

Data Path : Z:\HPCHEM1\BNA F\Data\BF032417\
 Data File : BF093916.D
 Acq On : 24 Mar 2017 19:46
 Operator : SJ/MA
 Sample : I2394-03
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP3

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-BF032217.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	4.110	373	378	387	rVB	344200	435022	9.04%	1.046%
2	4.498	438	444	447	rBV	3769856	3893769	80.94%	9.364%
3	5.557	617	624	627	rBV	3320829	4094606	85.11%	9.847%
4	5.704	643	649	652	rBV	3776813	4117736	85.59%	9.903%
5	5.957	688	692	696	rBV	1106112	969543	20.15%	2.332%
6	6.139	718	723	726	rBV	3206502	3205275	66.63%	7.709%
7	6.604	796	802	806	rBV	2168114	2648063	55.04%	6.369%
8	7.463	942	948	954	rVB	1338670	1378717	28.66%	3.316%
9	8.222	1072	1077	1080	rBV	48791	59901	1.25%	0.144%
10	8.786	1164	1173	1177	rBV	4160882	4810892	100.00%	11.570%
11	8.922	1190	1196	1201	rBV	75208	83722	1.74%	0.201%
12	9.280	1251	1257	1260	rBV	261653	251945	5.24%	0.606%
13	9.504	1289	1295	1303	rVV3	112026	249843	5.19%	0.601%
14	9.575	1303	1307	1308	rVV	136446	124636	2.59%	0.300%
15	9.604	1308	1312	1322	rVB2	1497850	1499740	31.17%	3.607%
16	10.192	1407	1412	1416	rVV	182361	178036	3.70%	0.428%
17	10.469	1452	1459	1462	rBV	65199	99010	2.06%	0.238%
18	10.580	1471	1478	1481	rBV	2334012	2722801	56.60%	6.548%
19	10.780	1508	1512	1514	rBV	196143	215099	4.47%	0.517%
20	11.333	1602	1606	1609	rBV	148231	129782	2.70%	0.312%
21	11.427	1616	1622	1626	rBV	1413689	1463682	30.42%	3.520%
22	11.863	1692	1696	1699	rBV	82921	77531	1.61%	0.186%
23	12.368	1778	1782	1785	rBV	60731	61477	1.28%	0.148%
24	12.851	1860	1864	1867	rVB	57080	56674	1.18%	0.136%
25	13.310	1938	1942	1945	rBV	59322	57747	1.20%	0.139%
26	13.410	1953	1959	1963	rBV	3502713	4389709	91.25%	10.557%
27	13.751	2013	2017	2020	rVB	66011	65316	1.36%	0.157%
28	14.174	2085	2089	2092	rBV	90804	85110	1.77%	0.205%
29	14.562	2151	2155	2156	rBV	152160	152968	3.18%	0.368%
30	14.580	2156	2158	2167	rVB	167932	171705	3.57%	0.413%
31	14.680	2170	2175	2179	rBV	1384472	1423876	29.60%	3.424%
32	14.974	2220	2225	2229	rBV	175197	192609	4.00%	0.463%
33	15.351	2285	2289	2295	rBV	198059	203724	4.23%	0.490%
34	15.668	2340	2343	2347	rBV	50812	53790	1.12%	0.129%

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Integration Parameters: rteint.p
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Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

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35	15.715	2347	2351	2354	rVB	174885	178025	3.70%	0.428%
36	16.068	2407	2411	2416	rBV	157647	174237	3.62%	0.419%
37	16.315	2448	2453	2463	rVB	963645	1140120	23.70%	2.742%
38	16.439	2470	2474	2478	rVB	126052	154245	3.21%	0.371%
39	16.850	2540	2544	2548	rBV	93578	138069	2.87%	0.332%
40	17.327	2621	2625	2629	rBV	64536	102169	2.12%	0.246%
41	18.527	2826	2829	2840	rVB9	31563	69607	1.45%	0.167%

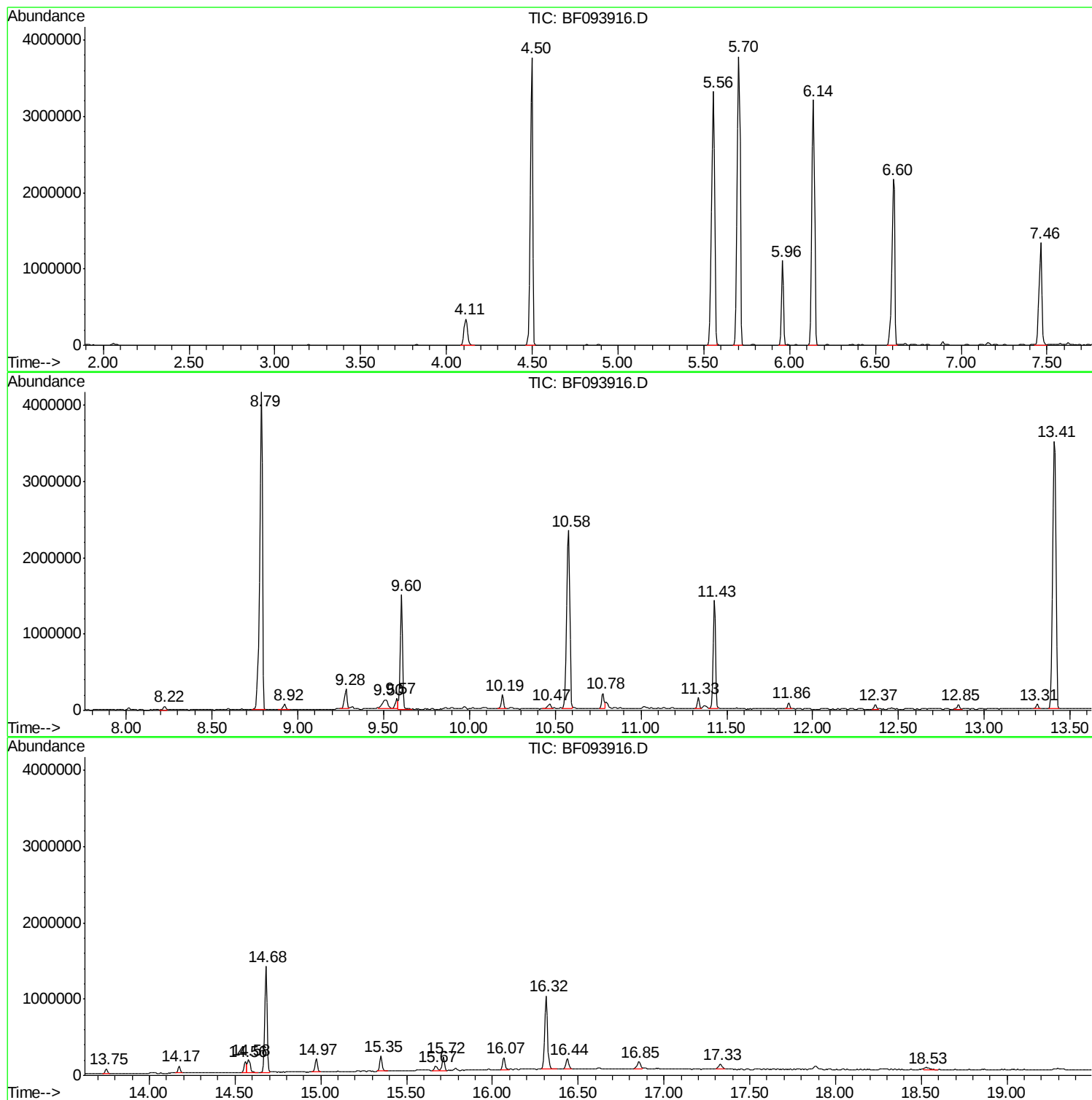
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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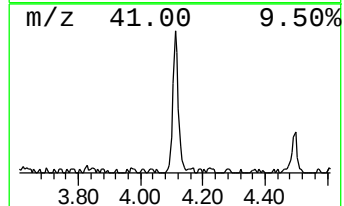
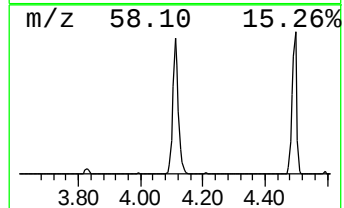
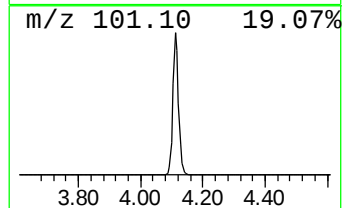
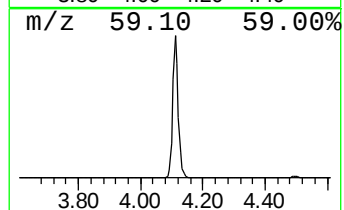
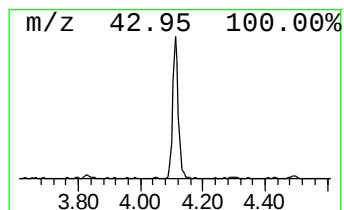
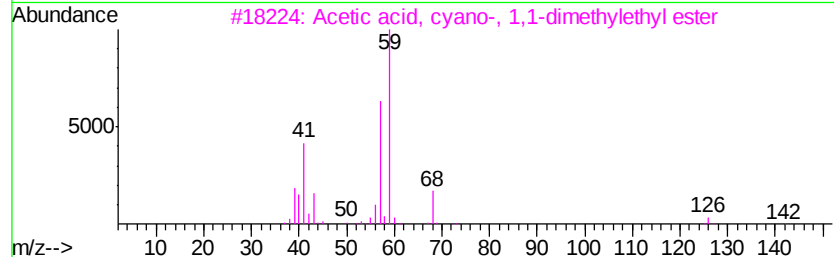
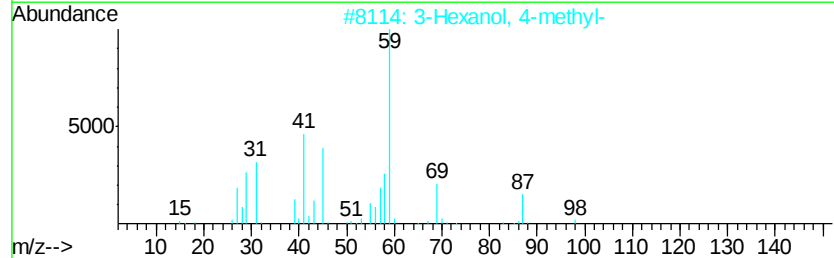
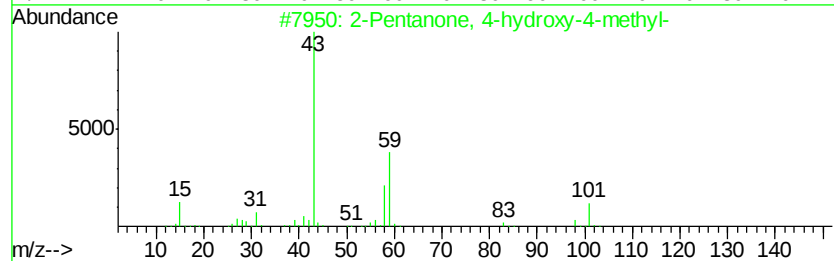
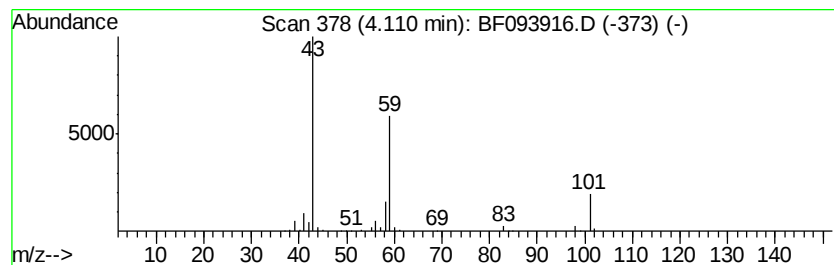
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.11	8.97 ng	435022	1,4-Dichlorobenzene-d4	5.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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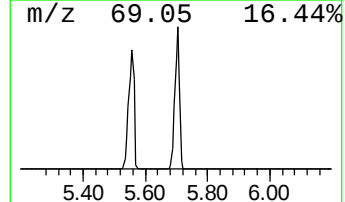
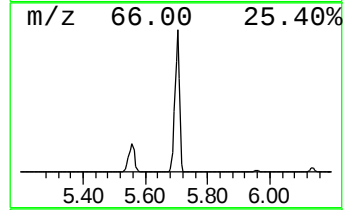
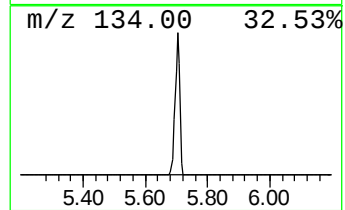
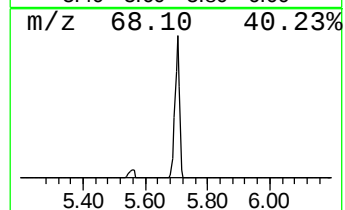
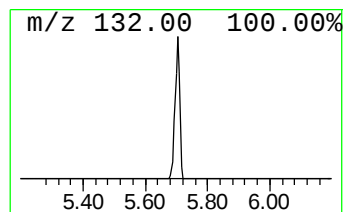
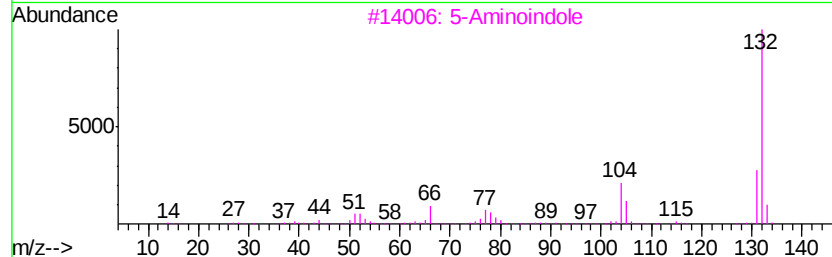
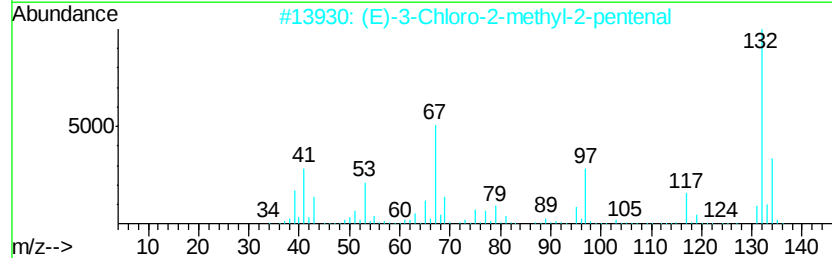
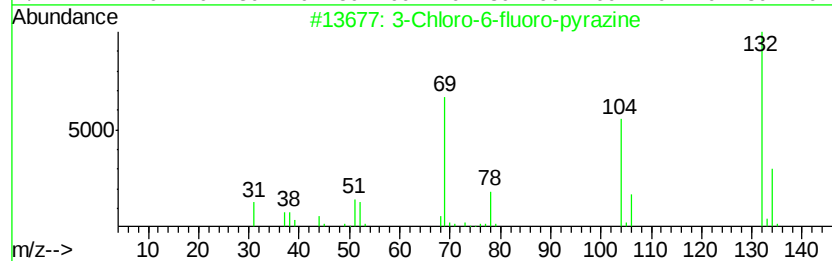
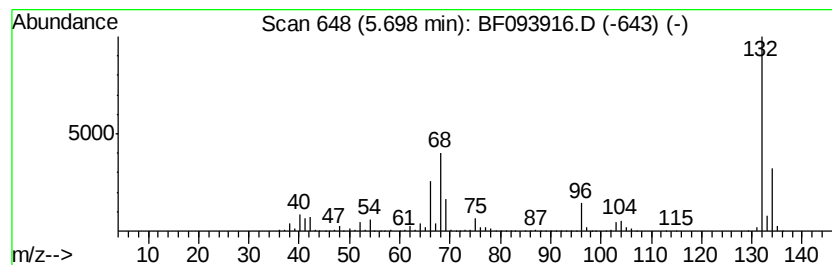
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Peak Number 2 unknown5.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.70	84.94 ng	4117740	1,4-Dichlorobenzene-d4	5.96

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	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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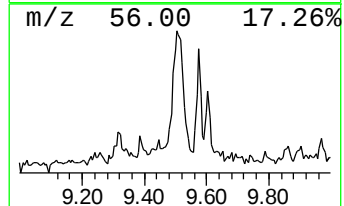
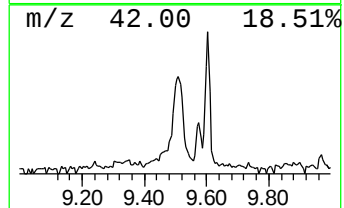
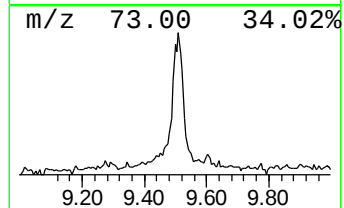
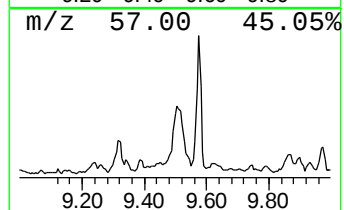
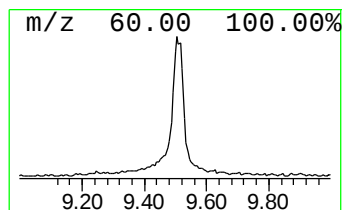
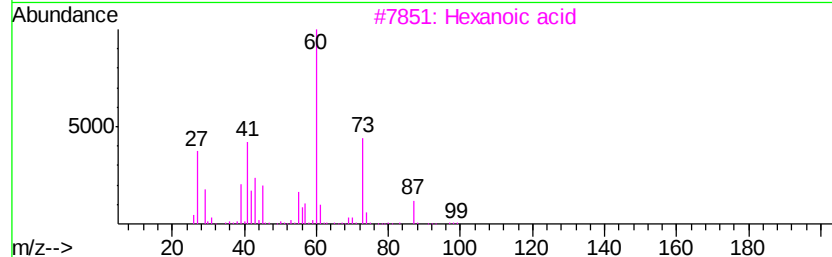
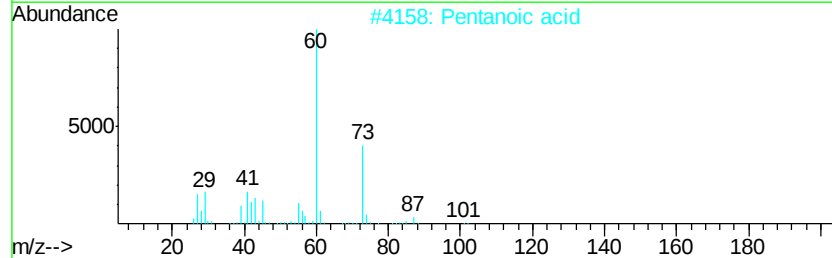
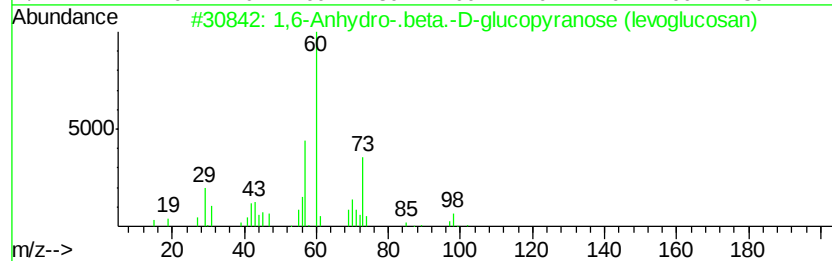
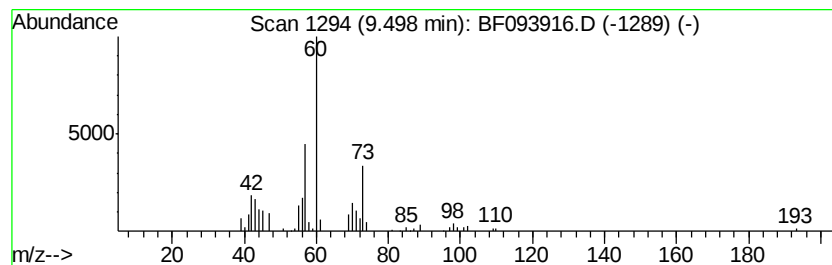
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1,6-Anhydro-.beta.-D-glucop... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.50	3.33 ng	249843	Acenaphthene-d10	9.60

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,6-Anhydro-.beta.-D-glucopyrano...	162	C6H10O5	000498-07-7	72
2		Pentanoic acid	102	C5H10O2	000109-52-4	53
3		Hexanoic acid	116	C6H12O2	000142-62-1	53
4		.beta.-D-Ribopyranoside, methyl	164	C6H12O5	017289-61-1	53
5		3,4-Altrosan	162	C6H10O5	1000129-76-4	42



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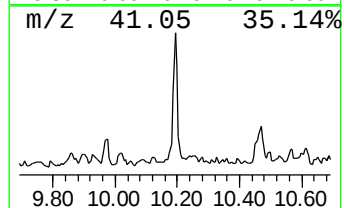
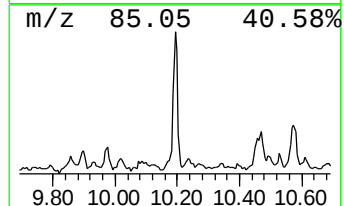
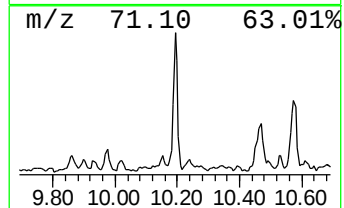
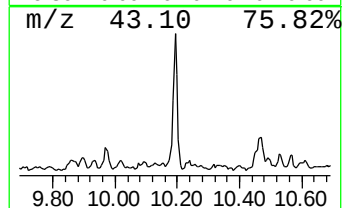
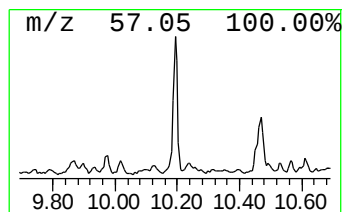
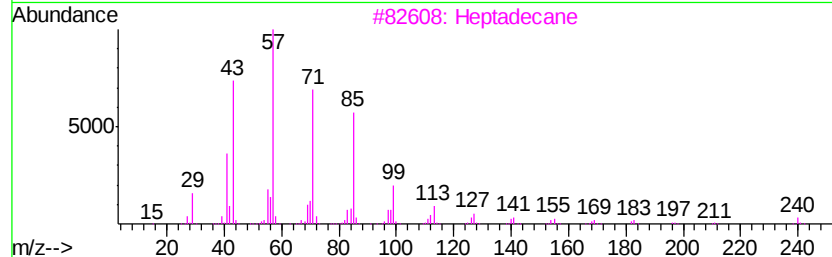
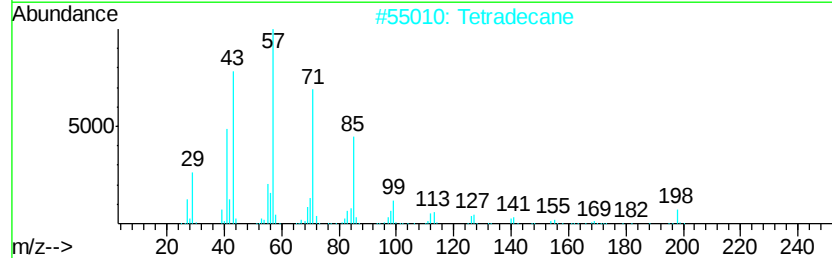
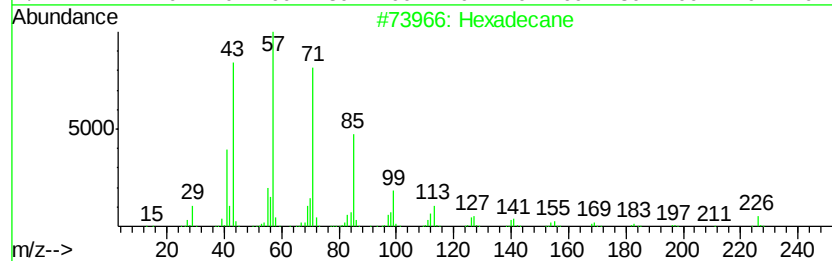
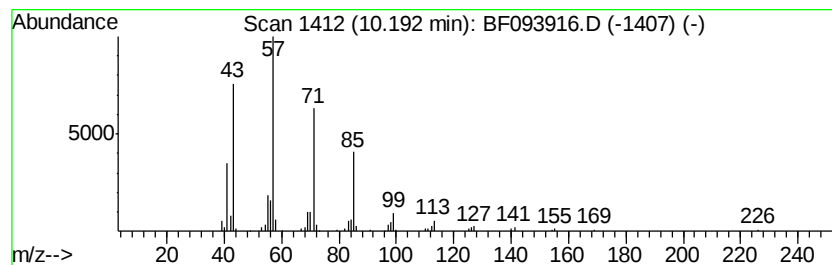
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Peak Number 5 Hexadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.19	2.37 ng	178036	Acenaphthene-d10	9.60
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecane	226 C16H34	000544-76-3	91
2	Tetradecane	198 C14H30	000629-59-4	86
3	Heptadecane	240 C17H36	000629-78-7	83
4	Pentadecane, 2-methyl-	226 C16H34	001560-93-6	80
5	Eicosane	282 C20H42	000112-95-8	80



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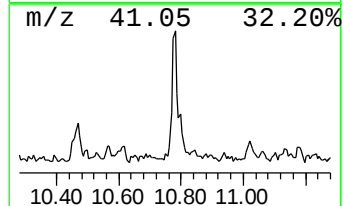
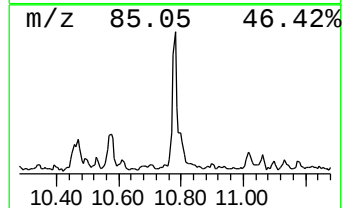
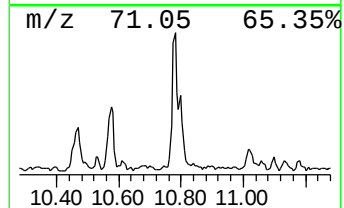
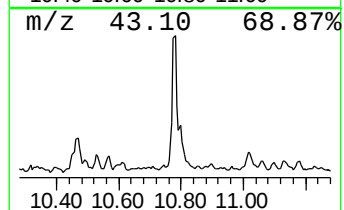
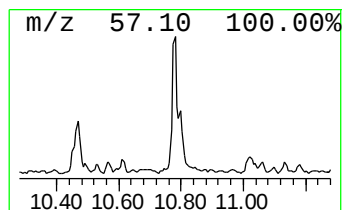
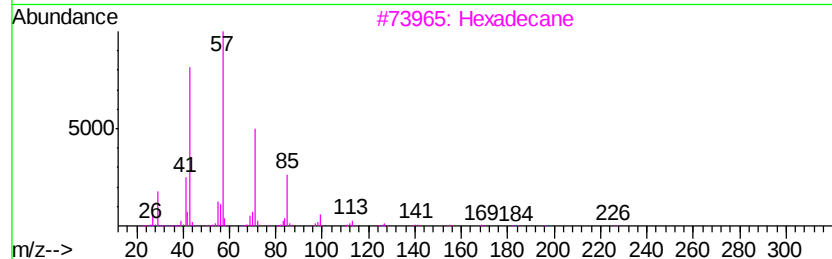
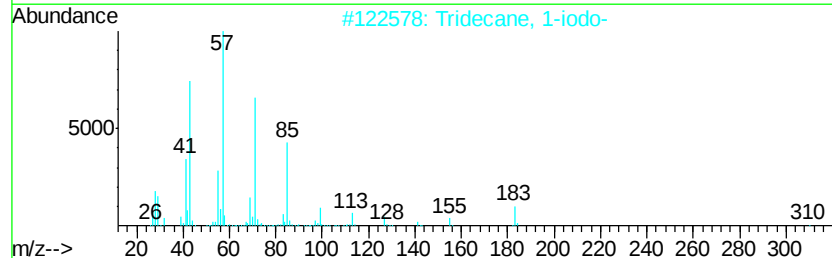
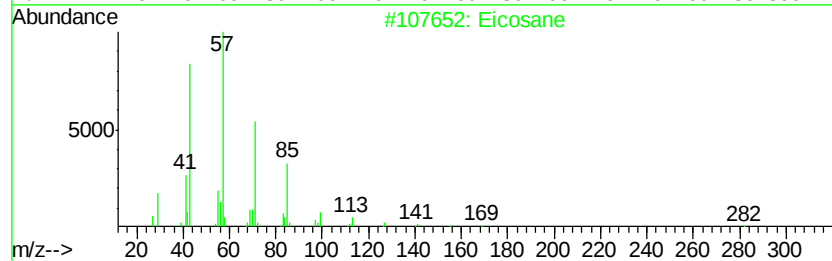
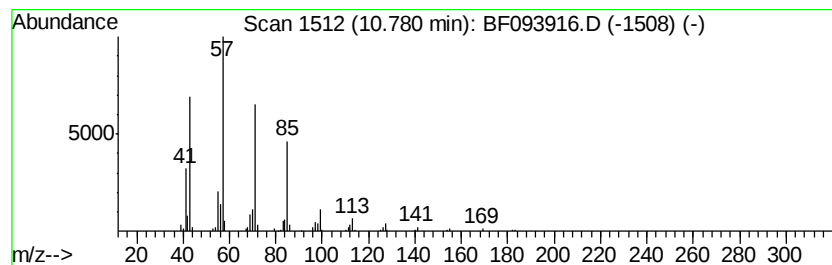
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TIC Integration Parameters: LSCINT.P

Peak Number 6 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.78	2.94 ng	215099	Phenanthrene-d10		11.43	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	91
2	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	90
3	Hexadecane		226	C16H34	000544-76-3	90
4	Heneicosane		296	C21H44	000629-94-7	90
5	Tridecane		184	C13H28	000629-50-5	90



Data Path : Z:\HPCHEM1\BNA F\Data\BF032417\
Data File : BF093916.D
Acq On : 24 Mar 2017 19:46
Operator : SJ/MA
Sample : I2394-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

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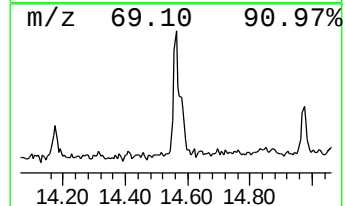
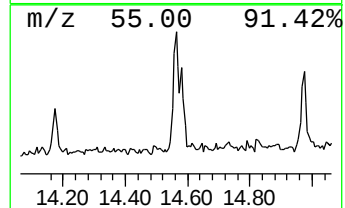
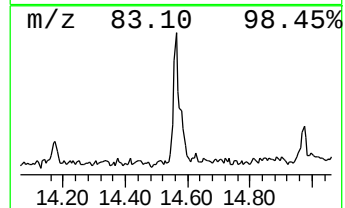
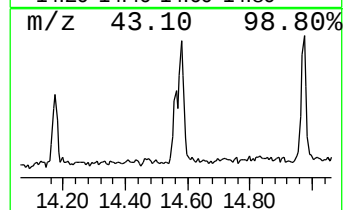
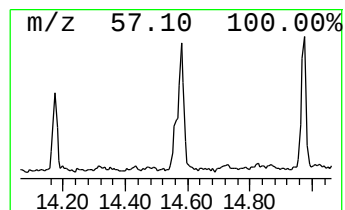
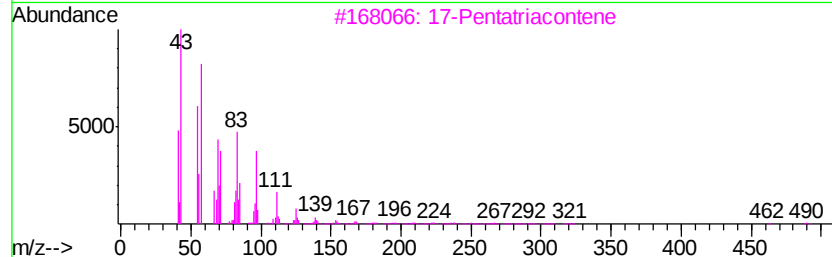
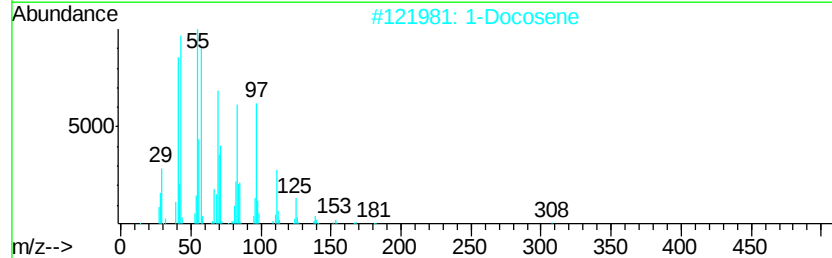
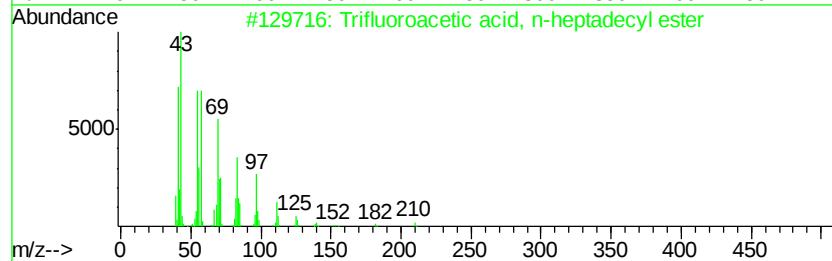
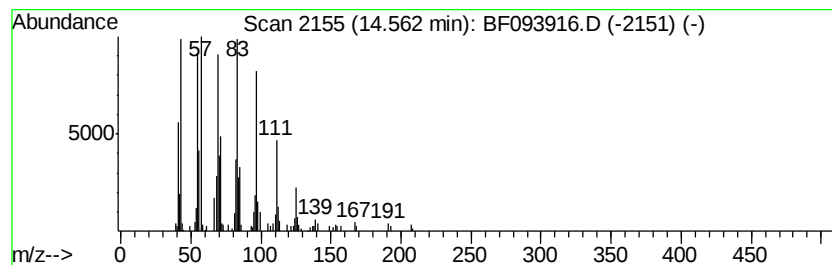
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Trifluoroacetic acid, n-hep... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.56	2.15 ng	152968	Chrysene-d12	14.68

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	90
2			1-Docosene	308	C22H44	001599-67-3	81
3			17-Pentatriacontene	491	C35H70	006971-40-0	80
4			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	76
5			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	76



Data Path : Z:\HPCHEM1\BNA F\Data\BF032417\
Data File : BF093916.D
Acq On : 24 Mar 2017 19:46
Operator : SJ/MA
Sample : I2394-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

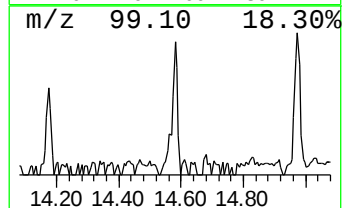
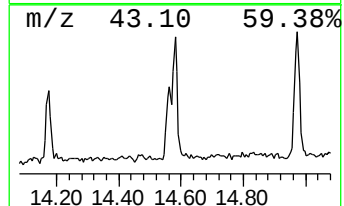
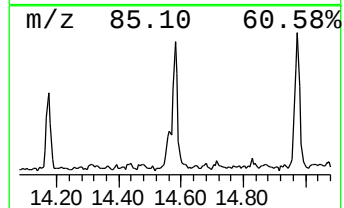
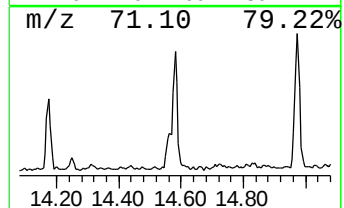
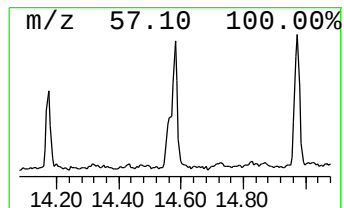
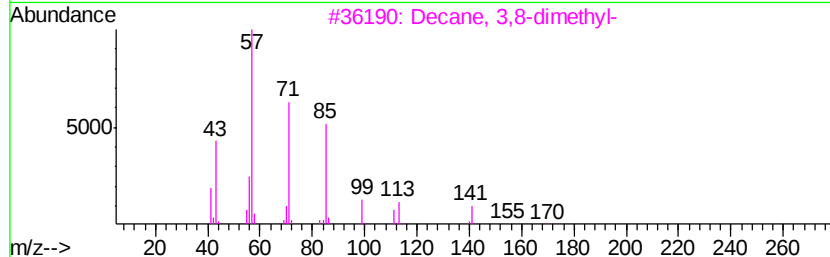
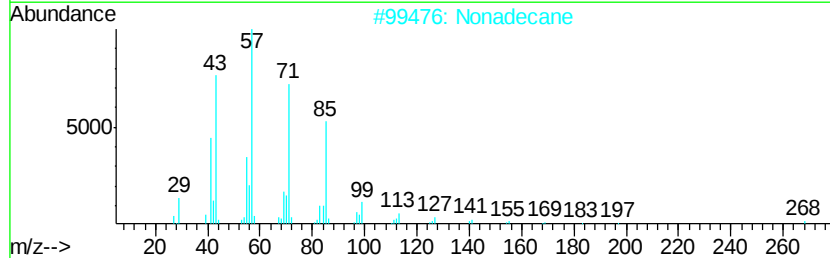
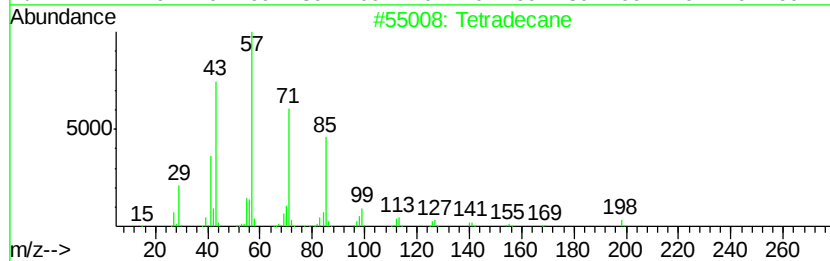
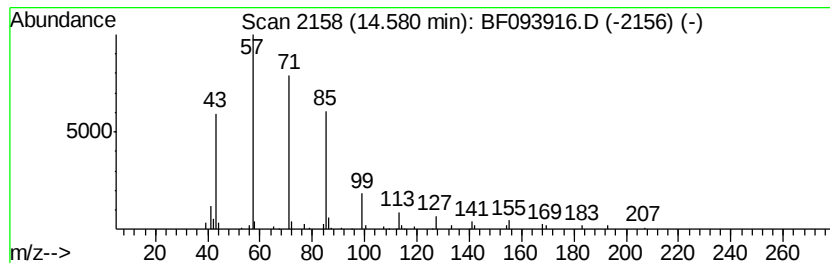
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Tetradecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.58	2.41 ng	171705	Chrysene-d12	14.68
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Tetradecane	198 C14H30	000629-59-4 83
2		Nonadecane	268 C19H40	000629-92-5 78
3		Decane, 3,8-dimethyl-	170 C12H26	017312-55-9 78
4		Tridecane	184 C13H28	000629-50-5 78
5		Dodecane	170 C12H26	000112-40-3 78



Data Path : Z:\HPCHEM1\BNA_F\Data\BF032417\
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Acq On : 24 Mar 2017 19:46
Operator : SJ/MA
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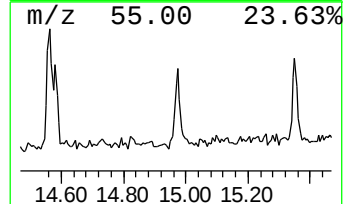
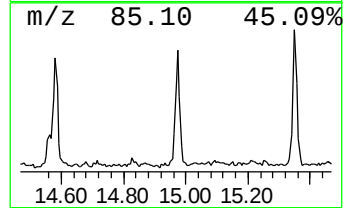
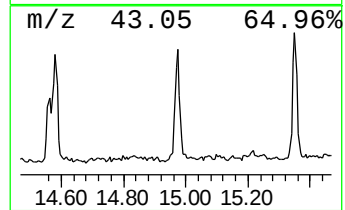
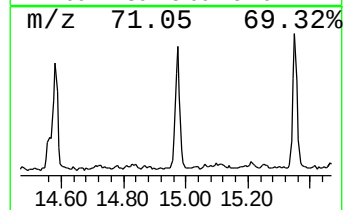
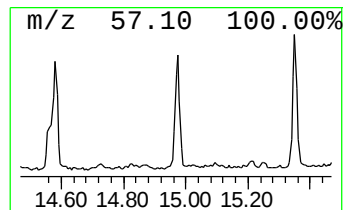
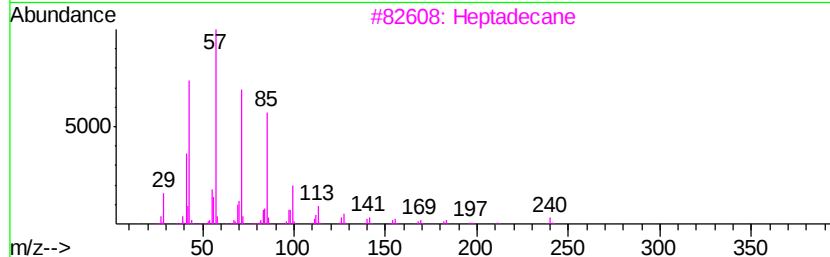
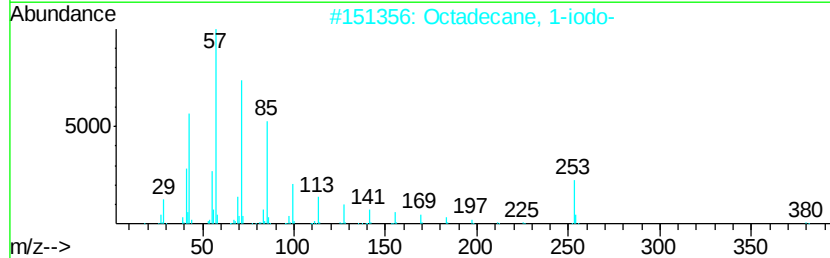
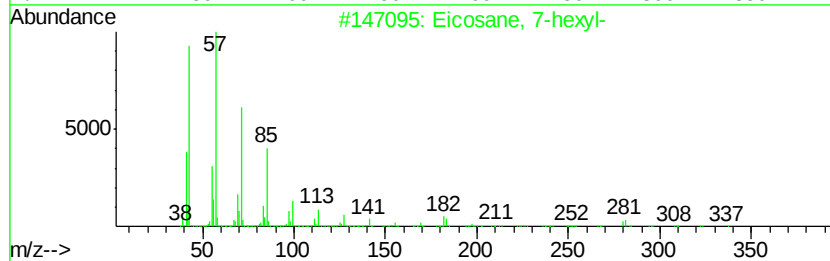
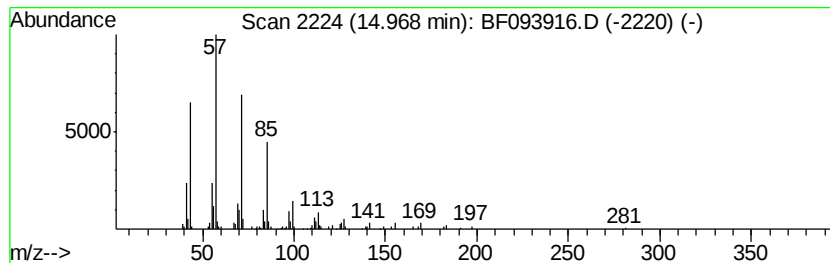
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Eicosane, 7-hexyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.97	2.71 ng	192609	Chrysene-d12	14.68	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
2	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	91
3	Heptadecane	240	C17H36	000629-78-7	91
4	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	91
5	Tetracosane	338	C24H50	000646-31-1	91



Data Path : Z:\HPCHEM1\BNA_F\Data\BF032417\
Data File : BF093916.D
Acq On : 24 Mar 2017 19:46
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Misc :
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Instrument :
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ClientSampleId :
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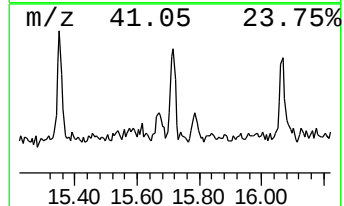
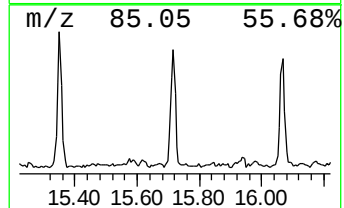
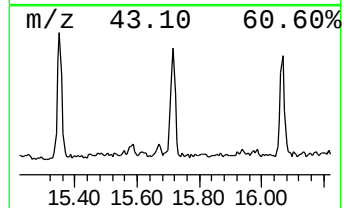
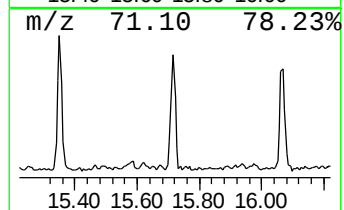
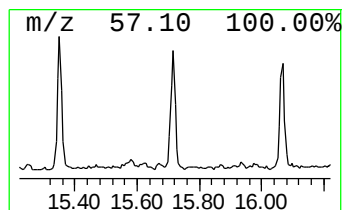
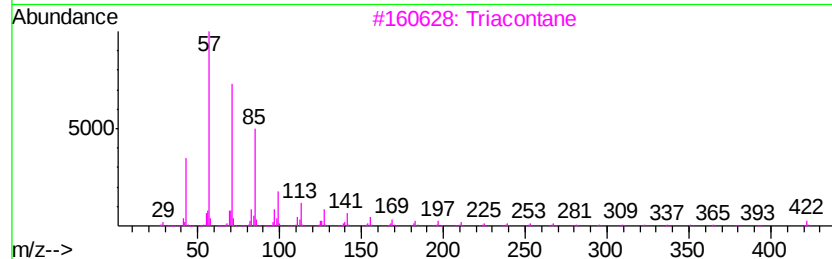
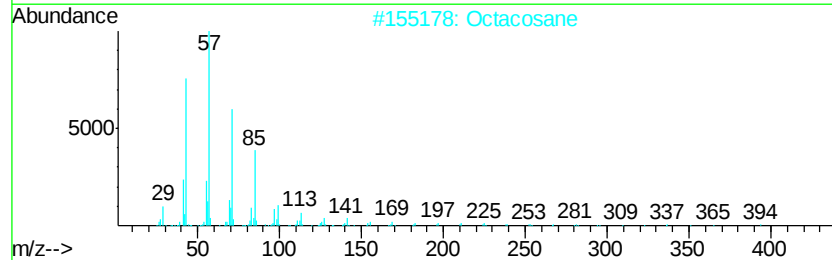
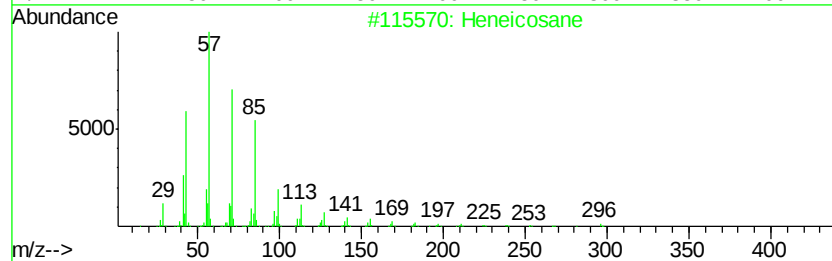
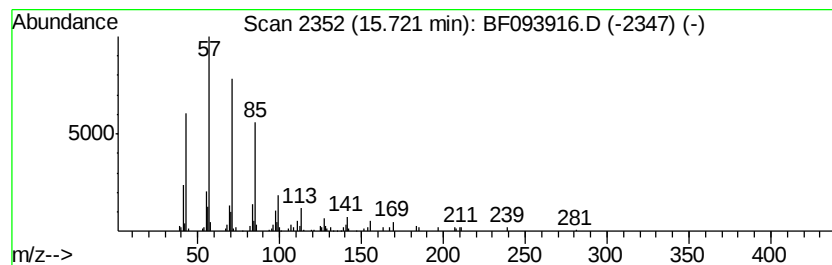
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	3.12 ng	178025	Perylene-d12	16.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Octacosane	394	C28H58	000630-02-4	91
3		Triacotane	422	C30H62	000638-68-6	91
4		Nonacosane	408	C29H60	000630-03-5	91
5		Tetracosane	338	C24H50	000646-31-1	91



Data Path : Z:\HPCHEM1\BNA F\Data\BF032417\
Data File : BF093916.D
Acq On : 24 Mar 2017 19:46
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Sample : I2394-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

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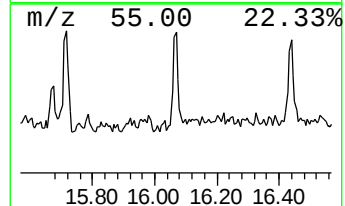
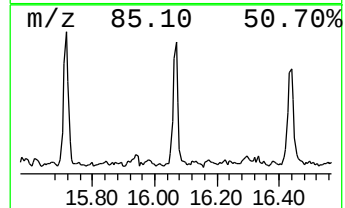
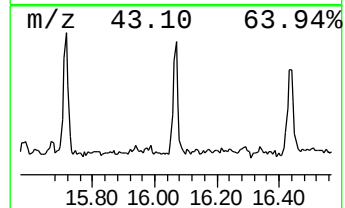
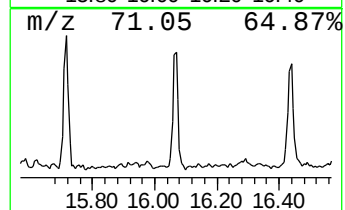
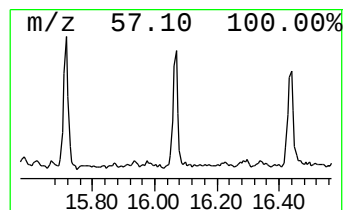
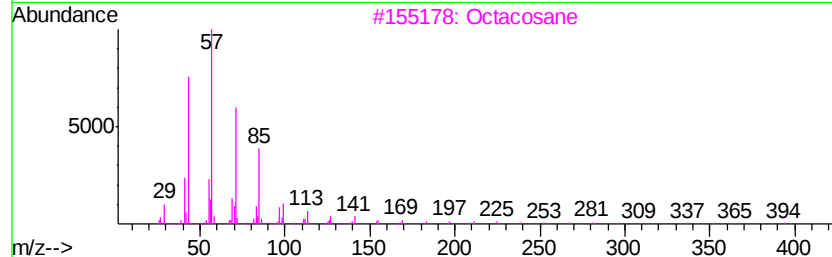
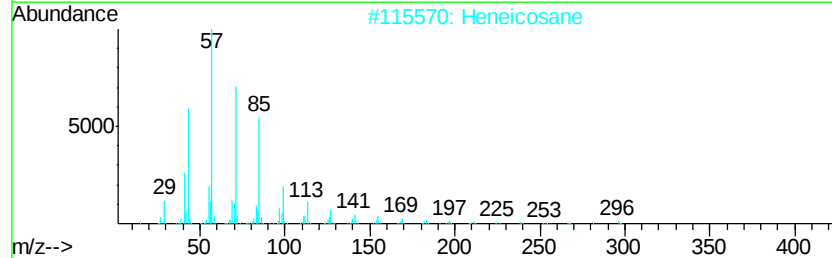
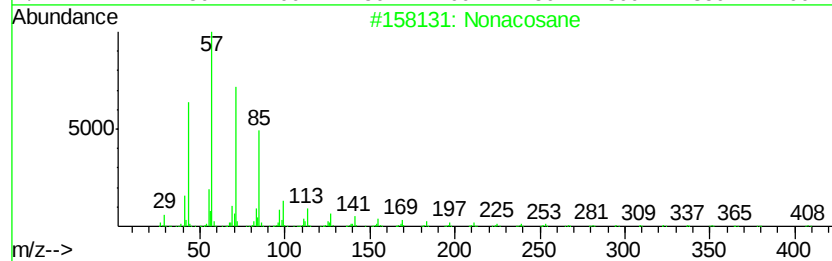
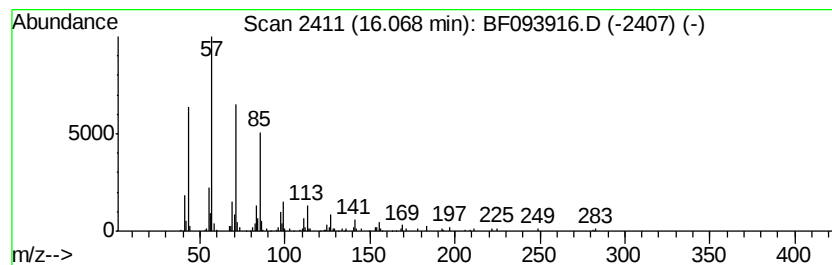
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Nonacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.07	3.06 ng	174237	Perylene-d12	16.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonacosane	408	C29H60	000630-03-5	90
2		Heneicosane	296	C21H44	000629-94-7	90
3		Octacosane	394	C28H58	000630-02-4	90
4		triacontane	422	C30H62	000638-68-6	87
5		Eicosane	282	C20H42	000112-95-8	87



Data Path : Z:\HPCHEM1\BNA_F\Data\BF032417\
Data File : BF093916.D
Acq On : 24 Mar 2017 19:46
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Sample : I2394-03
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ClientSampleId :
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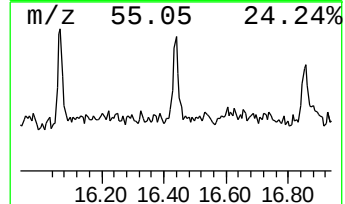
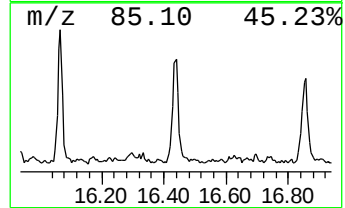
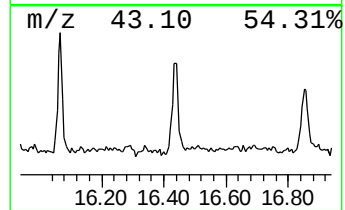
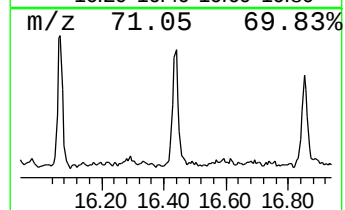
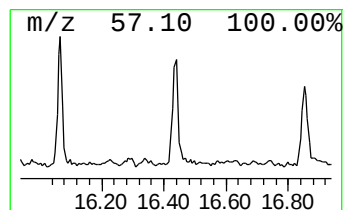
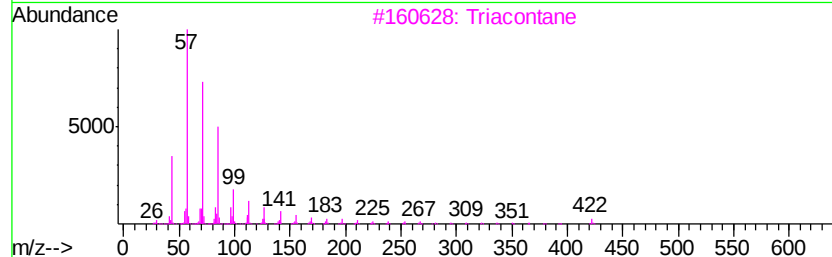
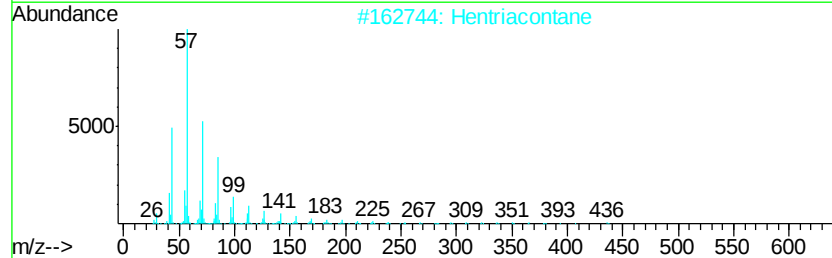
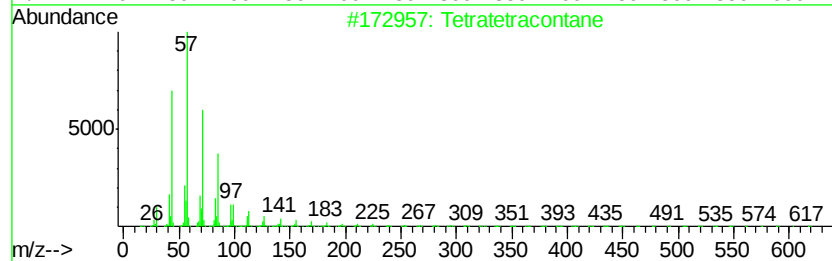
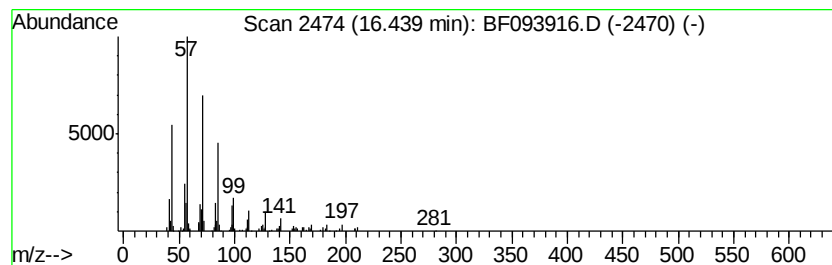
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Tetratetracontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.44	2.71 ng	154245	Perylene-d12	16.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetratetracontane	619	C44H90	007098-22-8	91
2		Hentriacontane	437	C31H64	000630-04-6	91
3		Triacontane	422	C30H62	000638-68-6	91
4		Nonacosane	408	C29H60	000630-03-5	91
5		Octacosane	394	C28H58	000630-02-4	87



Data Path : Z:\HPCHEM1\BNA_F\Data\BF032417\
Data File : BF093916.D
Acq On : 24 Mar 2017 19:46
Operator : SJ/MA
Sample : I2394-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

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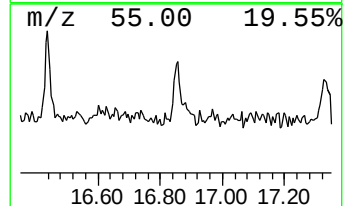
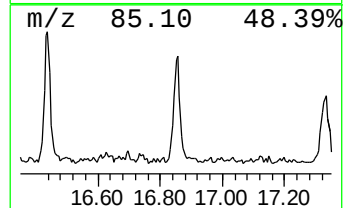
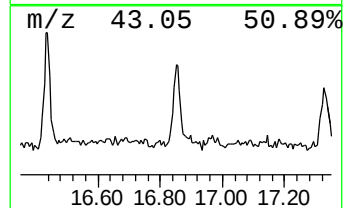
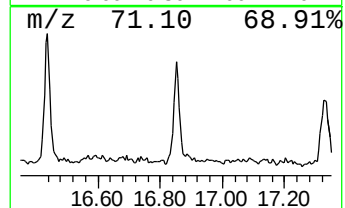
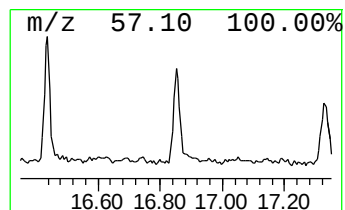
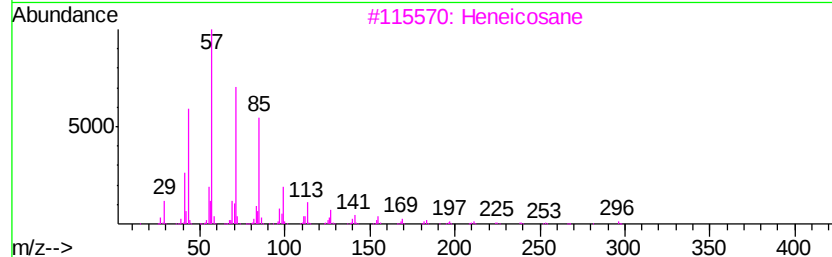
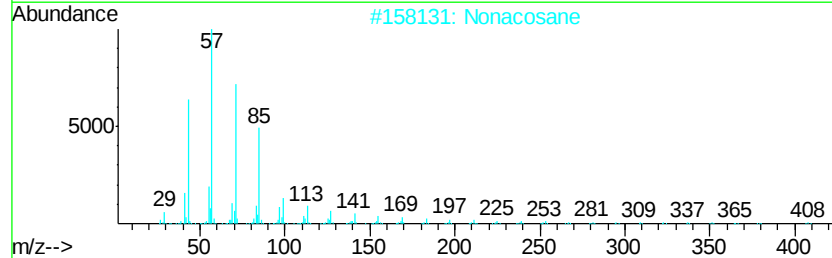
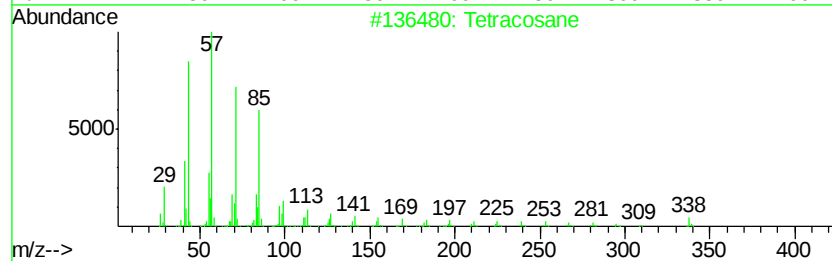
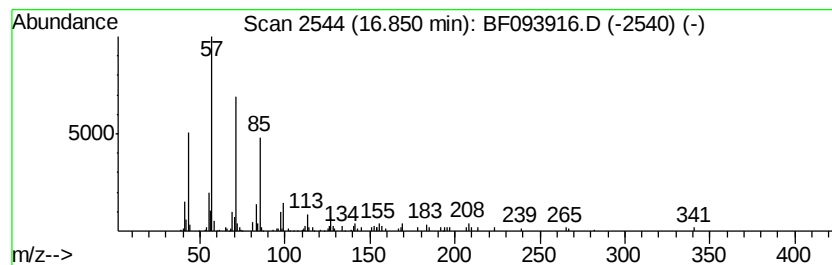
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Tetracosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.85	2.42 ng	138069	Perylene-d12	16.32

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	86
2			Nonacosane	408	C29H60	000630-03-5	83
3			Heneicosane	296	C21H44	000629-94-7	80
4			Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	80
5			Octadecane	254	C18H38	000593-45-3	72



Data Path : Z:\HPCHEM1\BNA_F\Data\BF032417\
Data File : BF093916.D
Acq On : 24 Mar 2017 19:46
Operator : SJ/MA
Sample : I2394-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.11	9.0 ng		435022	1	5.96	969543	20.0
unknown5.70	5.70	84.9 ng		4117740	1	5.96	969543	20.0
1,6-Anhydro-.beta...	9.50	3.3 ng		249843	3	9.60	1499740	20.0
Hexadecane	10.19	2.4 ng		178036	3	9.60	1499740	20.0
Eicosane	10.78	2.9 ng		215099	4	11.43	1463680	20.0
Trifluoroacetic a...	14.56	2.1 ng		152968	5	14.68	1423880	20.0
Tetradecane	14.58	2.4 ng		171705	5	14.68	1423880	20.0
Eicosane, 7-hexyl-	14.97	2.7 ng		192609	5	14.68	1423880	20.0
Heneicosane	15.72	3.1 ng		178025	6	16.32	1140120	20.0
Nonacosane	16.07	3.1 ng		174237	6	16.32	1140120	20.0
Tetratetracontane	16.44	2.7 ng		154245	6	16.32	1140120	20.0
Tetracosane	16.85	2.4 ng		138069	6	16.32	1140120	20.0