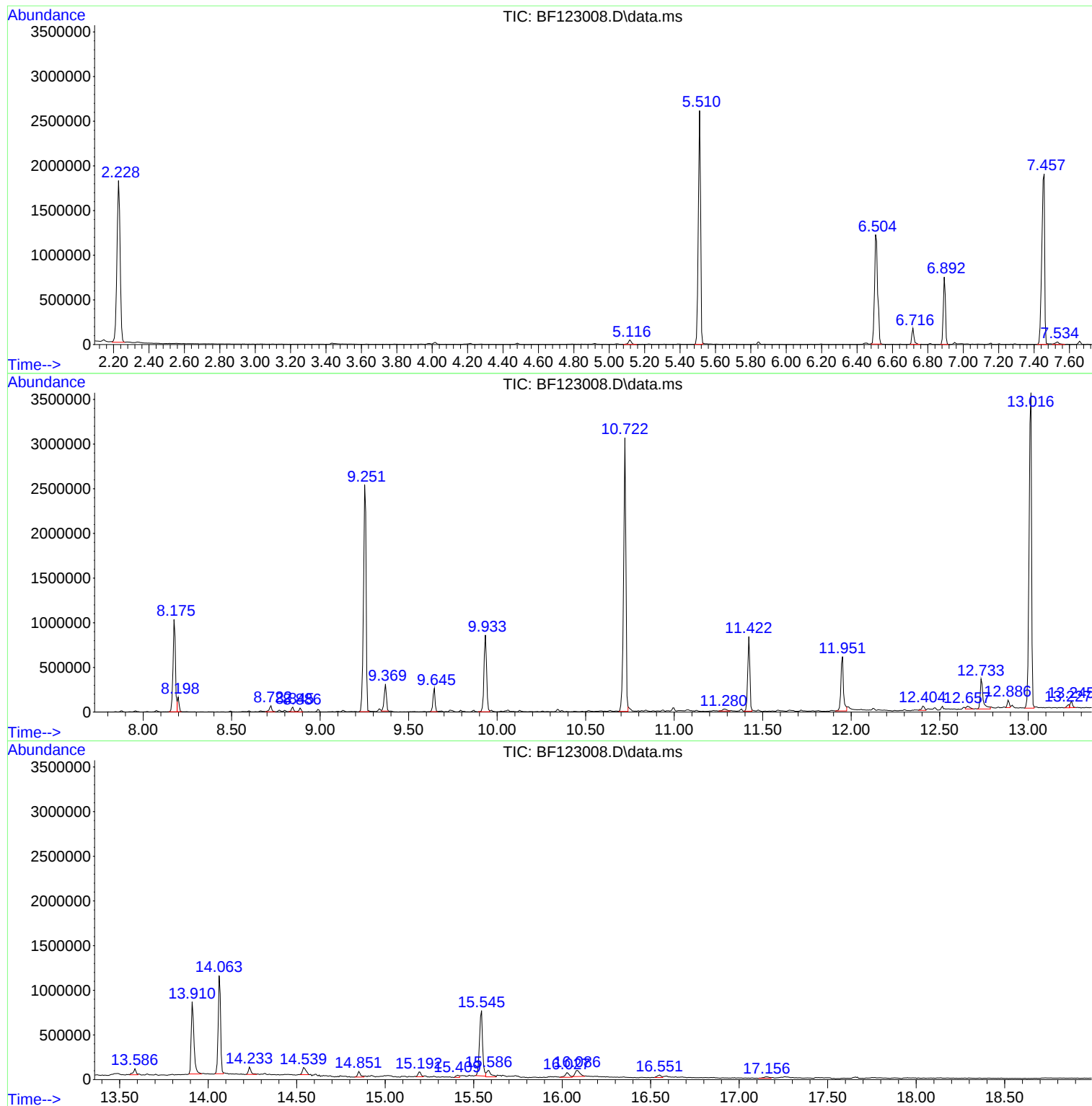
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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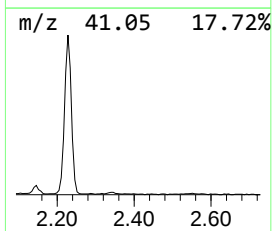
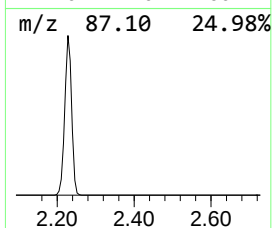
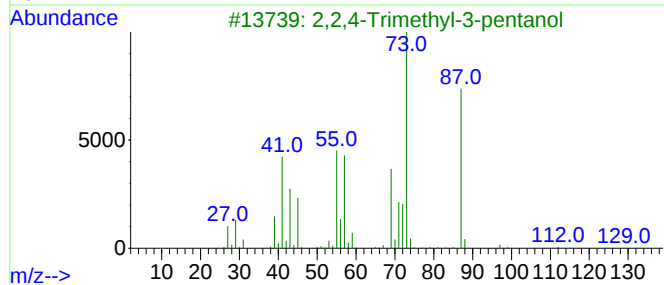
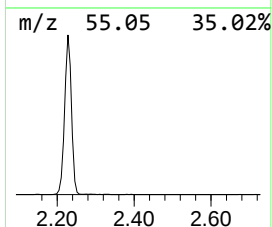
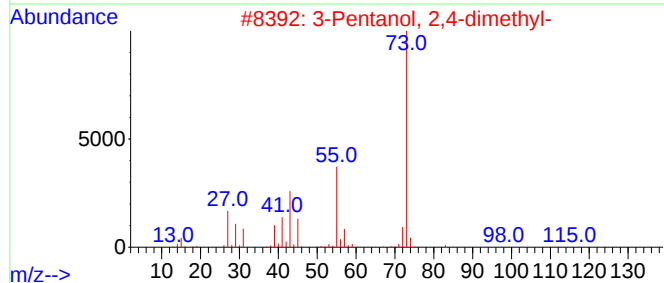
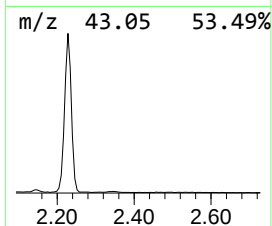
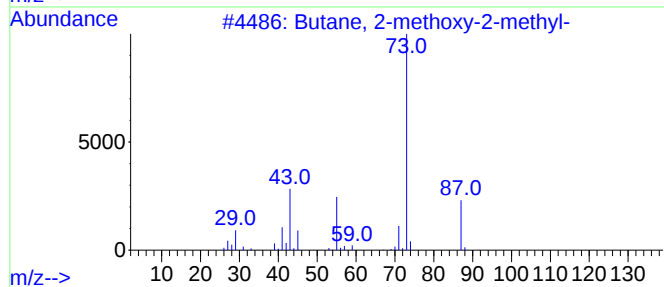
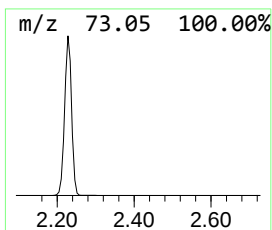
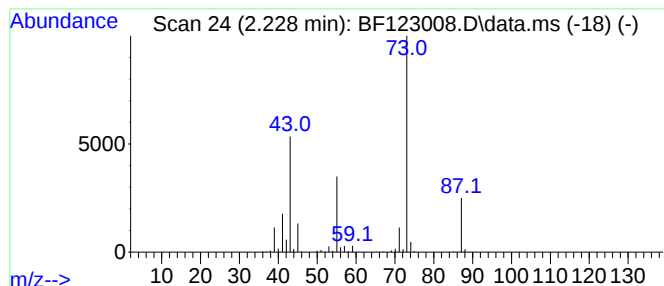
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.228	70.56 ng	2246620	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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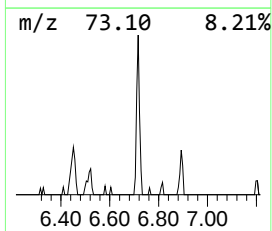
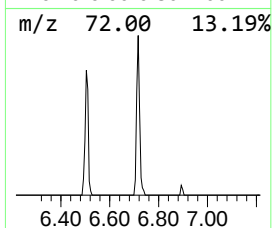
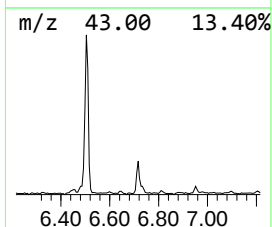
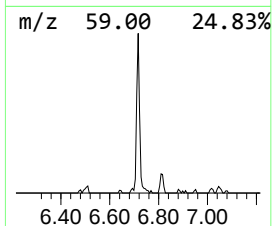
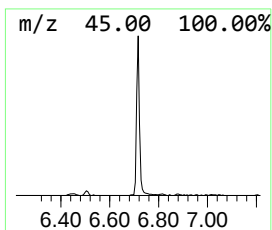
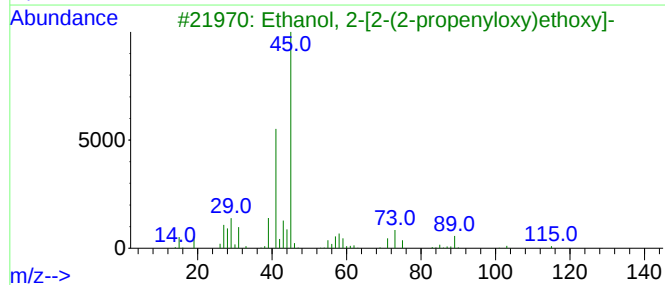
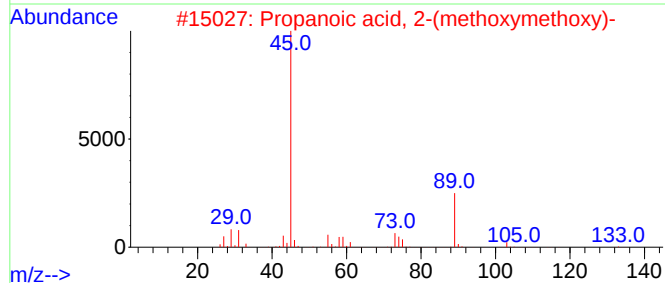
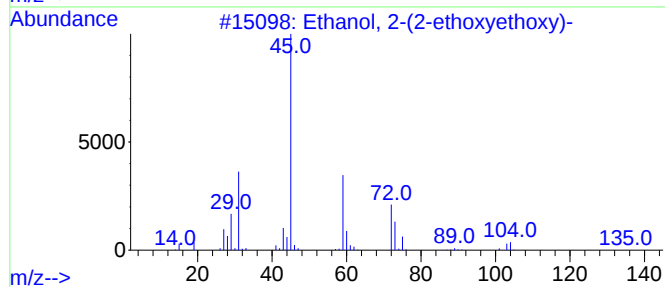
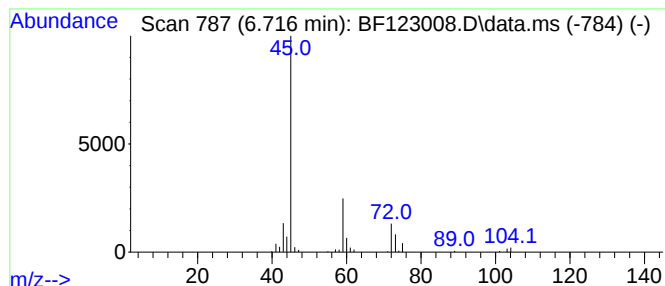
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011621.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.716	4.83 ng	153685	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	50
2			Propanoic acid, 2-(methoxymethoxy)-	134	C5H10O4	081327-29-9	42
3			Ethanol, 2-[2-(2-propenyloxy)etho...	146	C7H14O3	015075-50-0	38
4			2-Butanol	74	C4H10O	000078-92-2	38
5			Ethyl ether	74	C4H10O	000060-29-7	36



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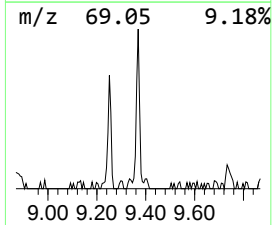
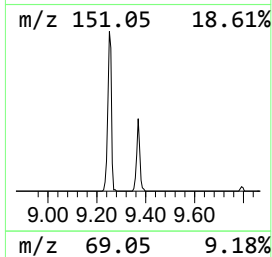
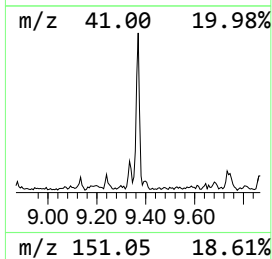
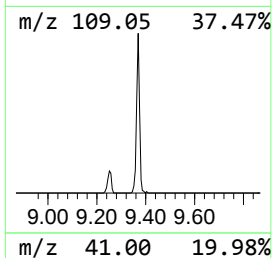
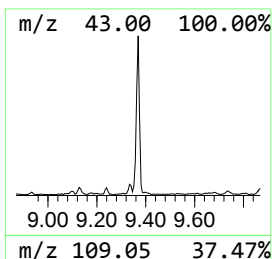
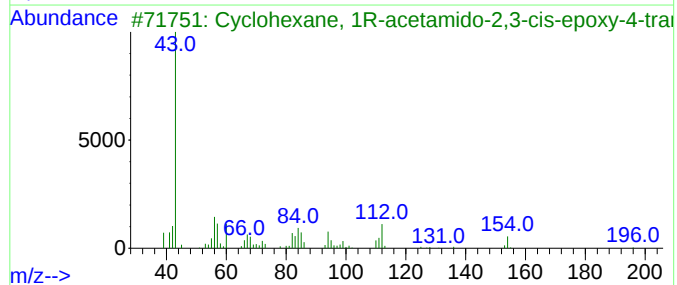
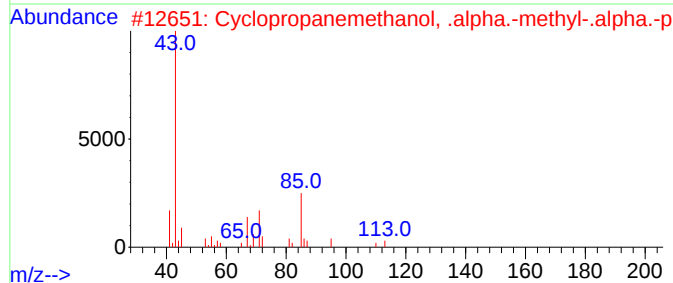
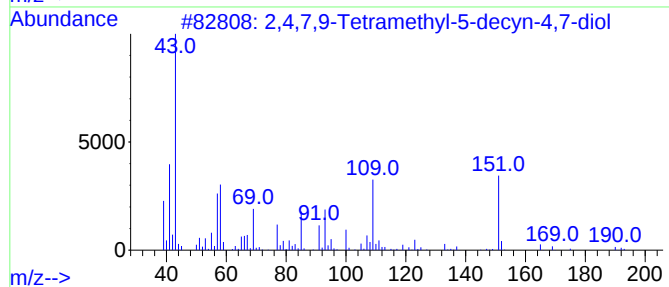
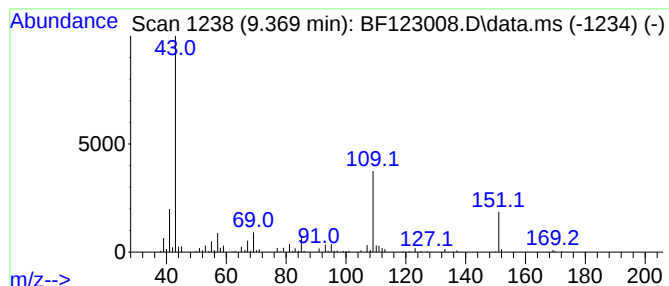
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011621.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown9.369 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.369	6.03 ng	264235	Acenaphthene-d10	9.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	28		
2	Cyclopropanemethanol, .alpha.-me...	128	C8H16O	024230-08-8	12		
3	Cyclohexane, 1R-acetamido-2,3-ci...	213	C10H15NO4	1000153-70-8	10		
4	1-Acetyl-3-amino-4-cyano-3-pyrro...	151	C7H9N3O	002125-74-8	9		
5	3-Hexyne-2,5-diol, 2,5-dimethyl-	142	C8H14O2	000142-30-3	9		



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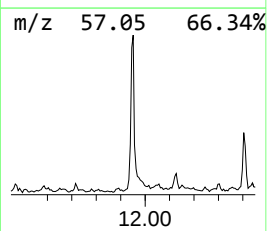
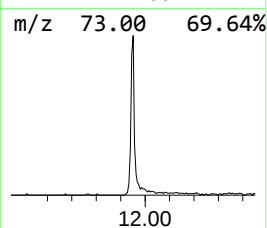
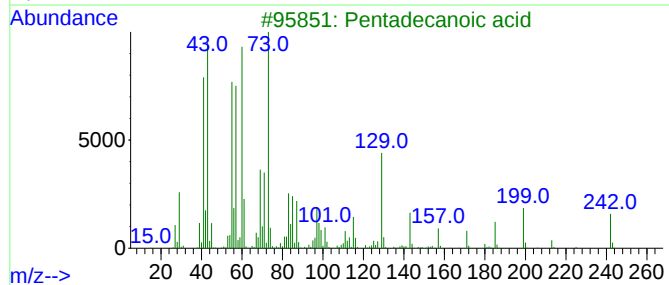
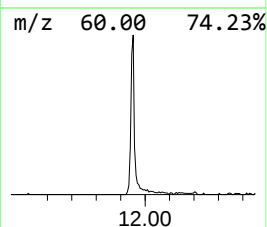
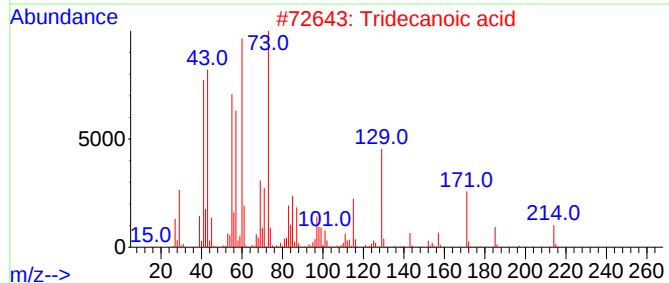
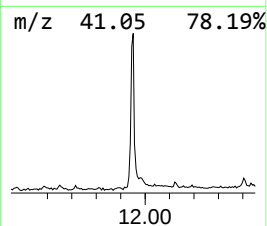
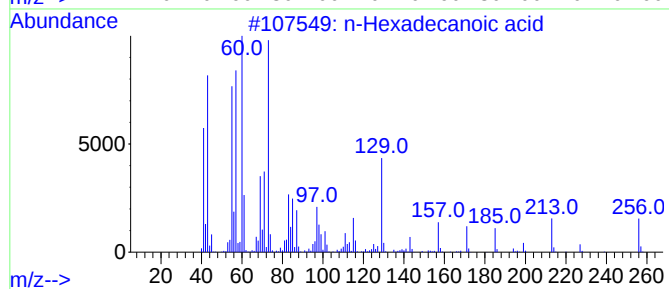
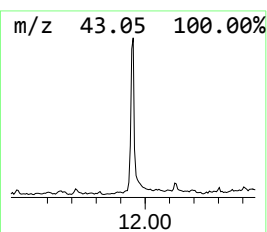
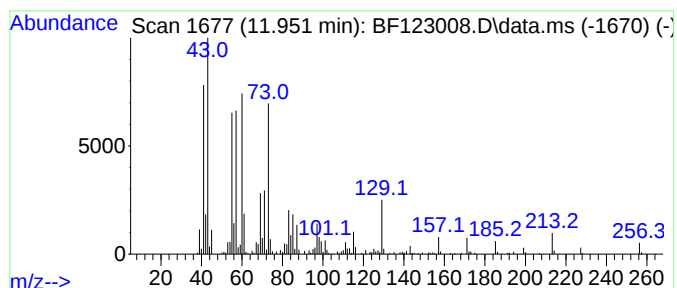
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.951	17.50 ng	613765	Phenanthrene-d10	11.422	
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	83
5	Dodecanoic acid	200	C12H24O2	000143-07-7	70



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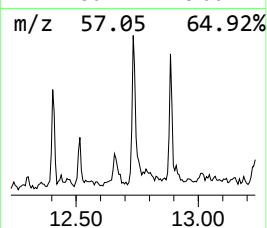
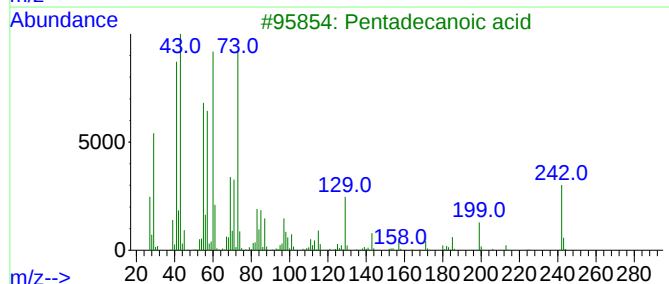
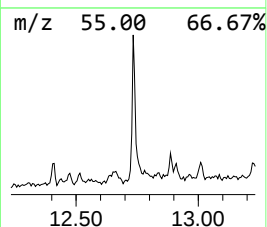
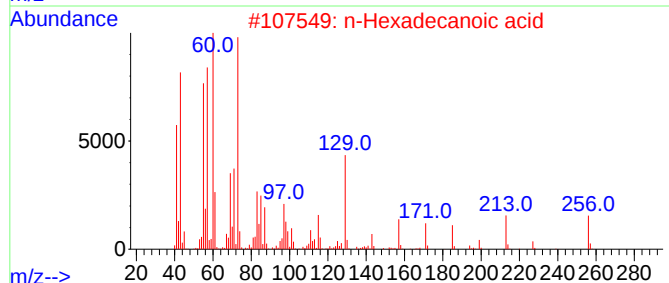
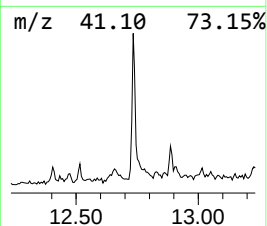
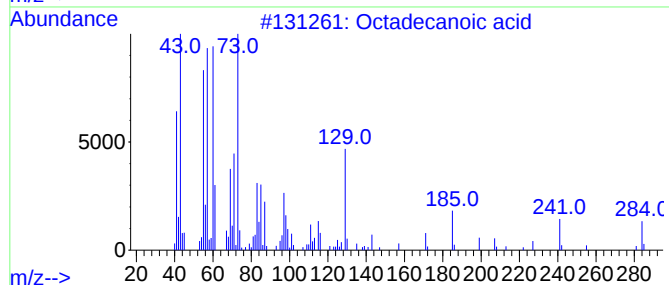
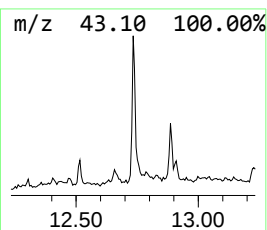
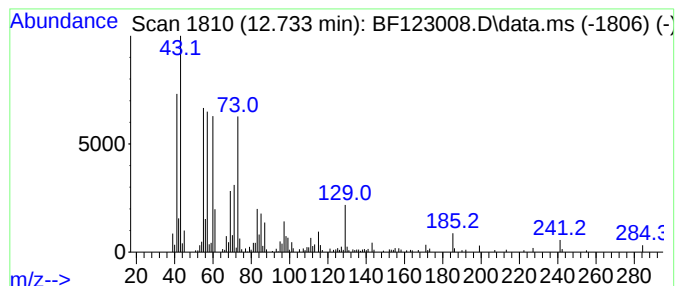
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.733	10.83 ng	379913	Phenanthrene-d10	11.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	97
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011821\
Data File : BF123008.D
Acq On : 19 Jan 2021 2:19
Operator : JU/CG
Sample : M1157-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-2

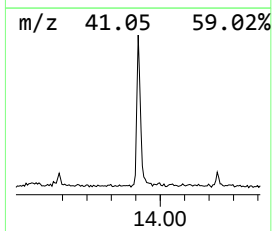
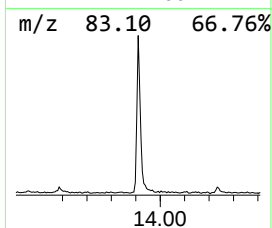
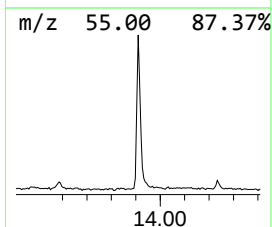
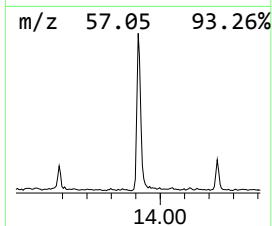
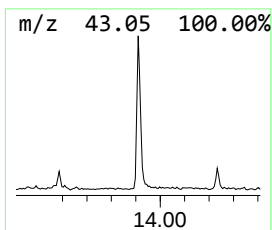
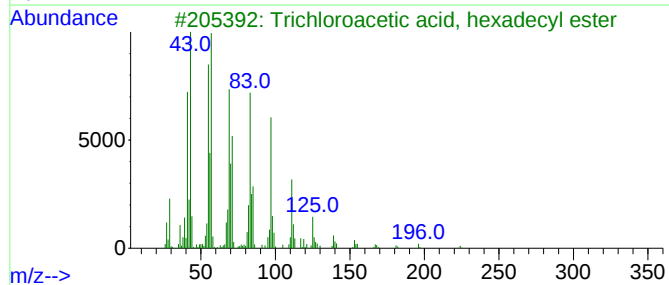
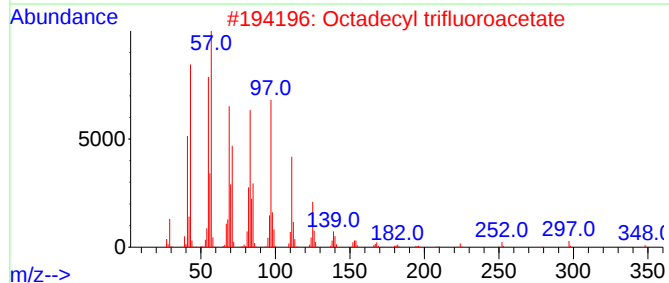
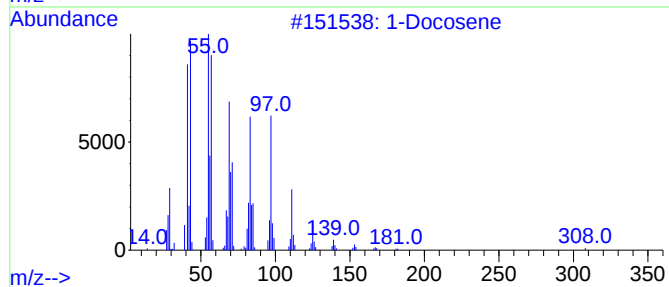
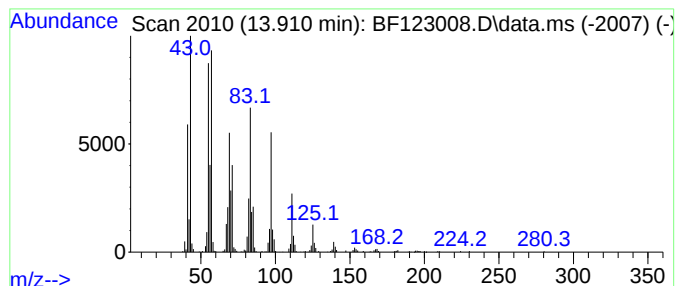
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	16.97 ng	868889	Chrysene-d12	14.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene			308	C22H44	001599-67-3	95
2	Octadecyl trifluoroacetate			366	C20H37F3O2	079392-43-1	94
3	Trichloroacetic acid, hexadecyl ...			386	C18H33Cl3O2	074339-54-1	94
4	Trifluoroacetoxy hexadecane			338	C18H33F3O2	006222-03-3	91
5	Heptafluorobutyric acid, hexadec...			438	C20H33F7O2	006385-15-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011821\
Data File : BF123008.D
Acq On : 19 Jan 2021 2:19
Operator : JU/CG
Sample : M1157-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-2

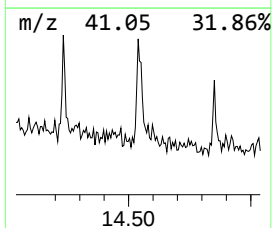
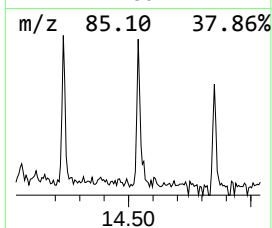
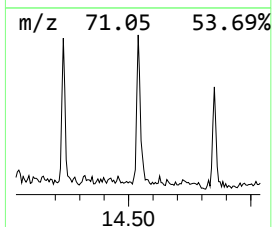
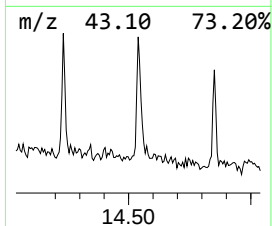
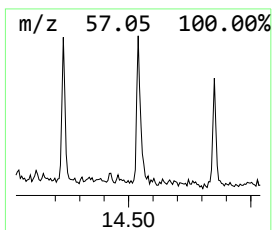
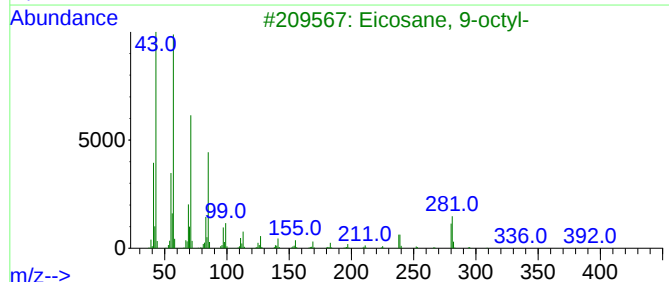
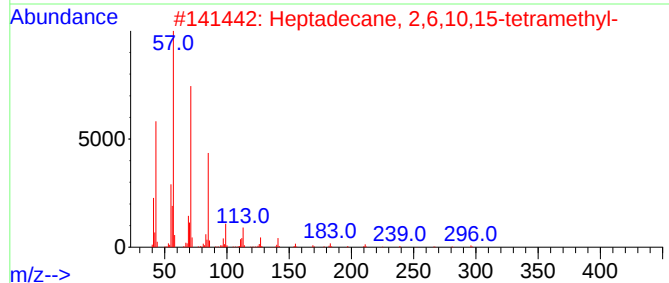
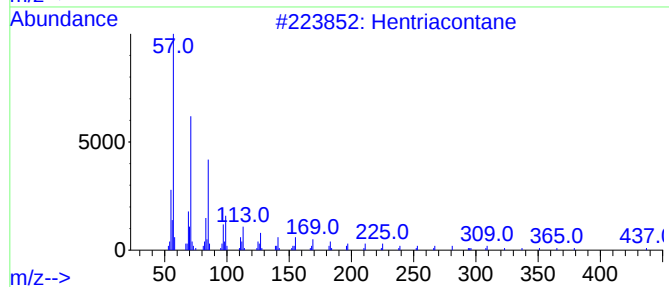
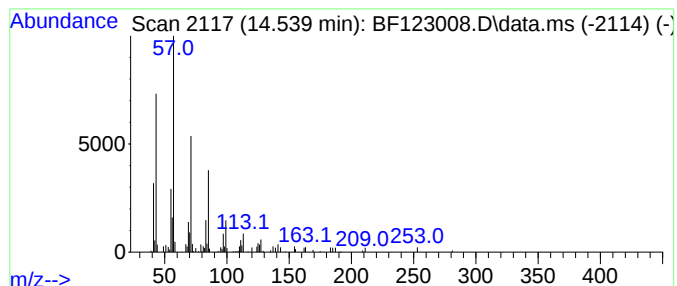
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hentriacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.539	2.19 ng	112336	Chrysene-d12	14.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hentriacontane	437	C31H64	000630-04-6	91
2			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90
3			Eicosane, 9-octyl-	394	C28H58	013475-77-9	87
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5			Tetratetracontane	619	C44H90	007098-22-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011821\
Data File : BF123008.D
Acq On : 19 Jan 2021 2:19
Operator : JU/CG
Sample : M1157-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
MW-2

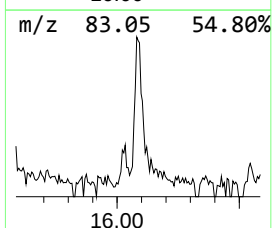
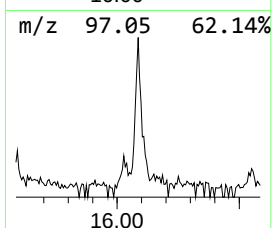
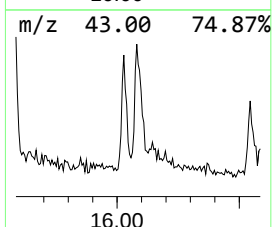
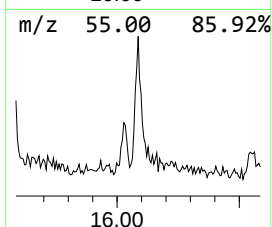
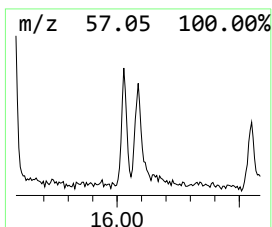
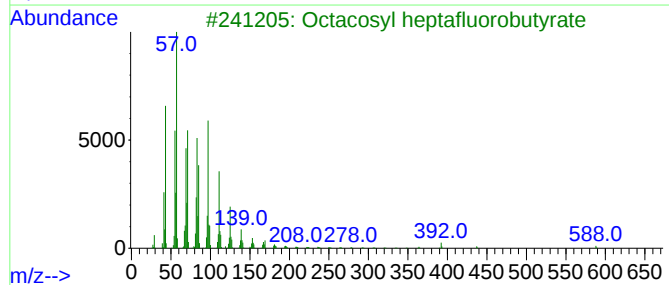
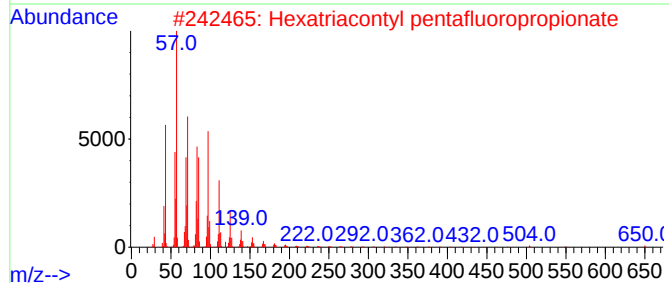
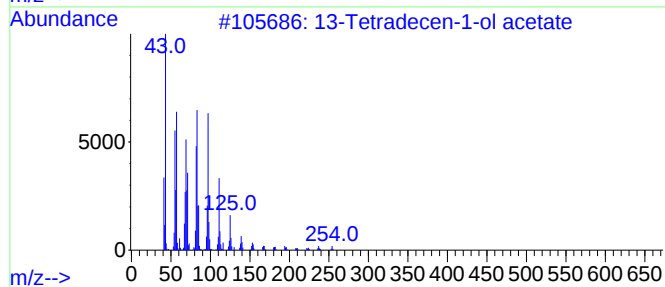
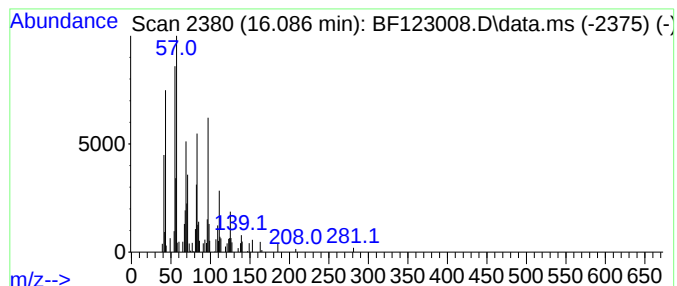
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 13-Tetradecen-1-ol acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.086	3.02 ng	134236	Perylene-d12	15.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	90
2			Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	87
3			Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	83
4			Heptacosyl pentafluoropropionate	542	C30H55F5O2	1000351-81-6	83
5			Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011821\
Data File : BF123008.D
Acq On : 19 Jan 2021 2:19
Operator : JU/CG
Sample : M1157-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011621.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...	2.228	70.6	ng	2246620	1	6.892	636790	20.0
Ethanol, 2-(2-e...	6.716	4.8	ng	153685	1	6.892	636790	20.0
unknown9.369	9.369	6.0	ng	264235	3	9.933	877072	20.0
n-Hexadecanoic ...	11.951	17.5	ng	613765	4	11.422	701581	20.0
Octadecanoic acid	12.733	10.8	ng	379913	4	11.422	701581	20.0
1-Docosene	13.910	17.0	ng	868889	5	14.063	1023810	20.0
Hentriacontane	14.539	2.2	ng	112336	5	14.063	1023810	20.0
13-Tetradecen-1...	16.086	3.0	ng	134236	6	15.545	887962	20.0