LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111717\
Data File : BF100667.D
Acq On : 17 Nov 2017 10:47
Operator : SJ/JU
Sample : I6289-05 5X
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-01-111417

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-BF110817.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	5.093	508	511	516	rBV	36181	34825	4.12%	0.367%
2	5.487	574	578	582	rBV	602120	510547	60.43%	5.378%
3	6.492	745	749	755	rBV	578020	539953	63.91%	5.688%
4	6.645	771	775	778	rBV	672108	545970	64.62%	5.752%
5	6.881	811	815	819	rVB	739232	586996	69.47%	6.184%
6	7.034	837	841	845	rBV	500954	409123	48.42%	4.310%
7	7.439	905	910	913	rBV	372468	319270	37.79%	3.363%
8	8.163	1026	1033	1036	rBV	994330	793541	93.92%	8.360%
9	9.233	1211	1215	1218	rBV	829869	640741	75.83%	6.750%
10	9.628	1279	1282	1286	rBV	19341	17055	2.02%	0.180%
11	9.916	1327	1331	1335	rBV2	957964	844923	100.00%	8.901%
12	9.945	1335	1336	1342	rVB	11670	9715	1.15%	0.102%
13	10.116	1359	1365	1369	rVB3	6453	10837	1.28%	0.114%
14	10.463	1421	1424	1426	rBV	13046	10917	1.29%	0.115%
15	10.622	1448	1451	1457	rVB	29357	26268	3.11%	0.277%
16	10.698	1461	1464	1472	rBV	377924	344642	40.79%	3.631%
17	11.404	1580	1584	1586	rBV	930394	822871	97.39%	8.669%
18	11.422	1586	1587	1591	rVV	70334	53413	6.32%	0.563%
19	11.474	1594	1596	1599	rVB	17744	12076	1.43%	0.127%
20	11.916	1666	1671	1672	rBV2	17951	22120	2.62%	0.233%
21	12.016	1685	1688	1690	rBV2	13488	14403	1.70%	0.152%
22	12.445	1758	1761	1764	rBV3	10007	11685	1.38%	0.123%
23	12.480	1764	1767	1773	rVV4	13045	18562	2.20%	0.196%
24	12.610	1787	1789	1792	rBV	80946	66265	7.84%	0.698%
25	12.698	1802	1804	1810	rBV5	6957	10274	1.22%	0.108%
26	12.839	1823	1828	1834	rBV	68285	83913	9.93%	0.884%
27	12.980	1848	1852	1856	rBV	608760	493366	58.39%	5.197%
28	13.057	1860	1865	1867	rBV5	8234	11211	1.33%	0.118%
29	13.168	1881	1884	1888	rVB3	18033	16948	2.01%	0.179%
30	13.210	1888	1891	1893	rBV3	8827	10261	1.21%	0.108%
31	13.551	1946	1949	1950	rBV2	9956	9532	1.13%	0.100%
32	13.792	1988	1990	1992	rVB3	12353	9594	1.14%	0.101%
33	13.874	2001	2004	2009	rVB4	26170	31789	3.76%	0.335%
34	14.039	2027	2032	2035	rBV	647240	628395	74.37%	6.620%

LSC Area Percent Report

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.063	2035	2036	2038	rVB	29818	15035	1.78%	0.158%
36	15.080	2205	2209	2212	rBV	33760	55857	6.61%	0.588%
37	15.145	2217	2220	2224	rVB3	24661	30600	3.62%	0.322%
38	15.445	2269	2271	2275	rBV	22966	28366	3.36%	0.299%
39	15.515	2277	2283	2292	rBV	483556	652323	77.21%	6.872%
40	15.739	2318	2321	2325	rBV6	26781	37193	4.40%	0.392%
41	15.962	2357	2359	2363	rVB4	22594	24978	2.96%	0.263%
42	16.221	2400	2403	2412	rVB5	45306	87834	10.40%	0.925%
43	16.798	2497	2501	2507	rVB8	31528	54529	6.45%	0.574%
44	17.315	2587	2589	2591	rBV3	11500	12874	1.52%	0.136%
45	17.774	2657	2667	2677	rVB10	59459	185149	21.91%	1.950%
46	18.133	2724	2728	2733	rVB9	13351	24054	2.85%	0.253%
47	18.250	2742	2748	2755	rVB7	34284	84641	10.02%	0.892%
48	18.739	2821	2831	2840	rBV4	67500	190619	22.56%	2.008%
49	19.180	2904	2906	2916	rVB4	14766	36576	4.33%	0.385%

Sum of corrected areas: 9492629

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Misc :
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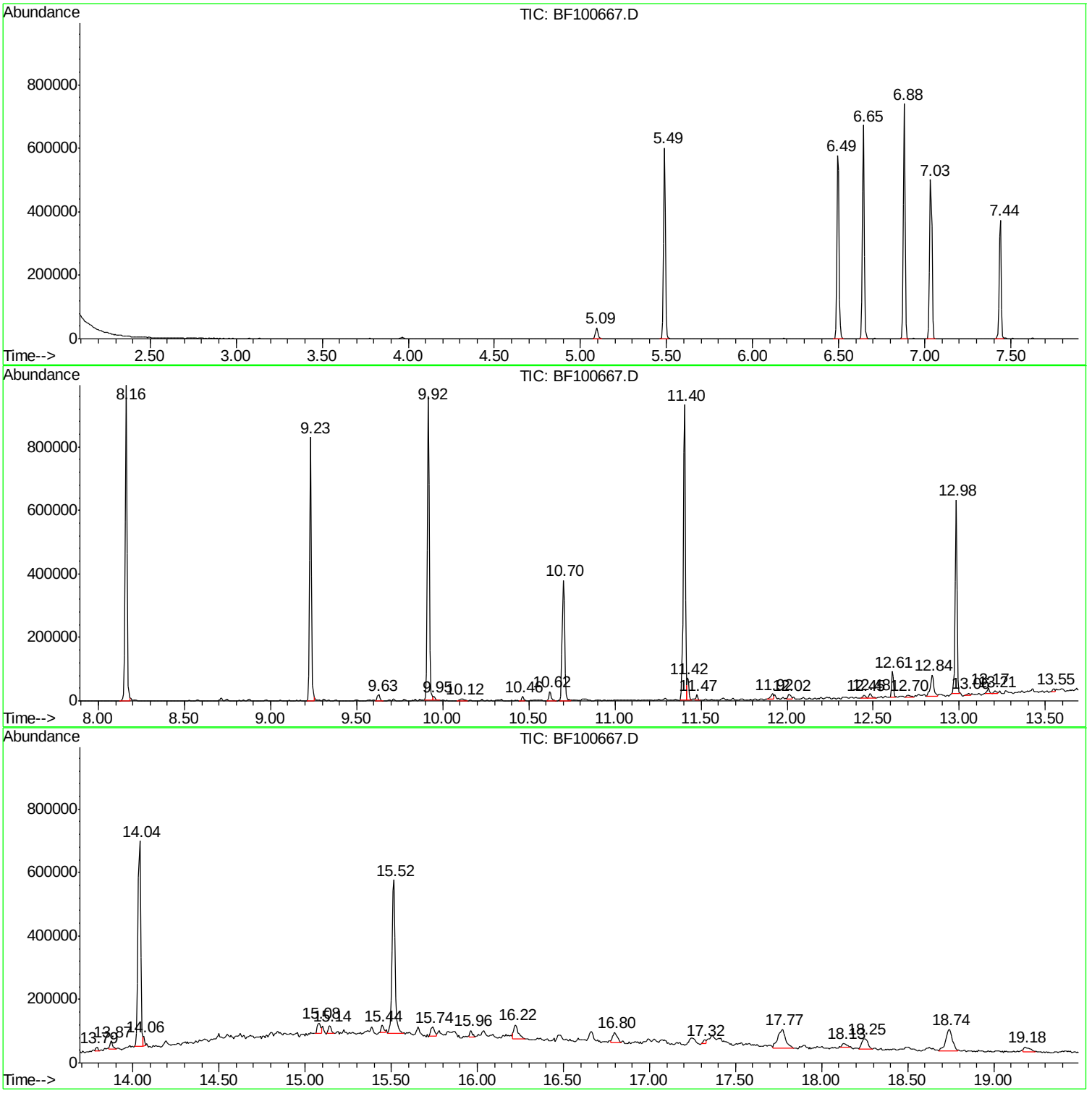
Instrument :
BNA_F
ClientSampleId :
SU-01-111417

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111717\
Data File : BF100667.D
Acq On : 17 Nov 2017 10:47
Operator : SJ/JU
Sample : I6289-05 5X
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-01-111417

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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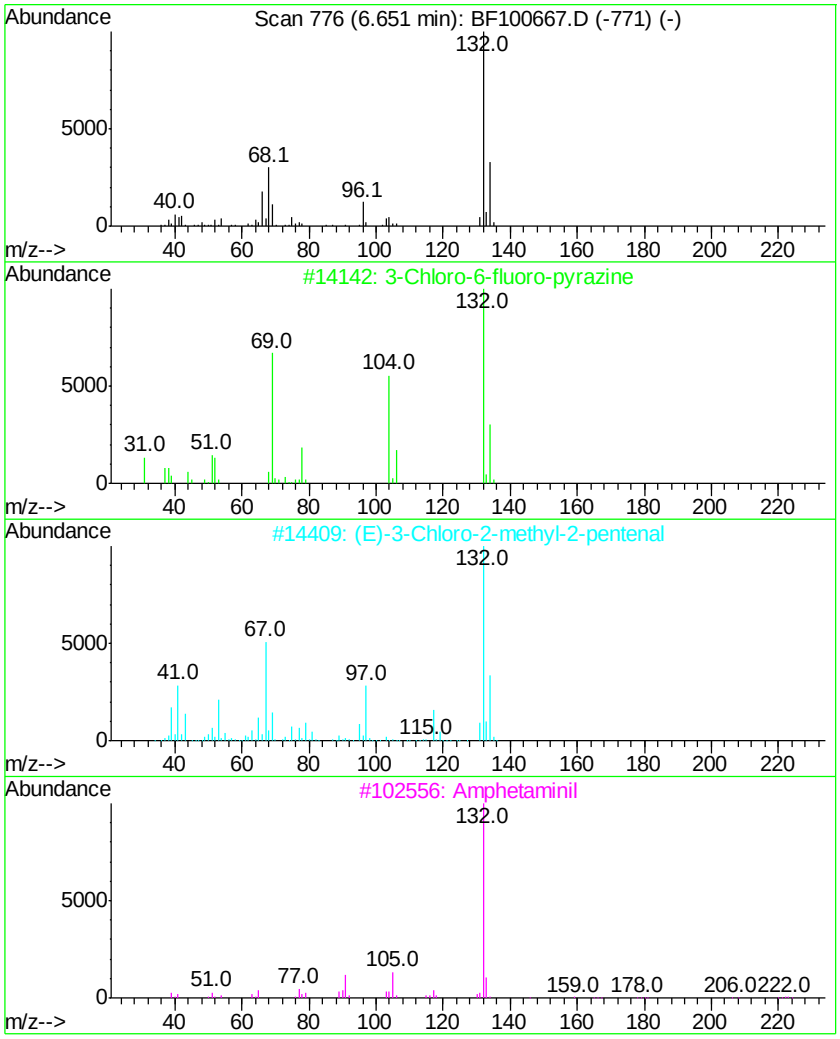
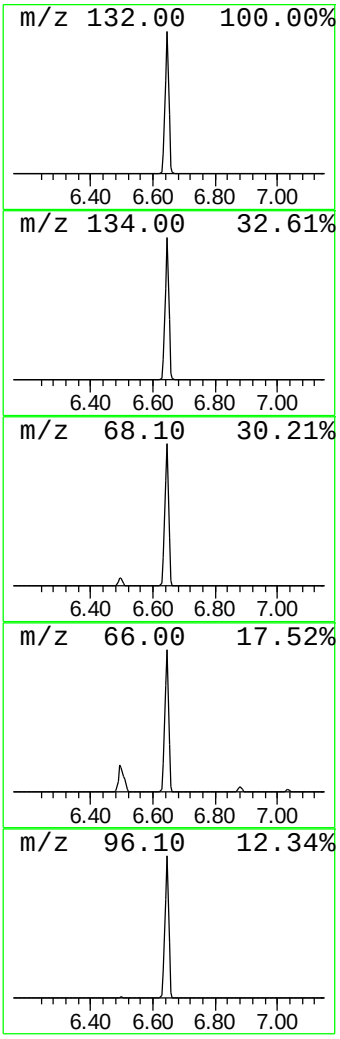
Peak Number 1 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	18.60 ng	545970	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Amphetaminil	250	C17H18N2	017590-01-1	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	5-Aminoindole	132	C8H8N2	005192-03-0	12





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ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-01-111417

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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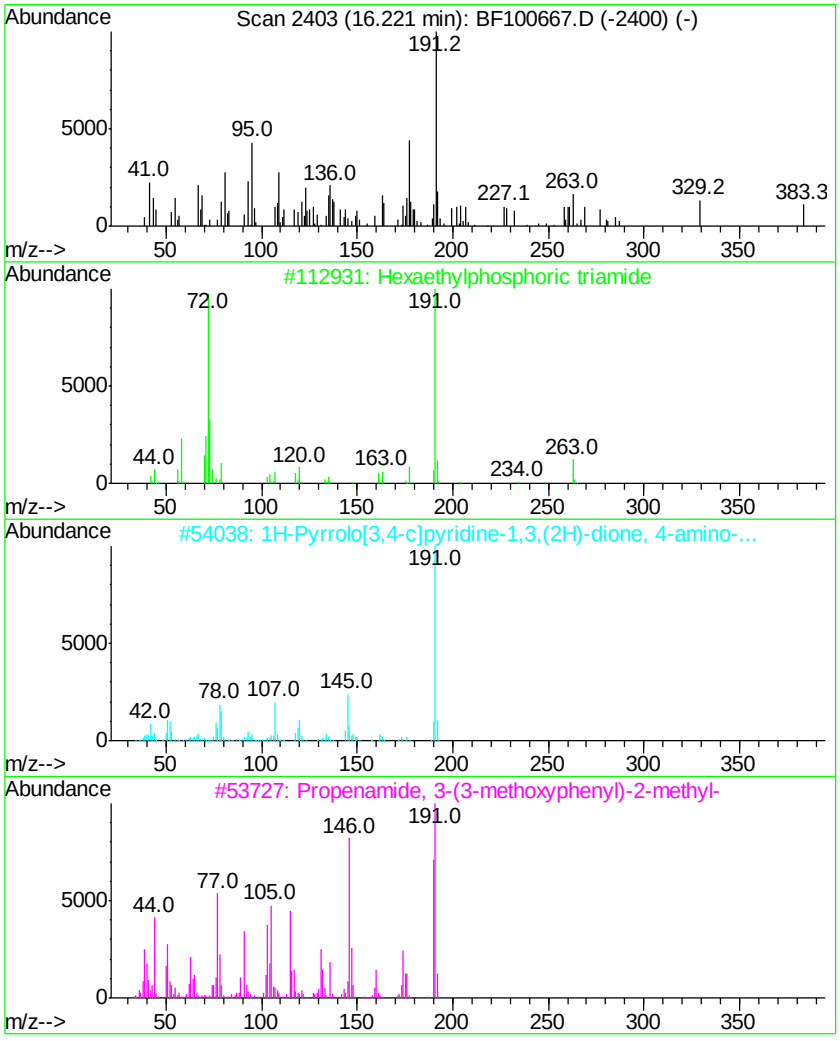
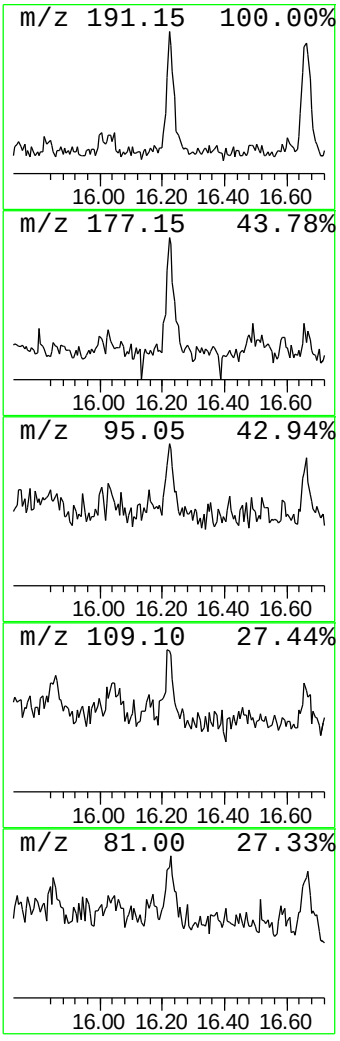
Peak Number 4 unknown16.22 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.22	2.69 ng	87834	Perylene-d12	15.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexaethylphosphoric triamide	263	C12H30N3OP	002622-07-3	35
2	1H-Pyrrolo[3,4-c]pyridine-1,3,(2...	191	C9H9N3O2	298688-32-1	30
3	Propenamide, 3-(3-methoxyphenyl)...	191	C11H13NO2	1000259-85-9	30
4	p-(Dimethylamino)cinnamic acid	191	C11H13NO2	001552-96-1	30
5	9H-Fluorene-9-carbonitrile	191	C14H9N	001529-40-4	27





Data Path : Z:\HPCHEM1\BNA F\DATA\BF111717\
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Operator : SJ/JU
Sample : I6289-05 5X
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-01-111417

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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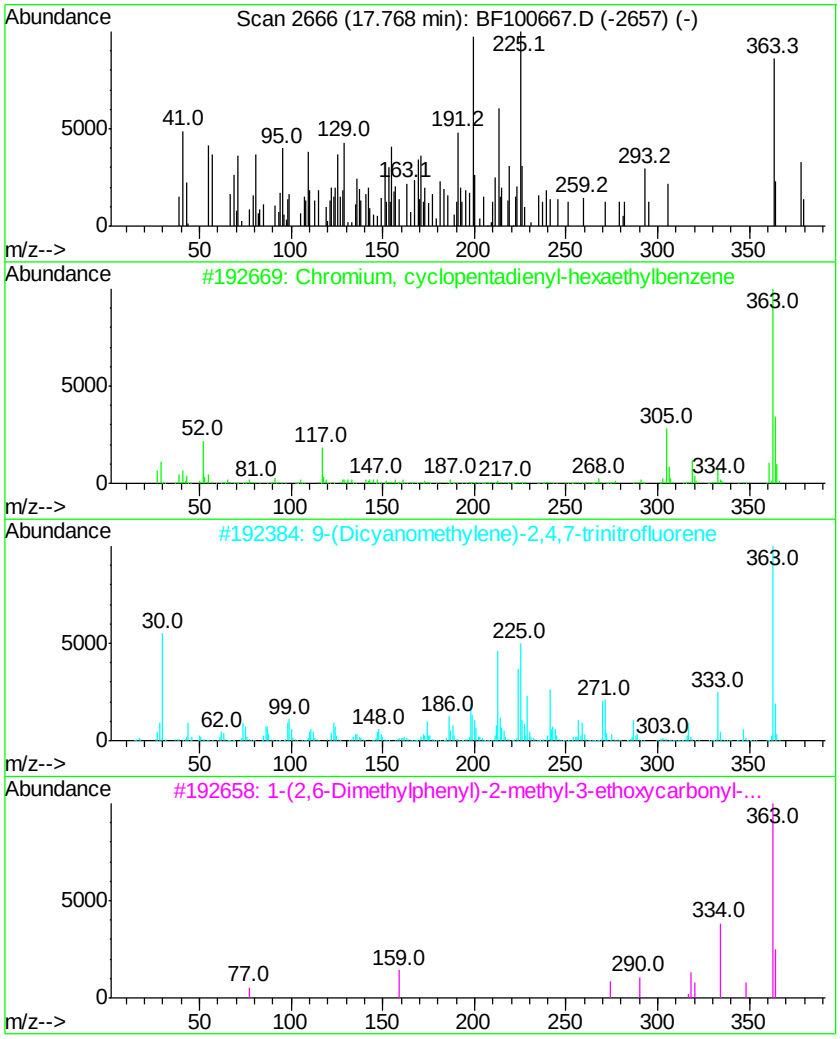
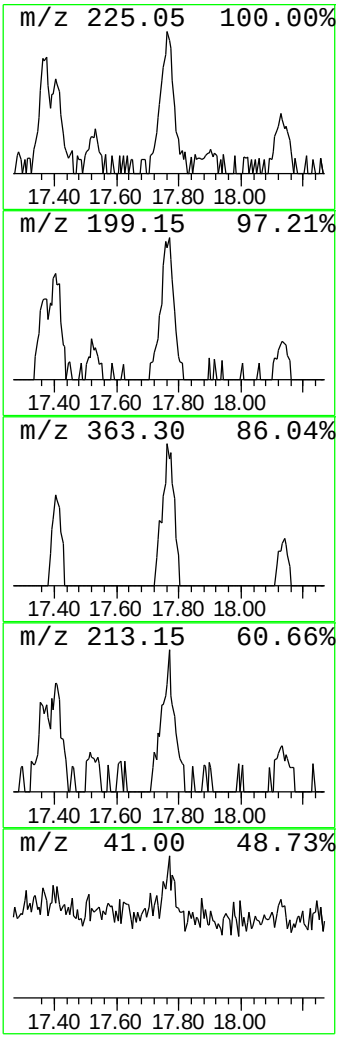
Peak Number 5 unknown17.77 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.77	5.68 ng	185149	Perylene-d12	15.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Chromium, cyclopentadienyl-hexae...	363	C23H35Cr	1000156-60-8	22
2	9-(Dicyanomethylene)-2,4,7-trini...	363	C16H5N5O6	001172-02-7	22
3	1-(2,6-Dimethylphenyl)-2-methyl-...	363	C23H25NO3	083490-98-6	22
4	4-Bromo-1-(4-methoxyphenyl)-1-(5...	318	C15H15BrN2O	1000292-95-2	18
5	3-(p-Ethoxyphenyl)-5-(1-naphthyl...	363	C22H21NO4	005256-09-7	14





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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-01-111417

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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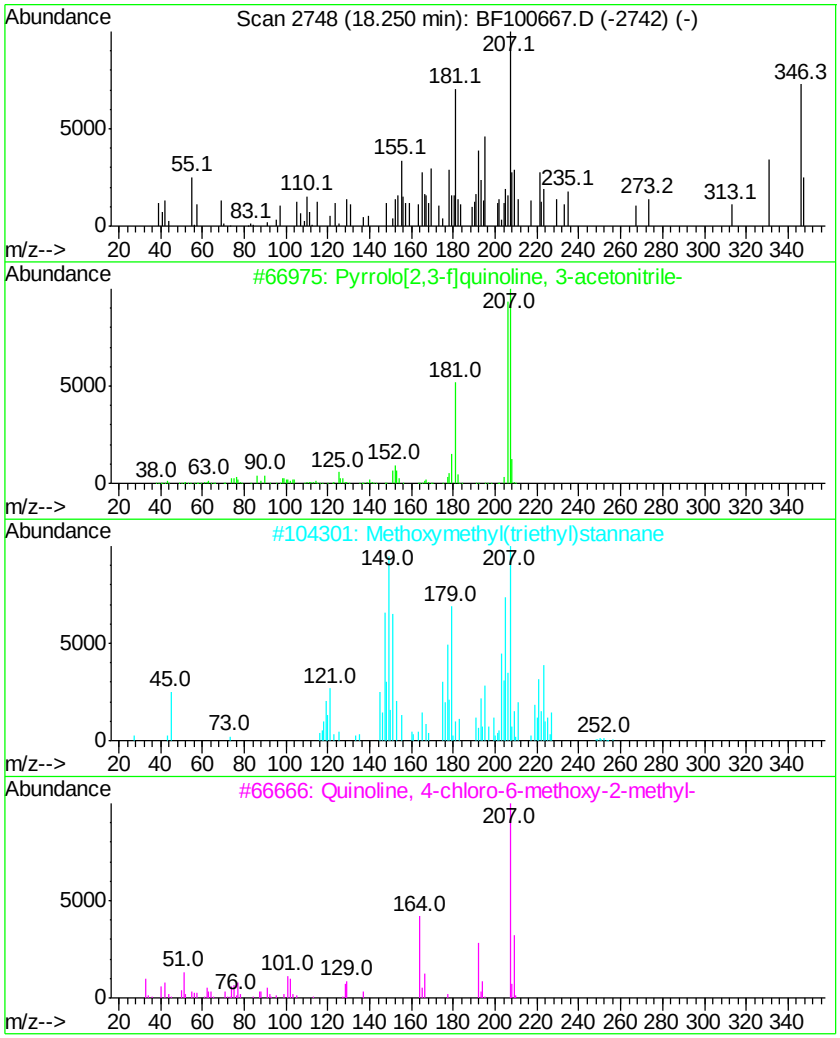
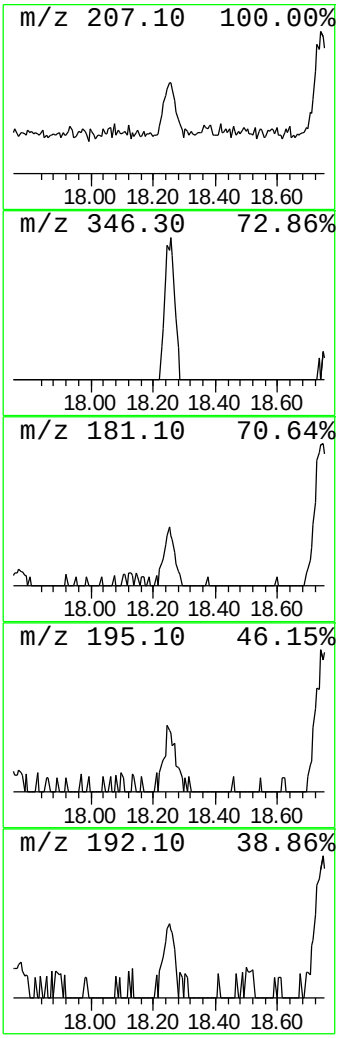
Peak Number 6 unknown18.25 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.25	2.60 ng	84641	Perylene-d12	15.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrrolo[2,3-f]quinoline, 3-aceto...	207	C13H9N3	087361-85-1	27
2	Methoxymethyl(triethyl)stannane	252	C8H20OSn	1000298-95-7	22
3	Quinoline, 4-chloro-6-methoxy-2-...	207	C11H10ClNO	050593-73-2	18
4	Pyrido[2,3-d]pyrimidine, 4-phenyl-	207	C13H9N3	028732-75-4	14
5	3,3-Diisopropoxy-1,1,1,5,5,5-hex...	324	C12H32O4Si3	018082-56-9	14





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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-01-111417

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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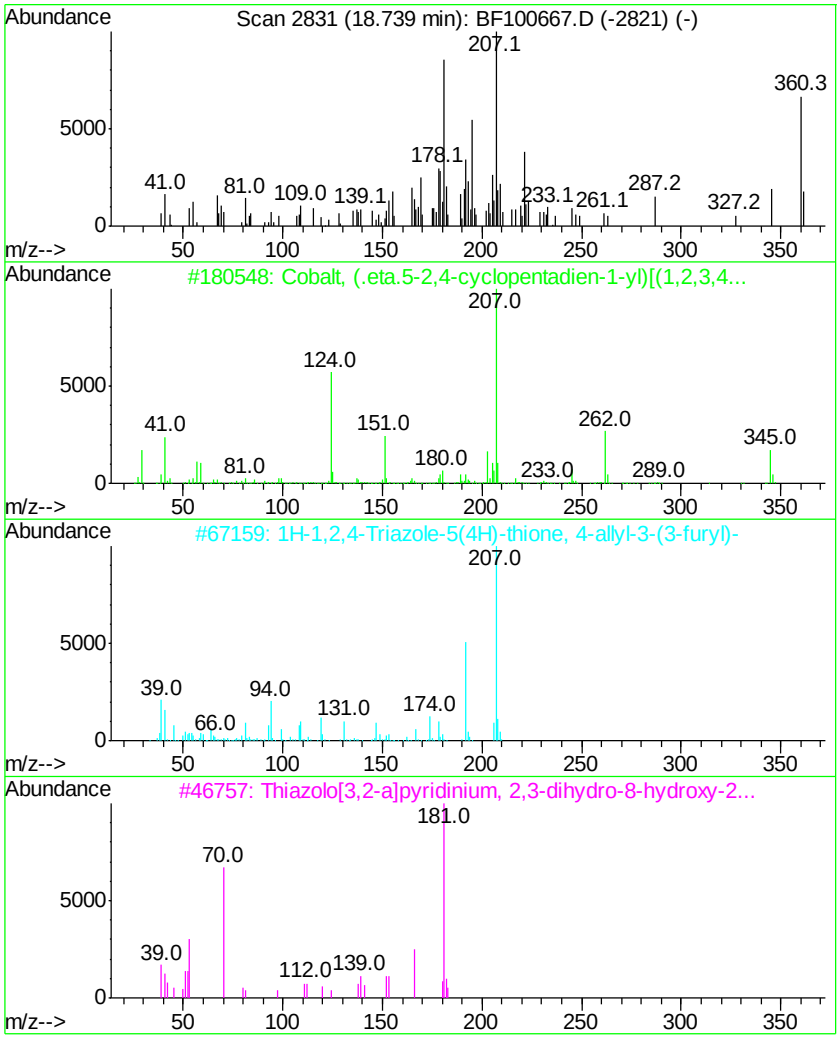
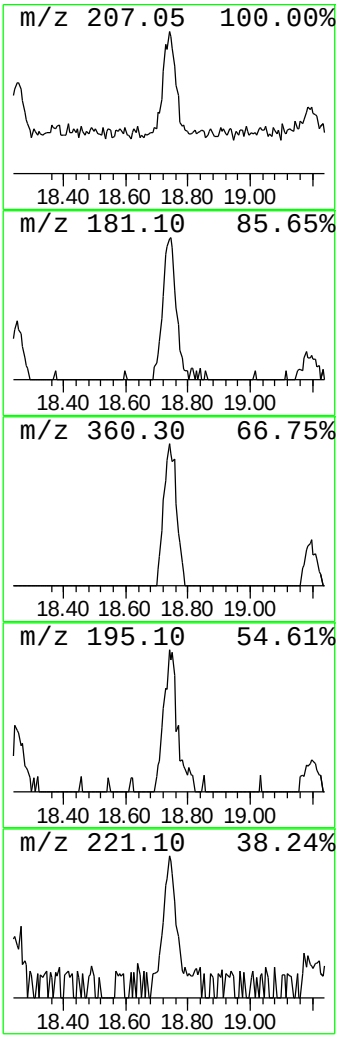
Peak Number 7 unknown18.74 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.74	5.84 ng	190619	Perylene-d12	15.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cobalt, (.eta.5-2,4-cyclopentadi...	345	C20H32CoN	117308-54-0	14
2	1H-1,2,4-Triazole-5(4H)-thione, ...	207	C9H9N3OS	1000277-38-2	14
3	Thiazolo[3,2-a]pyridinium, 2,3-d...	181	C9H11NOS	023933-08-6	11
4	Benzenecarboxamide, 2-methoxy-4-...	287	C16H17NO2S	335397-82-5	11
5	Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	11





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown6.65	6.65	18.6	ng	545970	1	6.88	586996	20.0
unknown16.22	16.22	2.7	ng	87834	6	15.52	652323	20.0
unknown17.77	17.77	5.7	ng	185149	6	15.52	652323	20.0
unknown18.25	18.25	2.6	ng	84641	6	15.52	652323	20.0
unknown18.74	18.74	5.8	ng	190619	6	15.52	652323	20.0