

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020717\
 Data File : BF092842.D
 Acq On : 7 Feb 2017 21:40
 Operator : SJ/MA
 Sample : I1745-03
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-1

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-BF013017.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	5.082	260	262	270	rBV	940386	1262876	35.10%	4.138%
2	5.516	297	300	302	rBV	2971901	3133525	87.09%	10.267%
3	6.545	387	390	393	rBV	2868531	2933453	81.53%	9.612%
4	6.670	399	401	404	rBV	2569735	2890521	80.34%	9.471%
5	6.899	419	421	424	rBV	799969	837306	23.27%	2.743%
6	7.059	433	435	438	rBV	2706896	2300574	63.94%	7.538%
7	7.470	468	471	473	rBV	2077483	1989276	55.29%	6.518%
8	8.190	531	534	536	rBV	1571397	1377873	38.30%	4.515%
9	9.265	625	628	630	rBV	4054356	3598002	100.00%	11.789%
10	9.653	660	662	665	rBV	433571	520169	14.46%	1.704%
11	9.871	678	681	683	rBV	62810	58936	1.64%	0.193%
12	9.939	685	687	690	rBV	1237607	1361312	37.84%	4.460%
13	10.351	721	723	724	rBV	38094	62994	1.75%	0.206%
14	10.373	724	725	726	rVB	105997	73556	2.04%	0.241%
15	10.591	741	744	747	rVB	37896	48401	1.35%	0.159%
16	10.728	754	756	759	rBV2	1147915	1579490	43.90%	5.175%
17	10.842	764	766	771	rVB	105327	132213	3.67%	0.433%
18	11.288	804	805	807	rBV	70744	79375	2.21%	0.260%
19	11.425	815	817	820	rBV2	893025	1009715	28.06%	3.308%
20	11.665	834	838	841	rBV5	18490	44501	1.24%	0.146%
21	11.722	841	843	845	rVV	75908	74949	2.08%	0.246%
22	12.122	877	878	881	rVB	42896	39875	1.11%	0.131%
23	12.637	922	923	926	rVB3	38260	44280	1.23%	0.145%
24	12.865	941	943	946	rBV2	34180	49384	1.37%	0.162%
25	13.014	953	956	959	rBV	2359807	2189280	60.85%	7.173%
26	13.917	1033	1035	1042	rBV	122777	215465	5.99%	0.706%
27	14.065	1046	1048	1053	rVB	871101	972750	27.04%	3.187%
28	14.545	1086	1090	1096	rBV2	84935	286259	7.96%	0.938%
29	14.694	1100	1103	1105	rBV	38101	53215	1.48%	0.174%
30	15.094	1136	1138	1142	rBV	32766	54509	1.51%	0.179%
31	15.163	1142	1144	1146	rBV	161627	201414	5.60%	0.660%
32	15.517	1172	1175	1180	rVB	556467	808527	22.47%	2.649%
33	15.963	1211	1214	1218	rVB	91443	131703	3.66%	0.432%
34	18.523	1435	1438	1446	rVB7	35897	104427	2.90%	0.342%

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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:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
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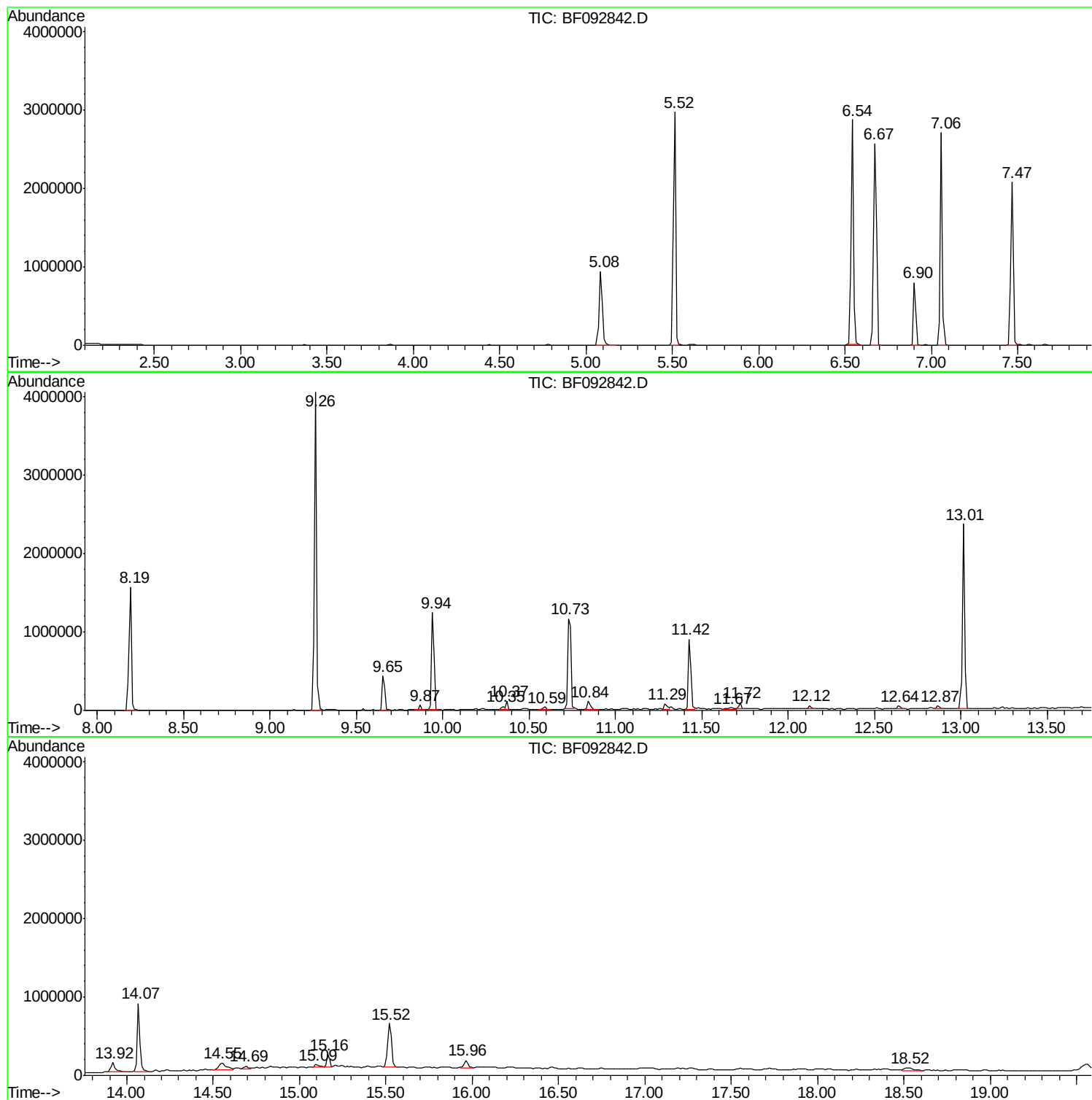
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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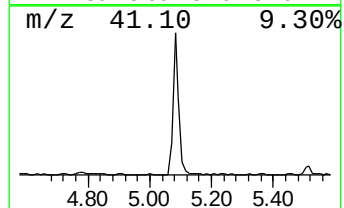
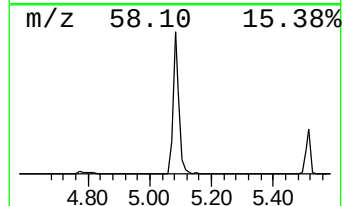
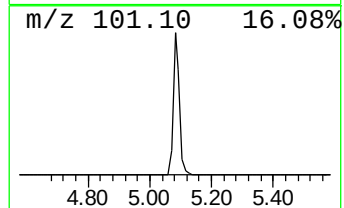
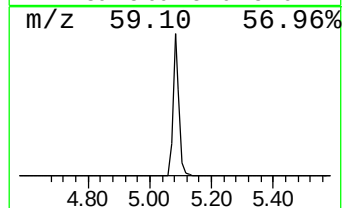
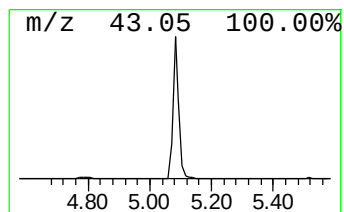
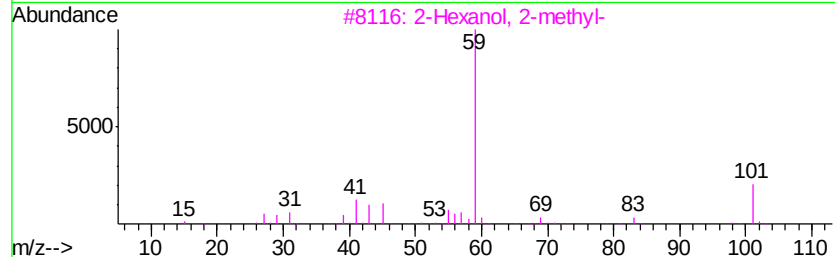
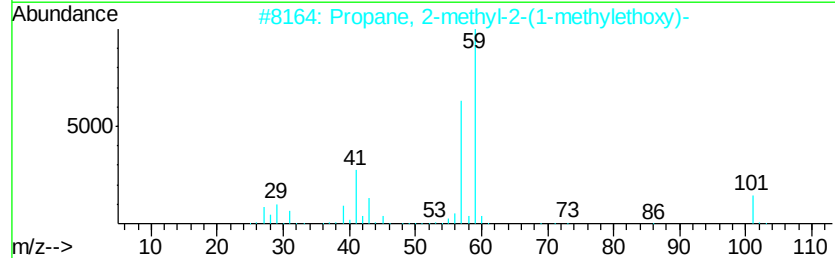
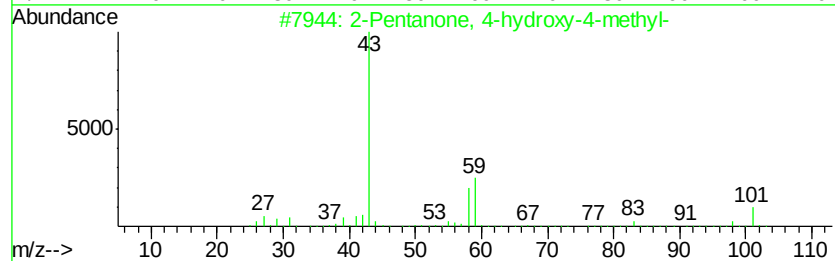
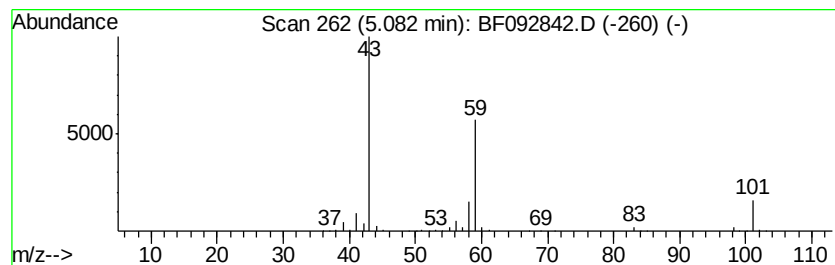
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	30.17 ng	1262880	1,4-Dichlorobenzene-d4	6.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32



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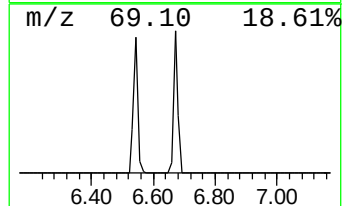
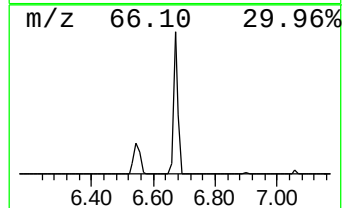
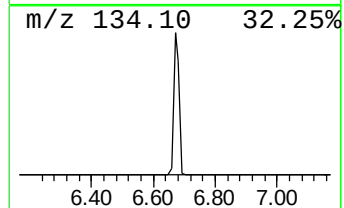
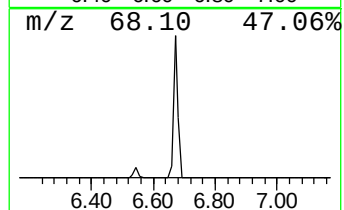
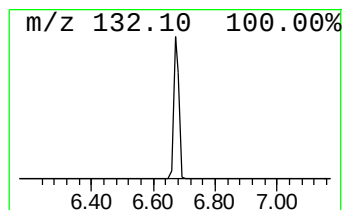
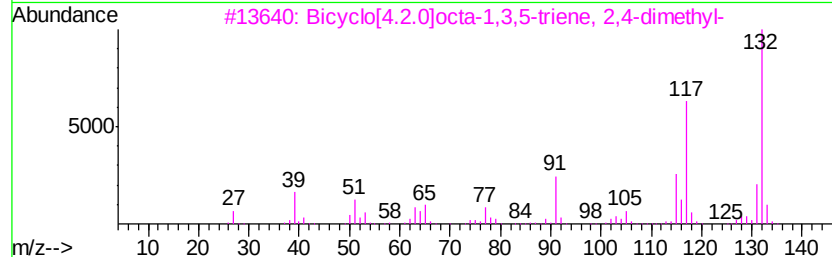
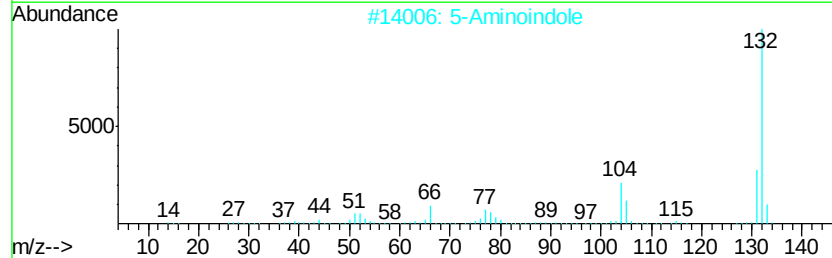
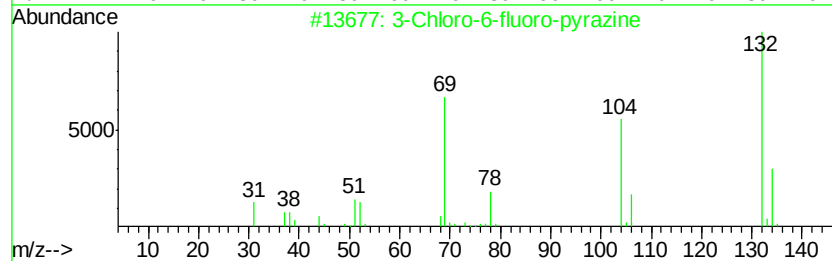
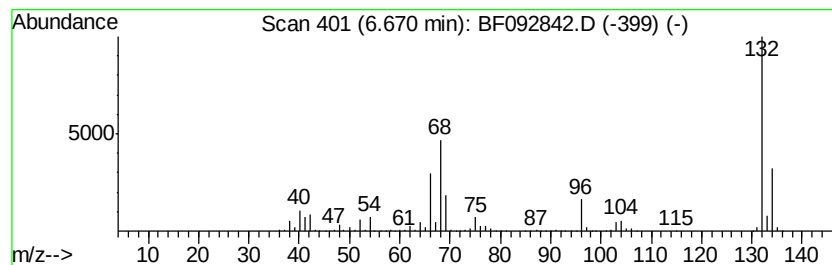
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	69.04 ng	2890520	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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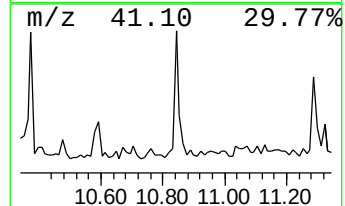
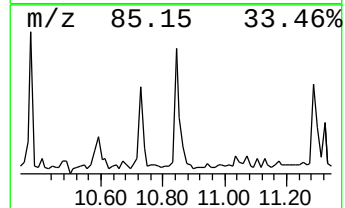
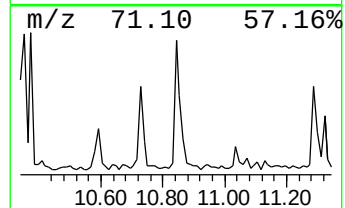
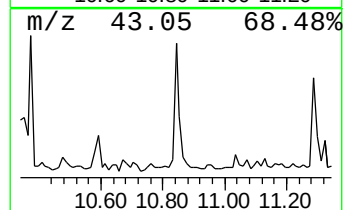
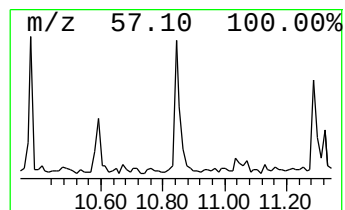
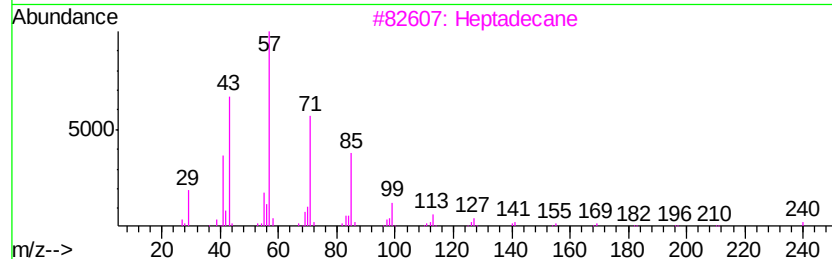
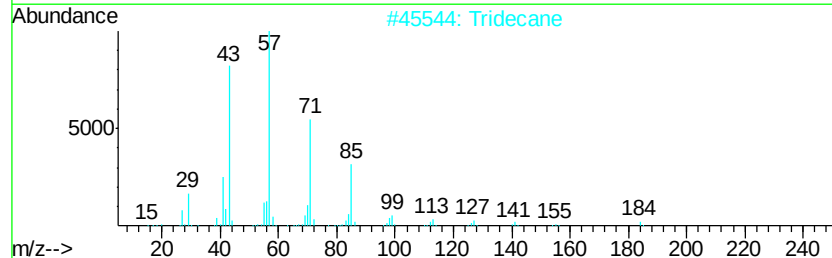
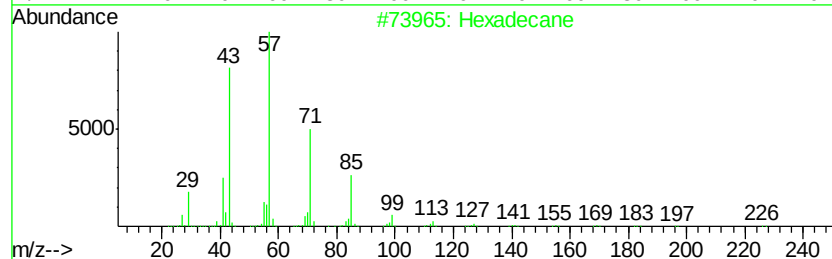
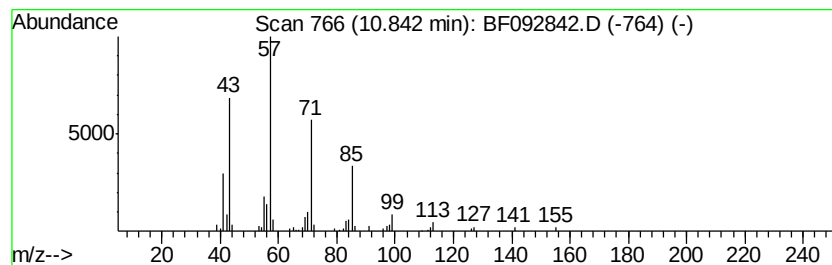
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.84	2.62 ng	132213	Phenanthrene-d10		11.43	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	91
2	Tridecane		184	C13H28	000629-50-5	90
3	Heptadecane		240	C17H36	000629-78-7	90
4	Pentadecane		212	C15H32	000629-62-9	86
5	Decane, 2,3,5-trimethyl-		184	C13H28	062238-11-3	78



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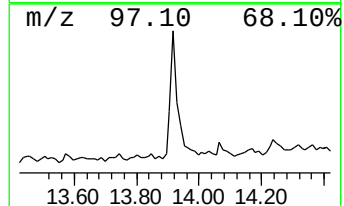
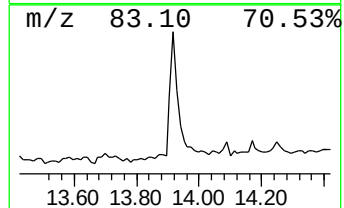
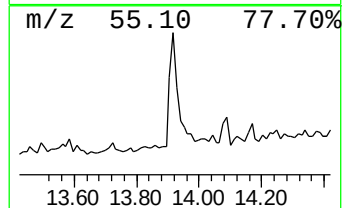
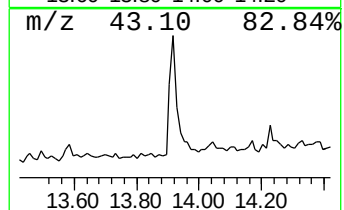
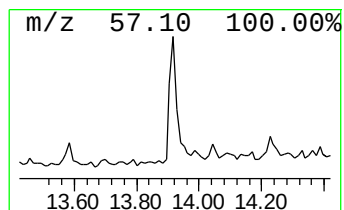
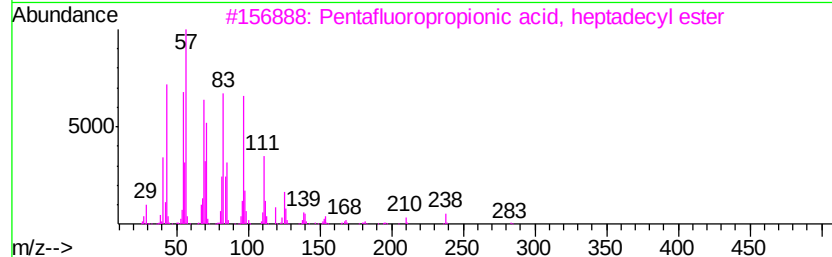
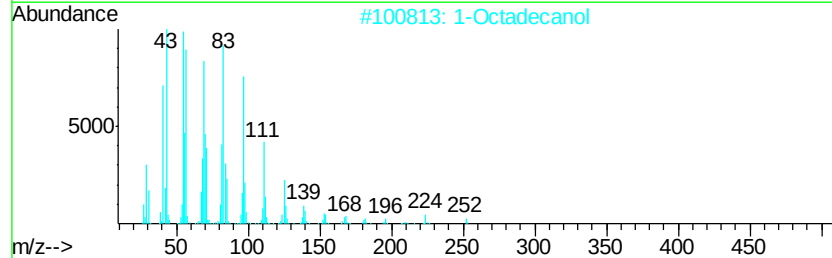
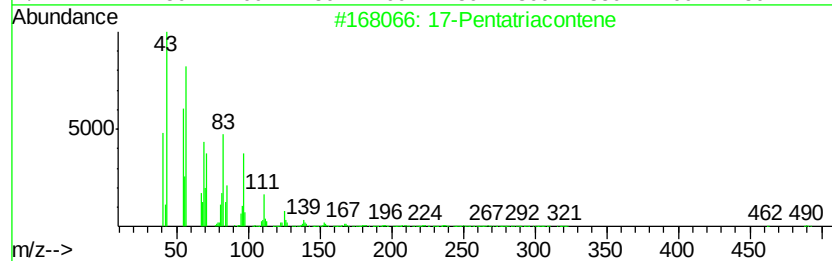
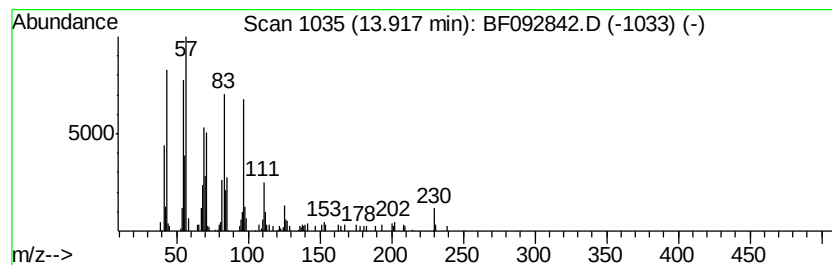
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 17-Pentatriacontene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.92	4.43 ng	215465	Chrysene-d12	14.07

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		17-Pentatriacontene	491	C35H70	006971-40-0	91
2		1-Octadecanol	270	C18H38O	000112-92-5	81
3		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	80
4		1-Heptadecanol	256	C17H36O	001454-85-9	76
5		Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	74



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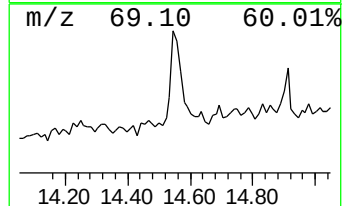
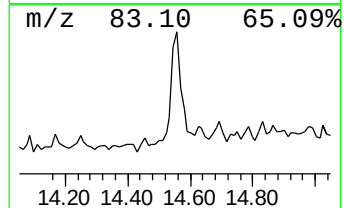
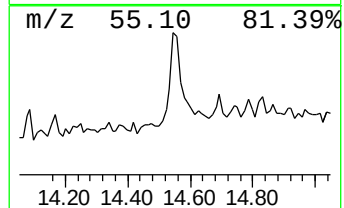
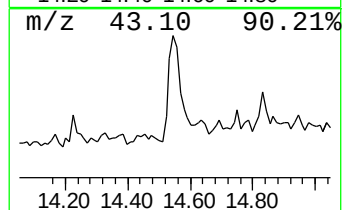
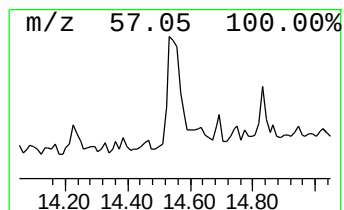
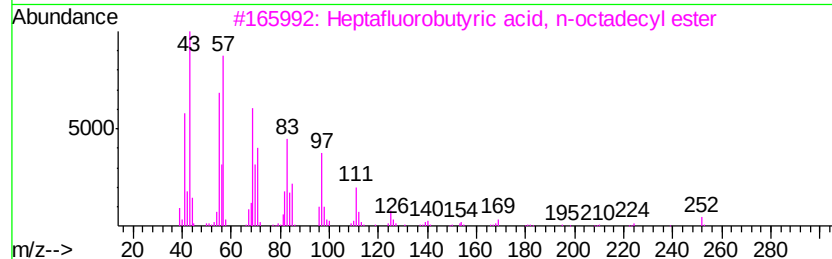
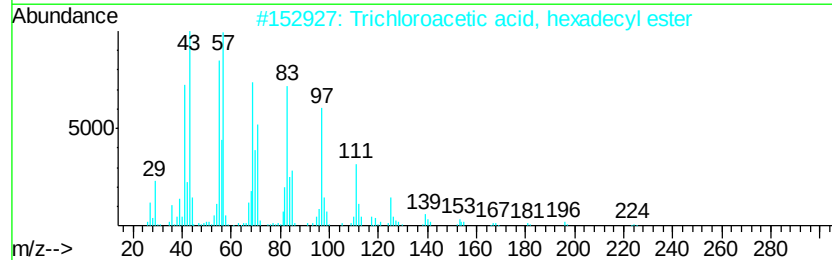
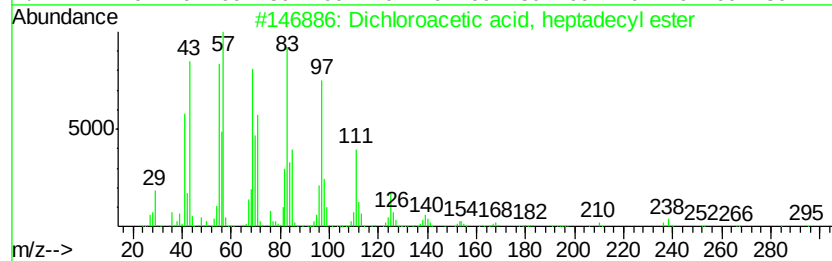
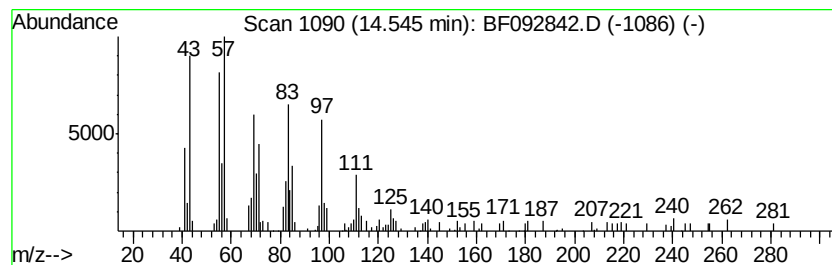
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Dichloroacetic acid, heptad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.55	5.89 ng	286259	Chrysene-d12	14.07	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
3	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	90
4	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	90
5	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	90



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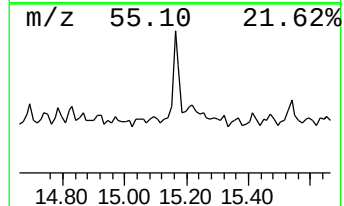
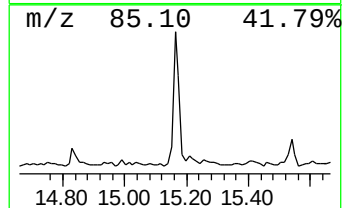
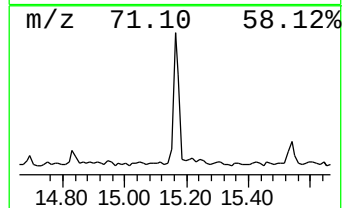
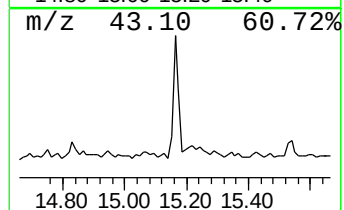
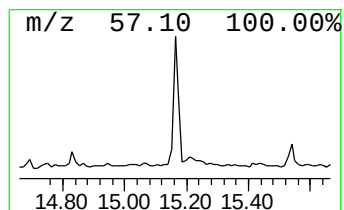
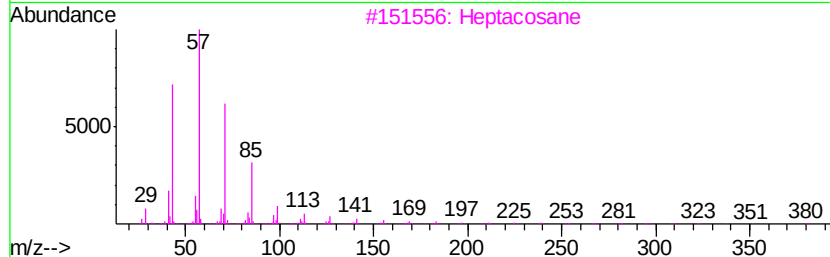
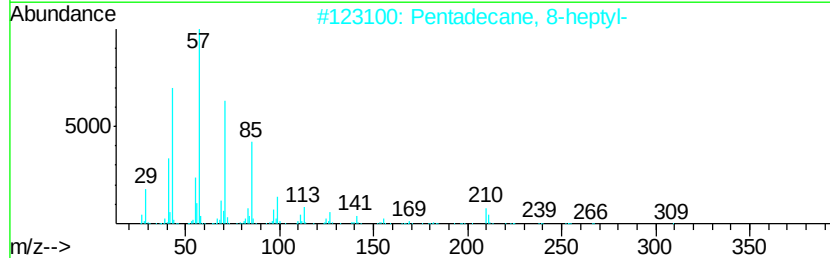
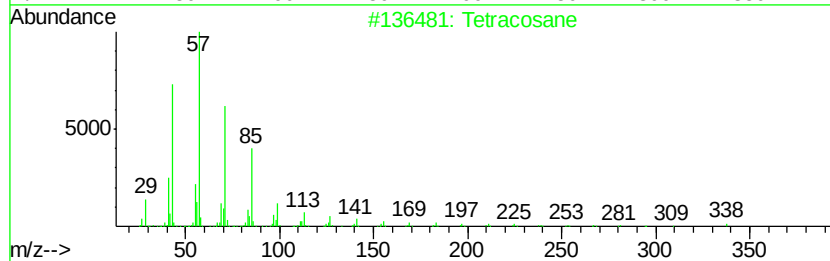
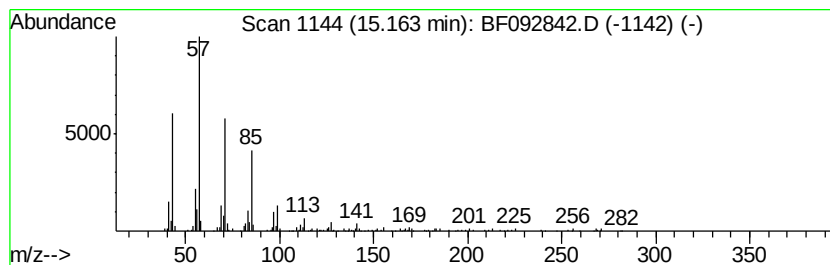
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.16	4.98 ng	201414	Perylene-d12	15.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	91
2		Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91
3		Heptacosane	380	C27H56	000593-49-7	90
4		Pentacosane	352	C25H52	000629-99-2	90
5		Triacontane	422	C30H62	000638-68-6	90



Data Path : Z:\HPCHEM1\BNA F\DATA\BF020717\
Data File : BF092842.D
Acq On : 7 Feb 2017 21:40
Operator : SJ/MA
Sample : I1745-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-1

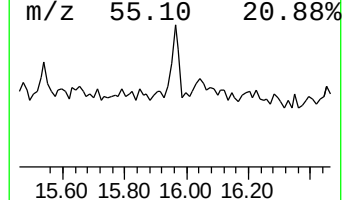
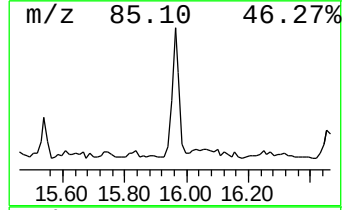
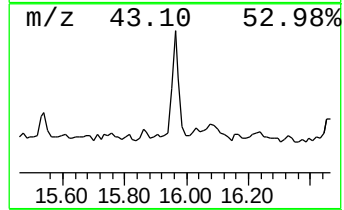
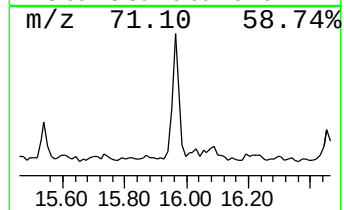
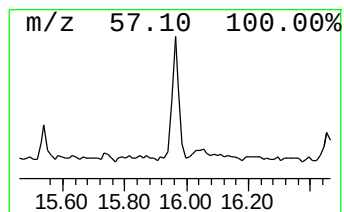
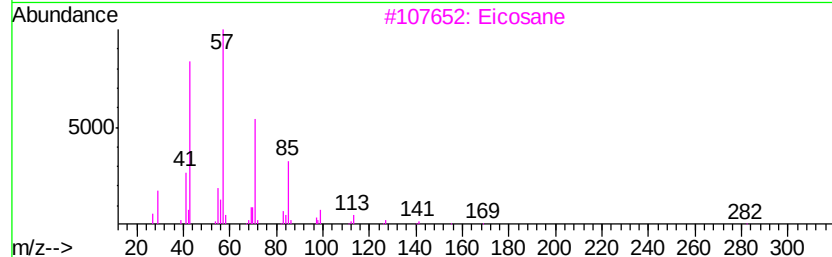
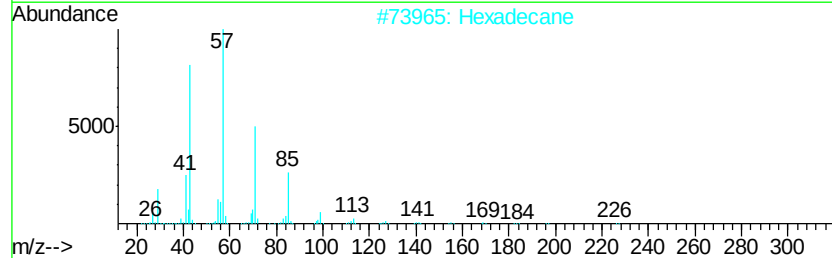
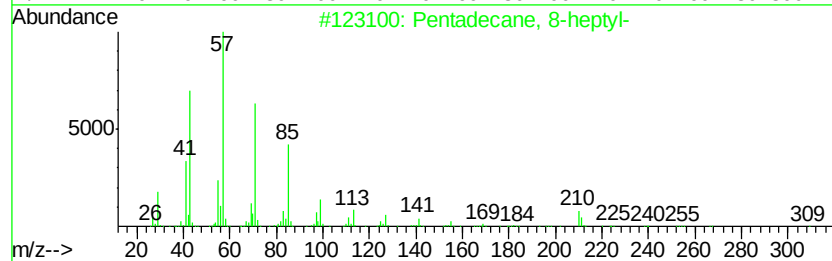
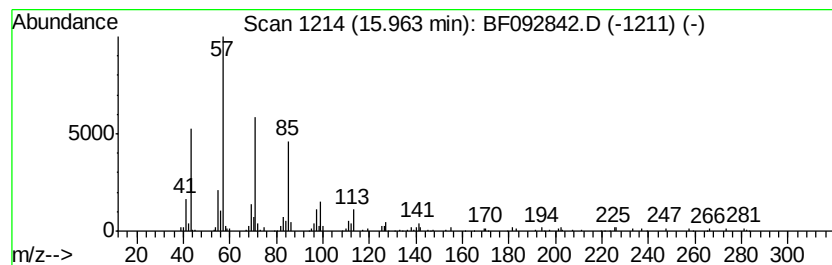
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentadecane, 8-heptyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.96	3.26 ng	131703	Perylene-d12	15.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	87
2		Hexadecane	226	C16H34	000544-76-3	87
3		Eicosane	282	C20H42	000112-95-8	87
4		Octacosane	394	C28H58	000630-02-4	86
5		2-Bromo dodecane	248	C12H25Br	013187-99-0	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020717\
Data File : BF092842.D
Acq On : 7 Feb 2017 21:40
Operator : SJ/MA
Sample : I1745-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

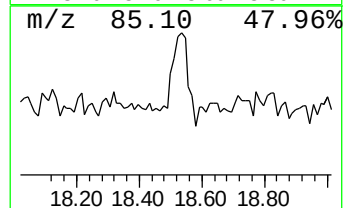
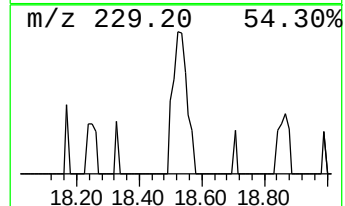
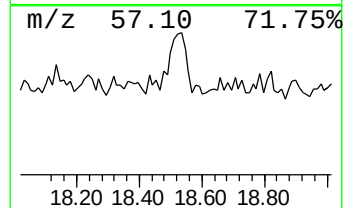
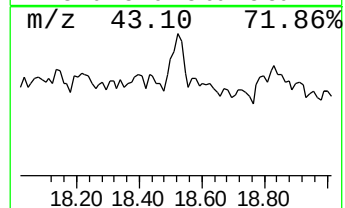
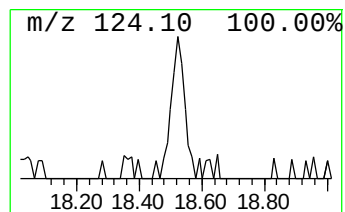
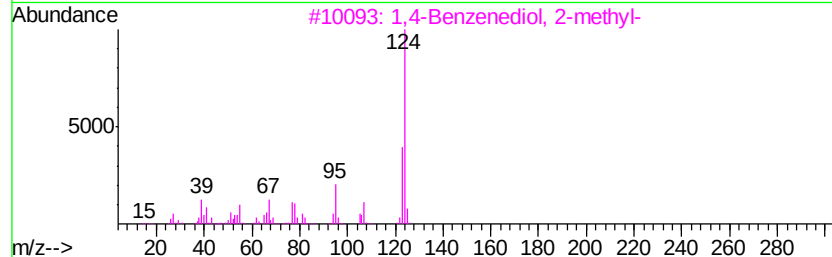
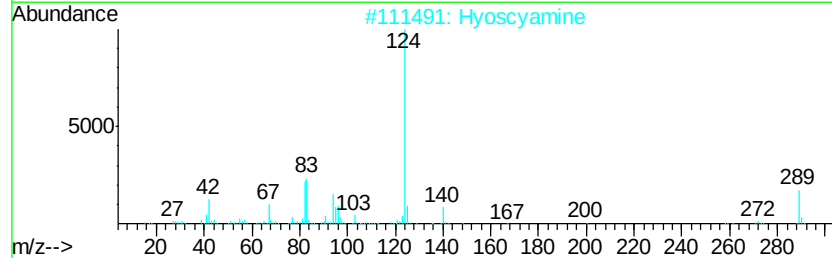
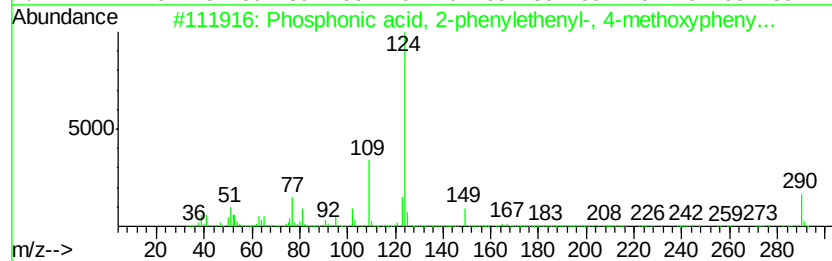
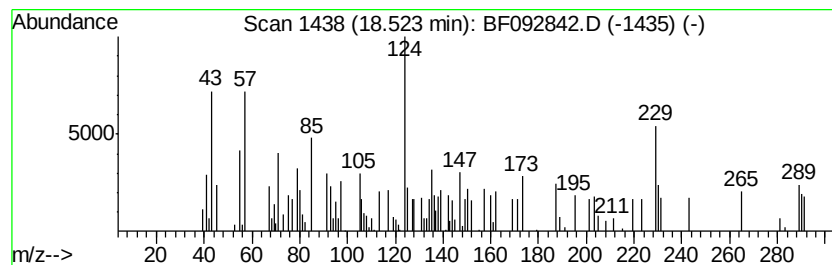
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown18.52 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.52	2.58 ng	104427	Perylene-d12	15.52
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Phosphonic acid, 2-phenylethenyl...	290 C15H15O4P	330855-58-8 22
2		Hyoscyamine	289 C17H23NO3	000101-31-5 22
3		1,4-Benzenediol, 2-methyl-	124 C7H8O2	000095-71-6 11
4		2H-1,3-Benzoxazine, octahydro-2-...	230 C14H18N2O	1000138-91-8 11
5		4-Methylmercaptoaniline	139 C7H9NS	000104-96-1 10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020717\
Data File : BF092842.D
Acq On : 7 Feb 2017 21:40
Operator : SJ/MA
Sample : I1745-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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...	5.08	30.2	ng	1262880	1	6.90	837306	20.0
unknown6.67	6.67	69.0	ng	2890520	1	6.90	837306	20.0
Hexadecane	10.84	2.6	ng	132213	4	11.43	1009720	20.0
17-Pentatriacontene	13.92	4.4	ng	215465	5	14.07	972750	20.0
Dichloroacetic ac...	14.55	5.9	ng	286259	5	14.07	972750	20.0
Tetracosane	15.16	5.0	ng	201414	6	15.52	808527	20.0
Pentadecane, 8-he...	15.96	3.3	ng	131703	6	15.52	808527	20.0
unknown18.52	18.52	2.6	ng	104427	6	15.52	808527	20.0