

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100416\
 Data File : BF090343.D
 Acq On : 4 Oct 2016 14:45
 Operator : UM/SJ
 Sample : H4998-19
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SUP-B057-6-9

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-BF100416.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	1.850	22	23	26	rBV	1441894	1881236	7.65%	1.231%
2	1.941	26	31	33	rVV	11456276	24598305	100.00%	16.101%
3	1.998	34	36	67	rVB	7231627	15769848	64.11%	10.322%
4	5.222	315	318	325	rBV	1654621	2524103	10.26%	1.652%
5	5.622	350	353	356	rBV	8647631	9999191	40.65%	6.545%
6	6.639	438	442	444	rVB	8766093	11975897	48.69%	7.839%
7	6.776	451	454	457	rBV	8527791	10801027	43.91%	7.070%
8	7.005	472	474	477	rBV	1953660	2296261	9.34%	1.503%
9	7.165	486	488	490	rVB	6443812	7297333	29.67%	4.777%
10	7.576	520	524	526	rBV	6493690	7444371	30.26%	4.873%
11	7.656	526	531	533	rVV	195806	270977	1.10%	0.177%
12	8.045	563	565	567	rVB	479742	461513	1.88%	0.302%
13	8.296	585	587	589	rBV	3967972	3275239	13.31%	2.144%
14	9.382	679	682	684	rBV	9095991	11111857	45.17%	7.274%
15	9.771	713	716	718	rBV	5450439	4659012	18.94%	3.050%
16	10.056	738	741	743	rBV	4481938	3684829	14.98%	2.412%
17	10.845	807	810	813	rBV	6732112	7695323	31.28%	5.037%
18	10.959	819	820	825	rVB	280965	386466	1.57%	0.253%
19	11.542	869	871	873	rBV	3243721	3208699	13.04%	2.100%
20	12.079	915	918	920	rBV	567951	817708	3.32%	0.535%
21	12.639	965	967	970	rBV	554713	487074	1.98%	0.319%
22	12.857	984	986	991	rBV	291874	457592	1.86%	0.300%
23	13.142	1008	1011	1013	rBV	9608992	9337552	37.96%	6.112%
24	13.371	1029	1031	1034	rVB	1231340	1088617	4.43%	0.713%
25	14.034	1087	1089	1093	rBV2	1864414	2309701	9.39%	1.512%
26	14.194	1100	1103	1105	rBV	2944310	2657123	10.80%	1.739%
27	14.674	1143	1145	1149	rBV	1435384	1471449	5.98%	0.963%
28	15.371	1202	1206	1210	rBV	624730	1028603	4.18%	0.673%
29	15.703	1231	1235	1237	rBV	1232195	1907936	7.76%	1.249%
30	16.251	1281	1283	1289	rVB	693976	1225341	4.98%	0.802%
31	17.451	1384	1388	1396	rBV	129335	380294	1.55%	0.249%
32	17.954	1428	1432	1438	rVB2	93530	261305	1.06%	0.171%

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Instrument :
BNA_F
ClientSampleId :
SUP-B057-6-9

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:\HPCHEM1\BNA_F\METHODS\8270-BF100416.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

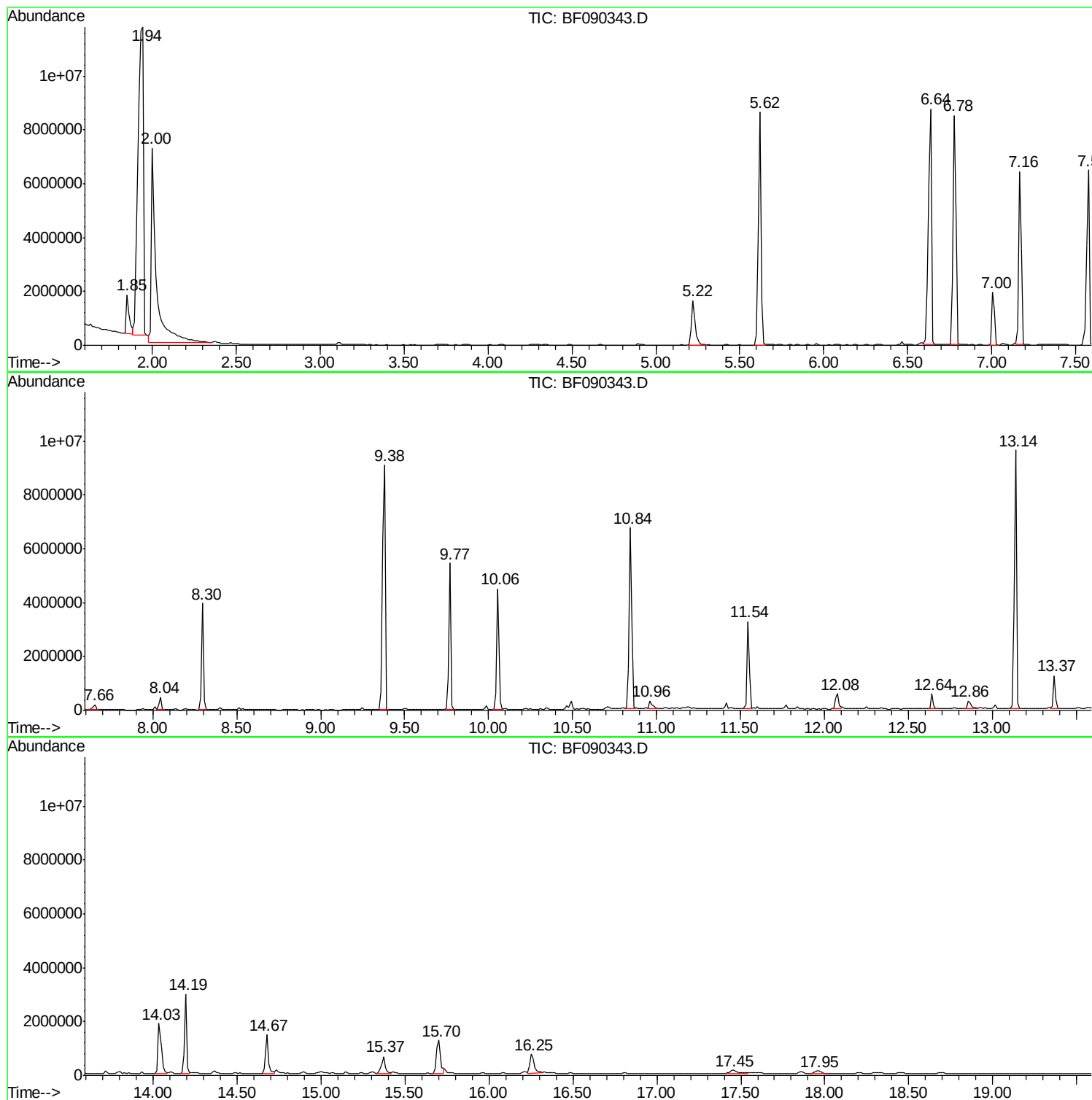
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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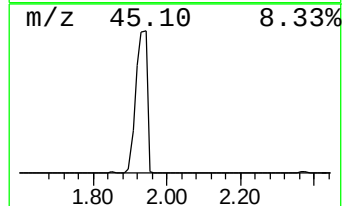
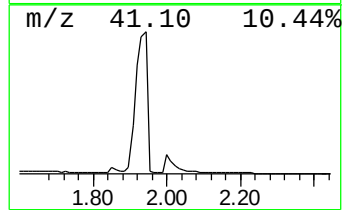
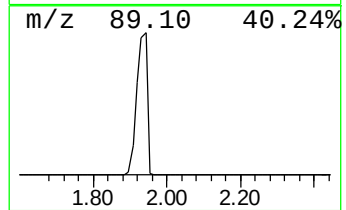
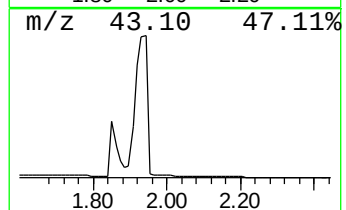
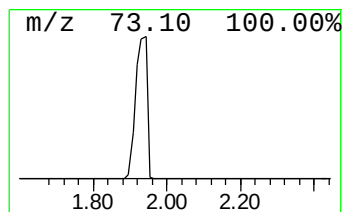
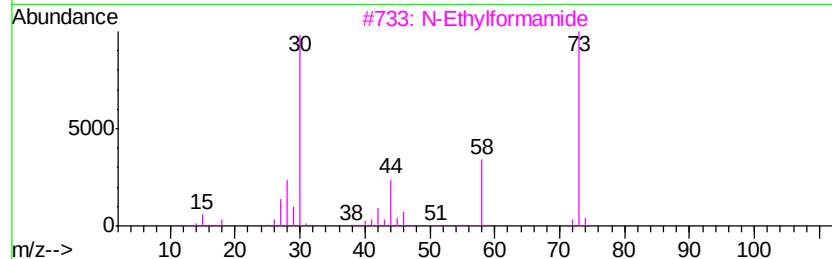
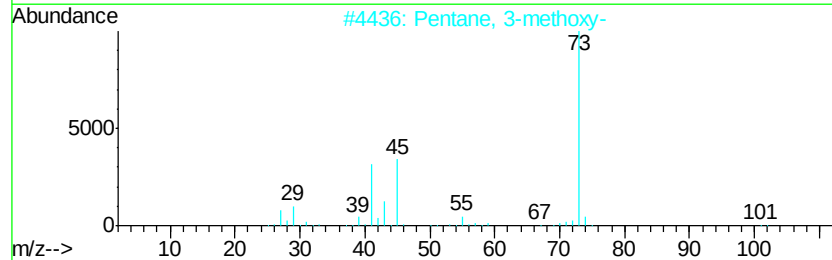
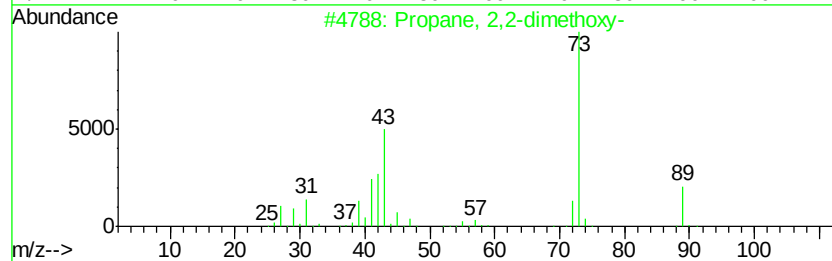
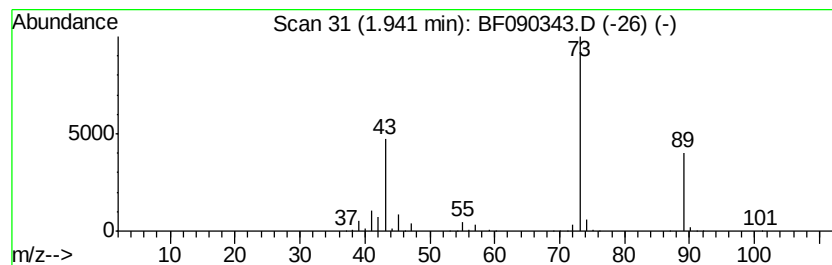
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100416.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.94	214.25 ng	24598300	1,4-Dichlorobenzene-d4	7.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	72
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
3		N-Ethylformamide	73	C3H7NO	000627-45-2	9
4		1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
5		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9



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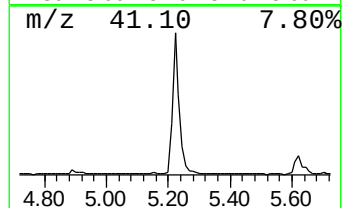
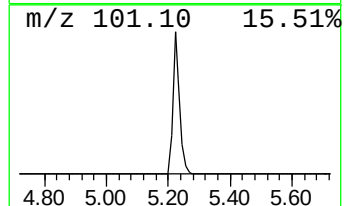
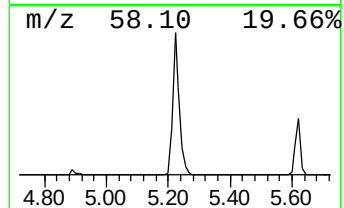
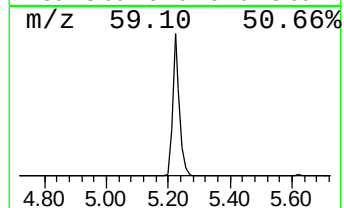
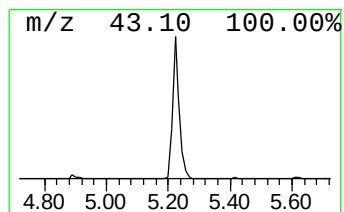
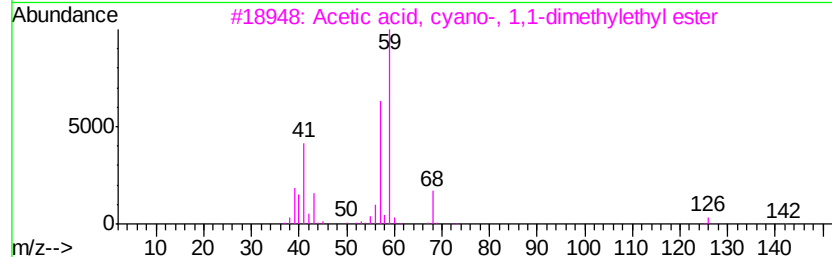
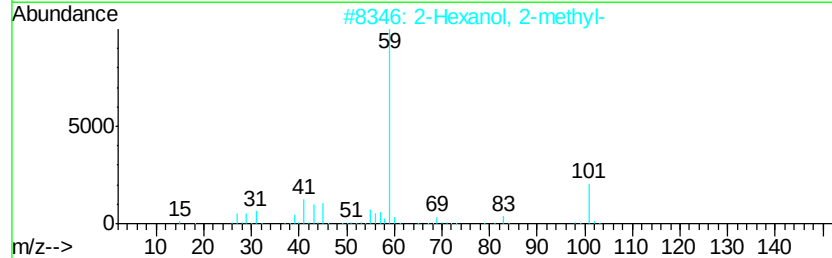
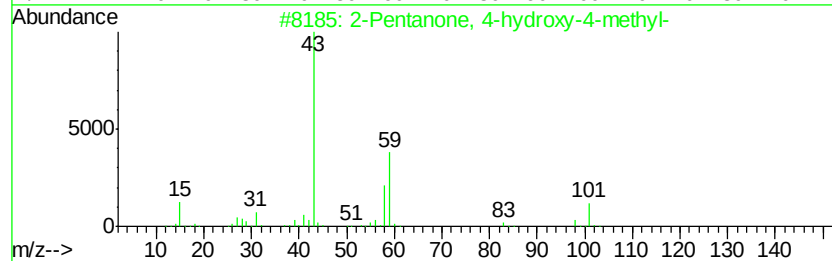
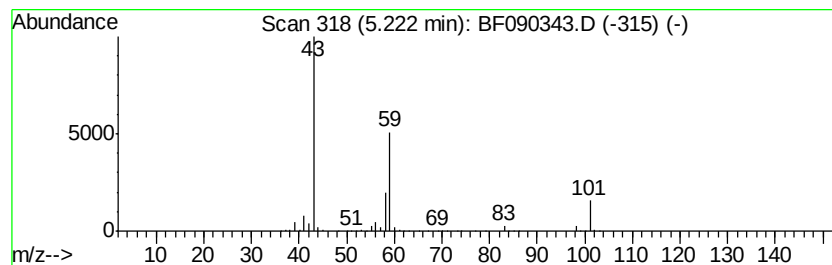
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	21.98 ng	2524100	1,4-Dichlorobenzene-d4	7.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	83
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
5		Acetone	58	C3H6O	000067-64-1	9



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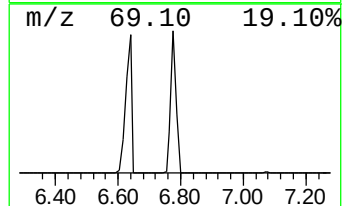
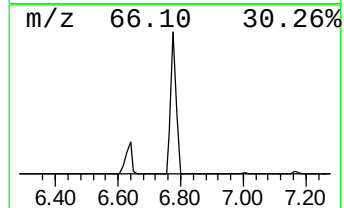
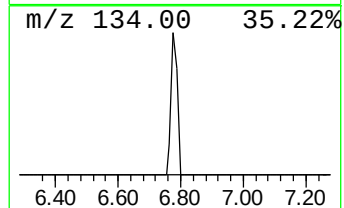
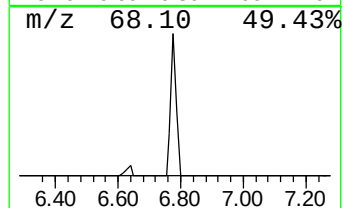
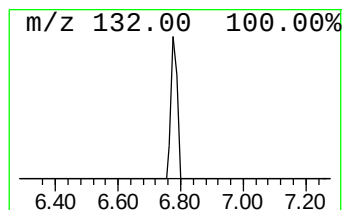
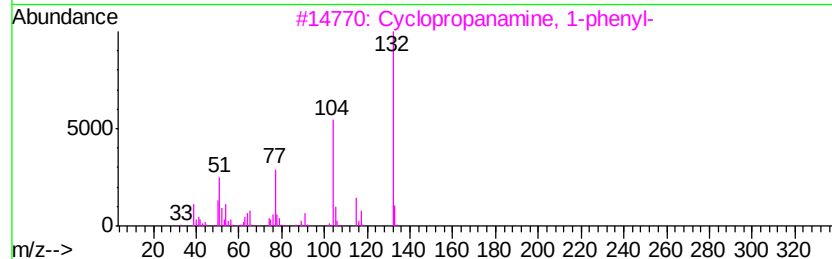
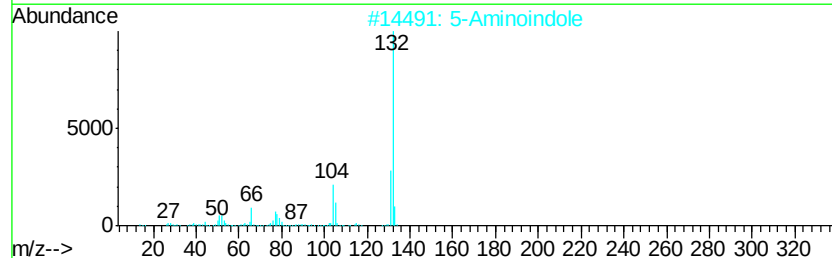
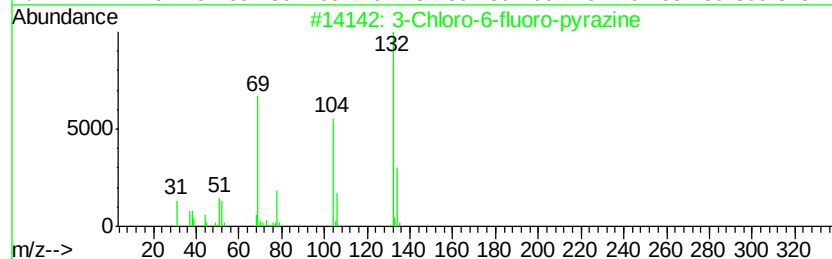
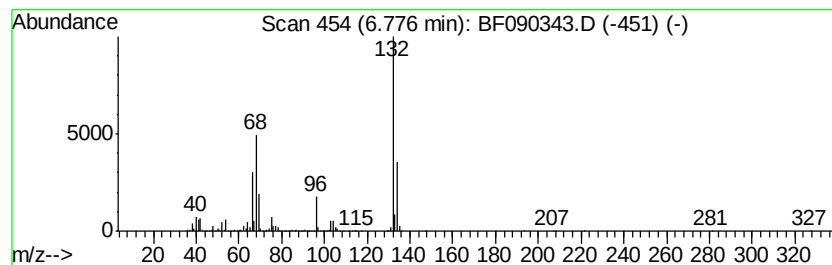
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown6.78 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.78	94.07 ng	10801000	1,4-Dichlorobenzene-d4	7.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	9
4		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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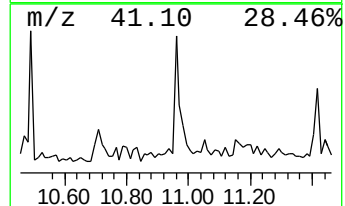
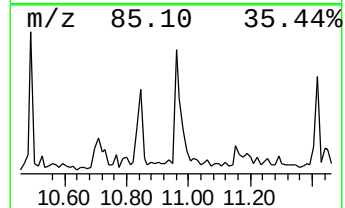
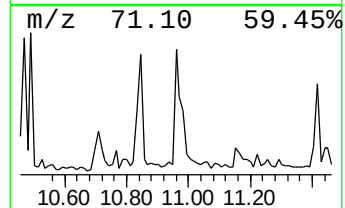
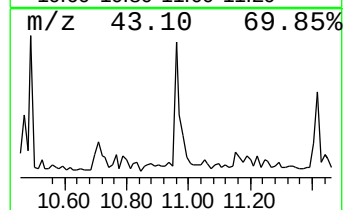
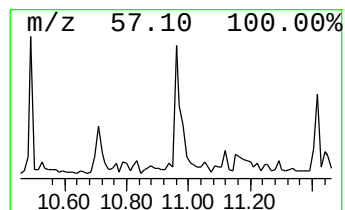
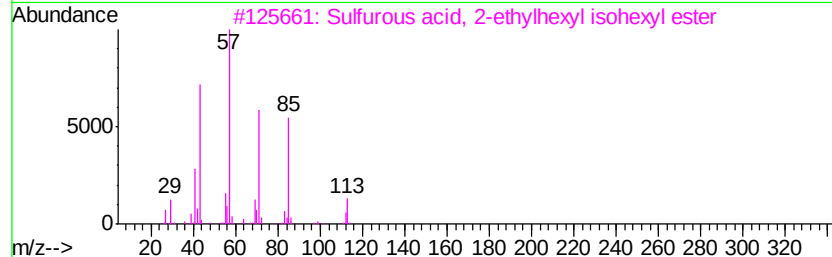
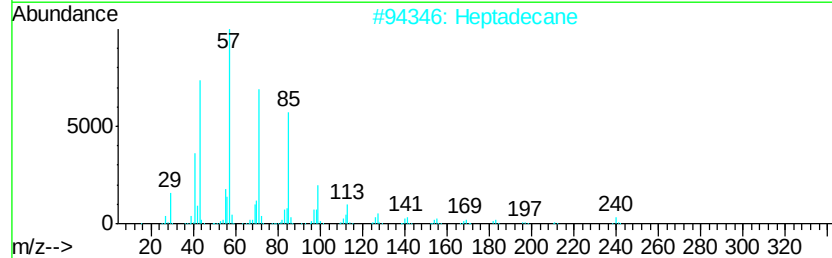
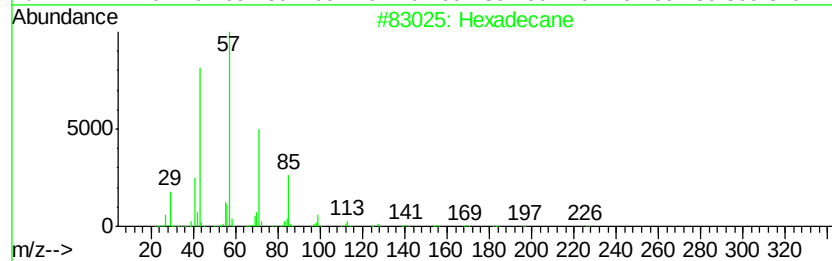
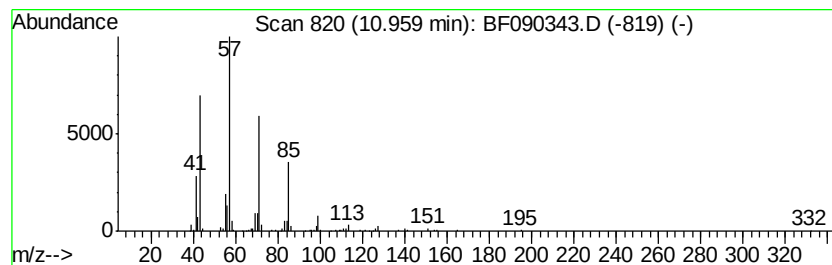
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Hexadecane Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.96	2.41 ng	386466	Phenanthrene-d10	11.54

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	90
2	Heptadecane		240	C17H36	000629-78-7	83
3	Sulfurous acid, 2-ethylhexyl iso...		278	C14H30O3S	1000309-19-0	78
4	Sulfurous acid, hexyl pentyl ester		236	C11H24O3S	1000309-14-1	72
5	Undecane, 6-ethyl-		184	C13H28	017312-60-6	72



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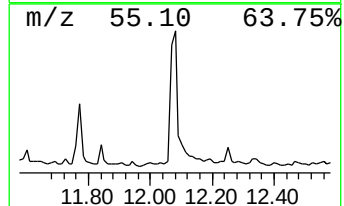
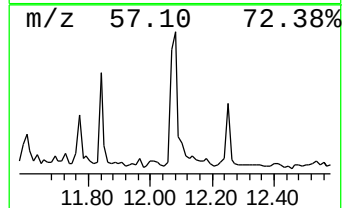
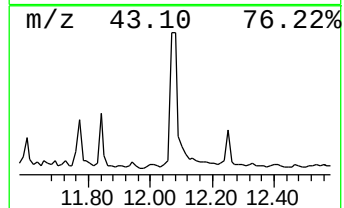
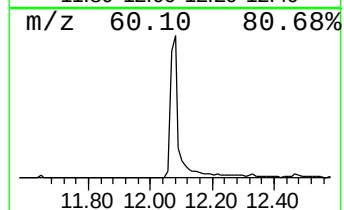
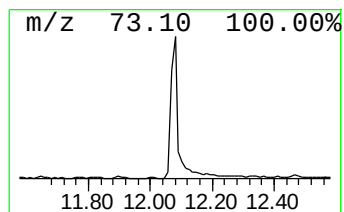
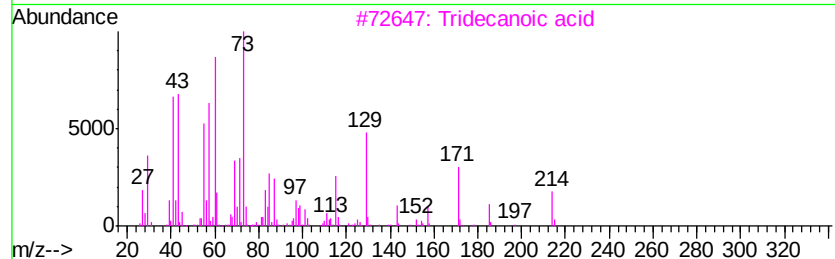
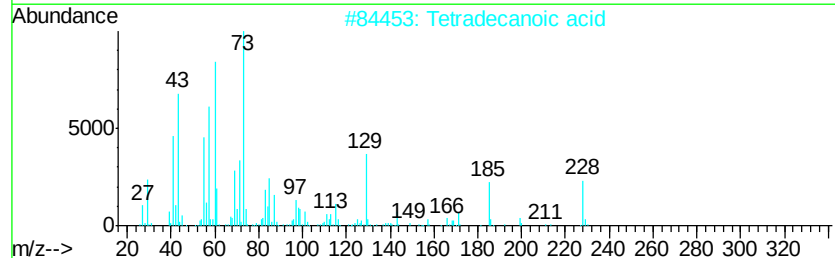
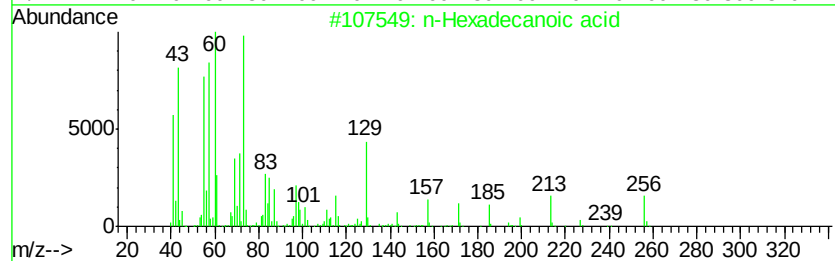
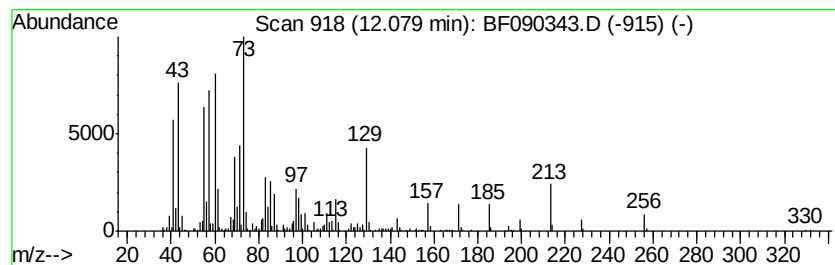
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 n-Hexadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.08	5.10 ng	817708	Phenanthrene-d10	11.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3		Tridecanoic acid	214	C13H26O2	000638-53-9	93
4		Octadecanoic acid	284	C18H36O2	000057-11-4	93
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	86



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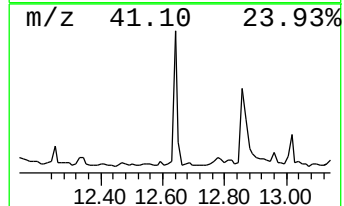
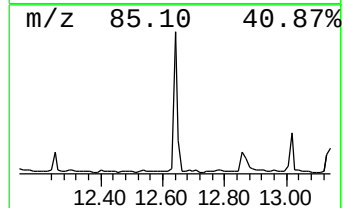
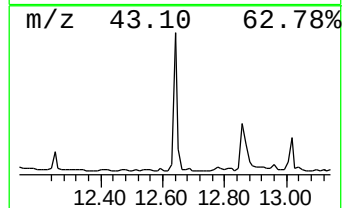
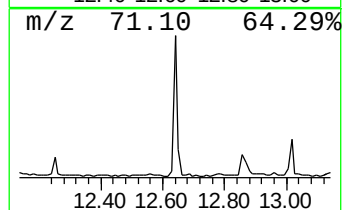
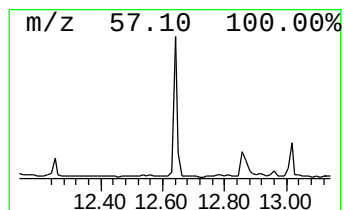
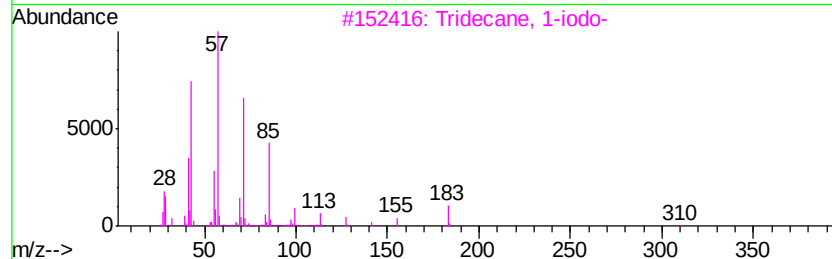
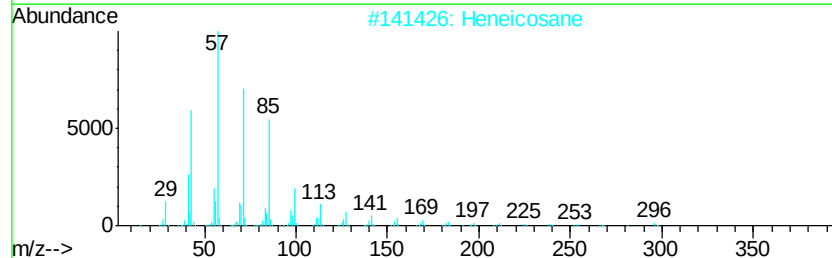
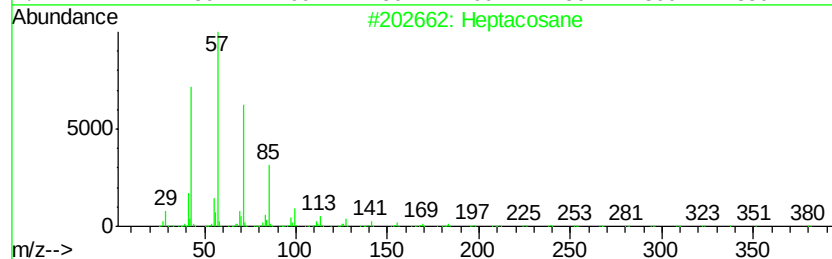
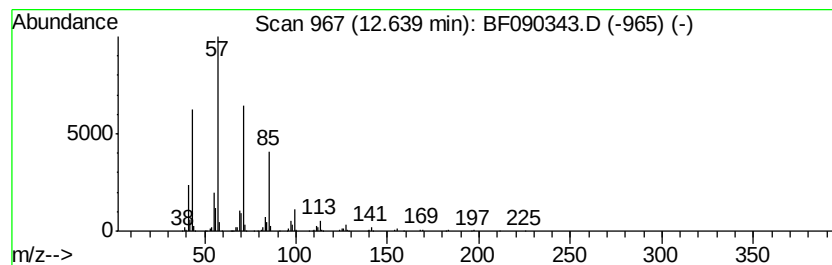
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptacosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	3.04 ng	487074	Phenanthrene-d10	11.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	91
2		Heneicosane	296	C21H44	000629-94-7	90
3		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
4		Pentacosane	352	C25H52	000629-99-2	86
5		Hexadecane	226	C16H34	000544-76-3	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100416\
Data File : BF090343.D
Acq On : 4 Oct 2016 14:45
Operator : UM/SJ
Sample : H4998-19
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-B057-6-9

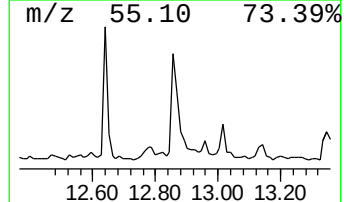
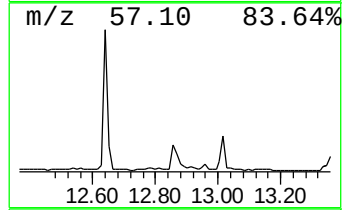
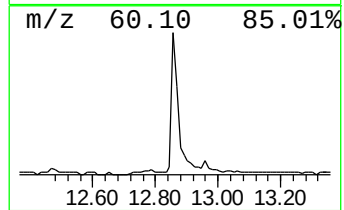
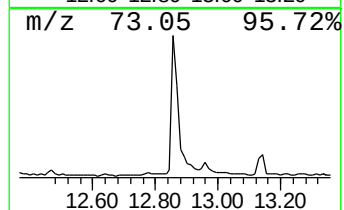
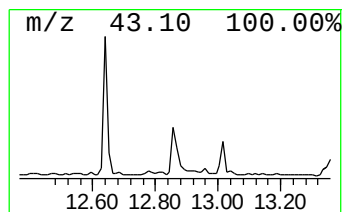
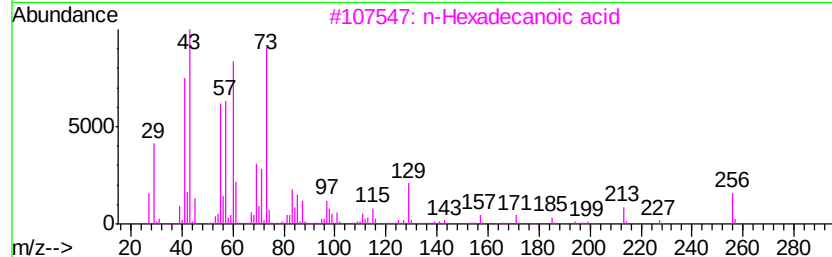
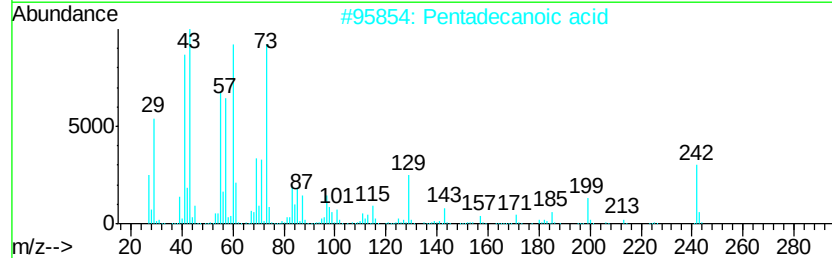
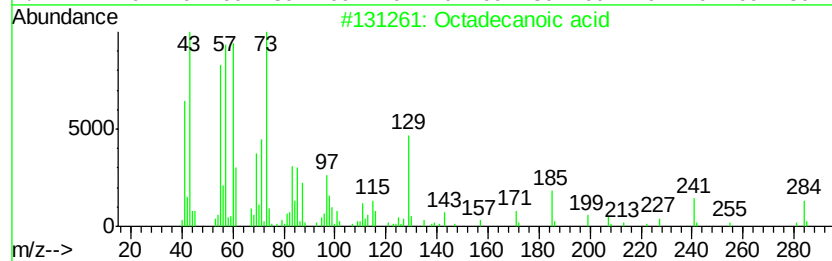
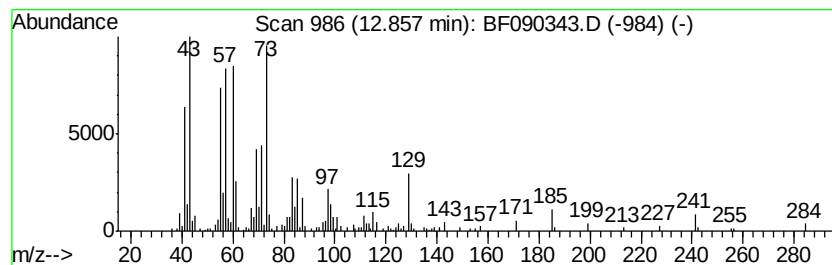
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octadecanoic acid Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.86	2.85 ng	457592	Phenanthrene-d10	11.54

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100416\
Data File : BF090343.D
Acq On : 4 Oct 2016 14:45
Operator : UM/SJ
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Misc :
ALS Vial : 11 Sample Multiplier: 1

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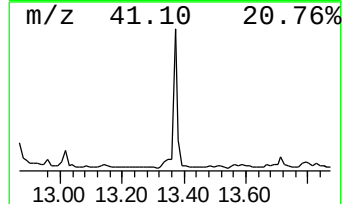
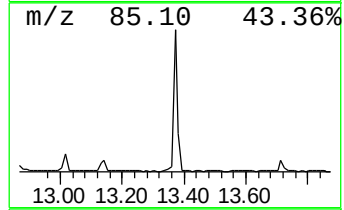
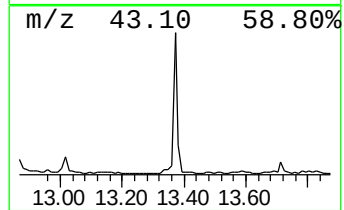
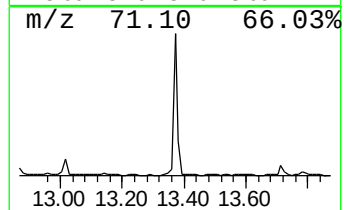
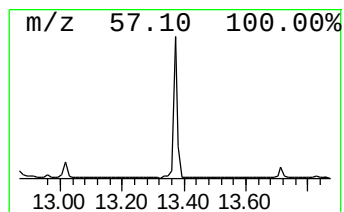
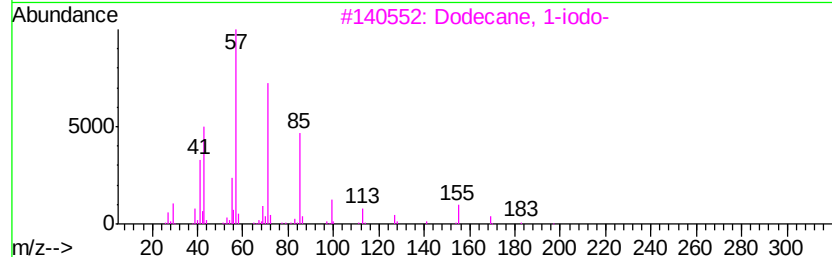
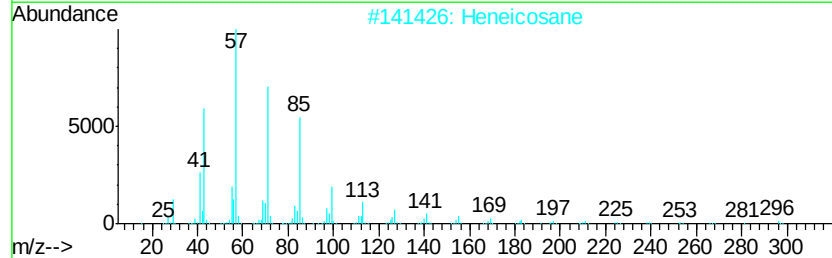
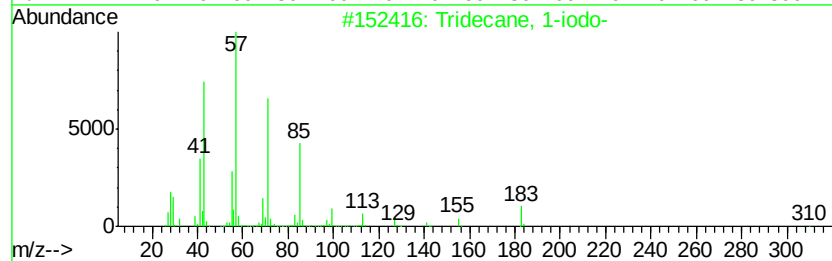
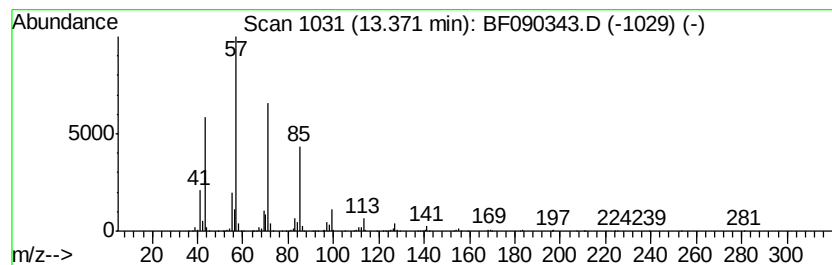
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Tridecane, 1-iodo- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.37	8.19 ng	1088620	Chrysene-d12	14.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	90
2		Heneicosane	296	C21H44	000629-94-7	90
3		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
4		Heptacosane	380	C27H56	000593-49-7	80
5		triacontane	422	C30H62	000638-68-6	78



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100416\
Data File : BF090343.D
Acq On : 4 Oct 2016 14:45
Operator : UM/SJ
Sample : H4998-19
Misc :
ALS Vial : 11 Sample Multiplier: 1

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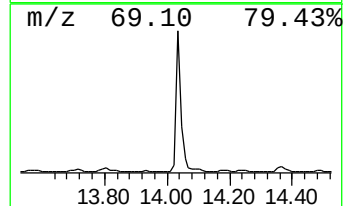
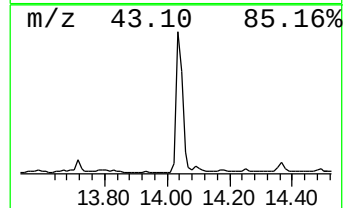
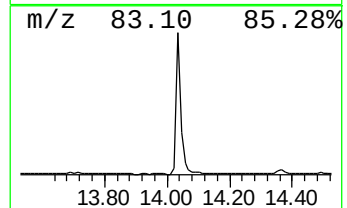
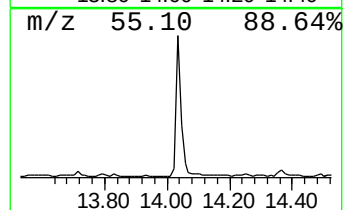
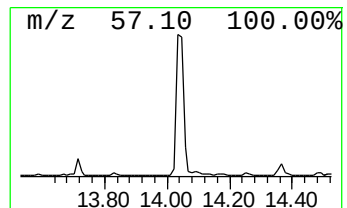
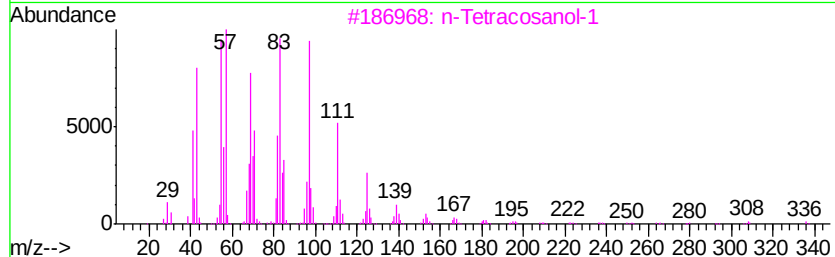
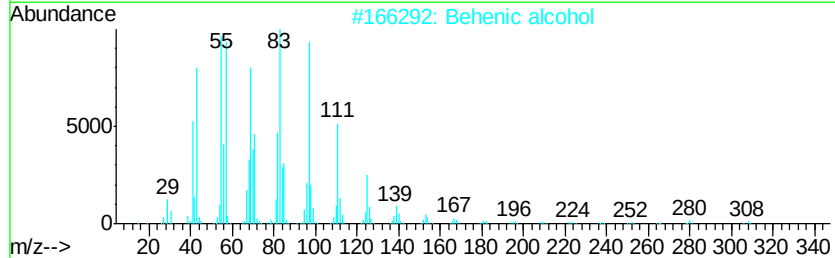
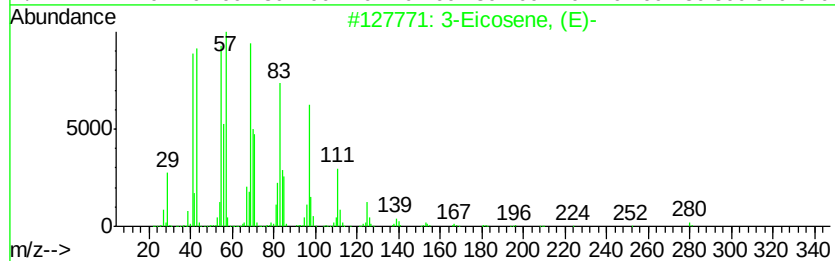
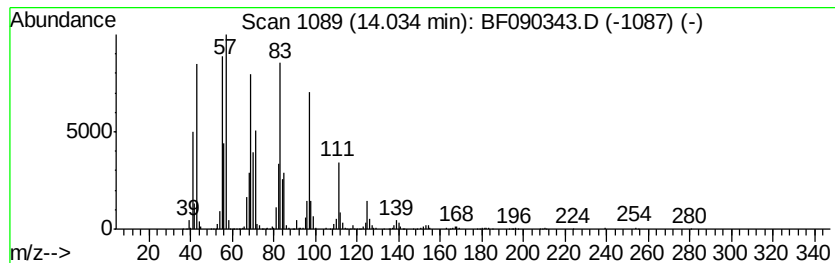
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 3-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.03	17.39 ng	2309700	Chrysene-d12	14.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Eicosene, (E)-	280	C20H40	074685-33-9	94
2		Behenic alcohol	326	C22H46O	000661-19-8	94
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4		2-Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	91
5		1-Heneicosanol	312	C21H44O	015594-90-8	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100416\
Data File : BF090343.D
Acq On : 4 Oct 2016 14:45
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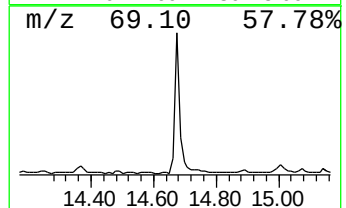
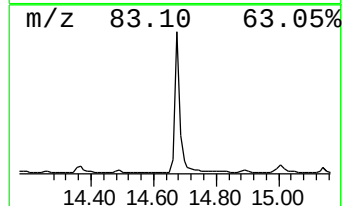
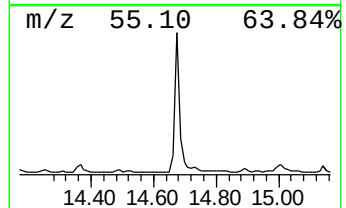
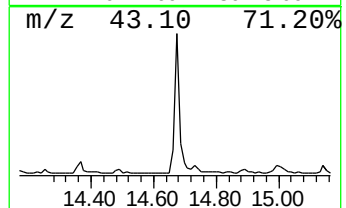
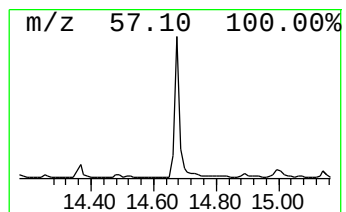
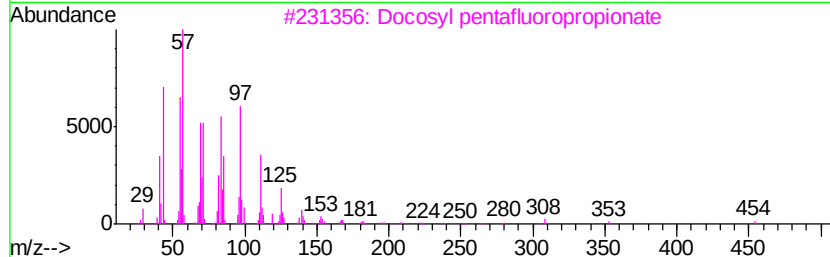
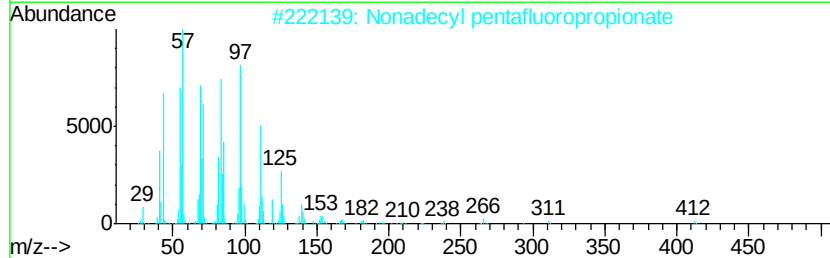
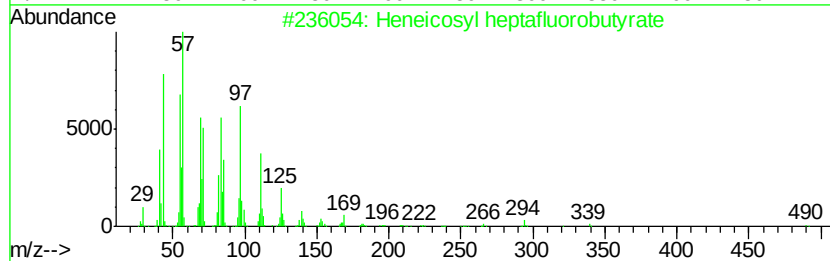
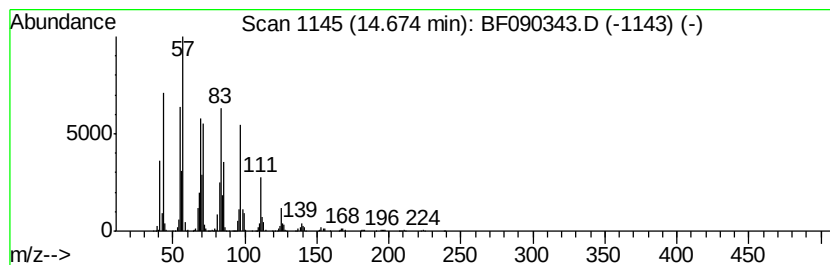
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Heneicosyl heptafluorobutyrate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.67	11.08 ng	1471450	Chrysene-d12	14.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
2		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
3		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
4		1-Heptacosanol	396	C27H56O	002004-39-9	90
5		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100416\
Data File : BF090343.D
Acq On : 4 Oct 2016 14:45
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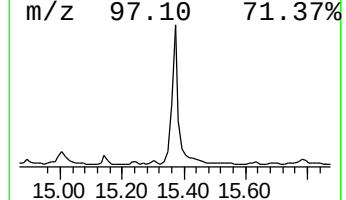
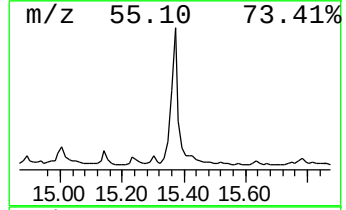
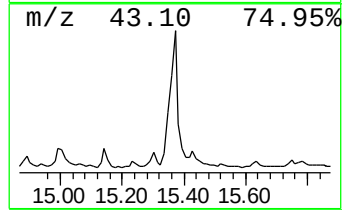
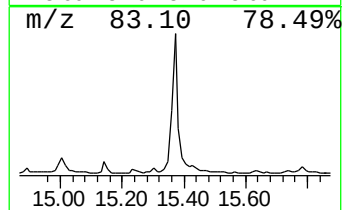
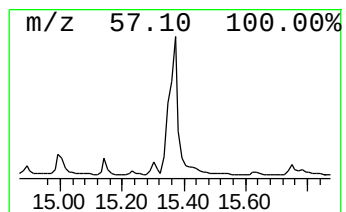
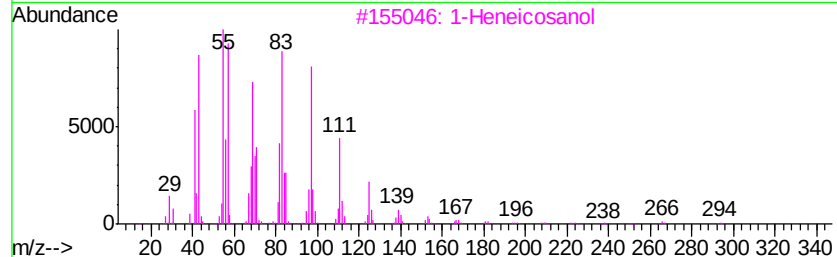
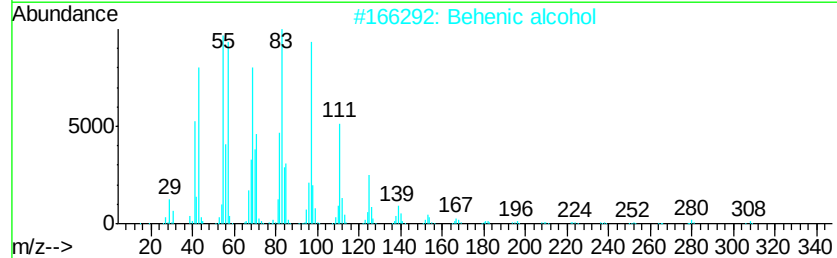
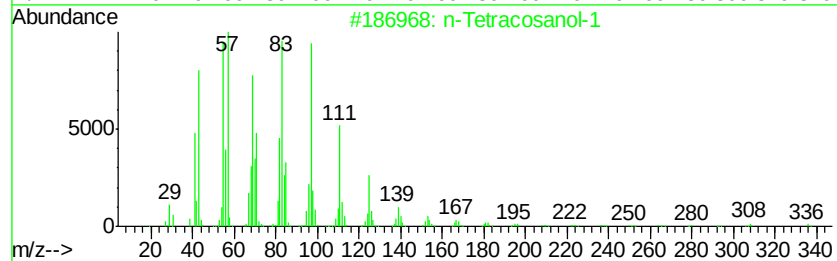
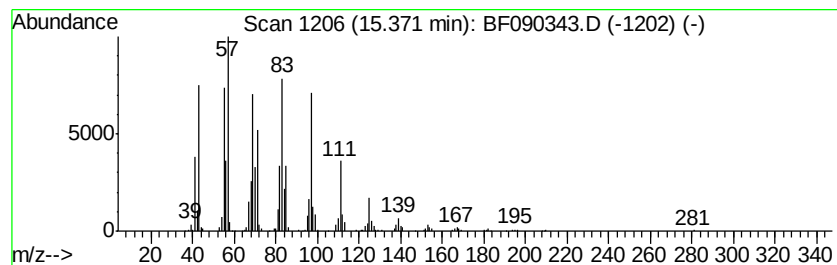
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 n-Tetracosanol-1 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.37	10.78 ng	1028600	Perylene-d12	15.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2		Behenic alcohol	326	C22H46O	000661-19-8	93
3		1-Heneicosanol	312	C21H44O	015594-90-8	93
4		1-Docosene	308	C22H44	001599-67-3	91
5		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100416\
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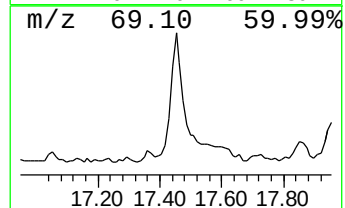
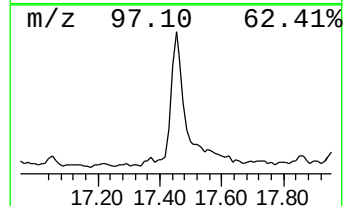
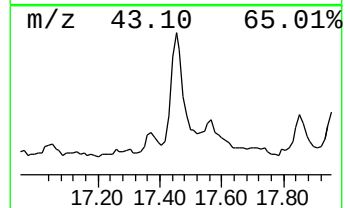
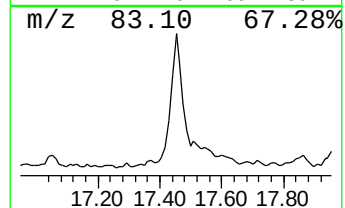
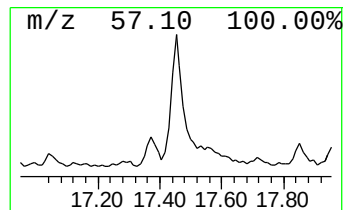
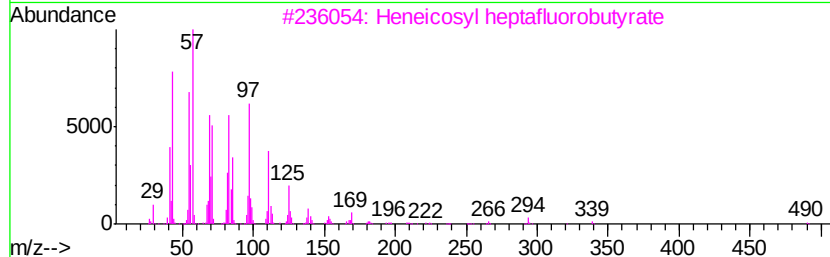
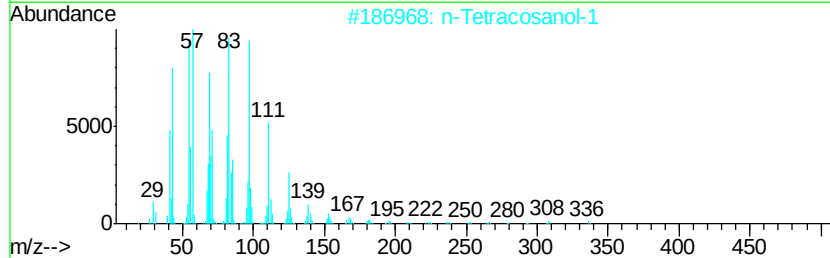
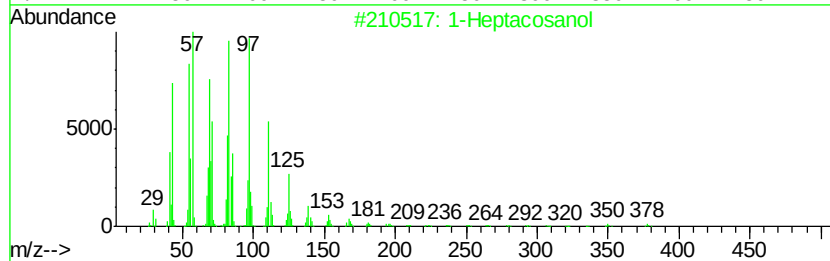
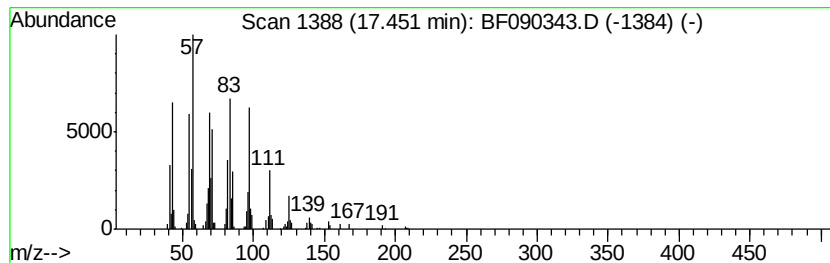
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 1-Heptacosanol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.45	3.99 ng	380294	Perylene-d12	15.70
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	Heneicosyl heptafluorobutyrate	508 C25H43F7O2	1000351-83-8	91
4	Docosyl pentafluoropropionate	472 C25H45F5O2	1000351-80-9	91
5	Tetracosyl heptafluorobutyrate	550 C28H49F7O2	1000351-83-7	91



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Misc :
ALS Vial : 11 Sample Multiplier: 1

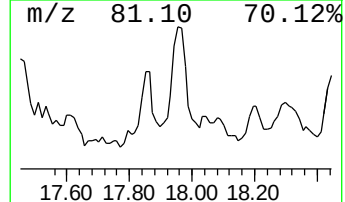
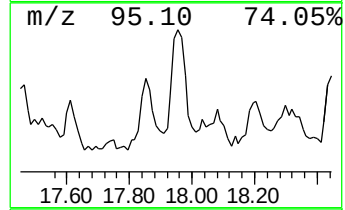
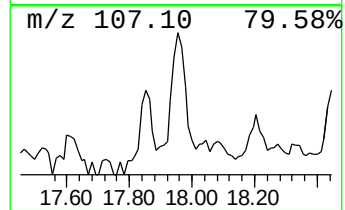
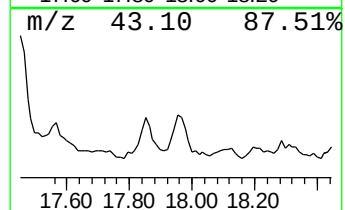
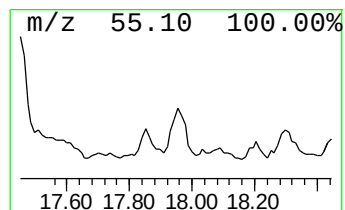
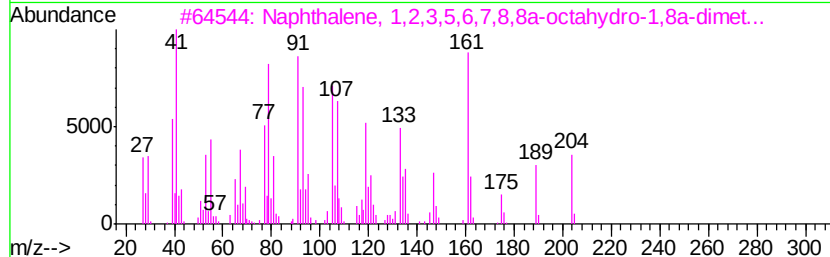
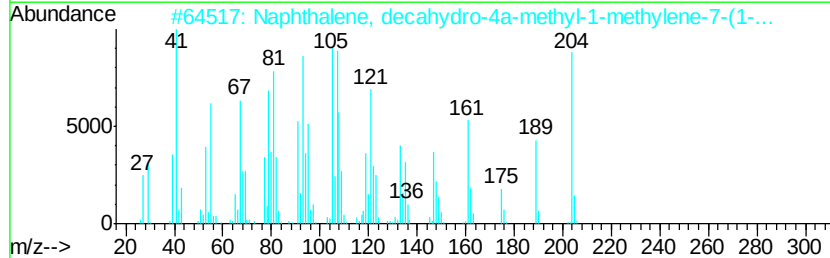
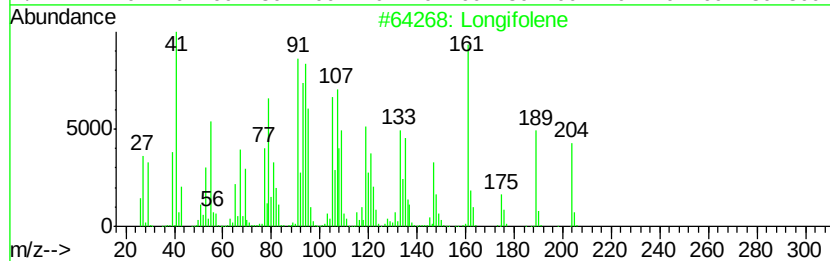
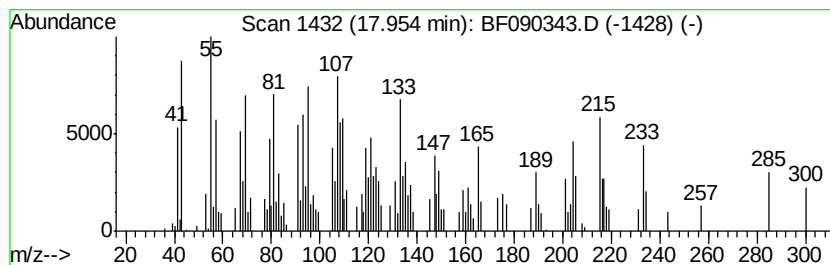
Instrument :
BNA_F
ClientSampleId :
SUP-B057-6-9

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Longifolene Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.95	2.74 ng	261305	Perylene-d12	15.70
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Longifolene	204 C15H24	000475-20-7 70
2		Naphthalene, decahydro-4a-methyl...	204 C15H24	017066-67-0 55
3		Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204 C15H24	004630-07-3 30
4		Azulene, 1,2,3,5,6,7,8,8a-octahy...	204 C15H24	003691-11-0 25
5		Isocaryophyllene	204 C15H24	1000140-07-2 25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100416\
 Data File : BF090343.D
 Acq On : 4 Oct 2016 14:45
 Operator : UM/SJ
 Sample : H4998-19
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SUP-B057-6-9

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100416.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
Propane, 2,2-dime...	1.94	214.3	ng	24598300	1	7.00	2296260	20.0
2-Pentanone, 4-hy...	5.22	22.0	ng	2524100	1	7.00	2296260	20.0
unknown6.78	6.78	94.1	ng	10801000	1	7.00	2296260	20.0
Hexadecane	10.96	2.4	ng	386466	4	11.54	3208700	20.0
n-Hexadecanoic acid	12.08	5.1	ng	817708	4	11.54	3208700	20.0
Heptacosane	12.64	3.0	ng	487074	4	11.54	3208700	20.0
Octadecanoic acid	12.86	2.9	ng	457592	4	11.54	3208700	20.0
Tridecane, 1-iodo-	13.37	8.2	ng	1088620	5	14.19	2657120	20.0
3-Eicosene, (E)-	14.03	17.4	ng	2309700	5	14.19	2657120	20.0
Heneicosyl heptaf...	14.67	11.1	ng	1471450	5	14.19	2657120	20.0
n-Tetracosanol-1	15.37	10.8	ng	1028600	6	15.70	1907940	20.0
1-Heptacosanol	17.45	4.0	ng	380294	6	15.70	1907940	20.0
Longifolene	17.95	2.7	ng	261305	6	15.70	1907940	20.0