LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020816\
Data File : BF084936.D
Acq On : 8 Feb 2016 18:47
Operator : SJ/IZ
Sample : H1311-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B006(0-2)

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-BF020116.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	4.796	234	237	247	rVB	858574	1197626	30.50%	2.846%
2	5.241	274	276	279	rBV	3552823	3685310	93.84%	8.758%
3	6.304	366	369	372	rBV	3486555	3751057	95.52%	8.914%
4	6.419	376	379	381	rBV	4231989	3927098	100.00%	9.332%
5	6.647	397	399	401	rBV	1348282	1104567	28.13%	2.625%
6	6.807	410	413	415	rBV	3067582	3055127	77.80%	7.260%
7	7.219	446	449	452	rBV	2424551	2456374	62.55%	5.837%
8	7.333	455	459	463	rVB	29340	44920	1.14%	0.107%
9	7.939	509	512	514	rBV	1349315	1521714	38.75%	3.616%
10	9.013	603	606	609	rBV	3805904	3296551	83.94%	7.834%
11	9.105	611	614	616	rBV	37953	42415	1.08%	0.101%
12	9.413	639	641	643	rBV	705535	573412	14.60%	1.363%
13	9.630	656	660	662	rBV	133591	138012	3.51%	0.328%
14	9.688	662	665	666	rVV	1453345	1520389	38.72%	3.613%
15	9.710	666	667	670	rVB	75404	75489	1.92%	0.179%
16	9.882	676	682	684	rBV2	59103	120049	3.06%	0.285%
17	10.133	702	704	705	rVB	138060	133671	3.40%	0.318%
18	10.225	711	712	715	rVB	85253	72892	1.86%	0.173%
19	10.350	721	723	724	rBV	53872	74791	1.90%	0.178%
20	10.385	724	726	729	rVB3	27696	53536	1.36%	0.127%
21	10.476	731	734	736	rBV2	1816006	2373656	60.44%	5.641%
22	10.602	743	745	750	rBV	207837	235717	6.00%	0.560%
23	10.773	757	760	761	rBV	29791	48292	1.23%	0.115%
24	10.968	776	777	779	rVB	46219	43513	1.11%	0.103%
25	11.013	779	781	782	rBV2	29020	41579	1.06%	0.099%
26	11.048	782	784	786	rVV2	561623	671667	17.10%	1.596%
27	11.105	787	789	791	rVV	241224	205045	5.22%	0.487%
28	11.162	791	794	795	rVV	1540109	1411391	35.94%	3.354%
29	11.231	798	800	802	rVB	162886	192651	4.91%	0.458%
30	11.402	812	815	819	rBV2	62611	102518	2.61%	0.244%
31	11.471	819	821	826	rVB2	44395	82976	2.11%	0.197%
32	11.665	835	838	839	rBV	89367	97315	2.48%	0.231%
33	11.688	839	840	843	rVV	146234	149262	3.80%	0.355%
34	11.733	843	844	846	rVV	61415	58981	1.50%	0.140%

LSC Area Percent Report

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Sample : H1311-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B006(0-2)

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-BF020116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.768	846	847	852	rVB	148866	235671	6.00%	0.560%
36	11.882	852	857	860	rBV5	26572	86541	2.20%	0.206%
37	11.962	861	864	868	rVB2	65225	129848	3.31%	0.309%
38	12.214	883	886	887	rBV	64563	90589	2.31%	0.215%
39	12.294	892	893	897	rVB2	66842	71929	1.83%	0.171%
40	12.362	897	899	902	rBV	534800	679452	17.30%	1.615%
41	12.511	909	912	916	rBV5	31955	51202	1.30%	0.122%
42	12.591	916	919	922	rVV	691720	735700	18.73%	1.748%
43	12.636	922	923	928	rVB3	44354	86639	2.21%	0.206%
44	12.716	928	930	931	rBV	45667	67994	1.73%	0.162%
45	12.751	931	933	935	rVB	2244584	2335069	59.46%	5.549%
46	12.819	935	939	940	rBV3	40322	52285	1.33%	0.124%
47	12.922	945	948	950	rVB	80863	133867	3.41%	0.318%
48	12.991	952	954	955	rVB	63136	49989	1.27%	0.119%
49	13.025	955	957	958	rBV	79364	73083	1.86%	0.174%
50	13.116	963	965	966	rVV	55879	54433	1.39%	0.129%
51	13.151	966	968	972	rVB2	43210	53815	1.37%	0.128%
52	13.334	978	984	989	rBV5	46201	131755	3.36%	0.313%
53	13.425	989	992	995	rBV3	45235	95542	2.43%	0.227%
54	13.539	999	1002	1003	rBV	61663	77302	1.97%	0.184%
55	13.654	1009	1012	1020	rBV2	283907	414927	10.57%	0.986%
56	13.791	1021	1024	1025	rBV2	1152341	1295260	32.98%	3.078%
57	13.974	1038	1040	1043	rBV3	34647	62454	1.59%	0.148%
58	14.179	1056	1058	1059	rVB	52669	57386	1.46%	0.136%
59	14.637	1096	1098	1103	rBV2	64359	87005	2.22%	0.207%
60	14.785	1108	1111	1115	rVV	257450	427611	10.89%	1.016%
61	14.877	1117	1119	1121	rVB	61378	61556	1.57%	0.146%
62	15.048	1132	1134	1137	rVB	132416	155626	3.96%	0.370%
63	15.105	1137	1139	1141	rVB	159862	219573	5.59%	0.522%
64	15.162	1141	1144	1146	rBV	576071	910371	23.18%	2.163%
65	15.574	1178	1180	1182	rBV	33463	56814	1.45%	0.135%
66	16.420	1251	1254	1258	rVB	89975	161650	4.12%	0.384%
67	16.797	1284	1287	1293	rVB	73047	157193	4.00%	0.374%
68	18.648	1444	1449	1453	rBV5	58404	161188	4.10%	0.383%

Sum of corrected areas: 42080882

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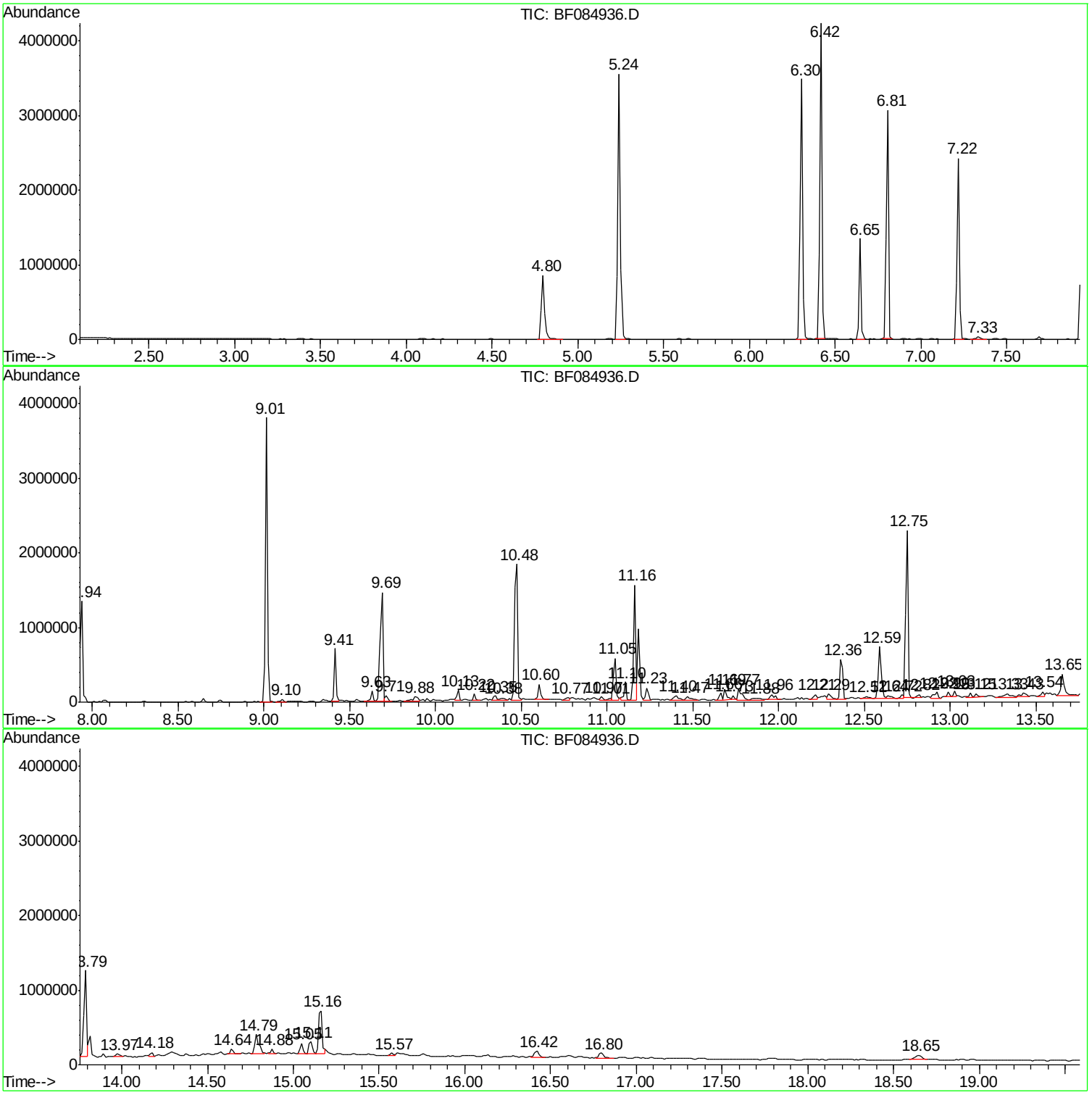
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-B006(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.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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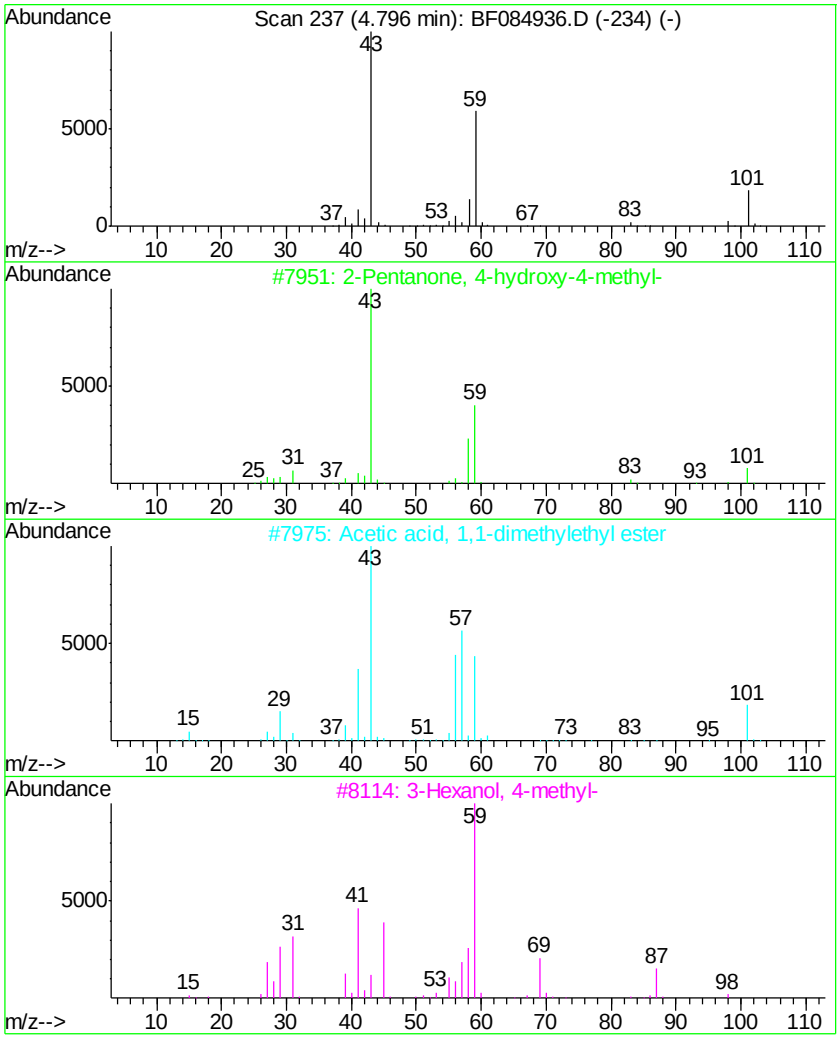
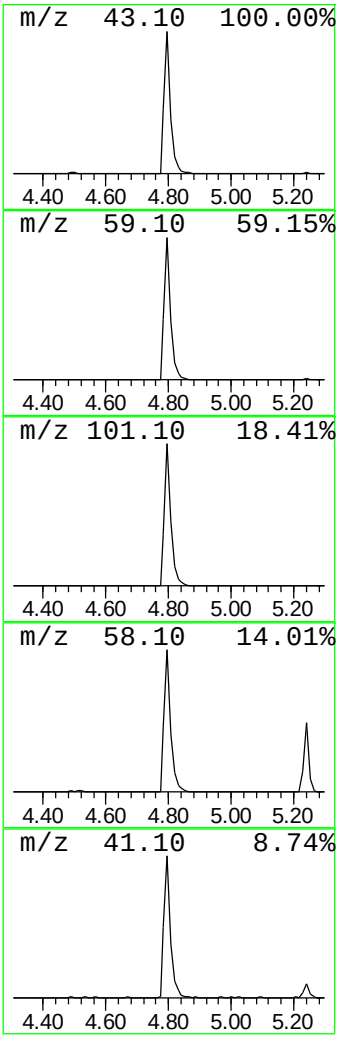
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	21.69 ng	1197630	1,4-Dichlorobenzene-d4	6.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Sample : H1311-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B006(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
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TIC Library : C:\DATABASE\NIST02.L
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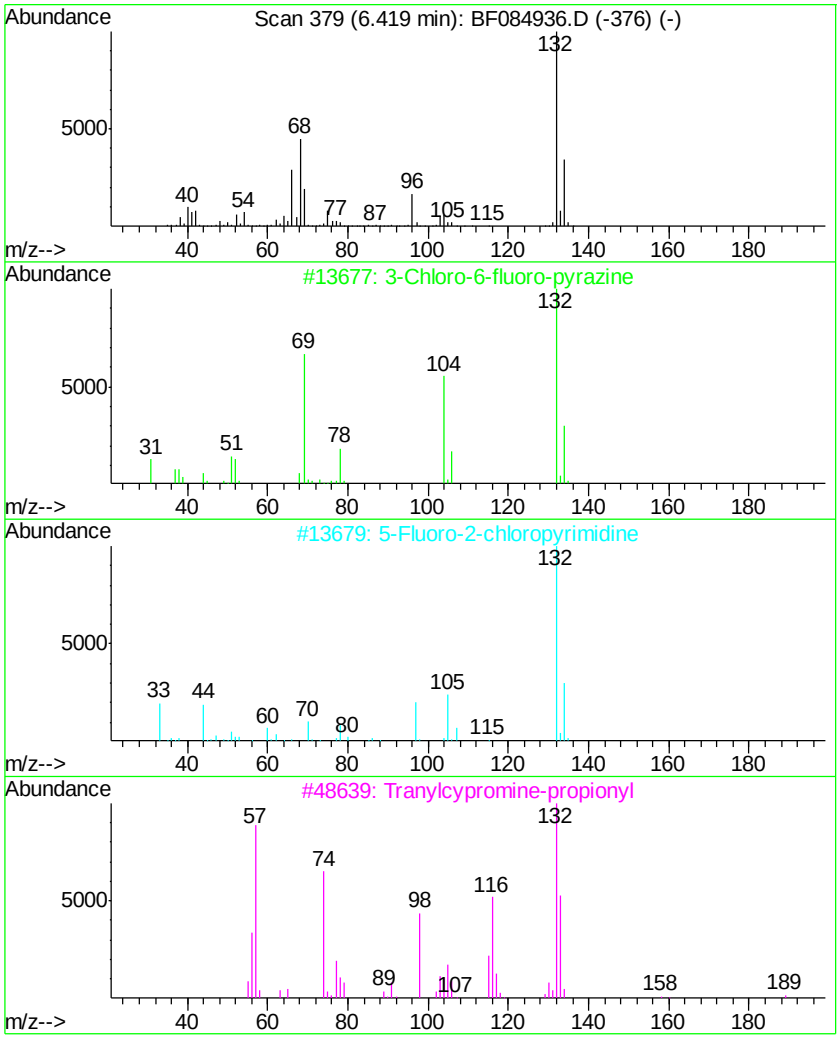
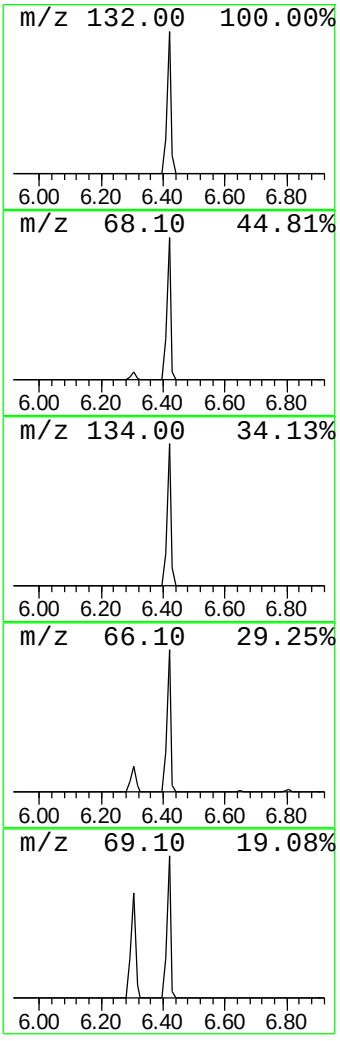
****

Peak Number 2 unknown6.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.42	71.11 ng	3927100	1,4-Dichlorobenzene-d4	6.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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Instrument : BNA_F
ClientSampleId : SUP-B006(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
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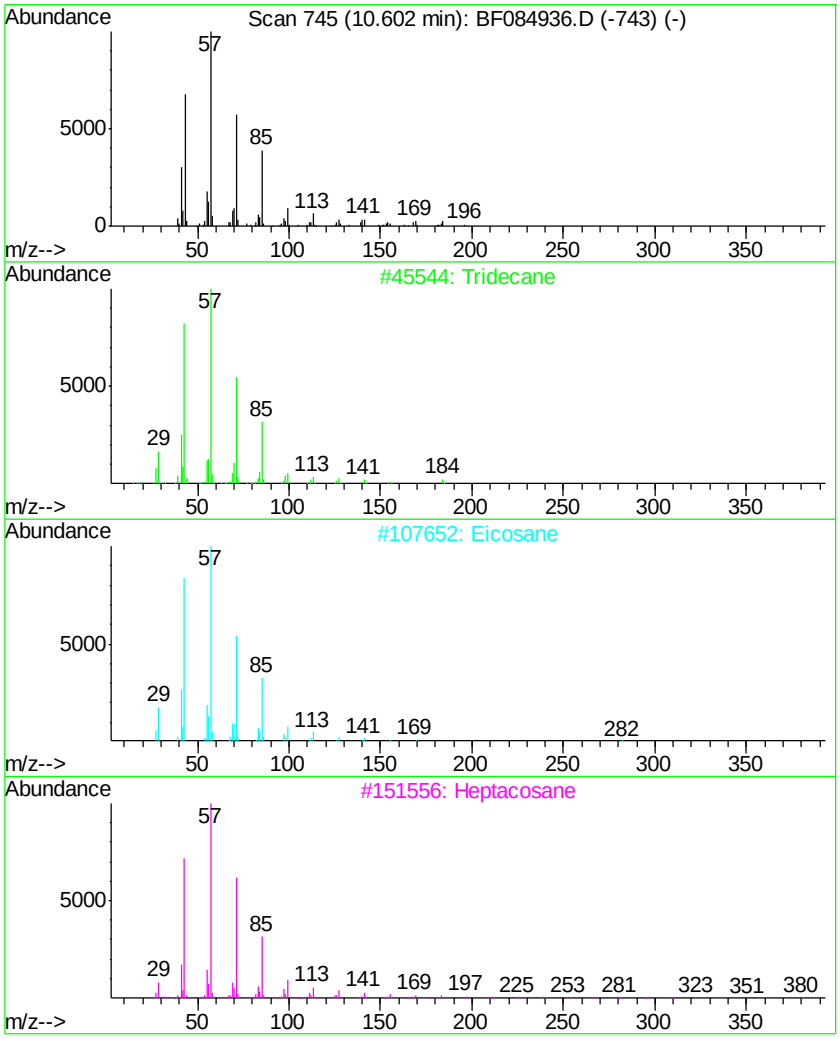
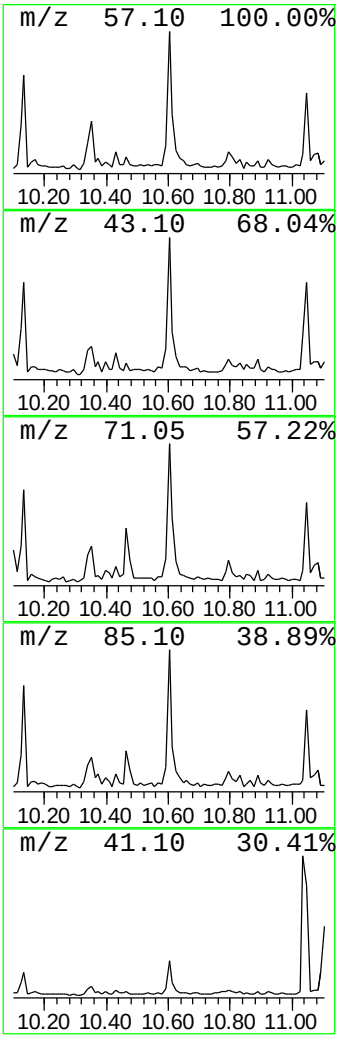
****

Peak Number 4 Tridecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.60	3.34 ng	235717	Phenanthrene-d10	11.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	94
2	Eicosane	282	C20H42	000112-95-8	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Hexadecane	226	C16H34	000544-76-3	90
5	Pentadecane	212	C15H32	000629-62-9	90





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Instrument : BNA_F
ClientSampleId : SUP-B006(0-2)

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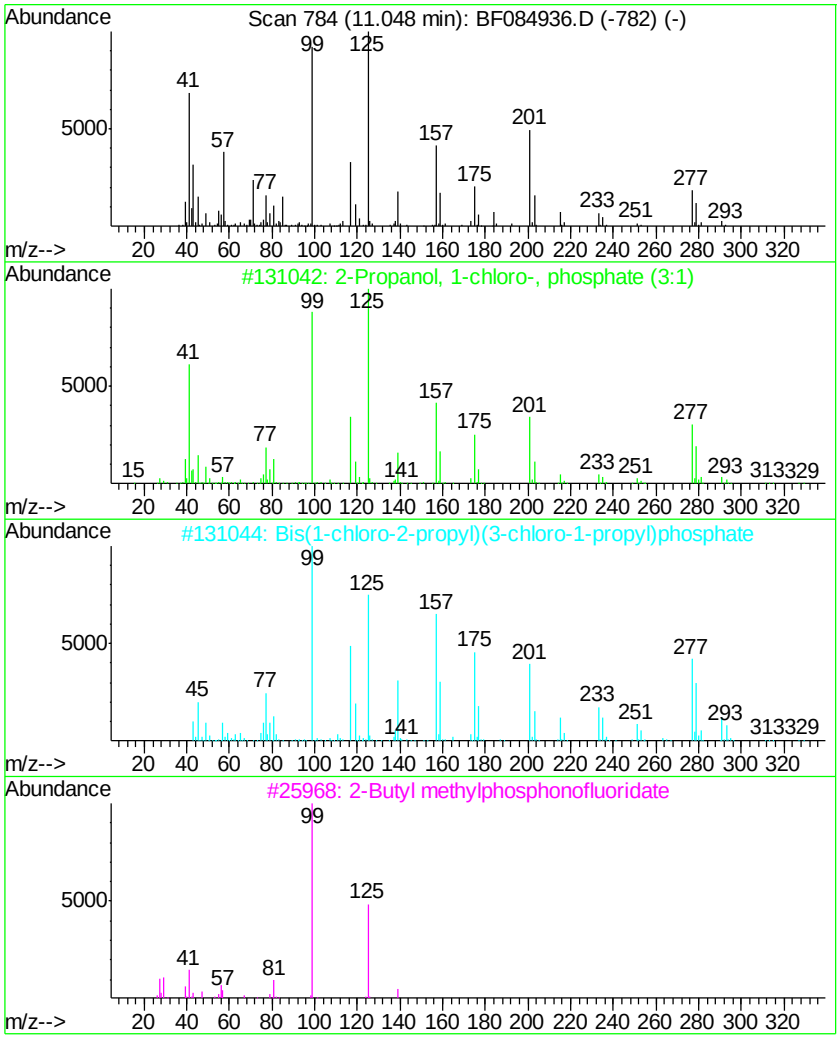
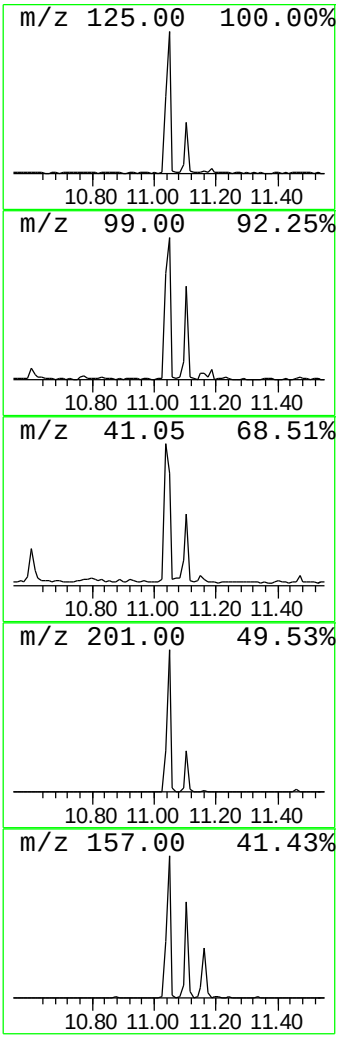
Peak Number 5 2-Propanol, 1-chloro-, phos... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.05	9.52 ng	671667	Phenanthrene-d10	11.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-chloro-, phosphate...	326	C9H18Cl3O4P	013674-84-5	64
2	Bis(1-chloro-2-propyl)(3-chloro-...	326	C9H18Cl3O4P	137909-40-1	49
3	2-Butyl methylphosphonofluoridate	154	C5H12FO2P	000352-52-3	32
4	Bis(3-chloro-1-propyl)(1-chloro-...	326	C9H18Cl3O4P	137888-35-8	28
5	4H-Imidazol-4-one, 2-amino-1,5-d...	99	C3H5N3O	000503-86-6	10





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Instrument : BNA_F
ClientSampleId : SUP-B006(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.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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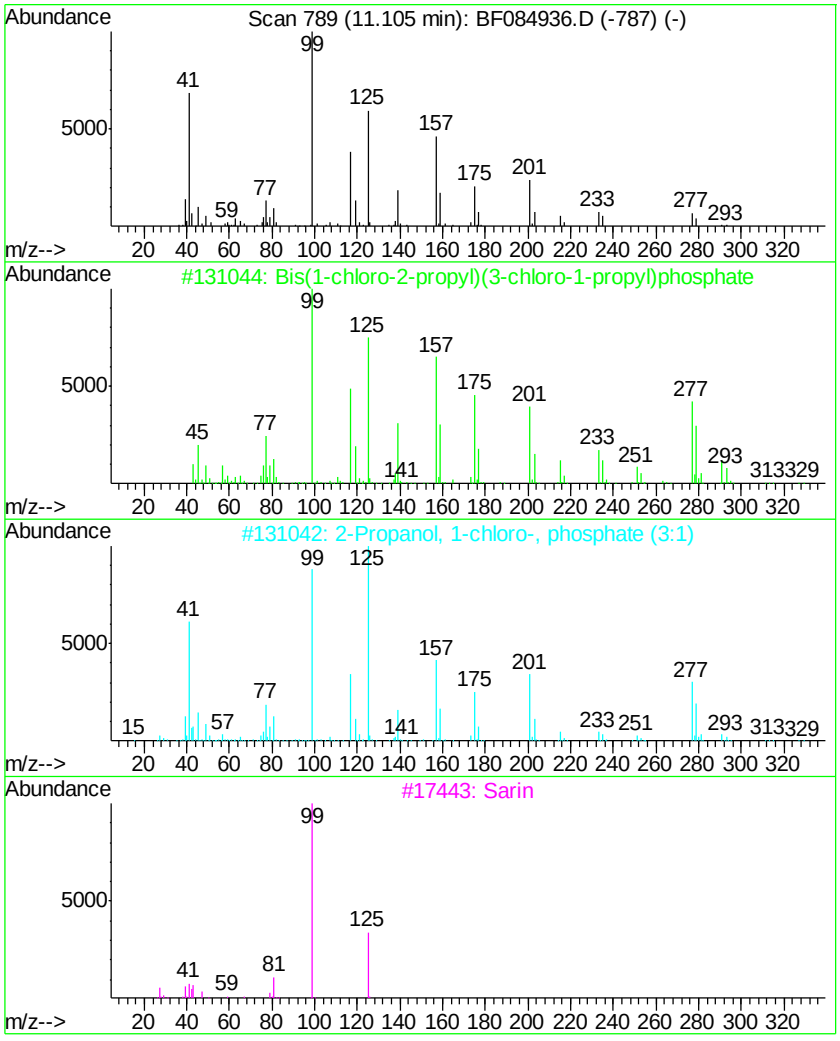
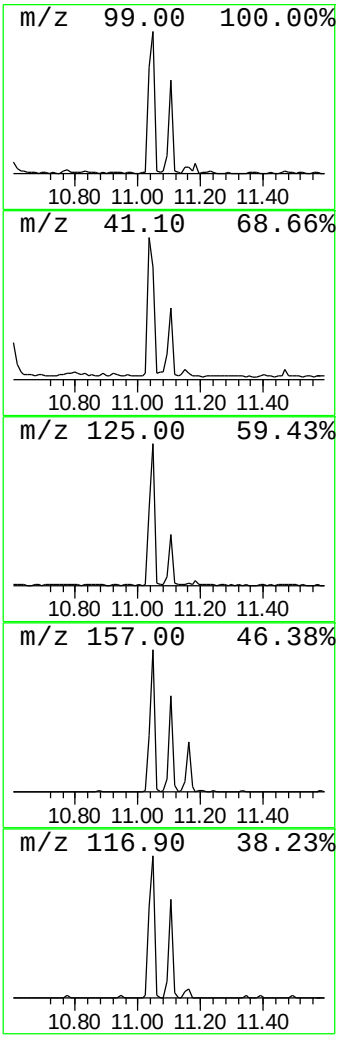
Peak Number 6 Bis(1-chloro-2-propyl)(3-ch... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.10	2.91 ng	205045	Phenanthrene-d10	11.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bis(1-chloro-2-propyl)(3-chloro-...	326	C9H18Cl3O4P	137909-40-1	80
2	2-Propanol, 1-chloro-, phosphate...	326	C9H18Cl3O4P	013674-84-5	59
3	Sarin	140	C4H10FO2P	000107-44-8	35
4	2-Butyl methylphosphonofluoridate	154	C5H12FO2P	000352-52-3	25
5	2-Heptyl methylphosphonofluoridate	196	C8H18FO2P	000674-95-3	17





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Instrument : BNA_F
ClientSampleId : SUP-B006(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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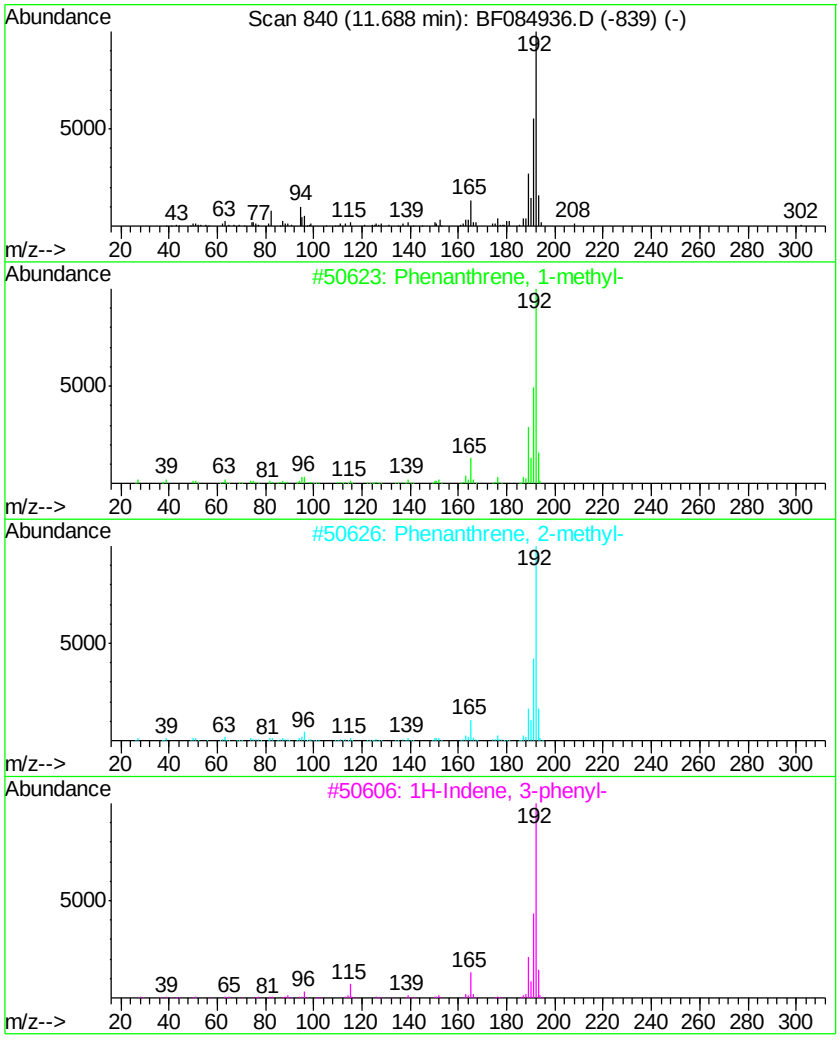
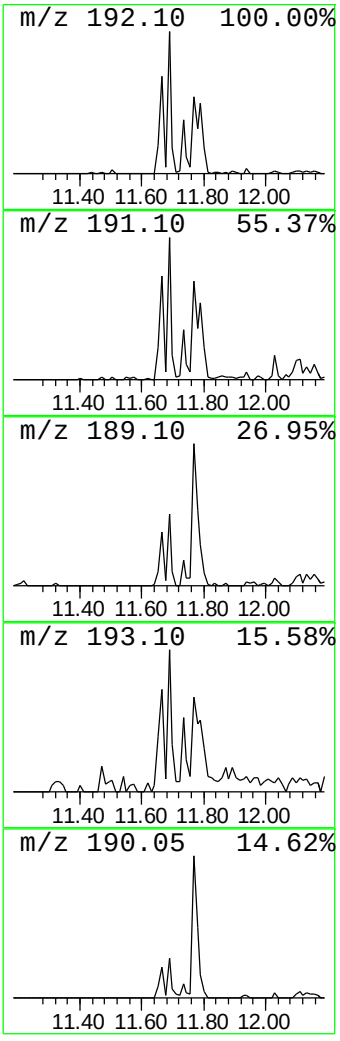
Peak Number 7 Phenanthrene, 1-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.69	2.12 ng	149262	Phenanthrene-d10	11.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	97
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	97
3	1H-Indene, 3-phenyl-	192	C15H12	001961-97-3	95
4	1H-Indene, 1-phenyl-	192	C15H12	001961-96-2	95
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	95





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020816\
Data File : BF084936.D
Acq On : 8 Feb 2016 18:47
Operator : SJ/IZ
Sample : H1311-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B006(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

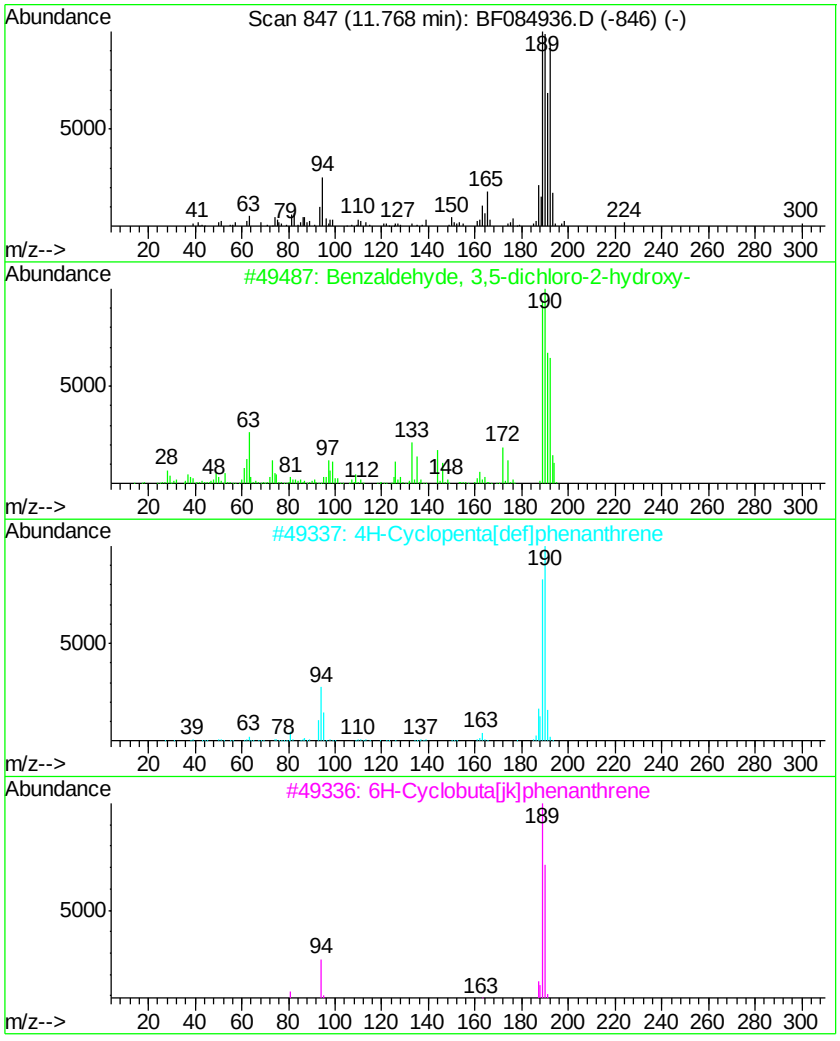
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

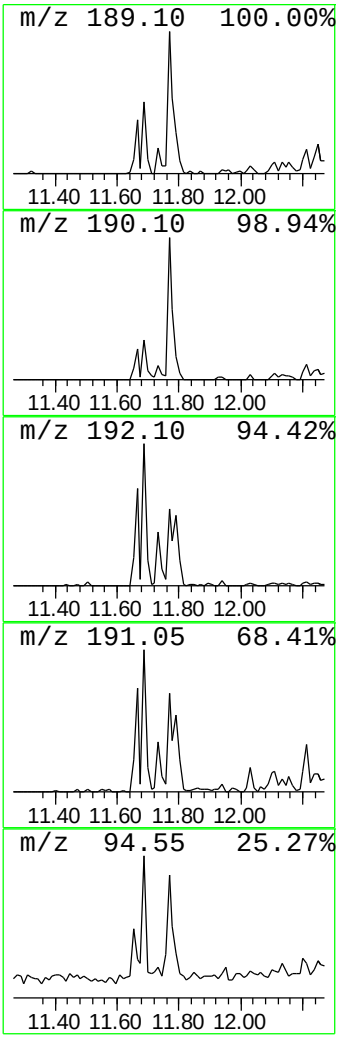
****

Peak Number 8 Benzaldehyde, 3,5-dichloro-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	3.34 ng	235671	Phenanthrene-d10	11.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	72
2	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	60
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	49
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	46
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	46





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Data File : BF084936.D
Acq On : 8 Feb 2016 18:47
Operator : SJ/IZ
Sample : H1311-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B006(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.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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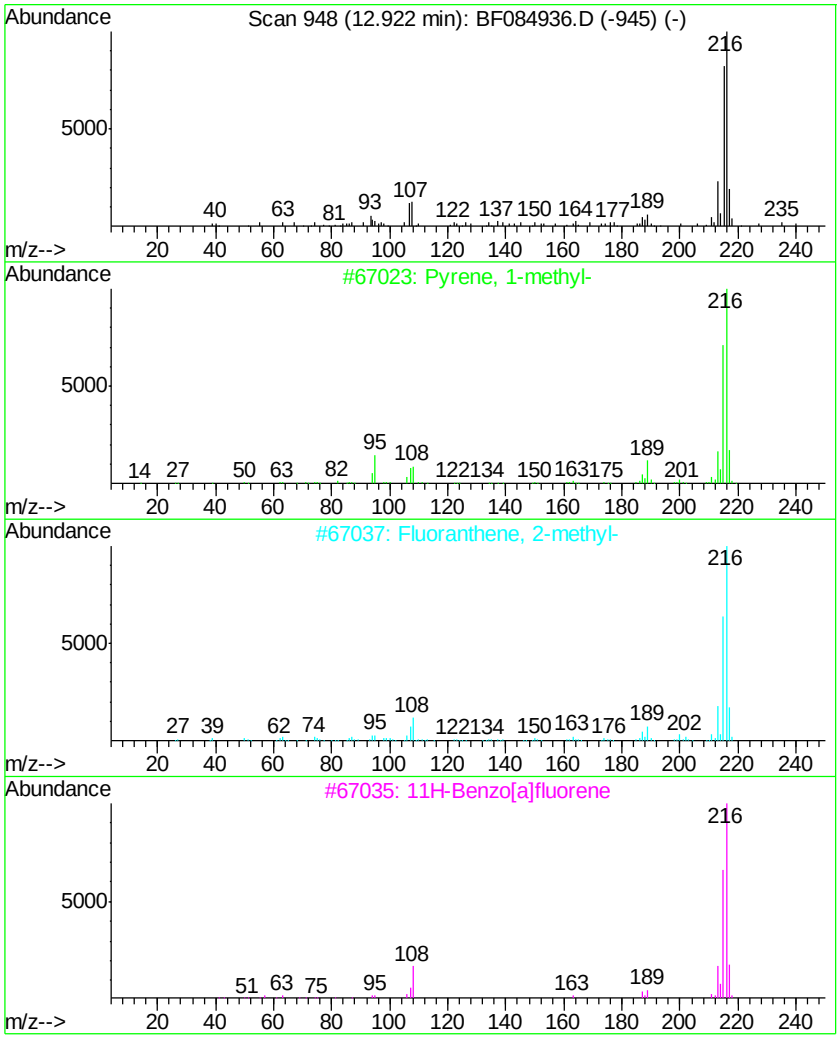
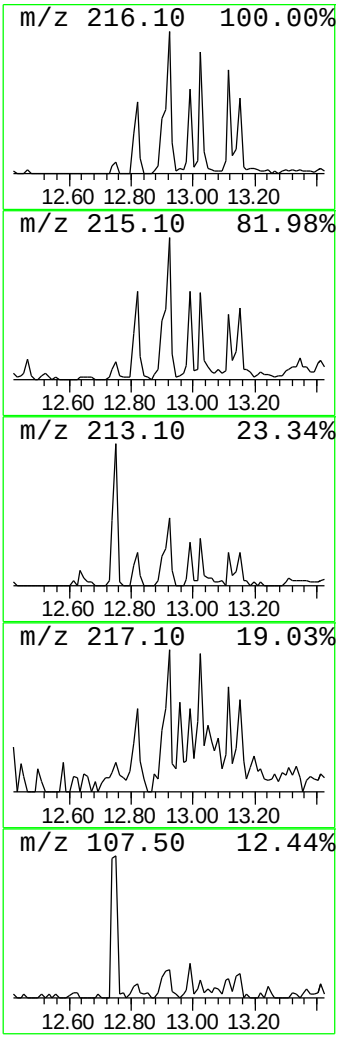
Peak Number 9 Pyrene, 1-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.92	2.07 ng	133867	Chrysene-d12	13.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	93
2	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	91
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	91
4	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	91
5	Pyrene, 2-methyl-	216	C17H12	003442-78-2	83





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Instrument : BNA_F
ClientSampleId : SUP-B006(0-2)

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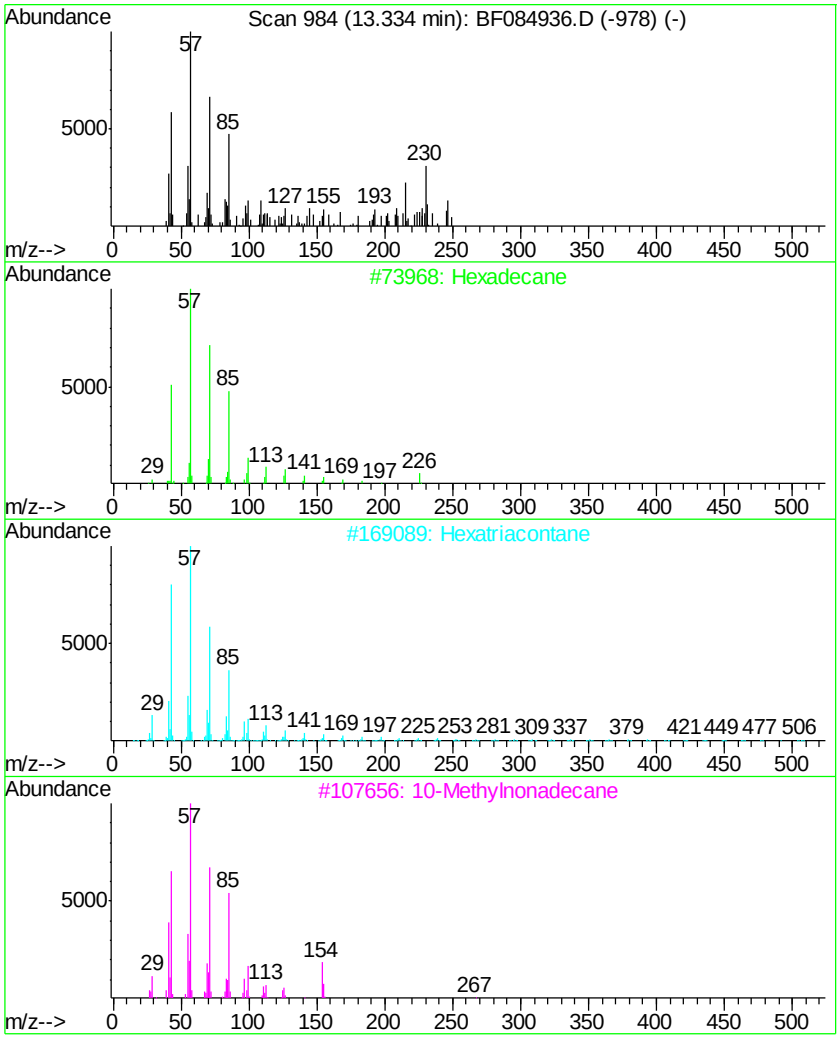
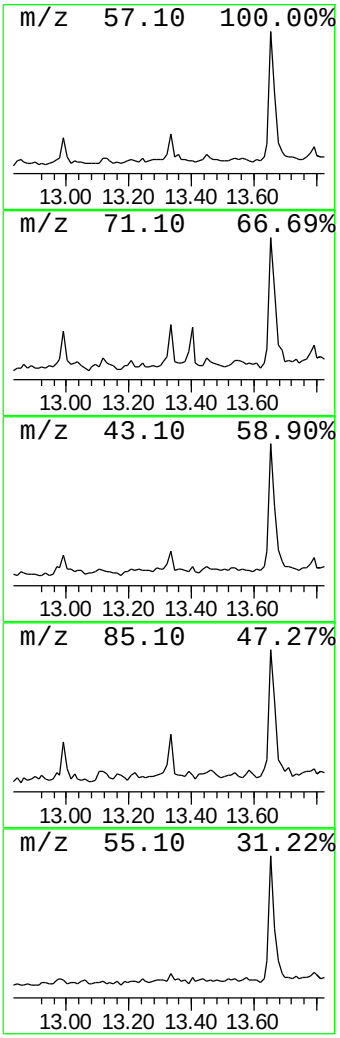
Peak Number 10 Hexadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.33	2.03 ng	131755	Chrysene-d12	13.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	62
2	Hexatriacontane	507	C36H74	000630-06-8	41
3	10-Methylnonadecane	282	C20H42	056862-62-5	38
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	38
5	Octacosane	394	C28H58	000630-02-4	38





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Operator : SJ/IZ
Sample : H1311-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B006(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
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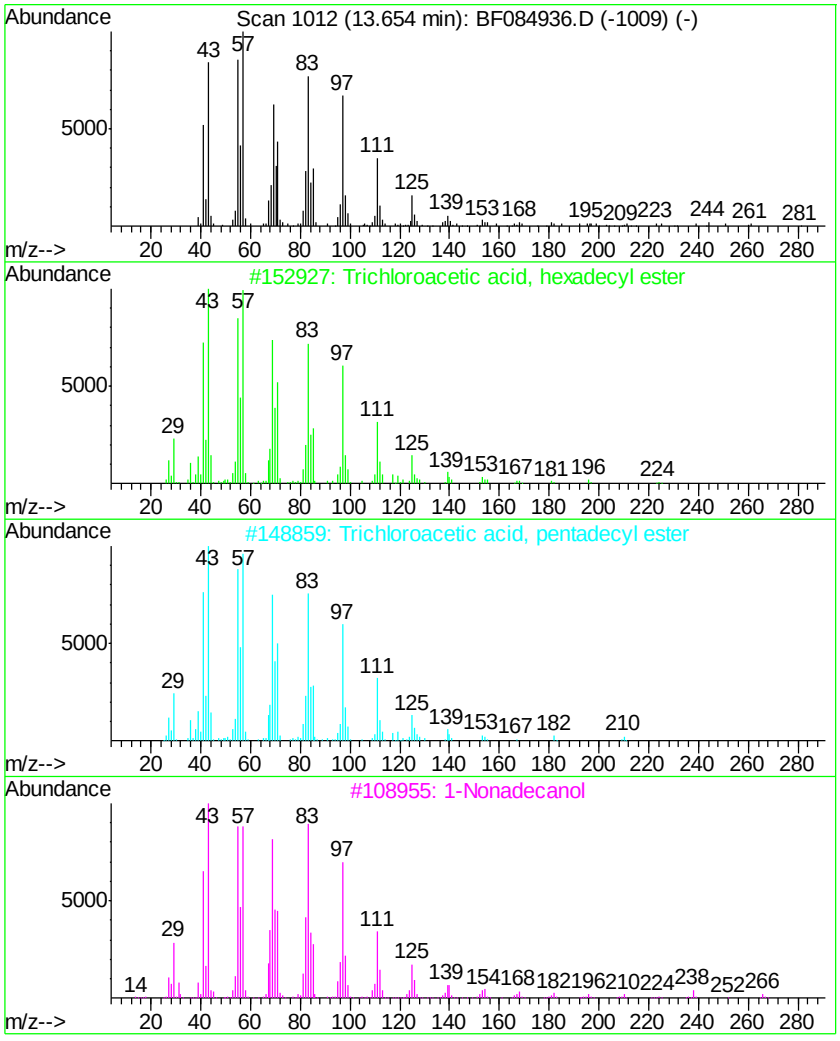
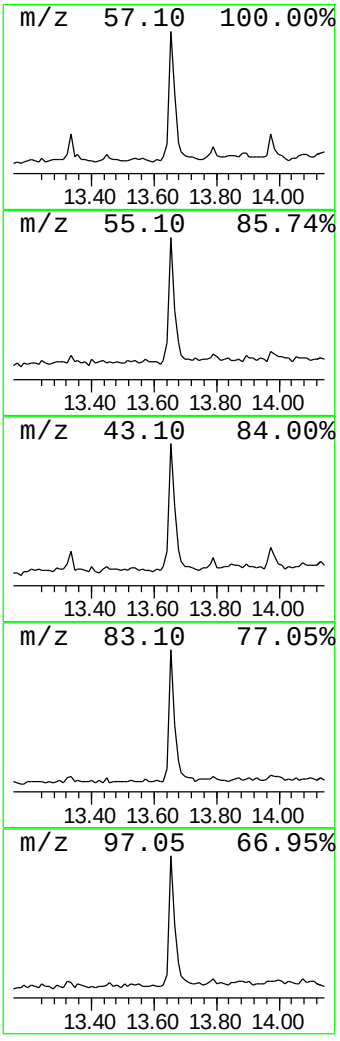
Peak Number 11 Trichloroacetic acid, hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.65	6.41 ng	414927	Chrysene-d12	13.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
3	1-Nonadecanol	284	C19H40O	001454-84-8	87
4	Cyclohexadecane	224	C16H32	000295-65-8	87
5	11-Tricosene	322	C23H46	052078-56-5	87





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ALS Vial : 11 Sample Multiplier: 1

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ClientSampleId : SUP-B006(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
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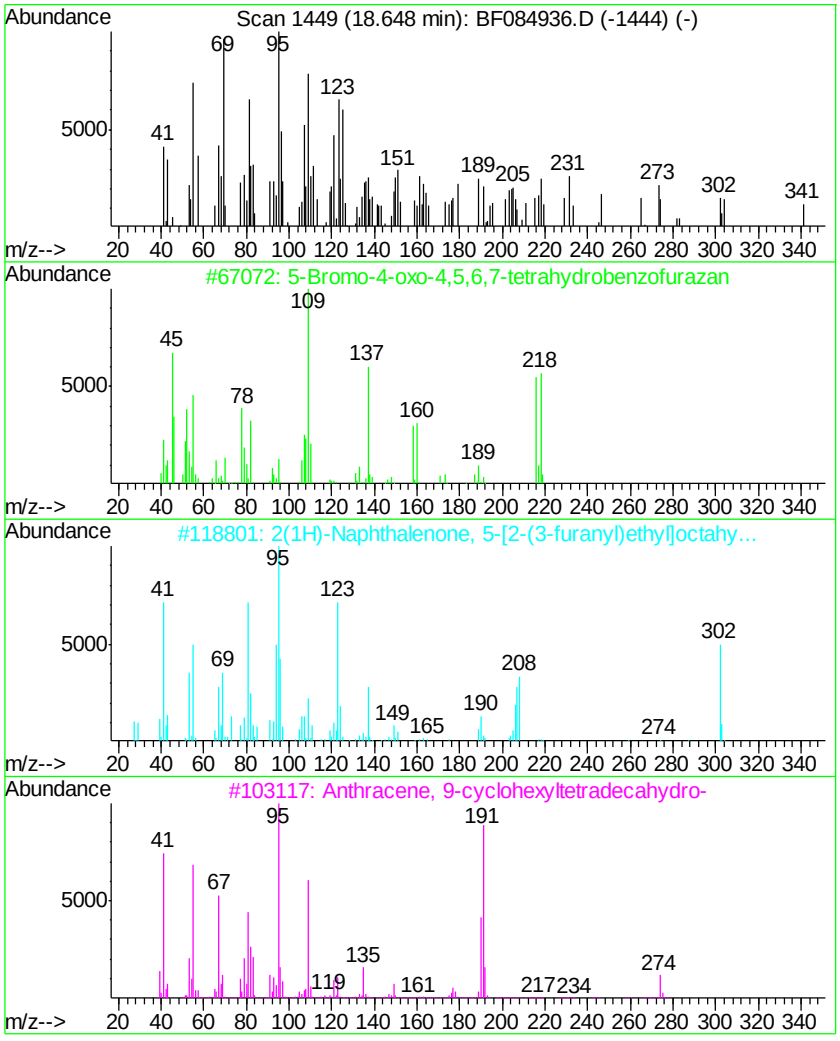
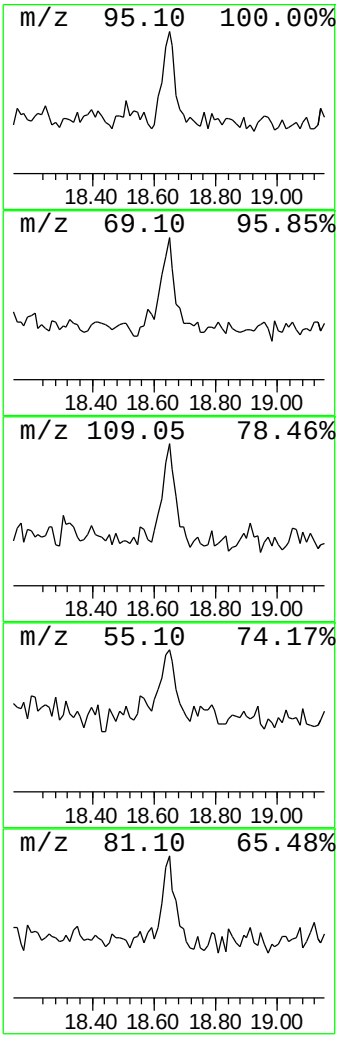
Peak Number 13 5-Bromo-4-oxo-4,5,6,7-tetra... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.65	3.54 ng	161188	Perylene-d12	15.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	60
2	2(1H)-Naphthalenone, 5-[2-(3-fur...	302	C20H30O2	059742-40-4	38
3	Anthracene, 9-cyclohexyltetradec...	274	C20H34	055255-70-4	38
4	Cyclopentanecarboxaldehyde, 2-me...	124	C8H12O	1000154-24-0	35
5	Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-41-8	30





Tentatively Identified Compound (LSC) summary

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Data File : BF084936.D
Acq On : 8 Feb 2016 18:47
Operator : SJ/IZ
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Misc :
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Instrument : BNA_F
ClientSampleId : SUP-B006(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.80	21.7	ng	1197630	1	6.65	1104570	20.0
unknown6.42	6.42	71.1	ng	3927100	1	6.65	1104570	20.0
Tridecane	10.60	3.3	ng	235717	4	11.16	1411390	20.0
2-Propanol, 1-chl...	11.05	9.5	ng	671667	4	11.16	1411390	20.0
Bis(1-chloro-2-pr...	11.10	2.9	ng	205045	4	11.16	1411390	20.0
Phenanthrene, 1-m...	11.69	2.1	ng	149262	4	11.16	1411390	20.0
Benzaldehyde, 3,5...	11.77	3.3	ng	235671	4	11.16	1411390	20.0
Pyrene, 1-methyl-	12.92	2.1	ng	133867	5	13.79	1295260	20.0
Hexadecane	13.33	2.0	ng	131755	5	13.79	1295260	20.0
Trichloroacetic a...	13.65	6.4	ng	414927	5	13.79	1295260	20.0
5-Bromo-4-oxo-4,5...	18.65	3.5	ng	161188	6	15.16	910371	20.0