LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF090817\
Data File : BF098366.D
Acq On : 8 Sep 2017 22:30
Operator : SJ/JU
Sample : I5113-05 10X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-3-0-11.75

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-BF081517.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	4.851	467	470	481	rBB	11925	13772	1.04%	0.101%
2	5.281	540	543	550	rBV	156394	172073	13.03%	1.260%
3	6.328	718	721	736	rBV	183430	199970	15.14%	1.464%
4	6.451	739	742	749	rVB	246246	197148	14.92%	1.444%
5	6.681	777	781	785	rBV	663509	544701	41.23%	3.989%
6	6.834	804	807	811	rBV	174631	152503	11.54%	1.117%
7	7.245	874	877	882	rBV	124564	101859	7.71%	0.746%
8	7.963	995	999	1002	rBV	733105	653443	49.47%	4.785%
9	9.039	1179	1182	1189	rBV	262131	193832	14.67%	1.419%
10	9.716	1293	1297	1300	rBV2	702524	585193	44.30%	4.286%
11	9.745	1300	1302	1306	rVB	140175	123927	9.38%	0.908%
12	9.922	1329	1332	1340	rVB	59717	48030	3.64%	0.352%
13	10.263	1387	1390	1396	rBB	131459	101336	7.67%	0.742%
14	10.504	1428	1431	1437	rBV	92558	78251	5.92%	0.573%
15	11.057	1521	1525	1529	rBV3	12475	13630	1.03%	0.100%
16	11.098	1529	1532	1535	rVB	51796	43291	3.28%	0.317%
17	11.198	1546	1549	1551	rBV	568773	518810	39.27%	3.799%
18	11.227	1551	1554	1557	rVV	1076832	976887	73.95%	7.154%
19	11.274	1557	1562	1566	rVV	330756	273909	20.74%	2.006%
20	11.310	1566	1568	1572	rVB	29842	24968	1.89%	0.183%
21	11.433	1583	1589	1595	rBV	166931	145678	11.03%	1.067%
22	11.498	1597	1600	1603	rBV2	14951	14487	1.10%	0.106%
23	11.698	1631	1634	1637	rBV	53200	46666	3.53%	0.342%
24	11.727	1637	1639	1643	rVV	81273	65633	4.97%	0.481%
25	11.774	1644	1647	1650	rVV	28747	24158	1.83%	0.177%
26	11.810	1650	1653	1656	rVV	161067	152963	11.58%	1.120%
27	11.833	1656	1657	1663	rVB	35354	21336	1.62%	0.156%
28	11.998	1680	1685	1687	rBV	56841	49785	3.77%	0.365%
29	12.027	1687	1690	1693	rVB	23894	22418	1.70%	0.164%
30	12.251	1725	1728	1731	rBV3	16740	17928	1.36%	0.131%
31	12.286	1731	1734	1740	rVV3	13364	18695	1.42%	0.137%
32	12.333	1740	1742	1746	rVB3	11919	13368	1.01%	0.098%
33	12.410	1751	1755	1759	rBV	1266160	1204939	91.21%	8.824%
34	12.474	1761	1766	1769	rVV2	20976	20564	1.56%	0.151%

LSC Area Percent Report

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Acq On : 8 Sep 2017 22:30
Operator : SJ/JU
Sample : I5113-05 10X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-3-0-11.75

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-BF081517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.557	1774	1780	1784	rBV2	38283	46825	3.54%	0.343%
36	12.639	1788	1794	1797	rBV	1155311	1244221	94.19%	9.112%
37	12.686	1800	1802	1806	rVB2	36402	34725	2.63%	0.254%
38	12.757	1811	1814	1816	rBV	56457	50703	3.84%	0.371%
39	12.780	1816	1818	1825	rVB2	206251	217898	16.50%	1.596%
40	12.863	1826	1832	1834	rBV3	35122	62288	4.72%	0.456%
41	12.892	1834	1837	1840	rVB	32563	29563	2.24%	0.216%
42	12.945	1840	1846	1847	rBV3	34776	47943	3.63%	0.351%
43	12.968	1847	1850	1853	rVB	154199	136584	10.34%	1.000%
44	13.033	1857	1861	1864	rBV	180457	149776	11.34%	1.097%
45	13.068	1864	1867	1869	rBV	62028	58436	4.42%	0.428%
46	13.092	1869	1871	1874	rVB	40568	35944	2.72%	0.263%
47	13.127	1874	1877	1880	rBV3	16222	15660	1.19%	0.115%
48	13.163	1880	1883	1886	rBV	27089	22408	1.70%	0.164%
49	13.192	1886	1888	1891	rBV	30230	28468	2.16%	0.208%
50	13.357	1912	1916	1917	rBV4	12834	16704	1.26%	0.122%
51	13.392	1919	1922	1924	rVB2	24432	23643	1.79%	0.173%
52	13.451	1929	1932	1934	rBV3	23908	26111	1.98%	0.191%
53	13.474	1934	1936	1940	rVB3	16299	22310	1.69%	0.163%
54	13.586	1951	1955	1957	rBV	71714	74221	5.62%	0.544%
55	13.610	1957	1959	1961	rVV	81316	70076	5.30%	0.513%
56	13.633	1961	1963	1970	rVV3	79346	132701	10.05%	0.972%
57	13.686	1970	1972	1975	rVB	30302	27240	2.06%	0.199%
58	13.751	1979	1983	1988	rBV	28123	36811	2.79%	0.270%
59	13.833	1989	1997	2000	rBV2	891534	1320993	100.00%	9.674%
60	13.863	2000	2002	2010	rVB	512034	427389	32.35%	3.130%
61	13.939	2012	2015	2018	rBV	168124	132742	10.05%	0.972%
62	14.004	2024	2026	2028	rBV	23718	19324	1.46%	0.142%
63	14.027	2028	2030	2032	rVV	46724	38260	2.90%	0.280%
64	14.063	2032	2036	2039	rVB2	46844	59432	4.50%	0.435%
65	14.221	2059	2063	2066	rBV	55325	60393	4.57%	0.442%
66	14.257	2066	2069	2072	rVB2	24034	23271	1.76%	0.170%
67	14.315	2076	2079	2082	rVV4	40413	42631	3.23%	0.312%
68	14.345	2082	2084	2085	rVV	36525	27723	2.10%	0.203%
69	14.363	2085	2087	2090	rVB2	62382	58011	4.39%	0.425%
70	14.398	2091	2093	2094	rBV	21345	15401	1.17%	0.113%
71	14.527	2113	2115	2117	rBV3	36069	33822	2.56%	0.248%

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Instrument : BNA_F
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Integration Parameters: rteint.p
Integrator: RTE
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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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72	14.698	2142	2144	2148	rBV	23082	26891	2.04%	0.197%
73	14.845	2165	2169	2172	rBV	343499	488788	37.00%	3.580%
74	14.945	2183	2186	2189	rVB	70504	67656	5.12%	0.495%
75	15.127	2213	2217	2223	rVB	197041	237018	17.94%	1.736%
76	15.186	2223	2227	2232	rBV	289751	327689	24.81%	2.400%
77	15.245	2232	2237	2240	rBV	394547	477973	36.18%	3.500%
78	16.598	2462	2467	2475	rVB2	99904	178997	13.55%	1.311%
79	17.004	2531	2536	2547	rBV	74843	143349	10.85%	1.050%

Sum of corrected areas: 13655163

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF090817\
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Acq On : 8 Sep 2017 22:30
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Misc :
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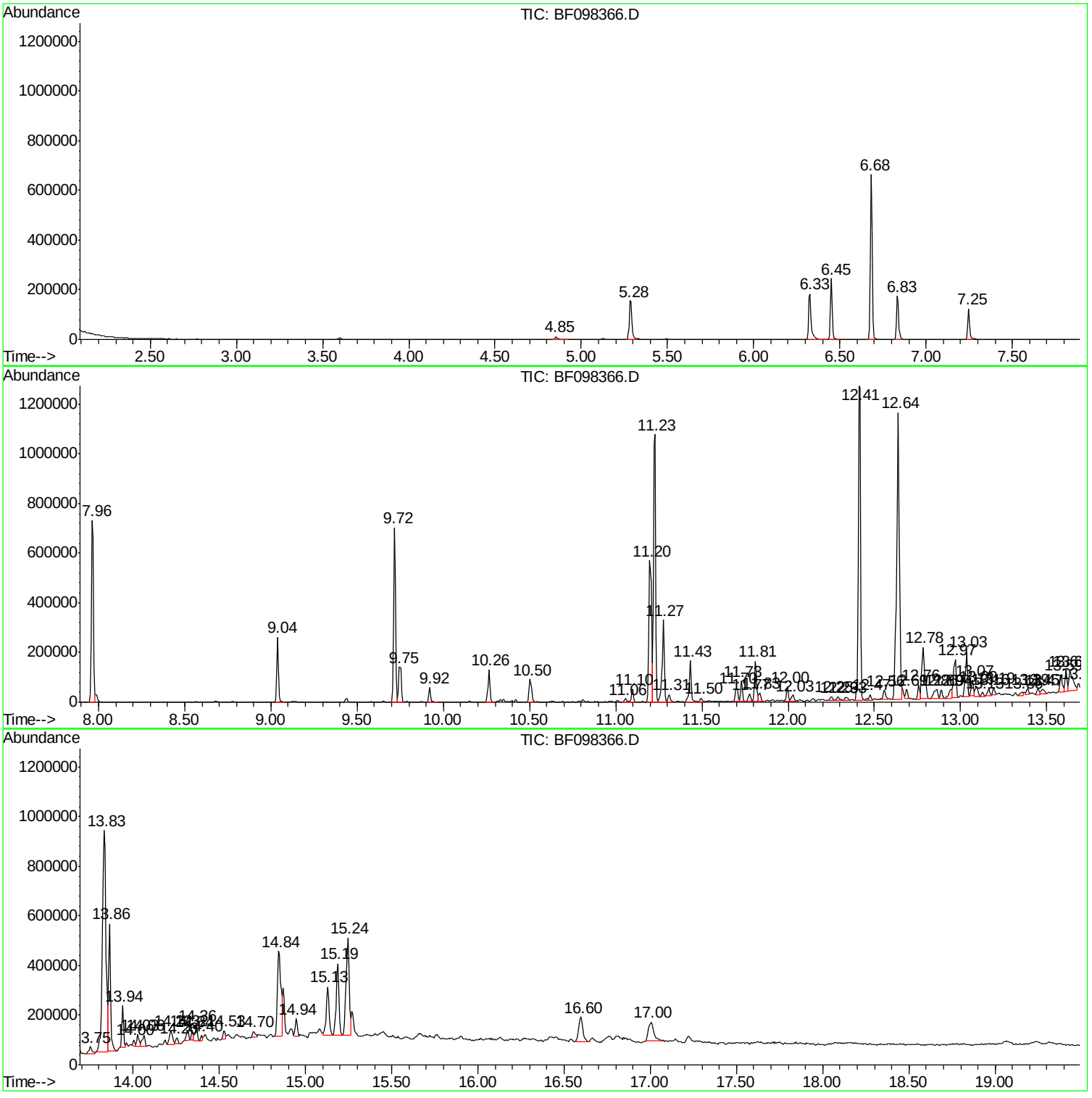
Instrument :
BNA_F
ClientSampleId :
RL-3-0-11.75

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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 : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF090817\
Data File : BF098366.D
Acq On : 8 Sep 2017 22:30
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Misc :
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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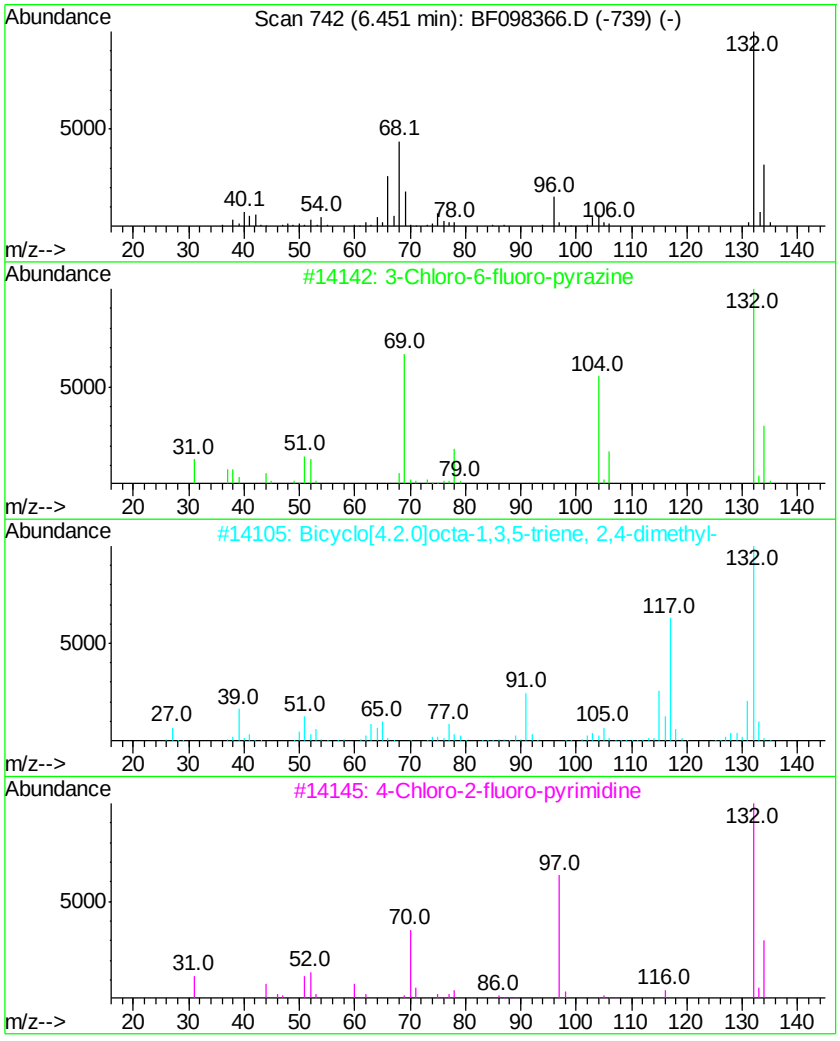
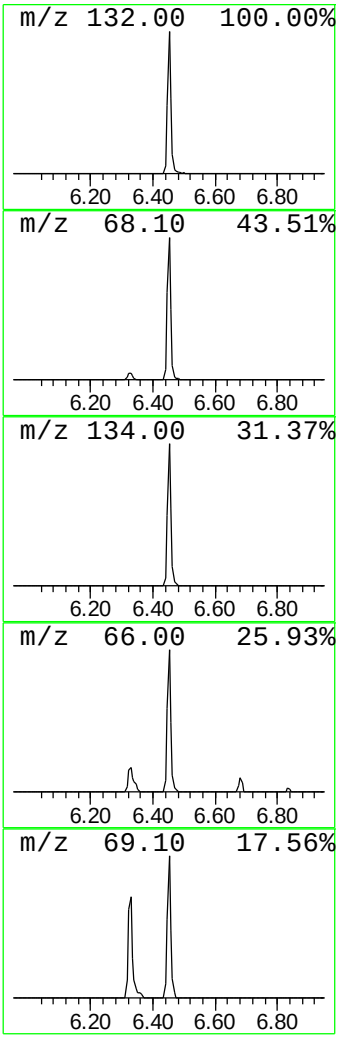
Peak Number 1 unknown6.45 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.45	7.24 ng	197148	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9





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Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-3-0-11.75

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TIC Library : C:\DATABASE\NIST11.L
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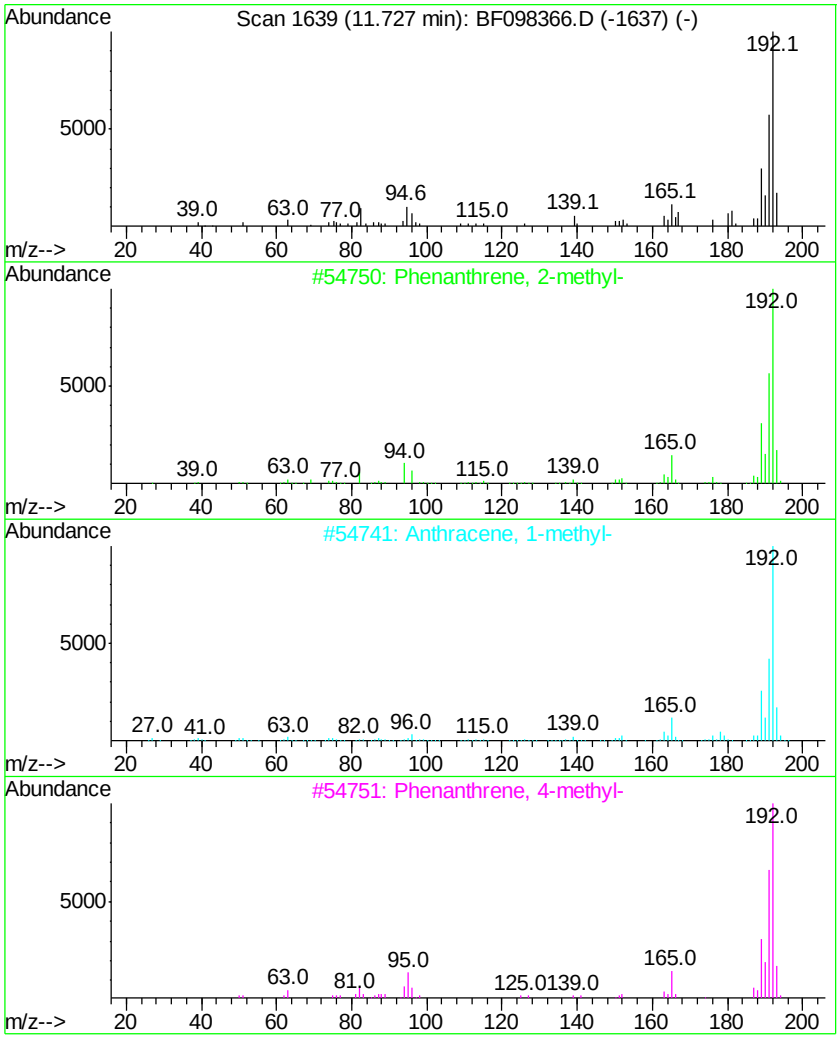
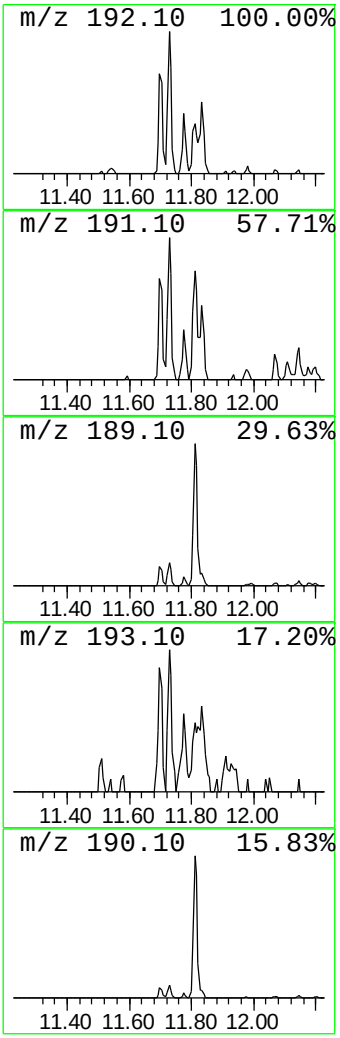
Peak Number 3 Phenanthrene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.73	2.53 ng	65633	Phenanthrene-d10	11.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	96
2	Anthracene, 1-methyl-	192	C15H12	000610-48-0	94
3	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	93
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	89
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	89





Library Search Compound Report

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ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-3-0-11.75

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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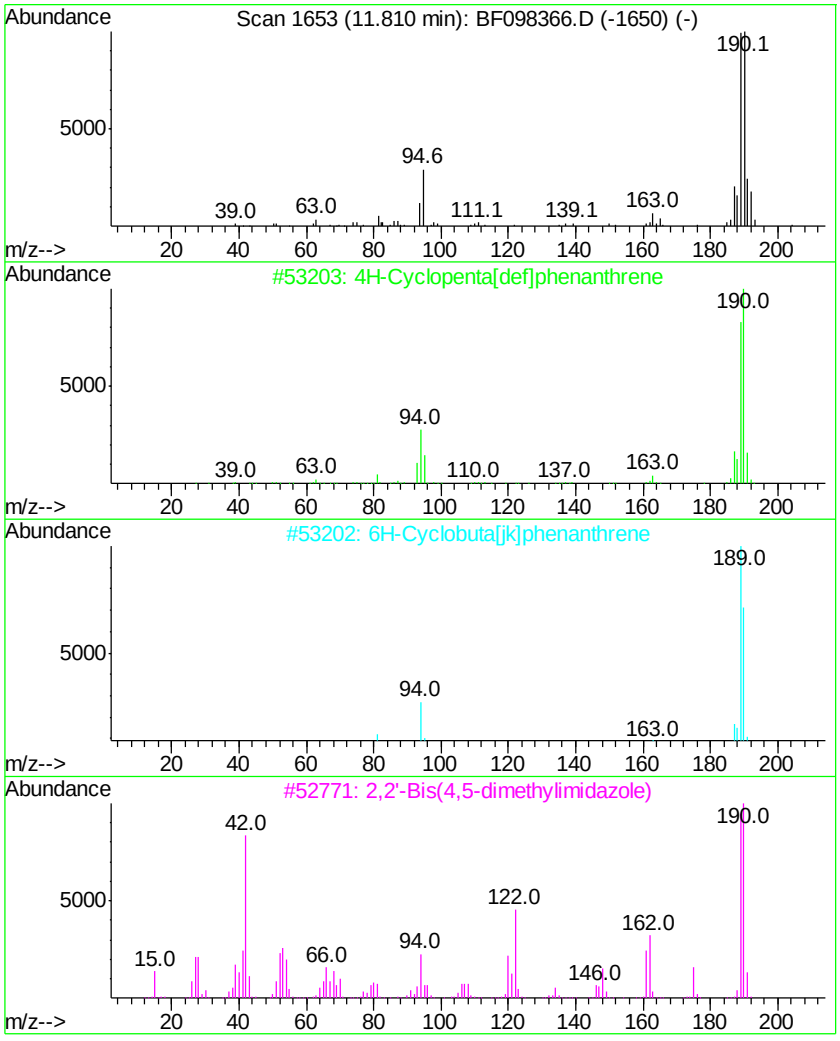
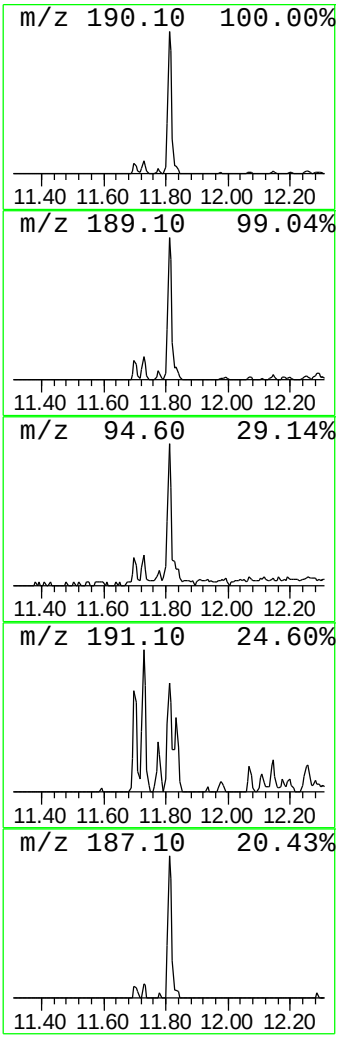
****

Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.81	5.90 ng	152963	Phenanthrene-d10	11.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	95
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	72
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45
4	Methyl diselenide	190	C2H6Se2	007101-31-7	38
5	1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	32





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ClientSampleId : RL-3-0-11.75

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TIC Library : C:\DATABASE\NIST11.L
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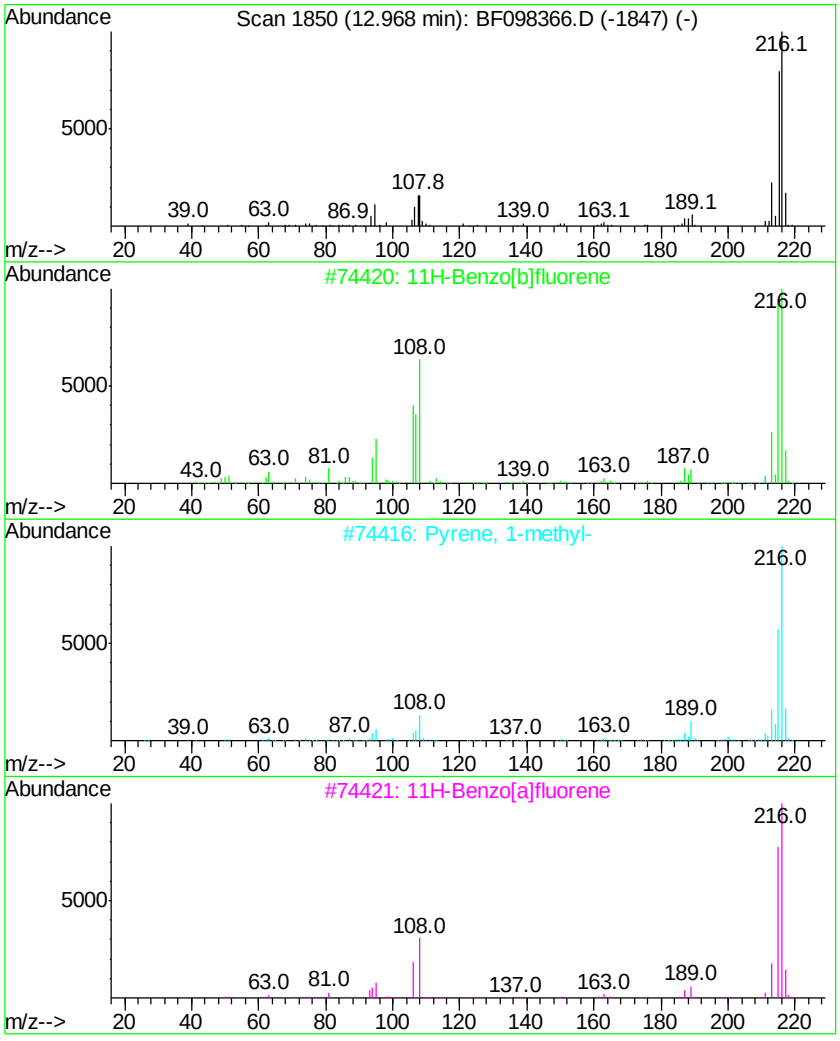
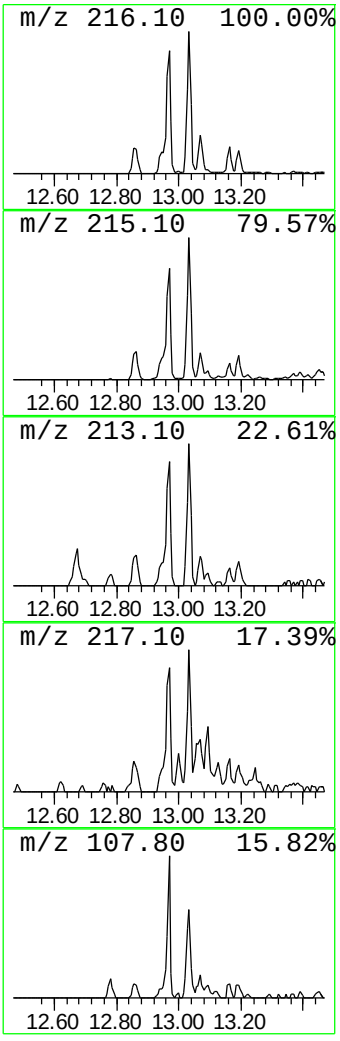
Peak Number 5 11H-Benzo[b]fluorene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.97	2.07 ng	136584	Chrysene-d12	13.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	95
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	86
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	81
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	74
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	64





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ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-3-0-11.75

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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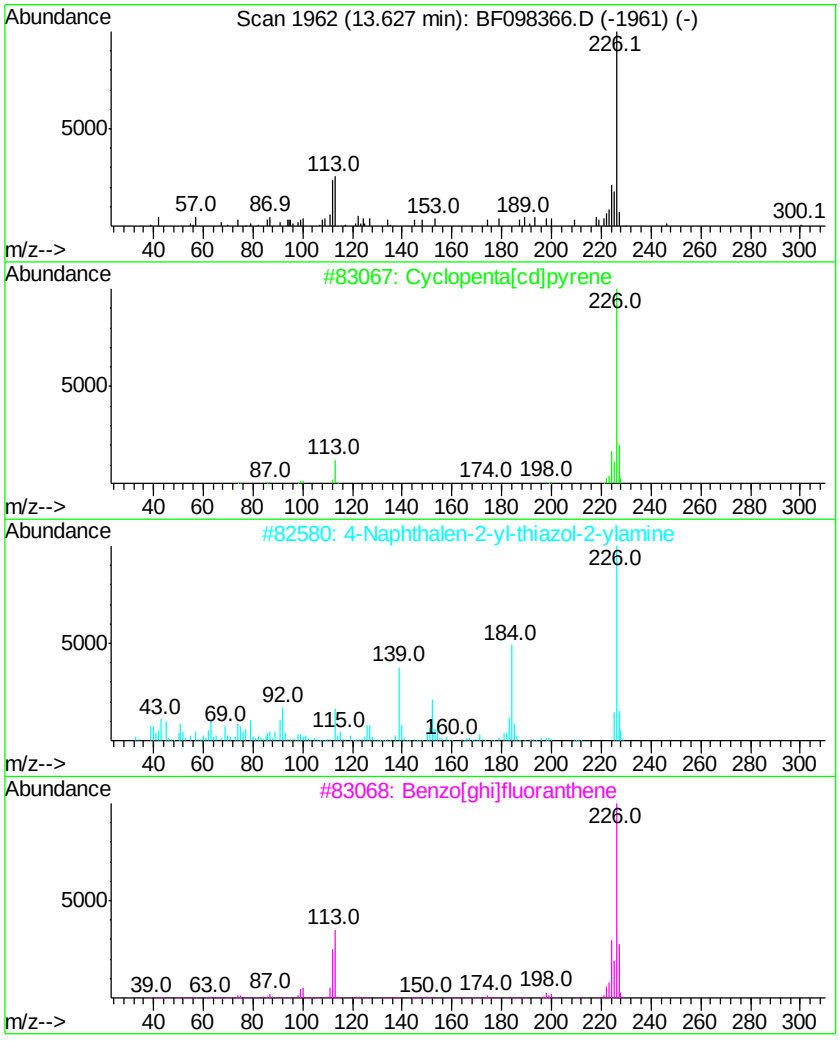
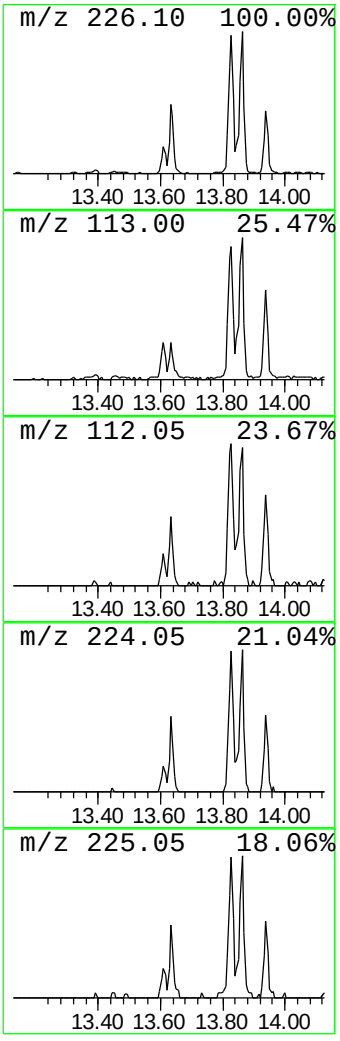
Peak Number 7 Cyclopenta[cd]pyrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.63	2.01 ng	132701	Chrysene-d12	13.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenta[cd]pyrene	226	C18H10	027208-37-3	76
2	4-Naphthalen-2-yl-thiazol-2-ylamine	226	C13H10N2S	1000300-53-4	59
3	Benzo[ghi]fluoranthene	226	C18H10	000203-12-3	43
4	9H-Thioxanthen-9-one, 2-methyl-	226	C14H10OS	015774-82-0	42
5	2-Thiazolamine, 4-(1-naphthalenyl)-	226	C13H10N2S	056503-96-9	40





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF090817\
Data File : BF098366.D
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Operator : SJ/JU
Sample : I5113-05 10X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-3-0-11.75

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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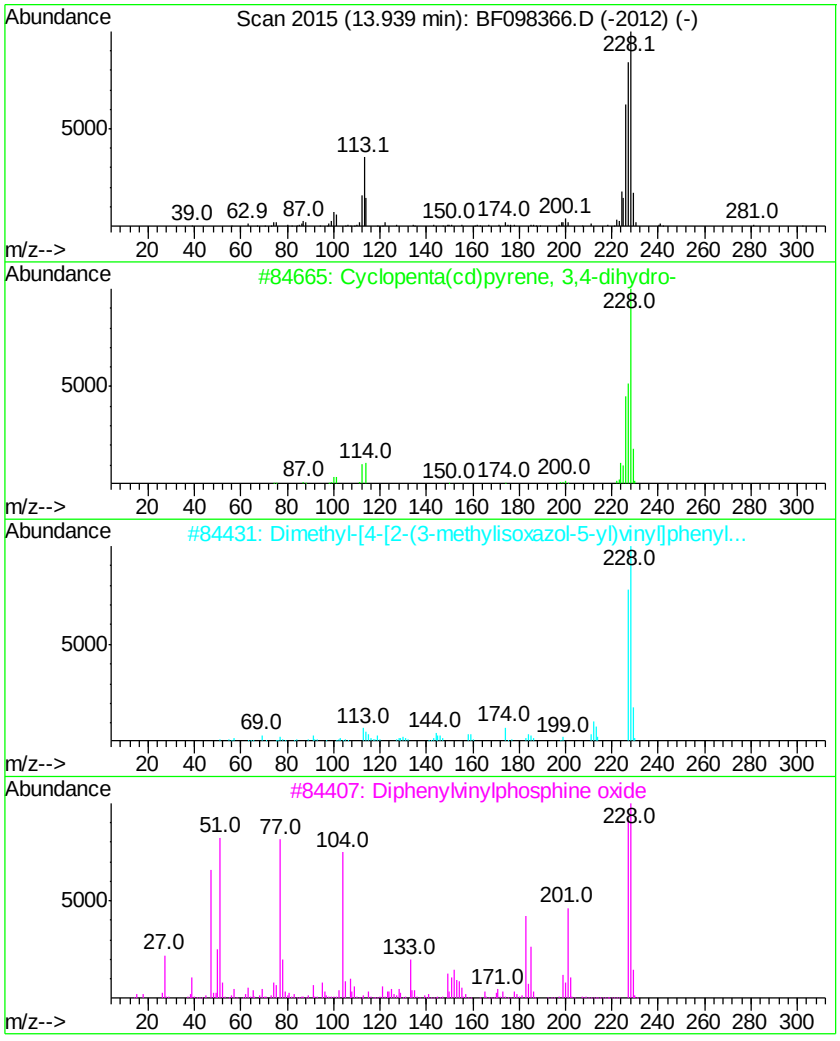
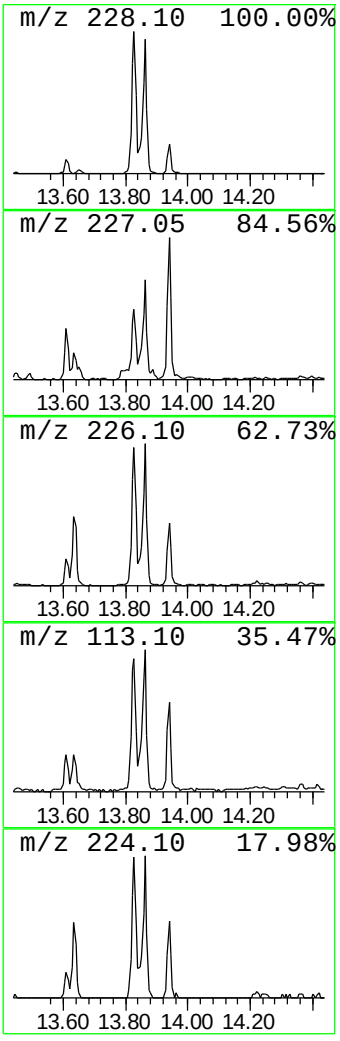
Peak Number 8 Cyclopenta(cd)pyrene, 3,4-d... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	2.01 ng	132742	Chrysene-d12	13.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenta(cd)pyrene, 3,4-dihydro-	228	C18H12	025732-74-5	55
2	Dimethyl-[4-[2-(3-methylisoxazol...	228	C14H16N2O	1000306-39-6	50
3	Diphenylvinylphosphine oxide	228	C14H13OP	002096-78-8	49
4	Benzo[c]phenanthrene	228	C18H12	000195-19-7	49
5	Isothiazol-5-amine, 4-bromo-3-ch...	226	C4H4BrClN2S	1000272-59-9	47





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Data File : BF098366.D
Acq On : 8 Sep 2017 22:30
Operator : SJ/JU
Sample : I5113-05 10X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-3-0-11.75

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

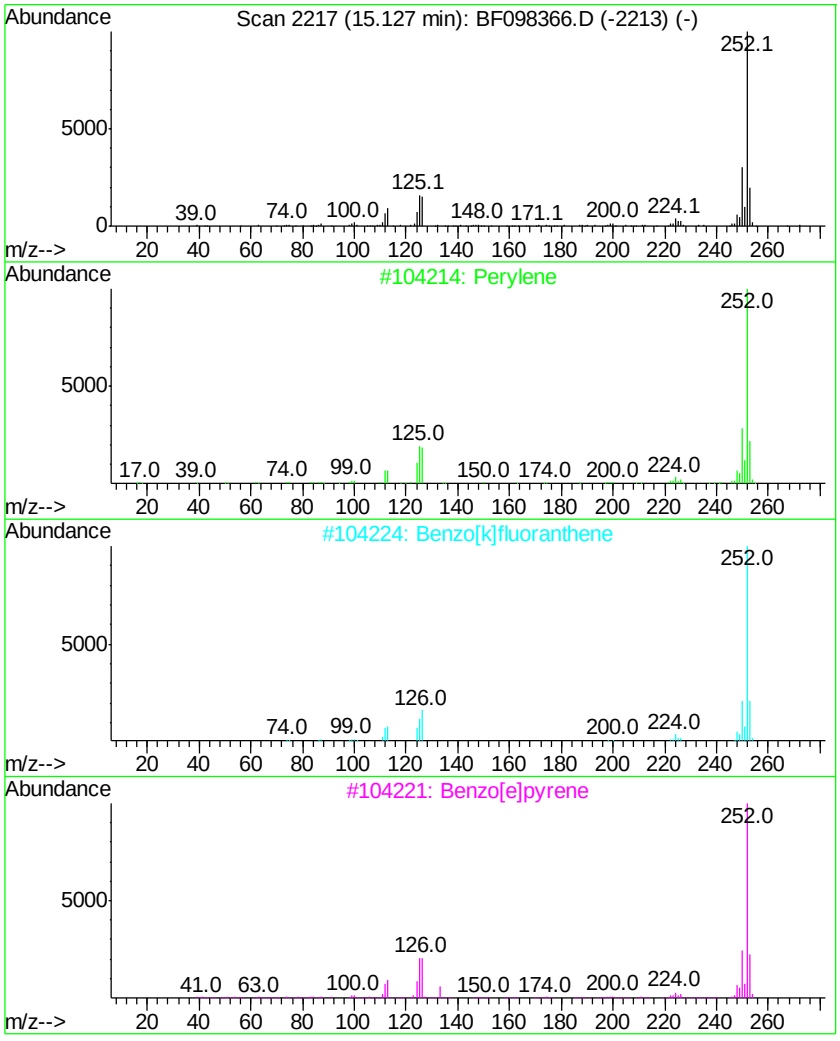
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

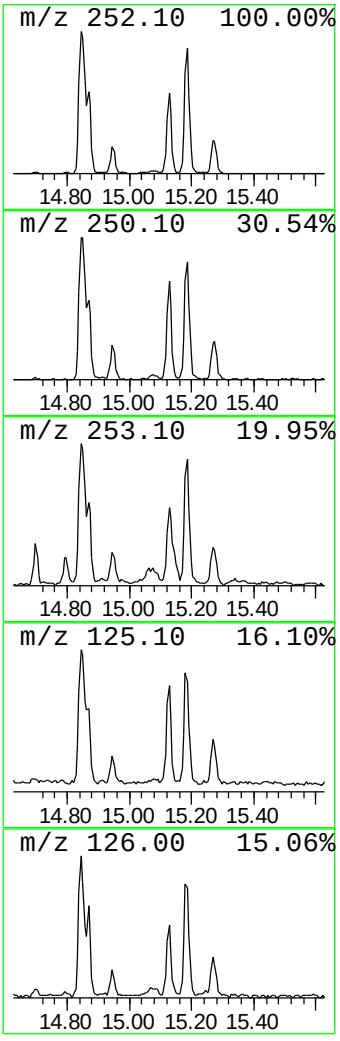
****

Peak Number 10 Perylene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.13	9.92 ng	237018	Perylene-d12	15.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	99
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	98
3	Benzo[e]pyrene	252	C20H12	000192-97-2	98
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	98
5	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	98





Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF090817\
Data File : BF098366.D
Acq On : 8 Sep 2017 22:30
Operator : SJ/JU
Sample : I5113-05 10X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-3-0-11.75

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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
unknown6.45	6.45	7.2	ng	197148	1	6.68	544701	20.0
Phenanthrene, 2-m...	11.73	2.5	ng	65633	4	11.20	518810	20.0
4H-Cyclopenta[def...	11.81	5.9	ng	152963	4	11.20	518810	20.0
11H-Benzo[b]fluorene	12.97	2.1	ng	136584	5	13.84	1320990	20.0
Cyclopenta[cd]pyrene	13.63	2.0	ng	132701	5	13.84	1320990	20.0
Cyclopenta(cd)pyr...	13.94	2.0	ng	132742	5	13.84	1320990	20.0
Perylene	15.13	9.9	ng	237018	6	15.24	477973	20.0