

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070517\
 Data File : BF096494.D
 Acq On : 5 Jul 2017 19:55
 Operator : SJ/MA
 Sample : I4052-01
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HR-03-070317-A

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.904	474	479	489	rVB	290674	431518	15.04%	1.800%
2	5.328	546	551	554	rBV	2672805	2829132	98.62%	11.798%
3	6.351	720	725	730	rBV	2610738	2868852	100.00%	11.964%
4	6.481	743	747	751	rBV	2761222	2714050	94.60%	11.318%
5	6.710	782	786	790	rBV	840556	674086	23.50%	2.811%
6	6.869	809	813	816	rBV	2336507	2090334	72.86%	8.717%
7	7.275	876	882	885	rBV	1753593	1694853	59.08%	7.068%
8	7.992	1000	1004	1007	rBV	1099765	873954	30.46%	3.645%
9	9.075	1182	1188	1191	rBV	3028640	2671358	93.12%	11.140%
10	9.463	1251	1254	1258	rBV	450226	360788	12.58%	1.505%
11	9.745	1298	1302	1306	rVB	934686	799184	27.86%	3.333%
12	10.192	1375	1378	1381	rVB	53335	40714	1.42%	0.170%
13	10.533	1431	1436	1439	rBV	1312988	1174293	40.93%	4.897%
14	10.663	1455	1458	1461	rBV	63786	64431	2.25%	0.269%
15	11.110	1531	1534	1538	rBV2	38357	40014	1.39%	0.167%
16	11.227	1550	1554	1556	rBV	710927	596010	20.78%	2.486%
17	11.251	1556	1558	1561	rVB	65911	52113	1.82%	0.217%
18	11.463	1589	1594	1598	rBV4	35863	40153	1.40%	0.167%
19	12.280	1730	1733	1736	rBV2	26869	32127	1.12%	0.134%
20	12.339	1740	1743	1745	rVB3	39067	36550	1.27%	0.152%
21	12.433	1756	1759	1763	rVB	84790	71619	2.50%	0.299%
22	12.663	1792	1798	1801	rBV	87986	113524	3.96%	0.473%
23	12.815	1819	1824	1827	rBV	1702115	1653377	57.63%	6.895%
24	13.715	1973	1977	1985	rVB2	119630	139316	4.86%	0.581%
25	13.857	1996	2001	2004	rBV	711154	672163	23.43%	2.803%
26	13.880	2004	2005	2010	rVB	45221	31249	1.09%	0.130%
27	14.351	2081	2085	2090	rBV	78456	93776	3.27%	0.391%
28	14.615	2127	2130	2134	rBV	125933	142445	4.97%	0.594%
29	14.715	2144	2147	2150	rVB	29743	34143	1.19%	0.142%
30	14.780	2155	2158	2162	rVB	42889	46180	1.61%	0.193%
31	14.862	2169	2172	2179	rBV	27327	58664	2.04%	0.245%
32	14.980	2186	2192	2200	rBV3	93188	174211	6.07%	0.727%
33	15.204	2227	2230	2235	rVB	26319	31565	1.10%	0.132%
34	15.268	2236	2241	2245	rBV	419362	517622	18.04%	2.159%

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ALS Vial : 24 Sample Multiplier: 1

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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

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35	15.727	2315	2319	2323	rBV2	55197	76714	2.67%	0.320%
36	16.751	2490	2493	2499	rVB4	24186	37870	1.32%	0.158%

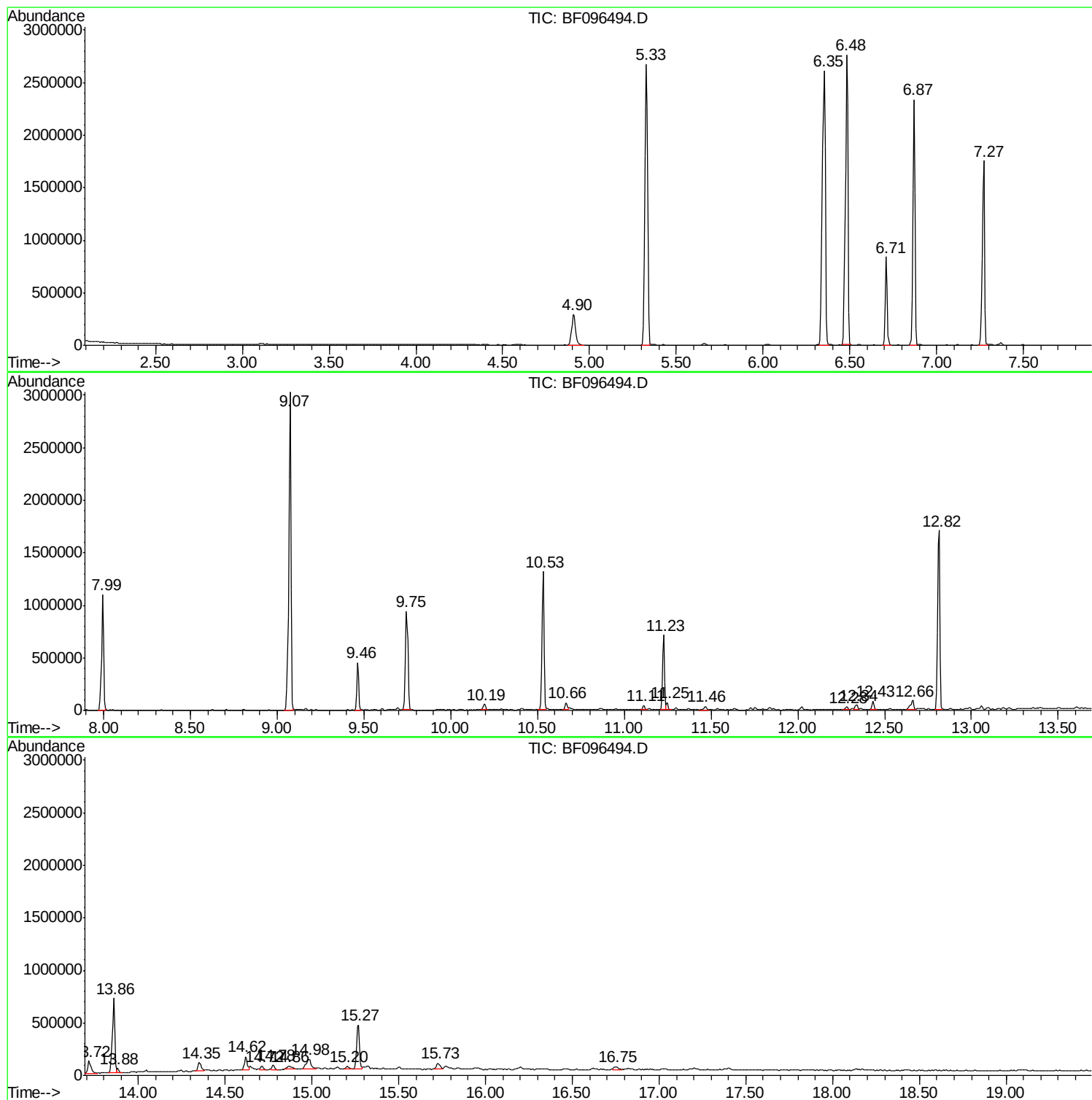
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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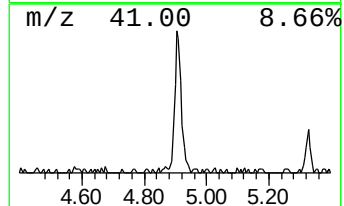
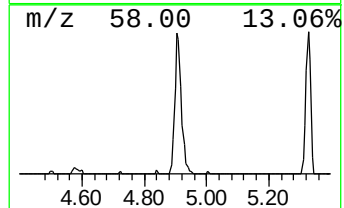
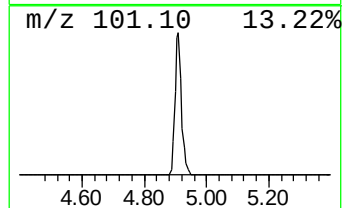
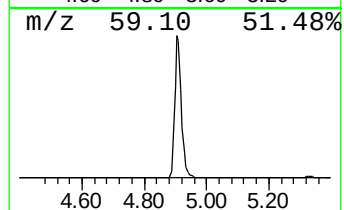
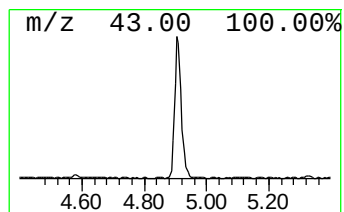
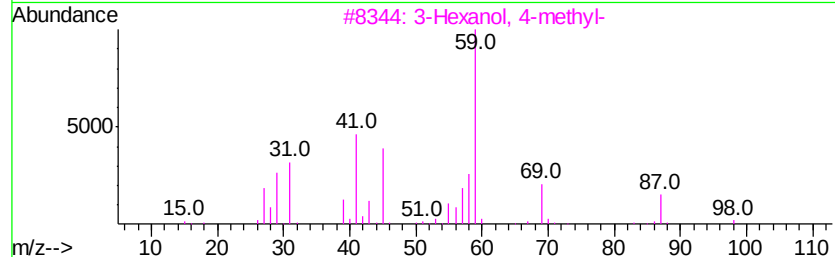
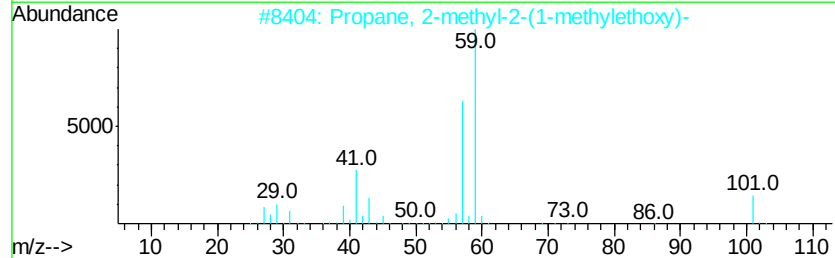
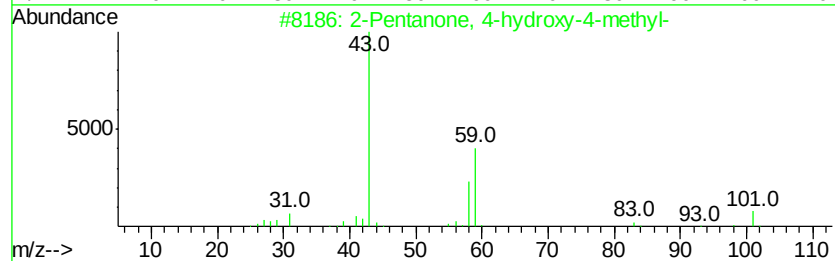
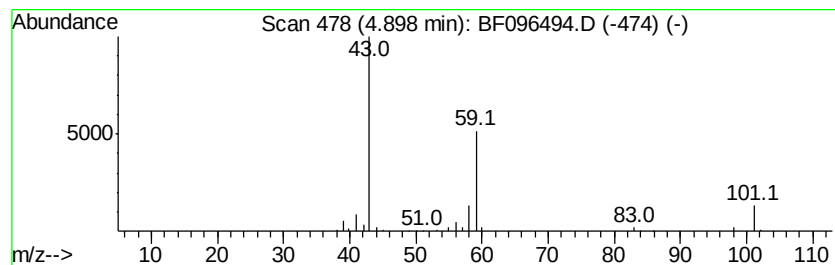
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
4.90	12.80 ng	431518	1,4-Dichlorobenzene-d4	6.71		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50	
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42	
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33	
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28	
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25	



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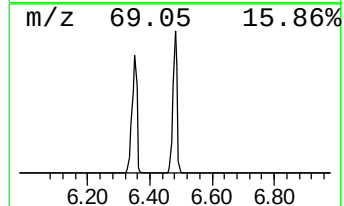
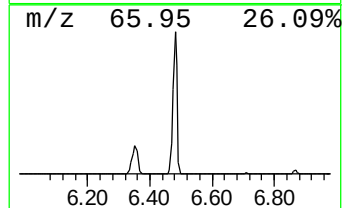
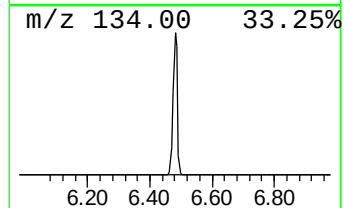
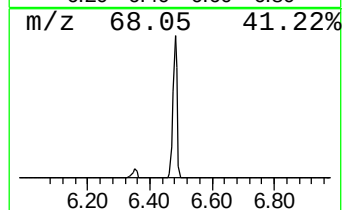
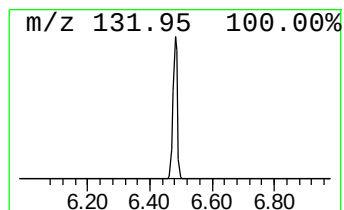
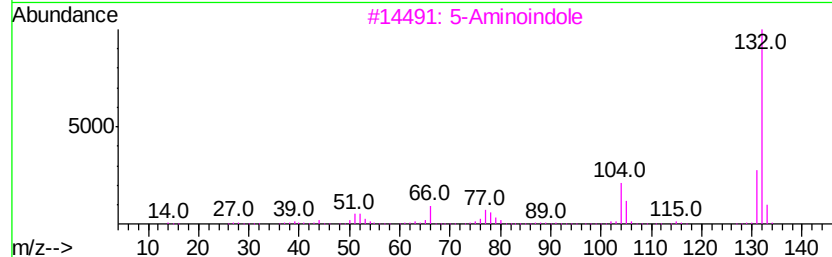
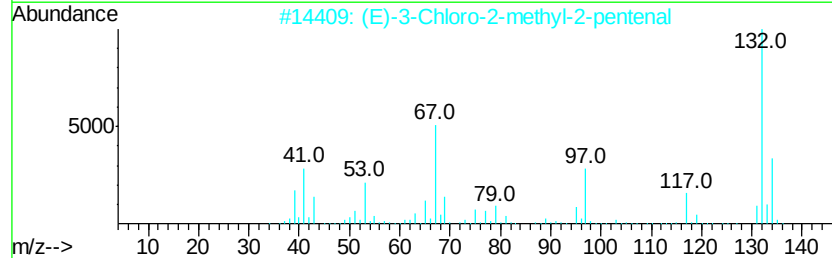
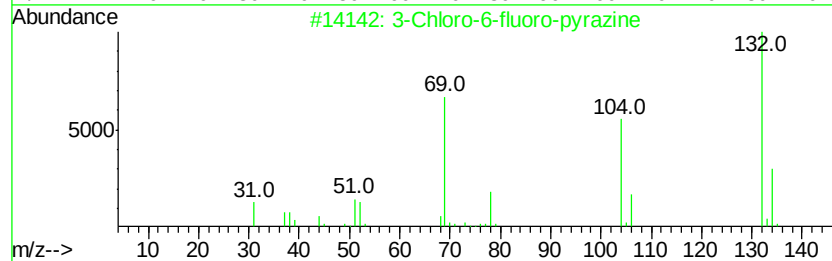
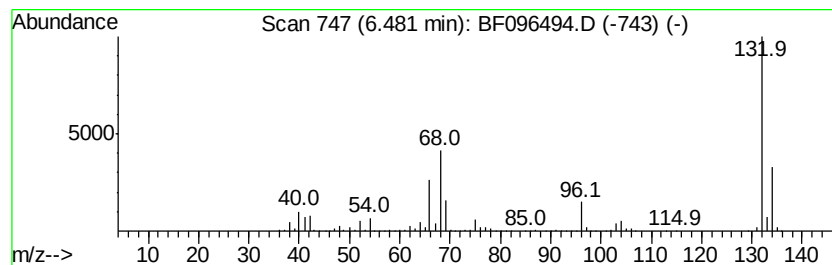
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	80.53 ng	2714050	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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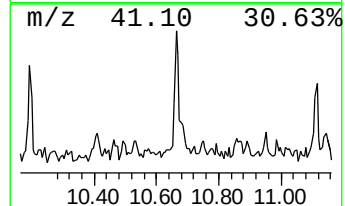
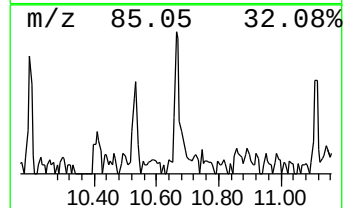
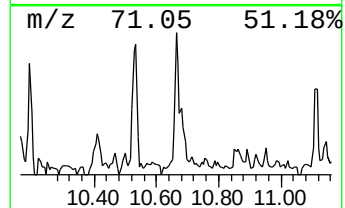
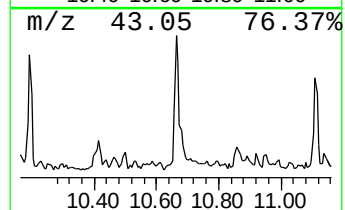
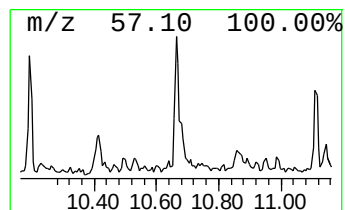
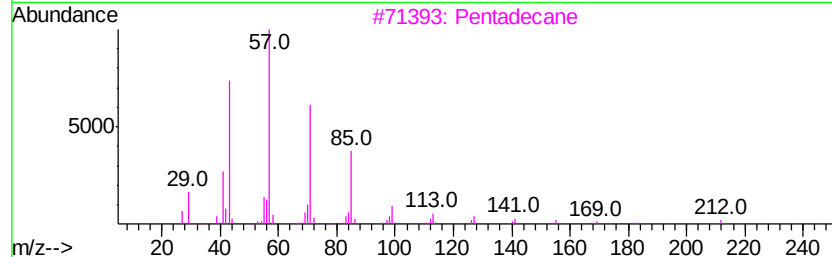
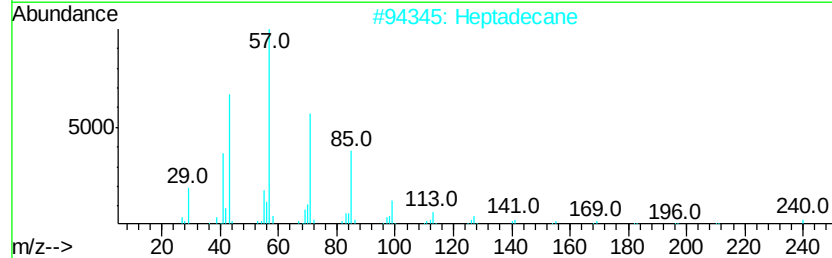
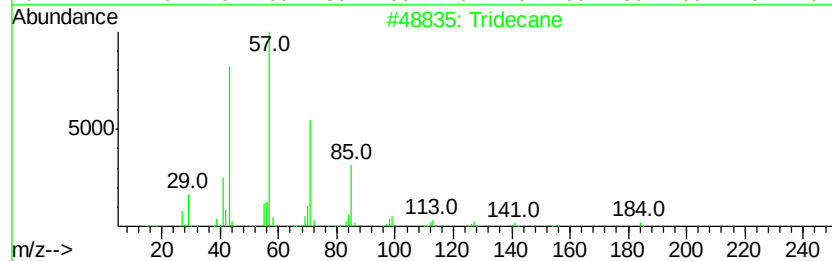
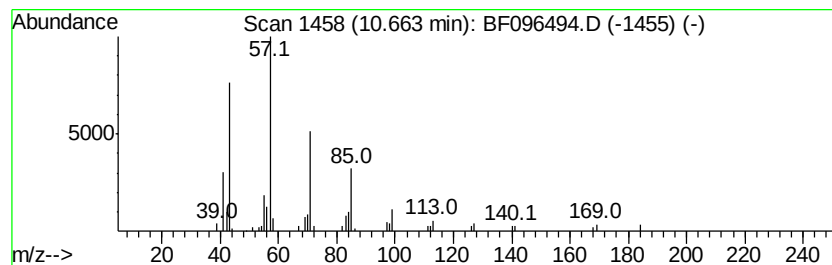
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tridecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.66	2.16 ng	64431	Phenanthrene-d10		11.23
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	94
2	Heptadecane	240	C17H36	000629-78-7	91
3	Pentadecane	212	C15H32	000629-62-9	90
4	Hexadecane	226	C16H34	000544-76-3	90
5	Tetradecane	198	C14H30	000629-59-4	87



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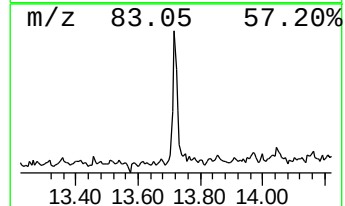
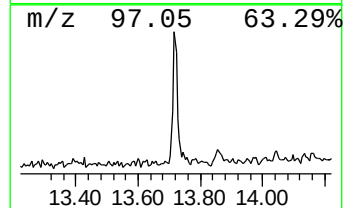
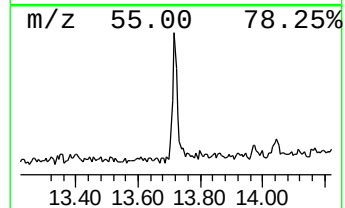
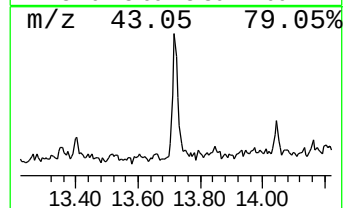
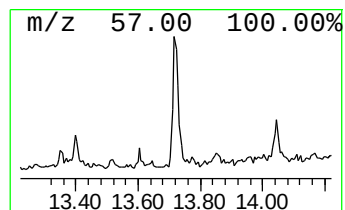
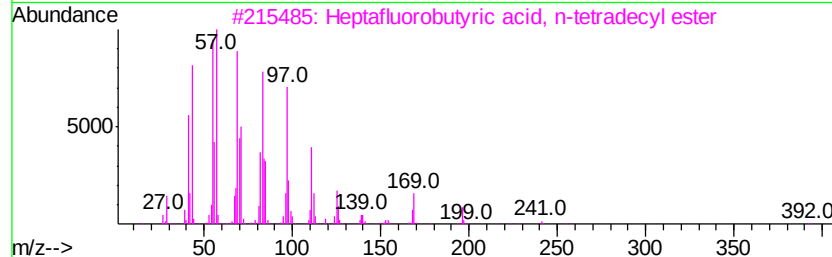
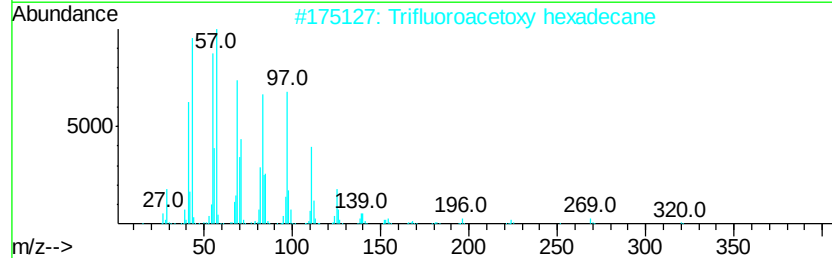
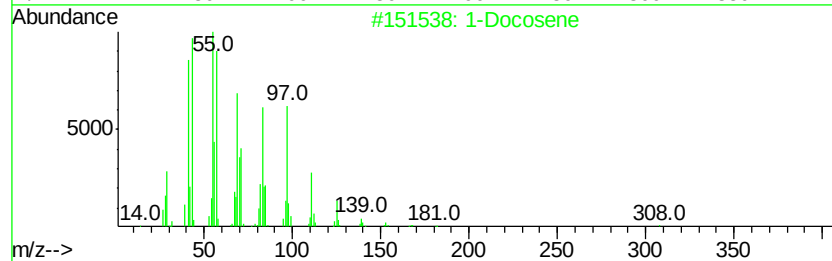
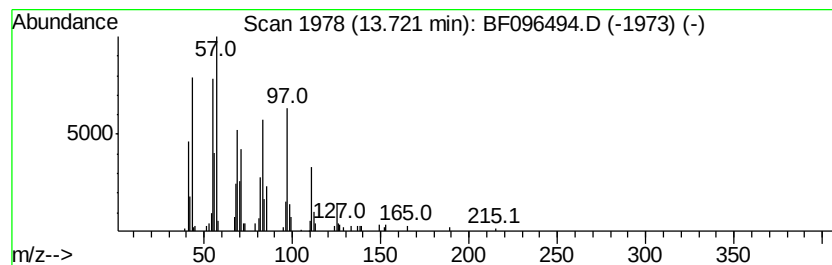
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Docosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	4.15 ng	139316	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	94
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91
4		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
5		3-Eicosene, (E)-	280	C20H40	074685-33-9	91



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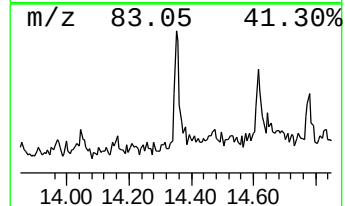
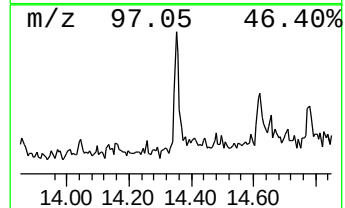
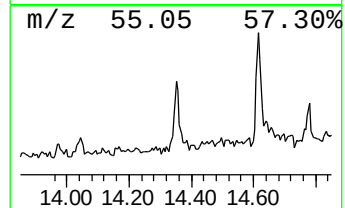
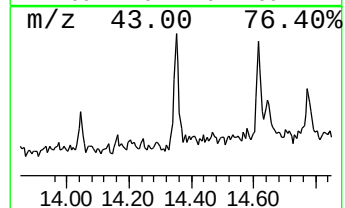
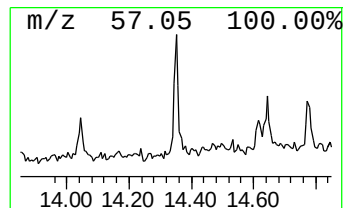
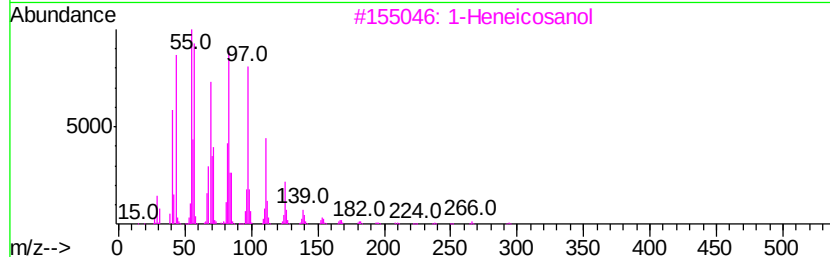
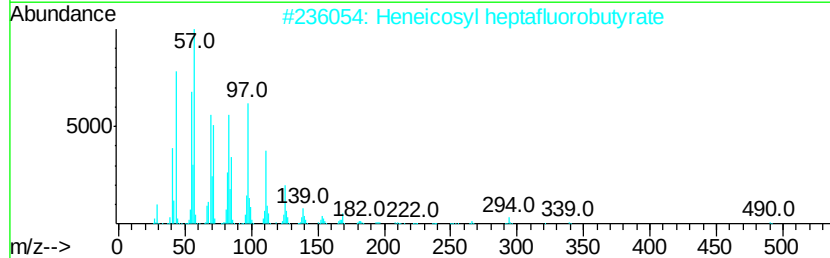
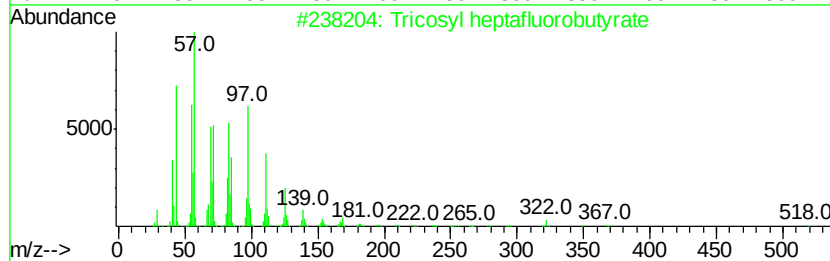
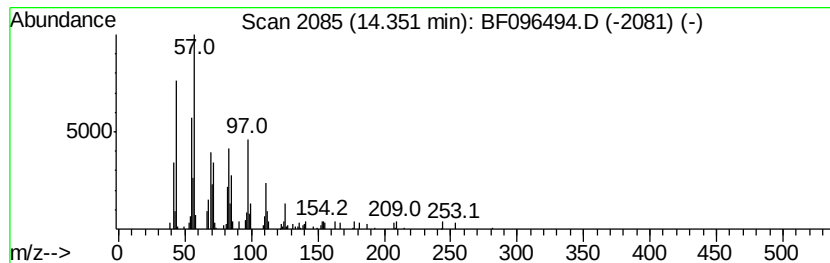
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Tricosyl heptafluorobutyrate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.35	2.79 ng	93776	Chrysene-d12	13.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	91
2		Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	90
3		1-Heneicosanol	312	C21H44O	015594-90-8	87
4		Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	87
5		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87



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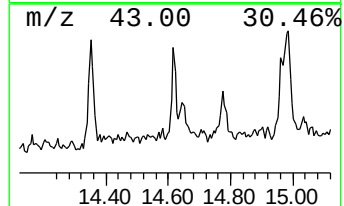
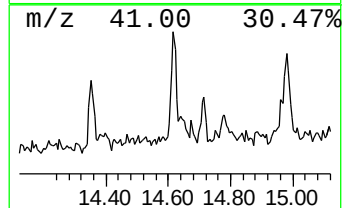
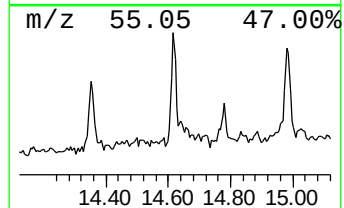
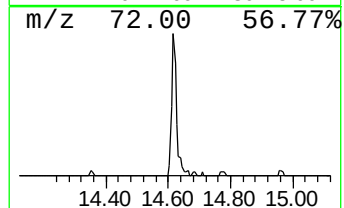
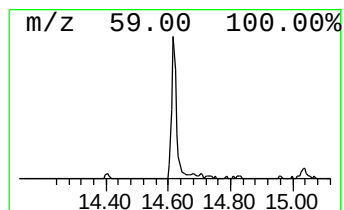
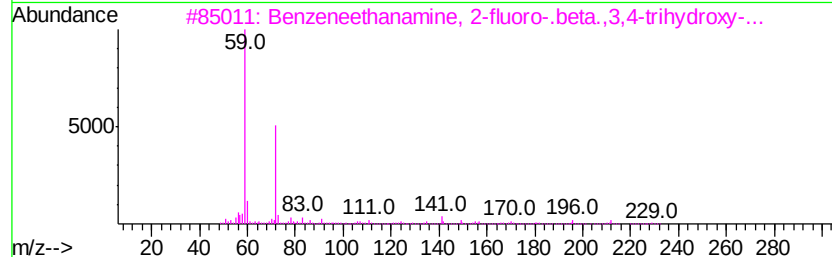
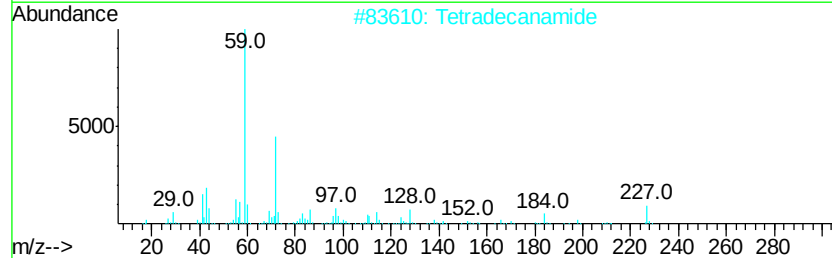
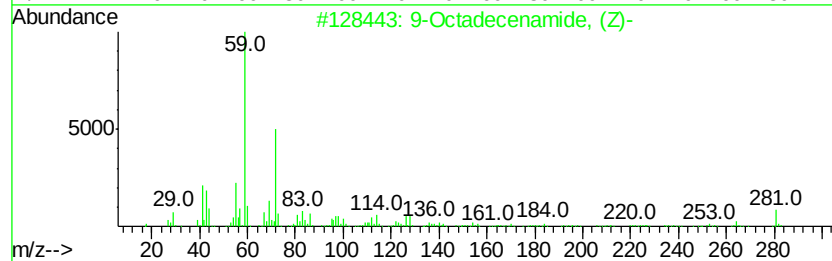
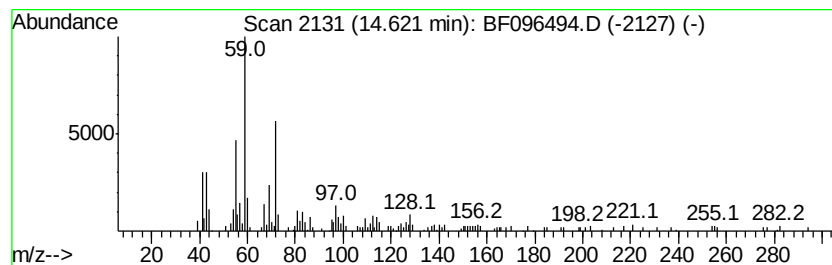
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	5.50 ng	142445	Perylene-d12	15.27

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
2		Tetradecanamide	227	C14H29NO	000638-58-4	80
3		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	72
4		Hexadecanamide	255	C16H33NO	000629-54-9	72
5		7-Nonenamide	155	C9H17NO	090949-53-4	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070517\
Data File : BF096494.D
Acq On : 5 Jul 2017 19:55
Operator : SJ/MA
Sample : I4052-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-03-070317-A

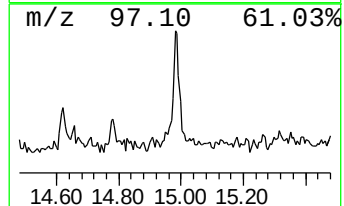
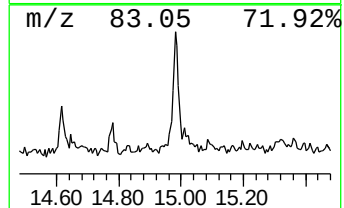
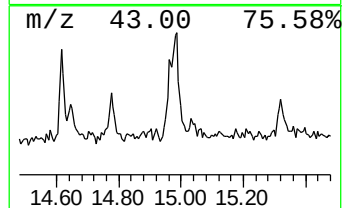
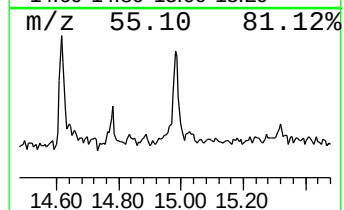
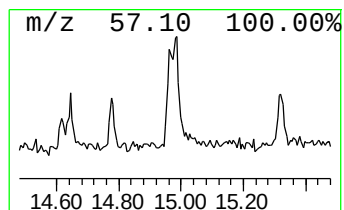
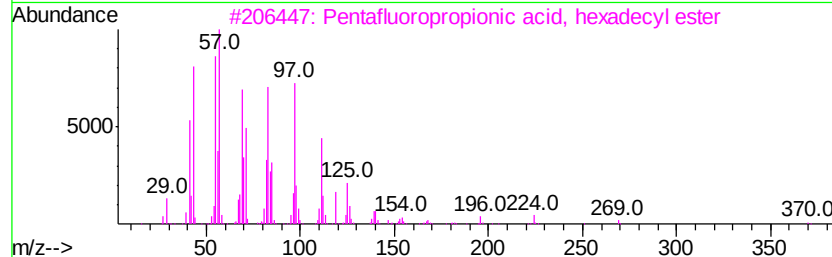
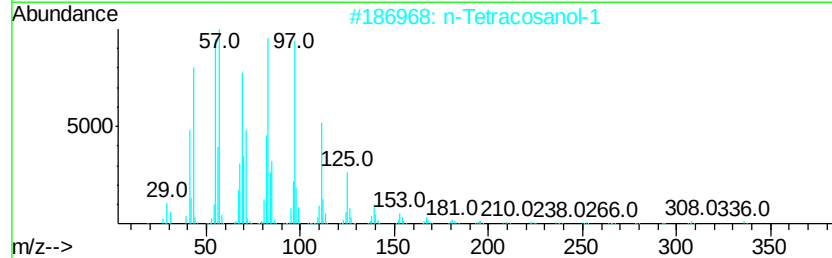
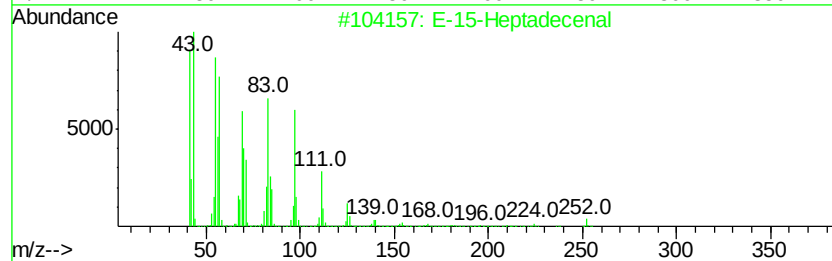
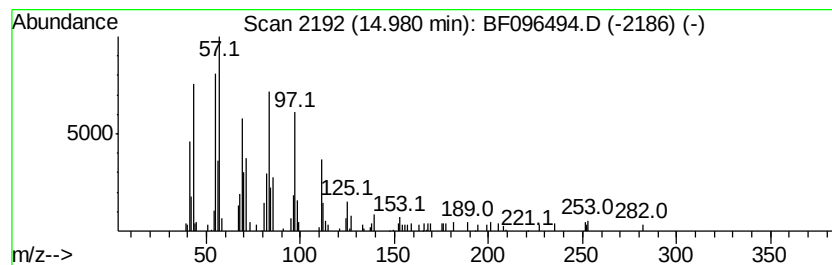
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 E-15-Heptadecenal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	6.73 ng	174211	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	E-15-Heptadecenal	252	C17H32O	1000130-97-9	96
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	93
3		Pentafluoropropionic acid, hexadecyl ester	388	C19H33F5O2	006222-07-7	90
4		Heptafluorobutyric acid, hexadecyl ester	438	C20H33F7O2	006385-15-5	90
5		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070517\
Data File : BF096494.D
Acq On : 5 Jul 2017 19:55
Operator : SJ/MA
Sample : I4052-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
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ClientSampleId :
HR-03-070317-A

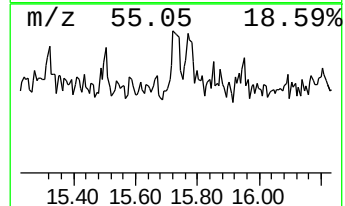
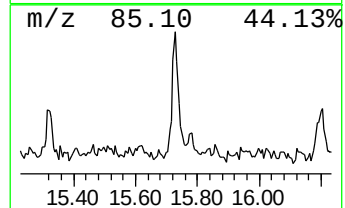
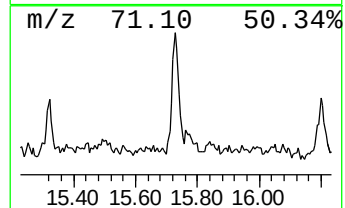
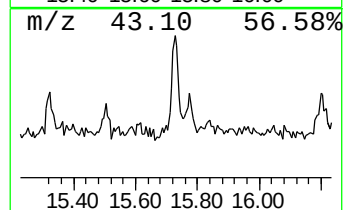
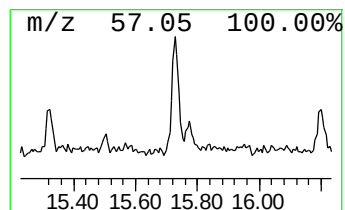
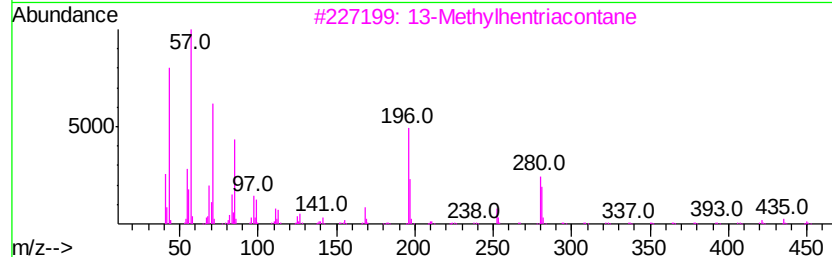
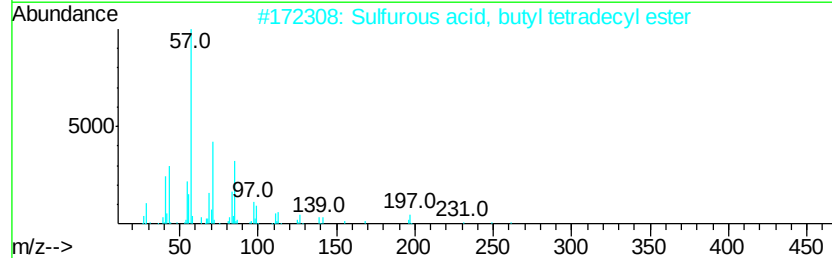
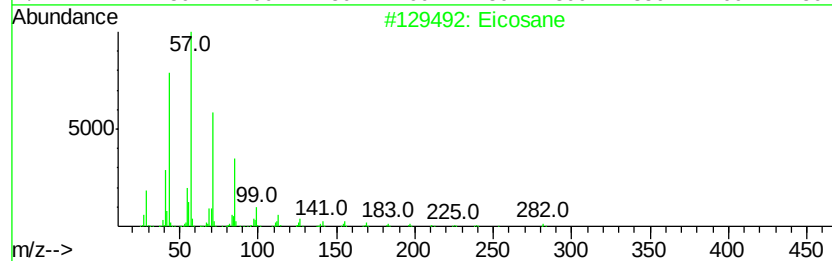
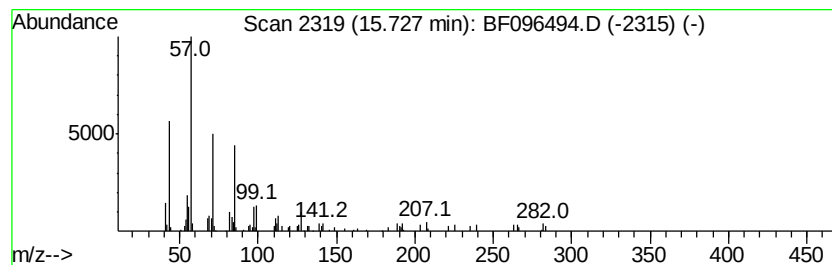
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.73	2.96 ng	76714	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	87
2		Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	80
3		13-Methylhentriacontane	451	C32H66	1000131-19-4	80
4		Tetratetracontane	619	C44H90	007098-22-8	72
5		Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070517\
Data File : BF096494.D
Acq On : 5 Jul 2017 19:55
Operator : SJ/MA
Sample : I4052-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-03-070317-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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
2-Pentanone, 4-hy...	4.90	12.8	ng	431518	1	6.71	674086	20.0
unknown6.48	6.48	80.5	ng	2714050	1	6.71	674086	20.0
Tridecane	10.66	2.2	ng	64431	4	11.23	596010	20.0
1-Docosene	13.72	4.2	ng	139316	5	13.86	672163	20.0
Tricosyl heptaflu...	14.35	2.8	ng	93776	5	13.86	672163	20.0
9-Octadecenamide,...	14.62	5.5	ng	142445	6	15.27	517622	20.0
E-15-Heptadecenal	14.98	6.7	ng	174211	6	15.27	517622	20.0
Eicosane	15.73	3.0	ng	76714	6	15.27	517622	20.0