

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020217\
 Data File : BF092748.D
 Acq On : 2 Feb 2017 21:15
 Operator : SJ/MA
 Sample : I1650-02
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-34-COMP

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	5.116	262	265	268	rBV	1101582	1602461	40.33%	4.925%
2	5.550	300	303	305	rBV	3458748	3696759	93.04%	11.363%
3	6.579	390	393	395	rBV	3462150	3973319	100.00%	12.213%
4	6.704	401	404	407	rBV	3560330	3274121	82.40%	10.064%
5	6.933	422	424	427	rBV	1222890	1011993	25.47%	3.111%
6	7.093	435	438	440	rBV	3054721	2696655	67.87%	8.289%
7	7.505	471	474	476	rBV	1809928	1948778	49.05%	5.990%
8	8.225	535	537	539	rBV	1254840	1084320	27.29%	3.333%
9	9.299	629	631	634	rBV	2366019	2999370	75.49%	9.219%
10	9.699	663	666	668	rBV	173383	182254	4.59%	0.560%
11	9.985	688	691	693	rBV	994190	1126625	28.35%	3.463%
12	10.408	724	728	729	rBV	57364	59464	1.50%	0.183%
13	10.762	757	759	762	rBV2	1127651	1478911	37.22%	4.546%
14	10.876	767	769	774	rVB	98478	117535	2.96%	0.361%
15	11.322	806	808	809	rBV	63019	53600	1.35%	0.165%
16	11.459	818	820	823	rBV	1027722	962444	24.22%	2.958%
17	13.048	956	959	961	rBV	2227485	2252832	56.70%	6.924%
18	13.939	1035	1037	1043	rBV2	78870	162204	4.08%	0.499%
19	14.100	1048	1051	1053	rBV	866766	869134	21.87%	2.671%
20	14.557	1089	1091	1092	rBV2	38290	46445	1.17%	0.143%
21	14.934	1123	1124	1127	rVB	38721	54585	1.37%	0.168%
22	15.197	1145	1147	1149	rBV	45818	60929	1.53%	0.187%
23	15.483	1168	1172	1173	rBV4	40856	79463	2.00%	0.244%
24	15.563	1176	1179	1182	rBV	629187	909895	22.90%	2.797%
25	16.008	1216	1218	1221	rVB	51009	67740	1.70%	0.208%
26	16.374	1246	1250	1251	rBV4	21479	46499	1.17%	0.143%
27	16.477	1255	1259	1260	rVV4	38264	91916	2.31%	0.283%
28	16.511	1260	1262	1266	rVB2	36951	68323	1.72%	0.210%
29	17.094	1310	1313	1318	rVB	32430	72776	1.83%	0.224%
30	17.791	1369	1374	1378	rBV4	33292	109596	2.76%	0.337%
31	18.088	1391	1400	1414	rVB3	202174	1373611	34.57%	4.222%

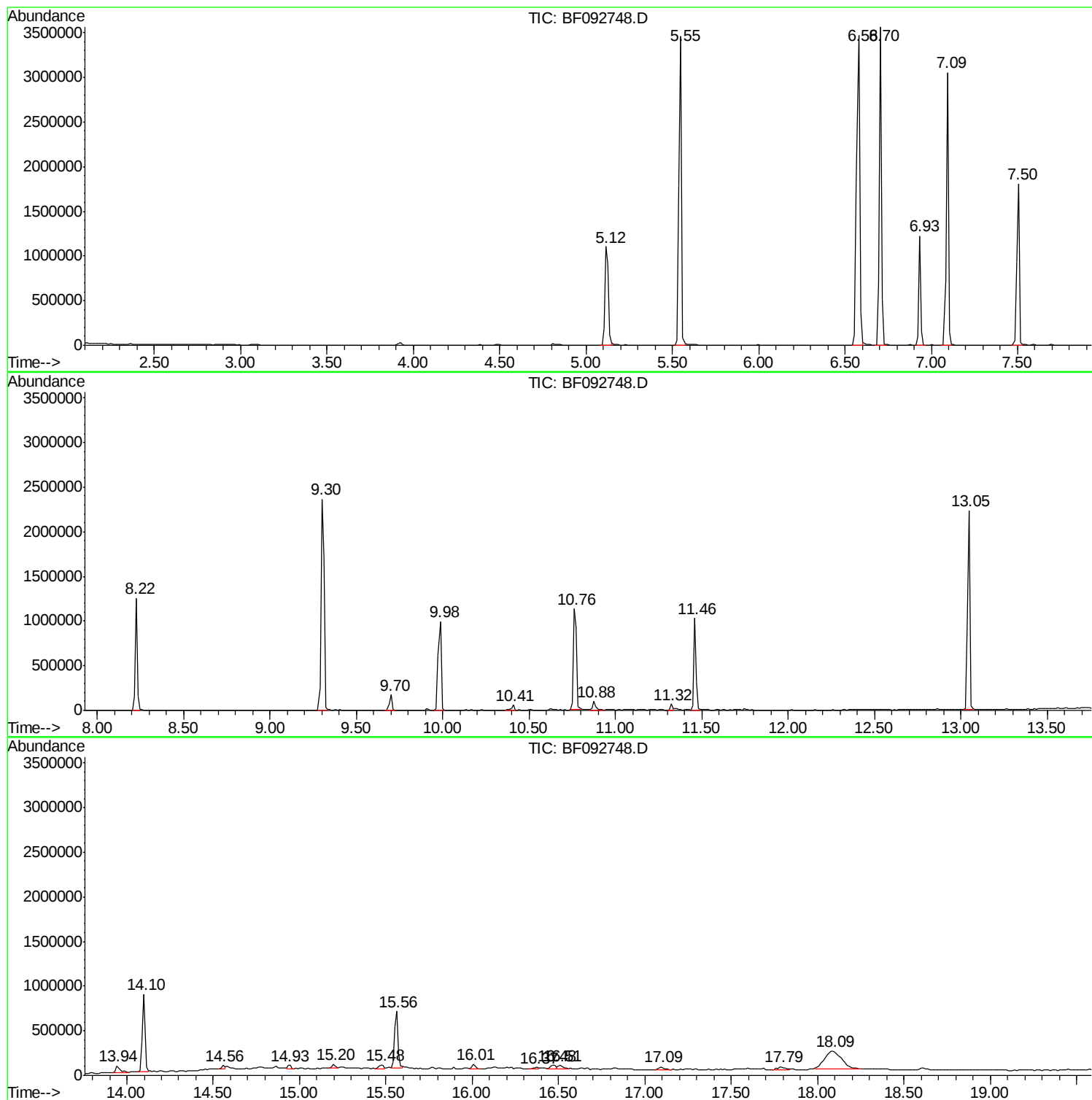
Sum of corrected areas: 32534557

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020217\
Data File : BF092748.D
Acq On : 2 Feb 2017 21:15
Operator : SJ/MA
Sample : I1650-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-34-COMP

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF020217\
Data File : BF092748.D
Acq On : 2 Feb 2017 21:15
Operator : SJ/MA
Sample : I1650-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-34-COMP

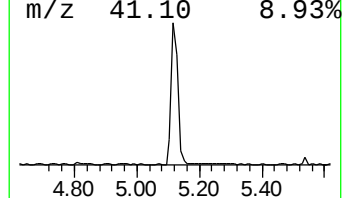
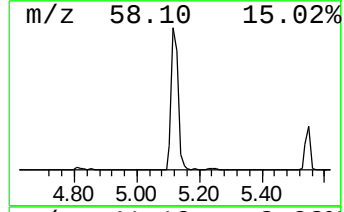
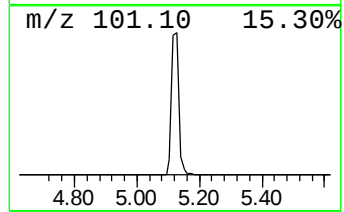
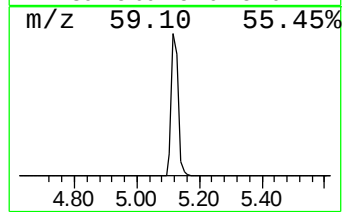
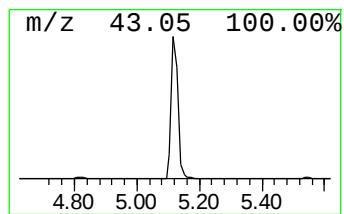
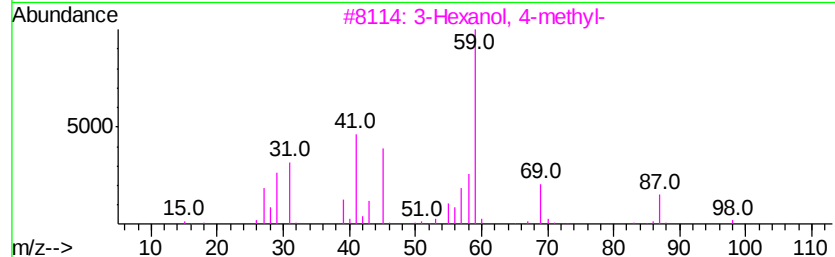
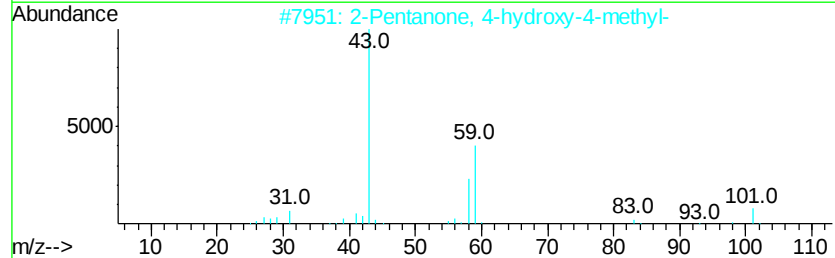
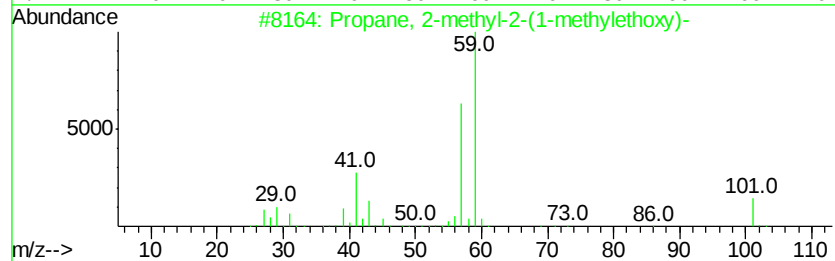
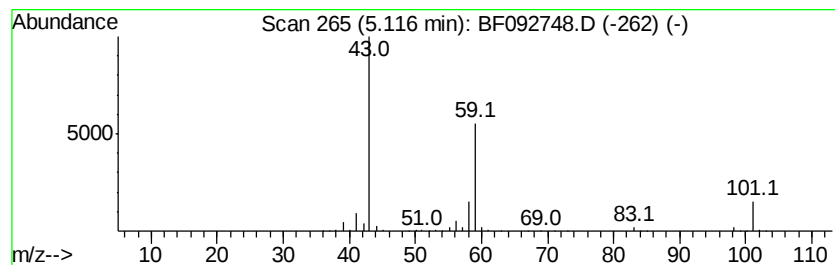
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2-methyl-2-(1-meth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	31.67 ng	1602460	1,4-Dichlorobenzene-d4	6.93

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53	
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50	
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33	
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33	
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32	



Data Path : Z:\HPCHEM1\BNA F\DATA\BF020217\
Data File : BF092748.D
Acq On : 2 Feb 2017 21:15
Operator : SJ/MA
Sample : I1650-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-34-COMP

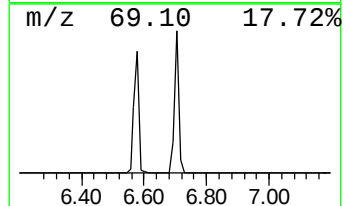
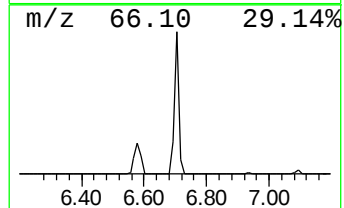
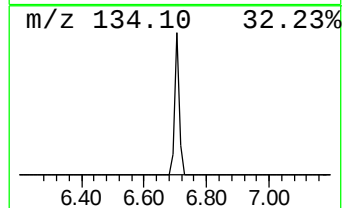
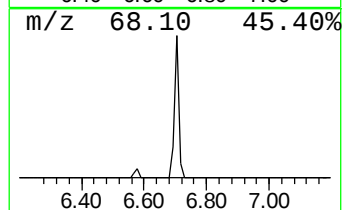
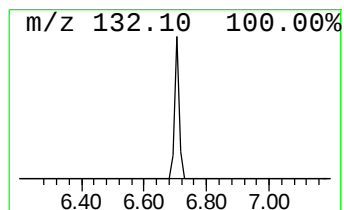
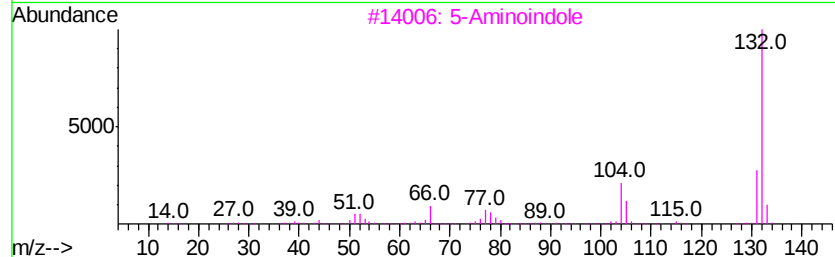
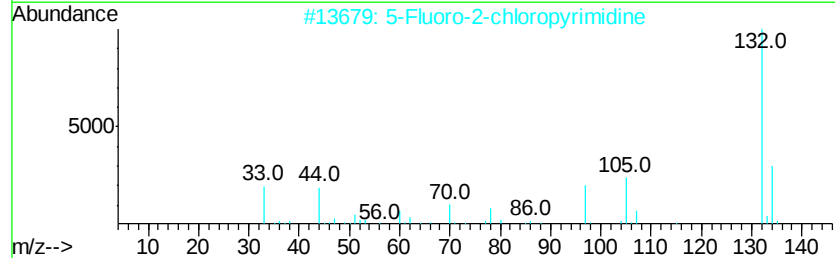
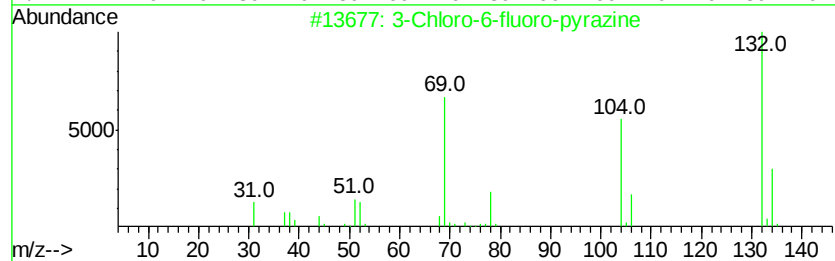
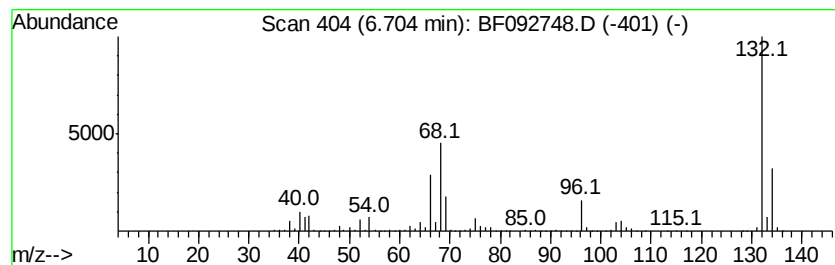
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	64.71 ng	3274120	1,4-Dichlorobenzene-d4	6.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020217\
Data File : BF092748.D
Acq On : 2 Feb 2017 21:15
Operator : SJ/MA
Sample : I1650-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-34-COMP

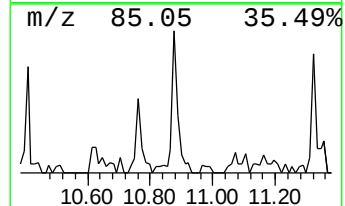
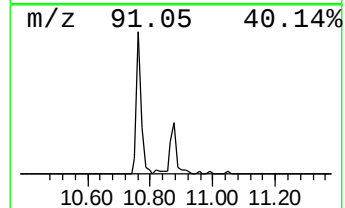
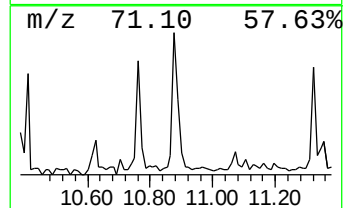
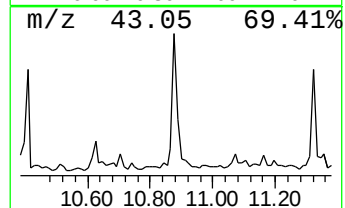
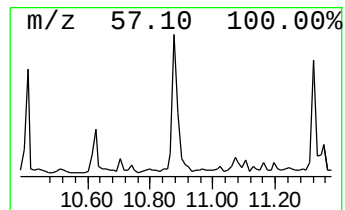
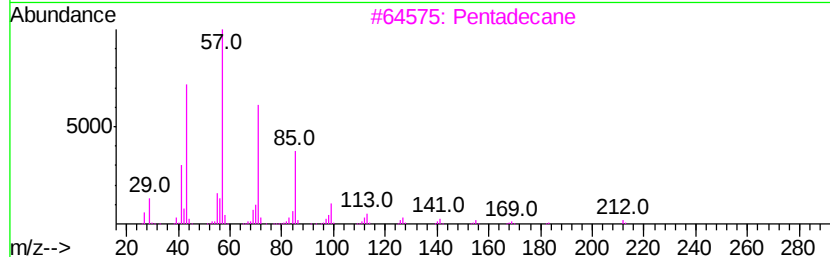
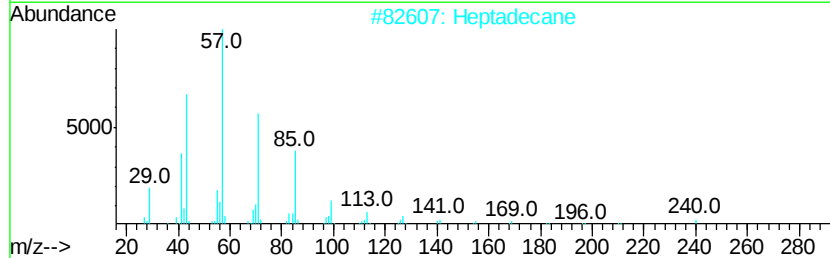
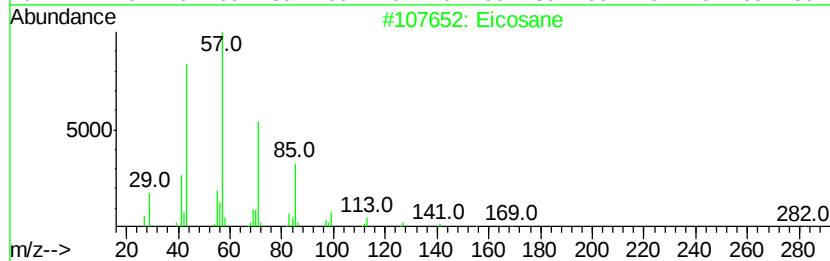
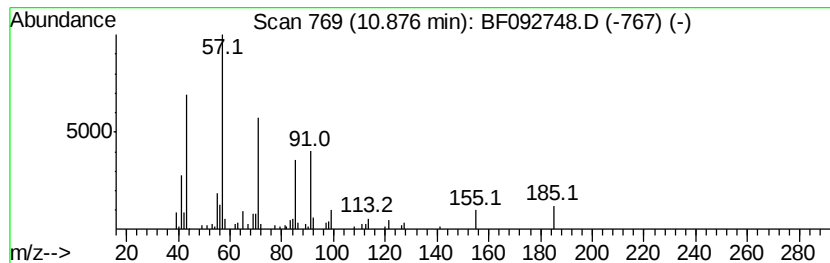
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.88	2.44 ng	117535	Phenanthrene-d10	11.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	74
2		Heptadecane	240	C17H36	000629-78-7	72
3		Pentadecane	212	C15H32	000629-62-9	72
4		Hexadecane	226	C16H34	000544-76-3	72
5		Tetradecane	198	C14H30	000629-59-4	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF020217\
Data File : BF092748.D
Acq On : 2 Feb 2017 21:15
Operator : SJ/MA
Sample : I1650-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-34-COMP

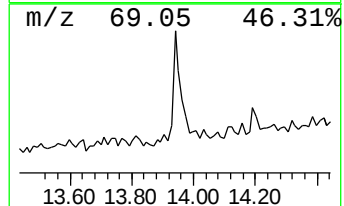
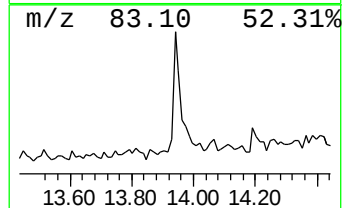
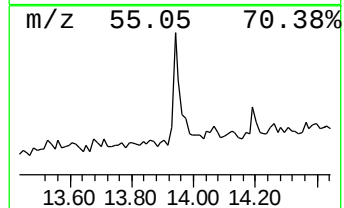
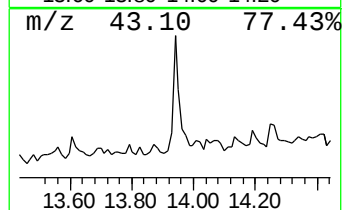
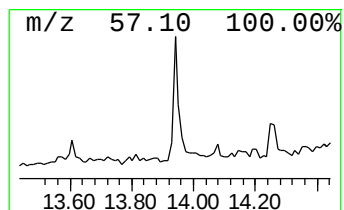
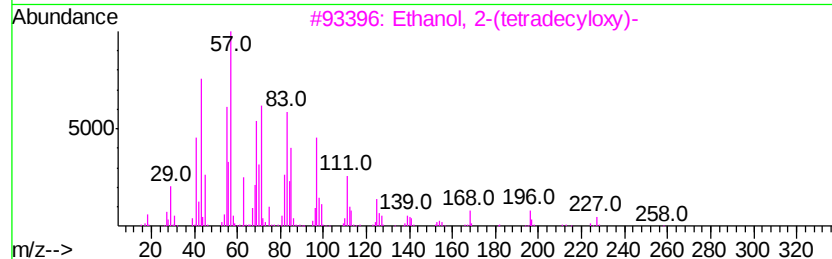
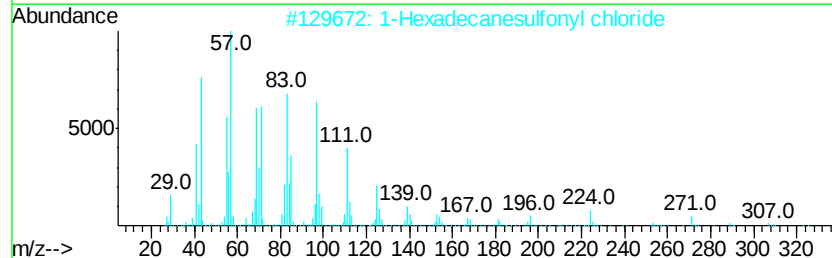
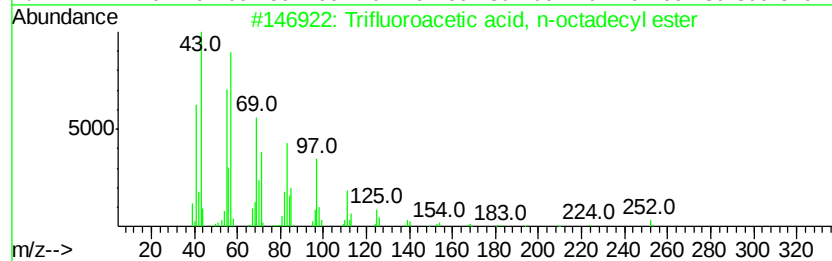
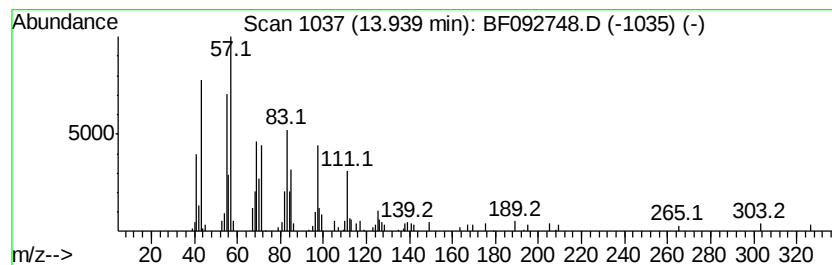
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Trifluoroacetic acid, n-oct... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	3.73 ng	162204	Chrysene-d12	14.10

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetic acid, n-octadecv...	366	C20H37F3O2	079392-43-1	91
2		1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
3		Ethanol, 2-(tetradecvloxv)-	258	C16H34O2	002136-70-1	90
4		1-Hexadecanol, 2-methyl-	256	C17H36O	002490-48-4	87
5		Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020217\
Data File : BF092748.D
Acq On : 2 Feb 2017 21:15
Operator : SJ/MA
Sample : I1650-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-34-COMP

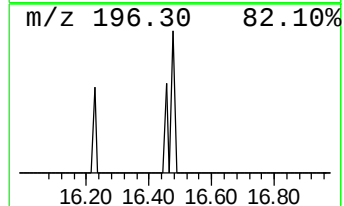
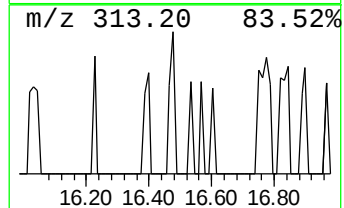
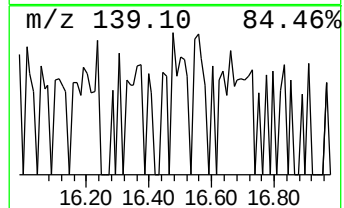
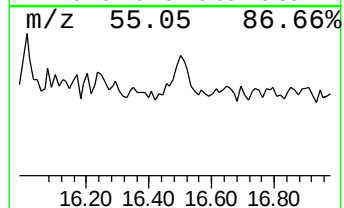
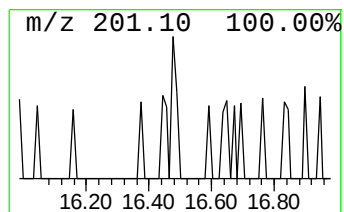
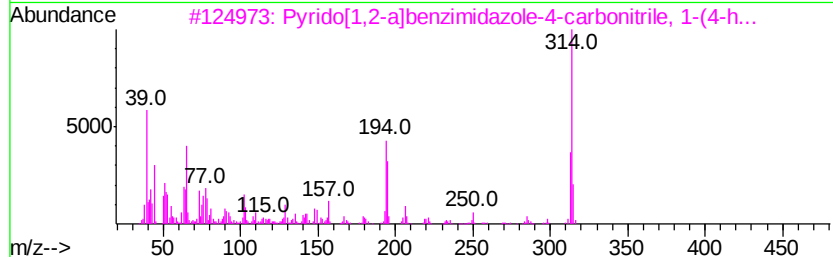
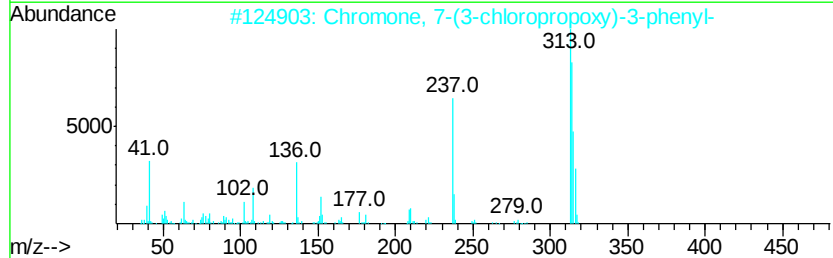
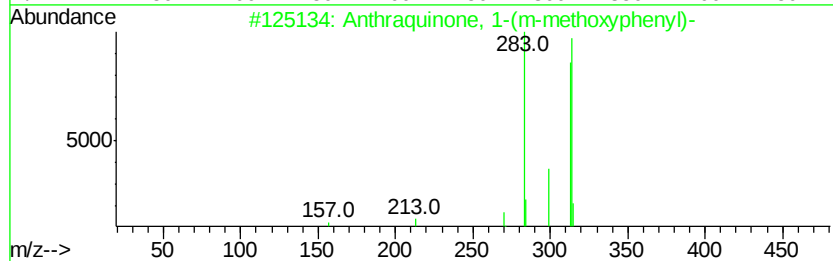
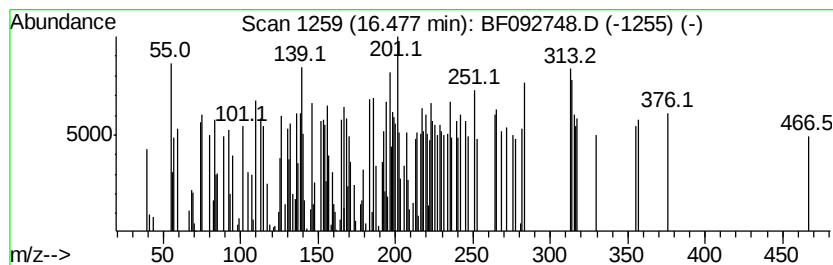
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown16.48 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.48	2.02 ng	91916	Perylene-d12	15.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Anthraquinone, 1-(m-methoxyphenyl)-	314	C21H14O3	020600-77-5	14
2		Chromone, 7-(3-chloropropoxy)-3-...	314	C18H15ClO3	035212-44-3	9
3		Pyrido[1,2-a]benzimidazole-4-car...	314	C19H14N4O	305333-73-7	9
4		9(10H)-Acridinone, 1,2,3,4-tetra...	329	C18H19NO5	000517-73-7	9
5		Phenol, 2-methoxy-4-(1,2,3,4-tet...	315	C18H21NO4	1000277-25-4	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020217\
Data File : BF092748.D
Acq On : 2 Feb 2017 21:15
Operator : SJ/MA
Sample : I1650-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-34-COMP

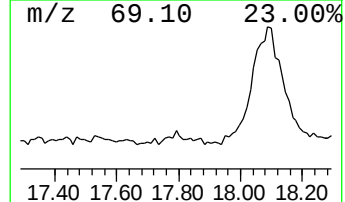
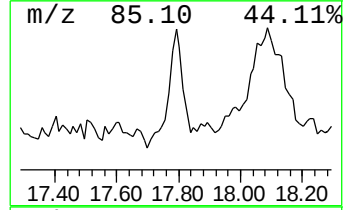
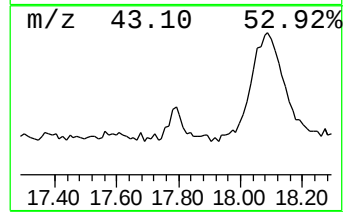
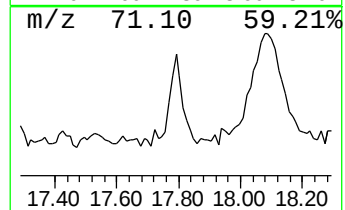
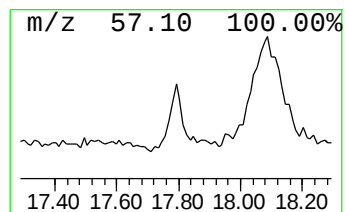
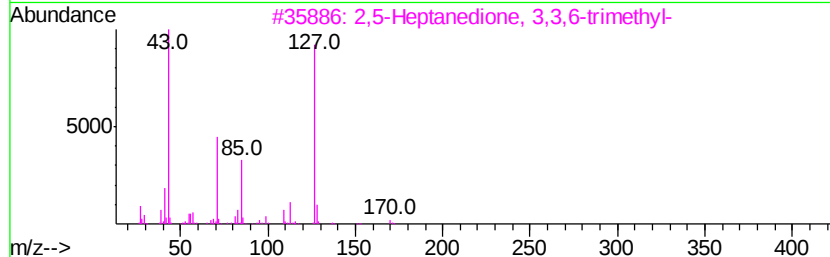
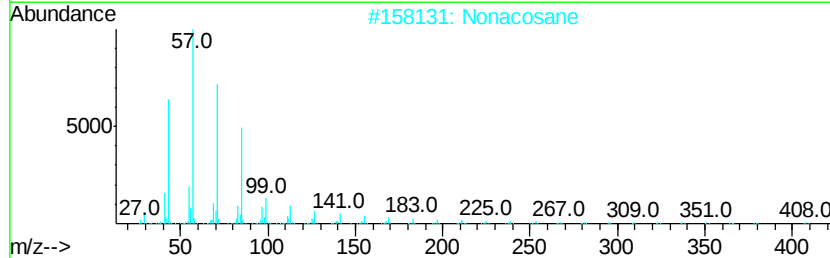
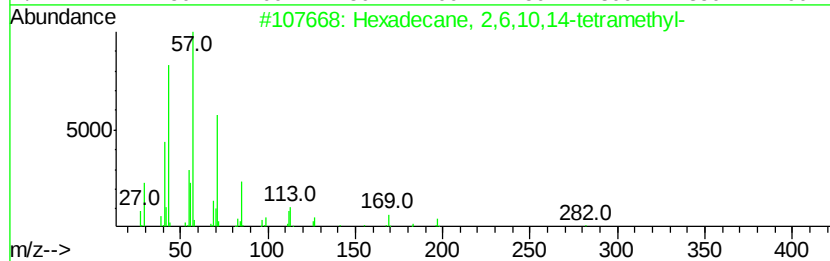
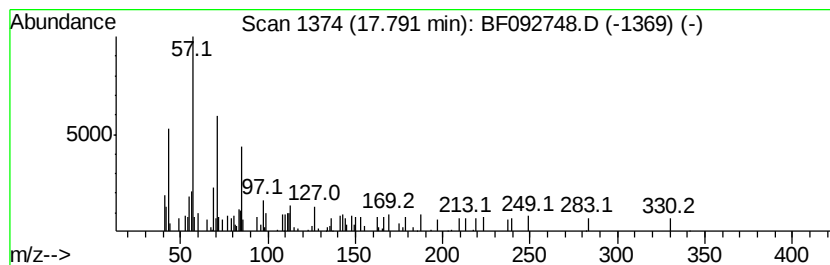
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecane, 2,6,10,14-tetra... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.79	2.41 ng	109596	Perylene-d12	15.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	58
2		Nonacosane	408	C29H60	000630-03-5	50
3		2,5-Heptanedione, 3,3,6-trimethyl-	170	C10H18O2	051513-40-7	50
4		Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	49
5		Eicosane	282	C20H42	000112-95-8	49



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020217\
Data File : BF092748.D
Acq On : 2 Feb 2017 21:15
Operator : SJ/MA
Sample : I1650-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-34-COMP

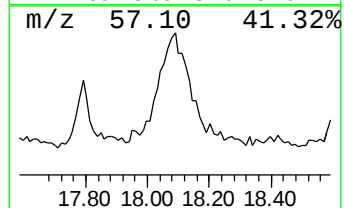
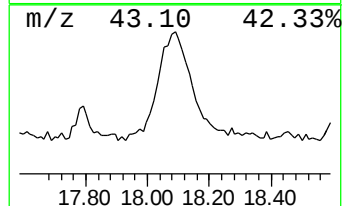
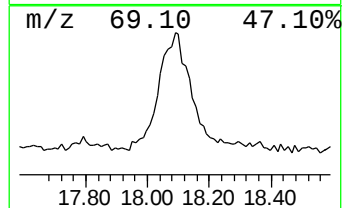
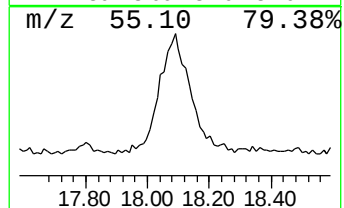
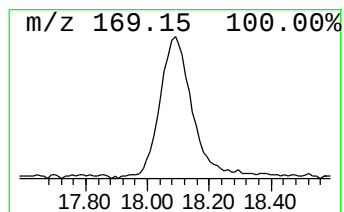
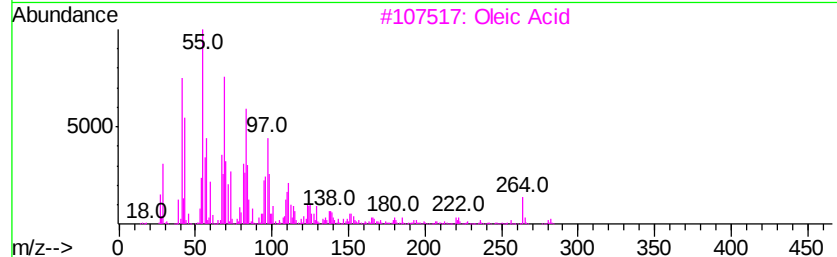
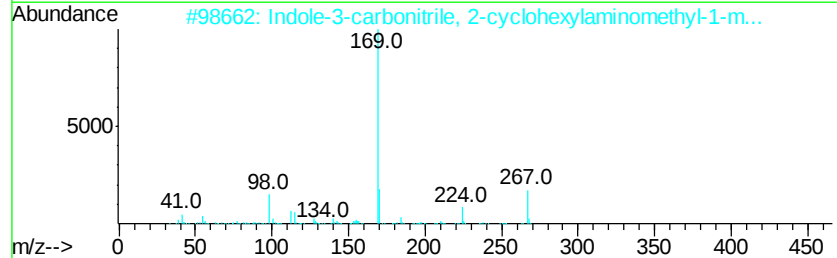
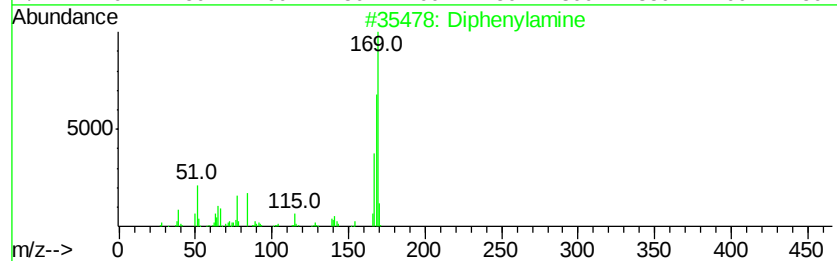
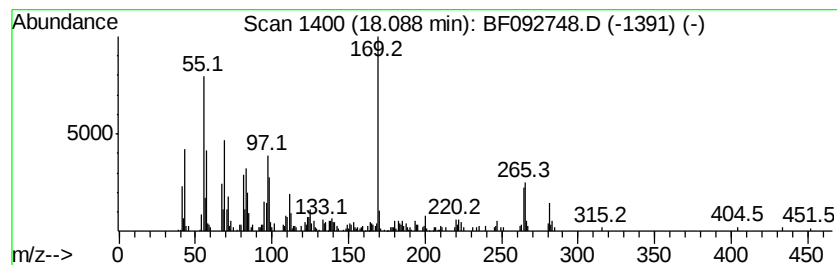
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown18.09 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.09	30.19 ng	1373610	Perylene-d12	15.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Diphenylamine	169	C12H11N	000122-39-4	38
2		Indole-3-carbonitrile, 2-cyclohe...	267	C17H21N3	296246-82-7	38
3		Oleic Acid	282	C18H34O2	000112-80-1	35
4		[1,1'-Biphenyl]-3-amine	169	C12H11N	002243-47-2	30
5		6-Octyloxy-naphthalene-2-carboni...	281	C19H23NO	342414-42-0	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020217\
Data File : BF092748.D
Acq On : 2 Feb 2017 21:15
Operator : SJ/MA
Sample : I1650-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-34-COMP

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
Propane, 2-methyl...	5.12	31.7	ng	1602460	1	6.93	1011990	20.0
unknown6.70	6.70	64.7	ng	3274120	1	6.93	1011990	20.0
Eicosane	10.88	2.4	ng	117535	4	11.46	962444	20.0
Trifluoroacetic a...	13.94	3.7	ng	162204	5	14.10	869134	20.0
unknown16.48	16.48	2.0	ng	91916	6	15.56	909895	20.0
Hexadecane, 2,6,1...	17.79	2.4	ng	109596	6	15.56	909895	20.0
unknown18.09	18.09	30.2	ng	1373610	6	15.56	909895	20.0