LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121217\
Data File : BF101343.D
Acq On : 12 Dec 2017 21:20
Operator : SJ/JU
Sample : I6822-10 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-9(13-15)

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-BF113017.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	5.028	497	500	506	rBV	12000	12975	2.55%	0.217%
2	5.440	567	570	594	rBV	198933	227631	44.78%	3.805%
3	6.457	740	743	756	rBV	226048	245861	48.37%	4.109%
4	6.592	762	766	774	rVB	307740	250987	49.38%	4.195%
5	6.822	802	805	814	rBB	291399	235807	46.39%	3.941%
6	6.975	828	831	842	rBB	211974	179772	35.37%	3.005%
7	7.386	898	901	912	rBV	146635	137268	27.00%	2.294%
8	8.104	1020	1023	1041	rVB	355886	297759	58.58%	4.977%
9	9.175	1202	1205	1216	rBV	318408	263739	51.88%	4.408%
10	9.575	1270	1273	1278	rBB	23781	19302	3.80%	0.323%
11	9.863	1318	1322	1326	rBV	329359	277193	54.53%	4.633%
12	9.892	1326	1327	1330	rVB	10268	6528	1.28%	0.109%
13	10.657	1453	1457	1464	rBV	128264	120776	23.76%	2.019%
14	10.757	1471	1474	1477	rBV	4368	5512	1.08%	0.092%
15	11.204	1544	1550	1553	rBV3	4758	5147	1.01%	0.086%
16	11.357	1572	1576	1578	rBV	285157	260615	51.27%	4.356%
17	11.380	1578	1580	1583	rVV	66815	53131	10.45%	0.888%
18	11.433	1584	1589	1593	rVV	26362	25391	5.00%	0.424%
19	11.592	1610	1616	1620	rBV2	9859	14540	2.86%	0.243%
20	11.857	1657	1661	1663	rBV	14893	14745	2.90%	0.246%
21	11.886	1663	1666	1669	rVB	22757	17330	3.41%	0.290%
22	11.933	1672	1674	1677	rVB	17792	12772	2.51%	0.213%
23	11.969	1677	1680	1683	rBV2	22135	29797	5.86%	0.498%
24	12.151	1709	1711	1714	rVB	8054	6192	1.22%	0.103%
25	12.404	1752	1754	1757	rBV	13981	12997	2.56%	0.217%
26	12.445	1760	1761	1763	rVV2	9219	7914	1.56%	0.132%
27	12.486	1766	1768	1774	rVB3	7707	11397	2.24%	0.190%
28	12.574	1779	1783	1786	rBV	142075	133160	26.20%	2.226%
29	12.721	1805	1808	1810	rBV3	7697	7424	1.46%	0.124%
30	12.786	1815	1819	1820	rBV2	50153	55240	10.87%	0.923%
31	12.804	1820	1822	1824	rVV	154487	126286	24.84%	2.111%
32	12.851	1828	1830	1837	rVB2	17474	22895	4.50%	0.383%
33	12.933	1837	1844	1847	rBV	236776	231046	45.45%	3.862%
34	12.963	1847	1849	1854	rVB	16434	16567	3.26%	0.277%

LSC Area Percent Report

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Acq On : 12 Dec 2017 21:20
Operator : SJ/JU
Sample : I6822-10 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-9(13-15)

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-BF113017.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.021	1854	1859	1862	rBV3	15590	25514	5.02%	0.426%
36	13.110	1870	1874	1875	rBV4	16370	21922	4.31%	0.366%
37	13.133	1875	1878	1881	rVB	43975	40580	7.98%	0.678%
38	13.168	1881	1884	1886	rBV4	4897	6791	1.34%	0.114%
39	13.198	1886	1889	1891	rVV	42583	37528	7.38%	0.627%
40	13.233	1891	1895	1898	rVV2	26402	35328	6.95%	0.590%
41	13.263	1898	1900	1903	rVB2	9880	8833	1.74%	0.148%
42	13.286	1903	1904	1907	rVB	7156	6145	1.21%	0.103%
43	13.333	1907	1912	1914	rBV2	15191	17103	3.36%	0.286%
44	13.363	1914	1917	1925	rVB2	19257	29841	5.87%	0.499%
45	13.480	1935	1937	1939	rBV2	10695	10229	2.01%	0.171%
46	13.533	1942	1946	1948	rVV5	10430	12905	2.54%	0.216%
47	13.557	1948	1950	1952	rVB2	10410	8735	1.72%	0.146%
48	13.616	1957	1960	1963	rBV4	15825	20385	4.01%	0.341%
49	13.651	1963	1966	1969	rBV5	10099	10613	2.09%	0.177%
50	13.704	1972	1975	1978	rVB5	5778	6904	1.36%	0.115%
51	13.739	1978	1981	1982	rBV3	5836	5452	1.07%	0.091%
52	13.757	1982	1984	1985	rBV	10146	7329	1.44%	0.122%
53	13.780	1985	1988	1990	rVB	22934	18128	3.57%	0.303%
54	13.810	1990	1993	1994	rBV	11215	11767	2.31%	0.197%
55	13.921	2007	2012	2017	rBV4	9874	21724	4.27%	0.363%
56	14.004	2017	2026	2029	rBV2	379497	508322	100.00%	8.496%
57	14.033	2029	2031	2034	rVB	144595	110966	21.83%	1.855%
58	14.110	2042	2044	2047	rVB	46349	40477	7.96%	0.677%
59	14.174	2051	2055	2057	rBV4	8687	12705	2.50%	0.212%
60	14.198	2057	2059	2061	rVV	19980	18418	3.62%	0.308%
61	14.239	2063	2066	2069	rVB	24775	26926	5.30%	0.450%
62	14.327	2078	2081	2083	rBV4	8556	9685	1.91%	0.162%
63	14.357	2083	2086	2088	rVV	24584	25607	5.04%	0.428%
64	14.392	2088	2092	2096	rVV	49810	56203	11.06%	0.939%
65	14.427	2096	2098	2100	rVB	16623	13126	2.58%	0.219%
66	14.492	2107	2109	2111	rVB	22824	17760	3.49%	0.297%
67	14.515	2111	2113	2115	rBV	24767	25339	4.98%	0.424%
68	14.539	2115	2117	2120	rVB2	22184	20967	4.12%	0.350%
69	14.639	2131	2134	2144	rVB2	19202	40266	7.92%	0.673%
70	14.715	2144	2147	2149	rBV4	9189	9577	1.88%	0.160%
71	14.815	2162	2164	2168	rVB5	10549	8189	1.61%	0.137%

LSC Area Percent Report

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Data File : BF101343.D
Acq On : 12 Dec 2017 21:20
Operator : SJ/JU
Sample : I6822-10 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-9(13-15)

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

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Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	14.862	2168	2172	2174	rVV5	11310	14780	2.91%	0.247%
73	14.892	2174	2177	2183	rVV5	22510	29209	5.75%	0.488%
74	14.945	2184	2186	2191	rVB6	8101	10226	2.01%	0.171%
75	15.051	2200	2204	2207	rBV	151027	208608	41.04%	3.487%
76	15.162	2219	2223	2226	rVB	46766	52990	10.42%	0.886%
77	15.245	2234	2237	2239	rBV4	14988	18642	3.67%	0.312%
78	15.292	2243	2245	2246	rBV2	12070	10927	2.15%	0.183%
79	15.357	2252	2256	2262	rVB	89490	115718	22.76%	1.934%
80	15.421	2262	2267	2272	rVV	160247	188420	37.07%	3.149%
81	15.480	2272	2277	2281	rVV	173153	224077	44.08%	3.745%
82	15.515	2281	2283	2289	rVB2	48824	63121	12.42%	1.055%
83	15.657	2304	2307	2309	rBV4	8458	11413	2.25%	0.191%
84	15.962	2356	2359	2362	rBV5	8814	12008	2.36%	0.201%
85	16.051	2370	2374	2378	rBV3	12365	19478	3.83%	0.326%
86	16.574	2461	2463	2465	rBV3	6783	6713	1.32%	0.112%
87	16.968	2523	2530	2537	rBV2	71170	133714	26.30%	2.235%
88	17.139	2553	2559	2564	rBV3	15931	36109	7.10%	0.604%
89	17.198	2566	2569	2574	rVB4	10980	18531	3.65%	0.310%
90	17.421	2601	2607	2614	rVB	44566	89871	17.68%	1.502%
91	17.551	2628	2629	2631	rBV2	7496	6163	1.21%	0.103%
92	17.662	2643	2648	2654	rBV3	22064	47904	9.42%	0.801%
93	18.574	2801	2803	2805	rBV3	4727	5335	1.05%	0.089%
94	18.786	2837	2839	2844	rBV6	3821	5089	1.00%	0.085%

Sum of corrected areas: 5983031

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Data File : BF101343.D
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Operator : SJ/JU
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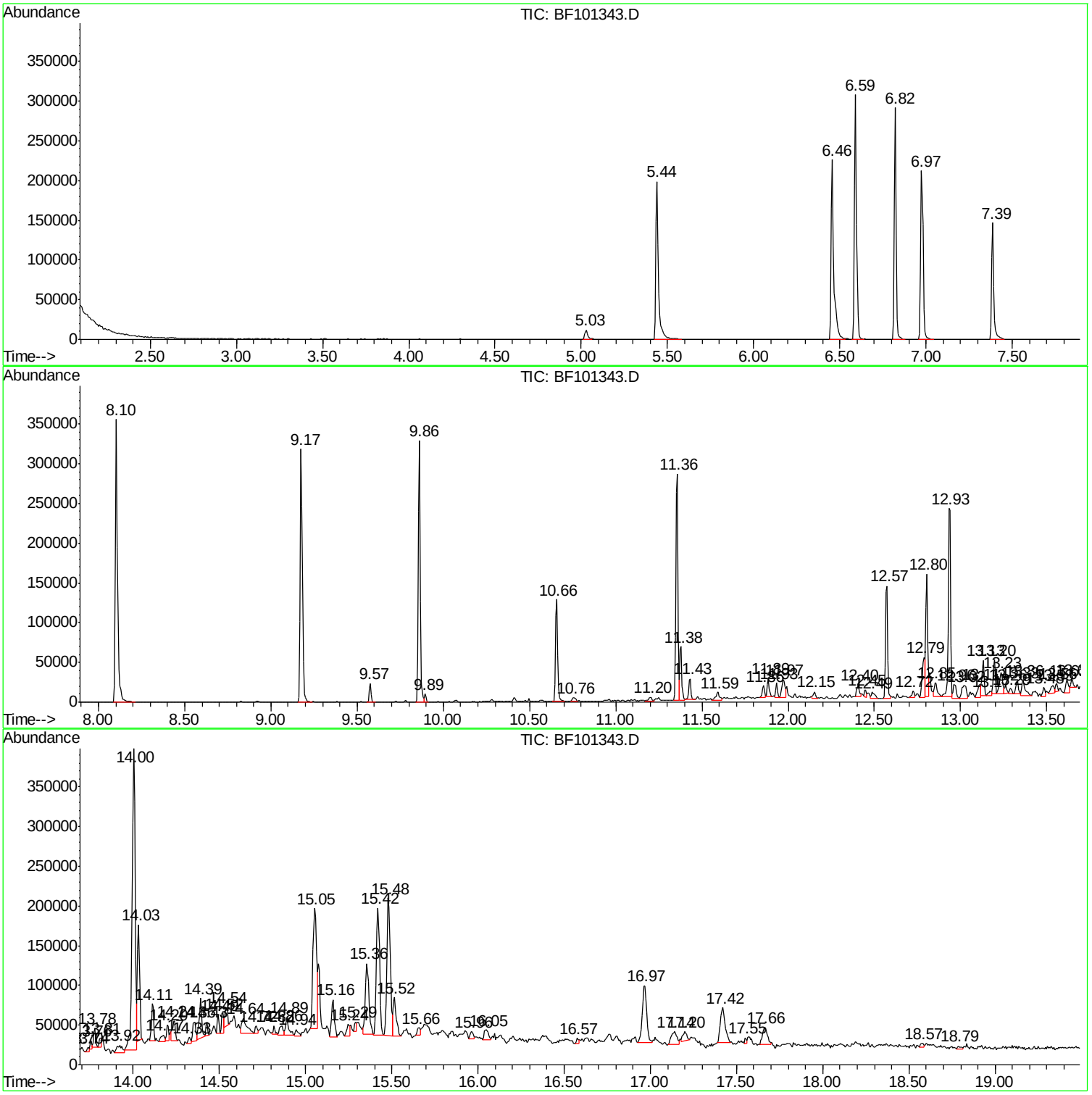
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-9(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121217\
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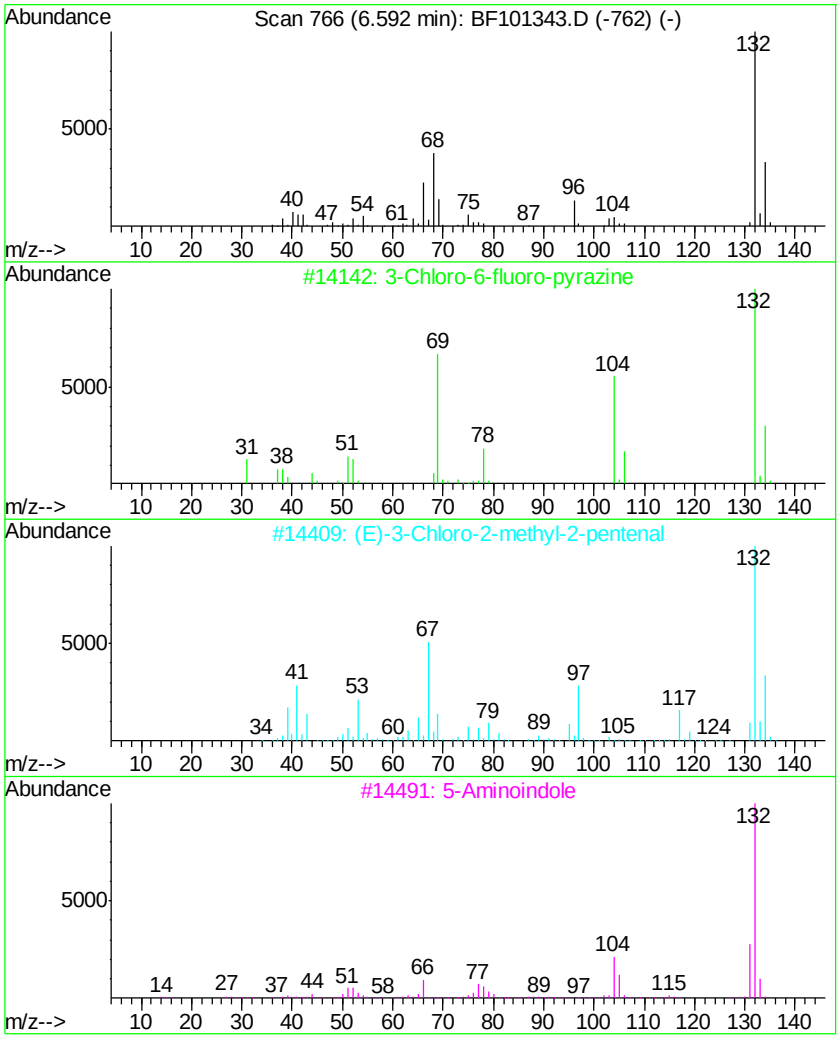
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

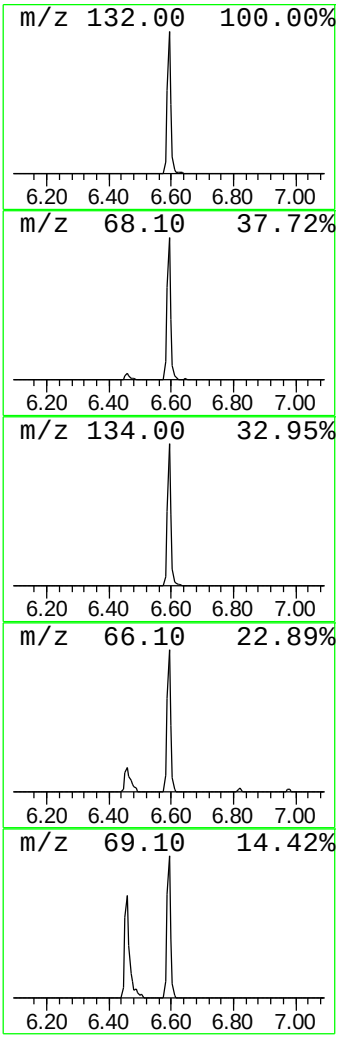
****

Peak Number 1 unknown6.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	21.29 ng	250987	1,4-Dichlorobenzene-d4	6.82

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	25
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121217\
Data File : BF101343.D
Acq On : 12 Dec 2017 21:20
Operator : SJ/JU
Sample : I6822-10 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-9(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

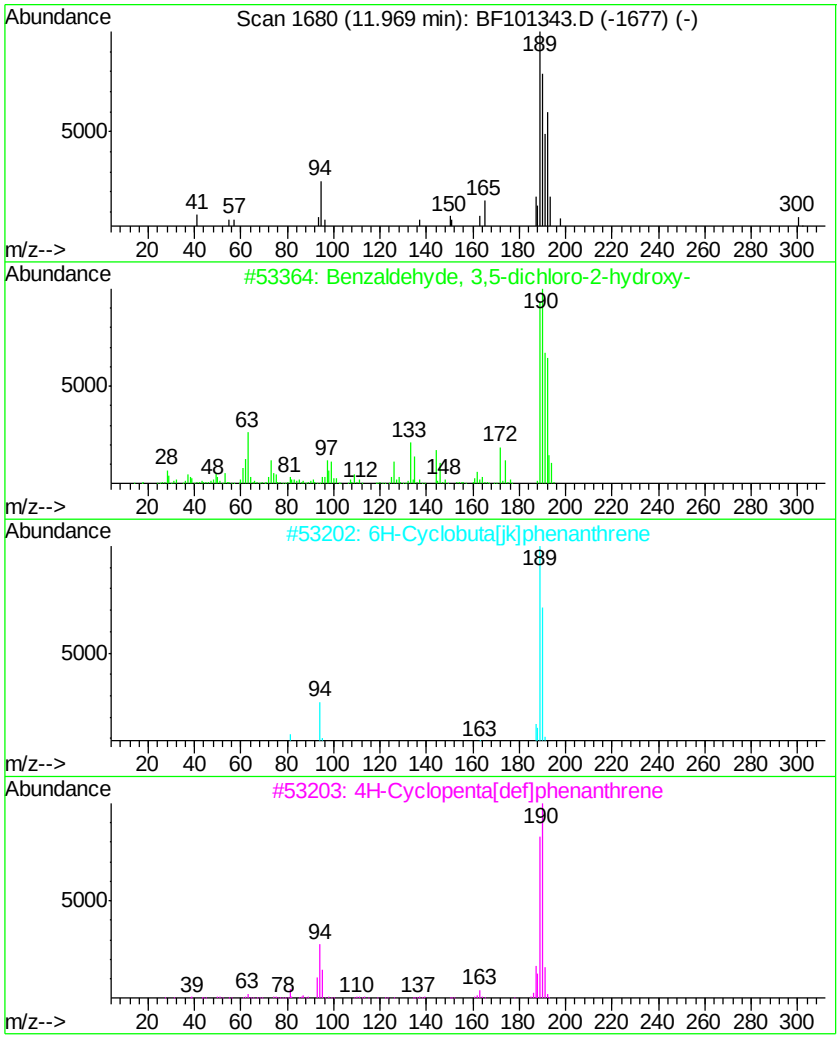
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

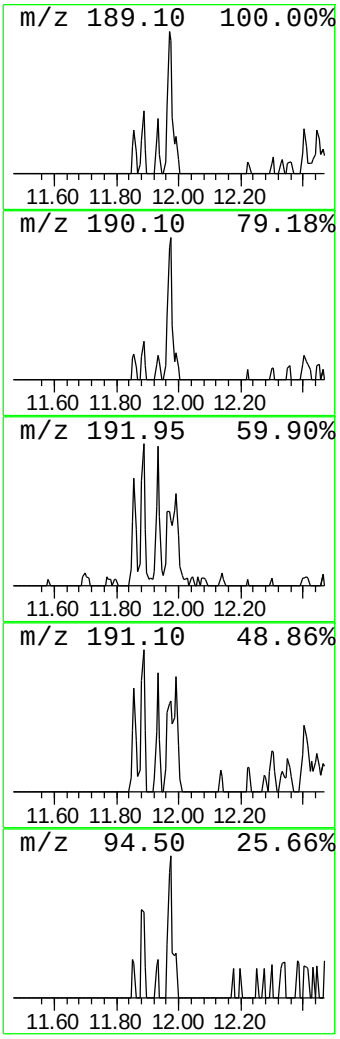
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.97	2.29 ng	29797	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	64
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	58
3	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	50
4	Isoquinoline, 1-chloro-3-ethyl-	191	C11H10ClN	055150-52-2	43
5	Methyl diselenide	190	C2H6Se2	007101-31-7	41





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Data File : BF101343.D
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Operator : SJ/JU
Sample : I6822-10 5X
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Instrument : BNA_F
ClientSampleId : SB-9(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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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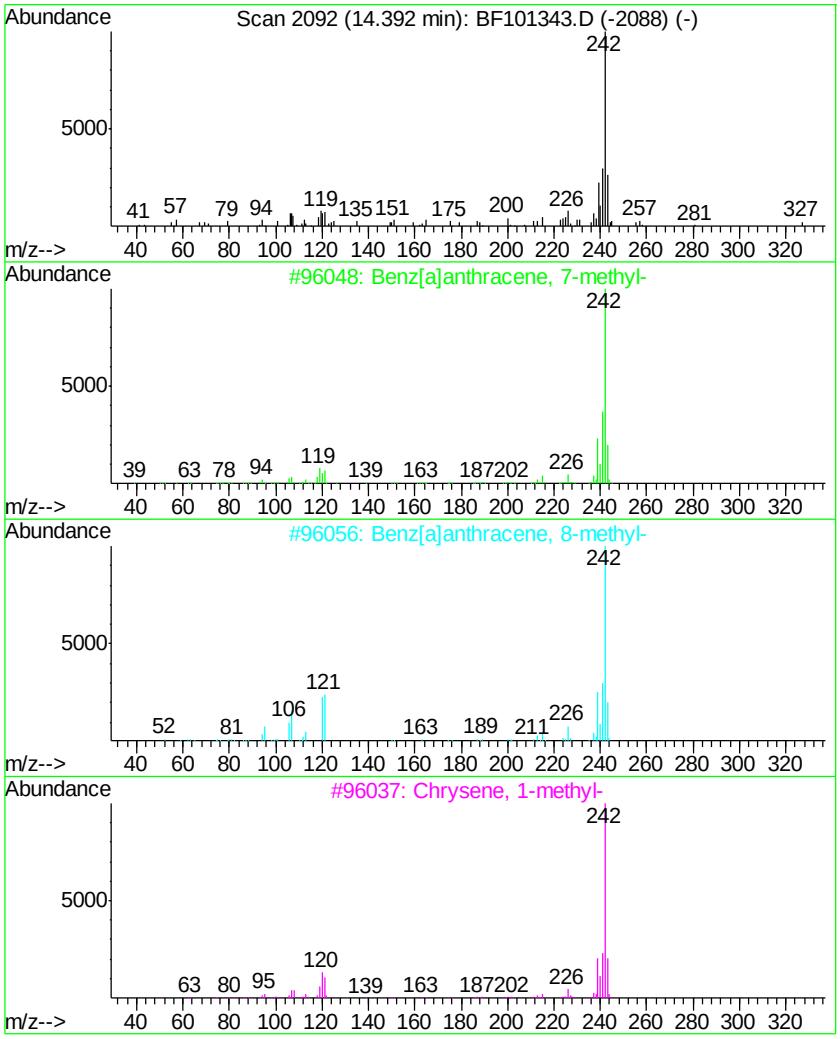
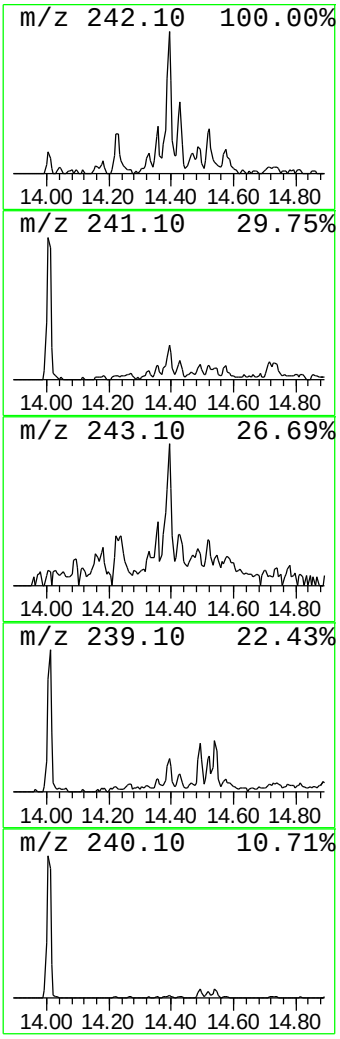
Peak Number 4 Benz[a]anthracene, 7-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.39	2.21 ng	56203	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benz[a]anthracene, 7-methyl-	242	C19H14	002541-69-7	91
2	Benz[a]anthracene, 8-methyl-	242	C19H14	002381-31-9	89
3	Chrysene, 1-methyl-	242	C19H14	003351-28-8	74
4	Benzo[c]phenanthrene, 3-methyl-	242	C19H14	002381-19-3	70
5	Chrysene, 6-methyl-	242	C19H14	001705-85-7	68





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Sample : I6822-10 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-9(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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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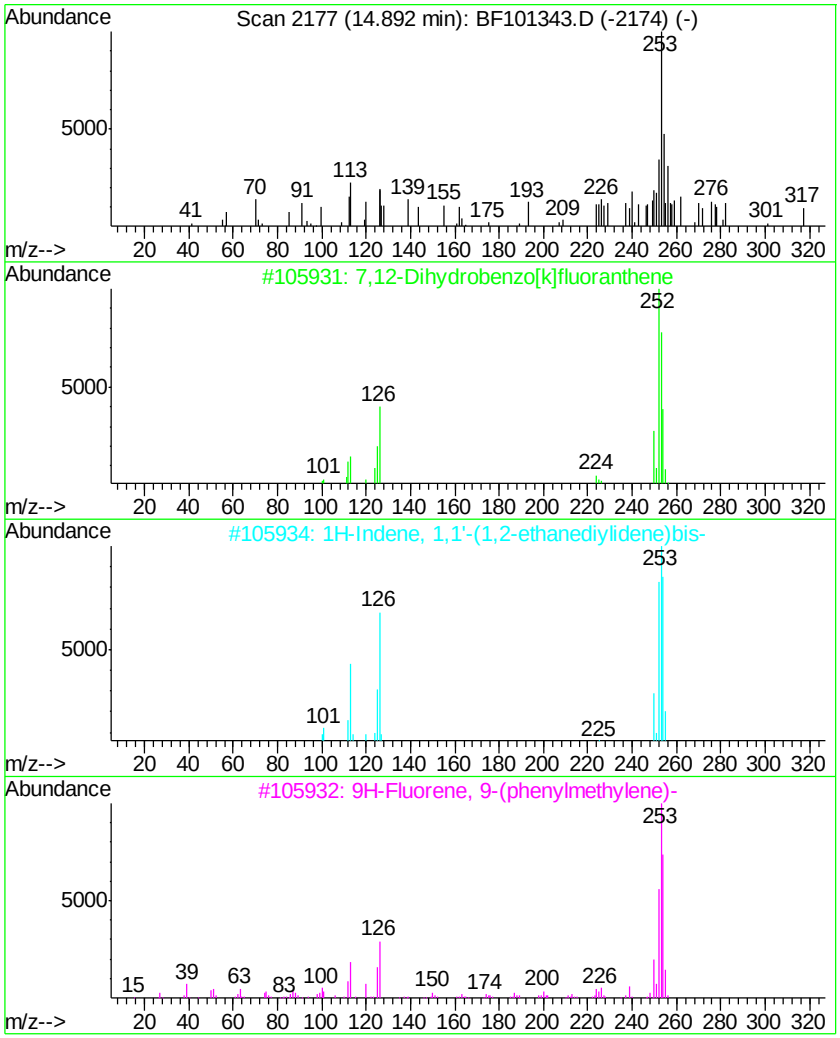
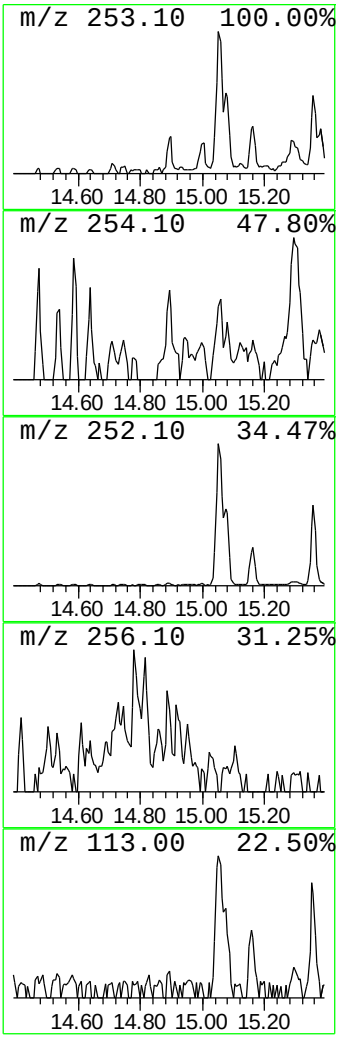
Peak Number 5 7,12-Dihydrobenzo[k]fluoran... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	2.61 ng	29209	Perylene-d12	15.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,12-Dihydrobenzo[k]fluoranthene	254	C20H14	1000080-17-7	52
2	1H-Indene, 1,1'-(1,2-ethanediyli...	254	C20H14	072088-04-1	43
3	9H-Fluorene, 9-(phenylmethylene)-	254	C20H14	001836-87-9	38
4	1H-Pyrrolo[2,3-f]quinolin-9-ol, ...	254	C16H18N2O	1000303-71-9	38
5	2-Chloro-4-iodoaniline	253	C6H5ClIN	042016-93-3	38





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121217\
Data File : BF101343.D
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Operator : SJ/JU
Sample : I6822-10 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-9(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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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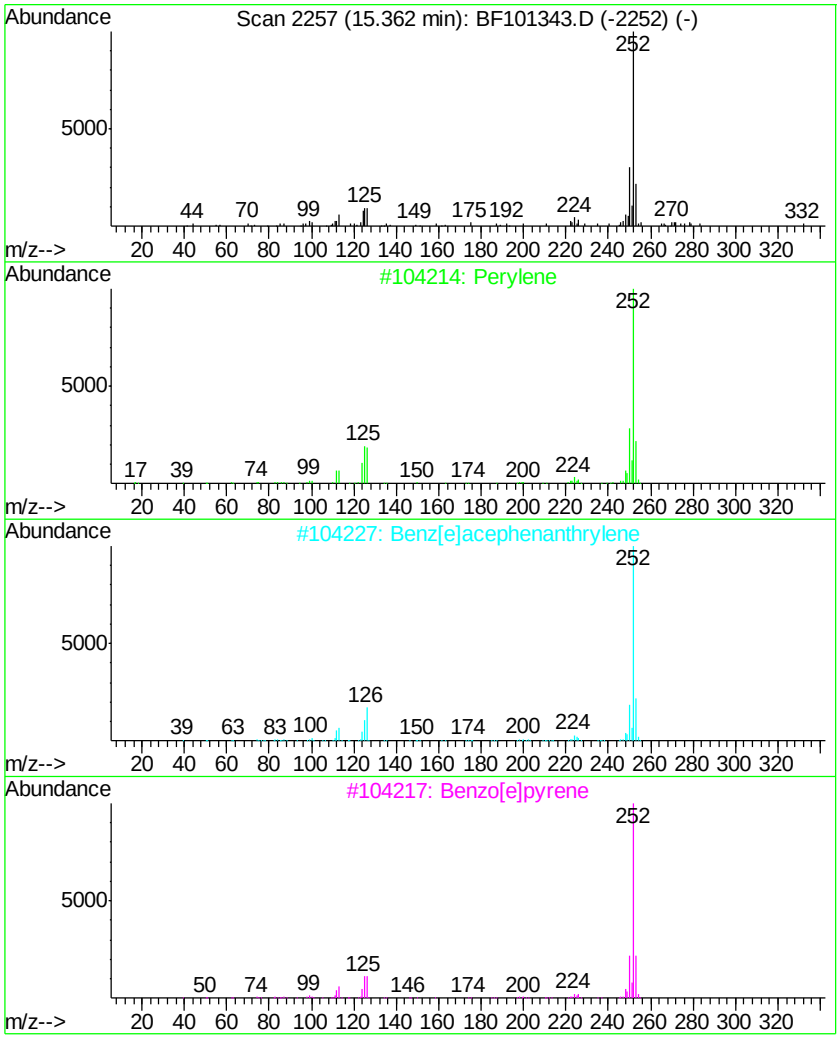
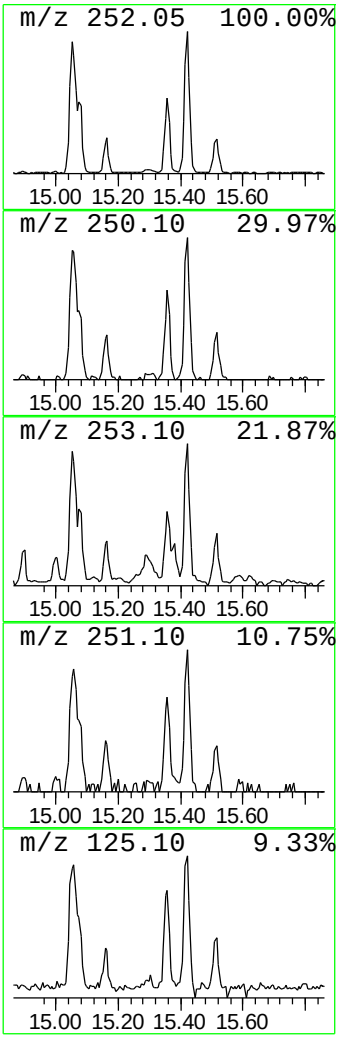
Peak Number 7 Perylene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.36	10.33 ng	115718	Perylene-d12	15.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	90
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	90
3	Benzo[e]pyrene	252	C20H12	000192-97-2	90
4	Benzo[a]pyrene	252	C20H12	000050-32-8	81
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	81





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121217\
Data File : BF101343.D
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Operator : SJ/JU
Sample : I6822-10 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-9(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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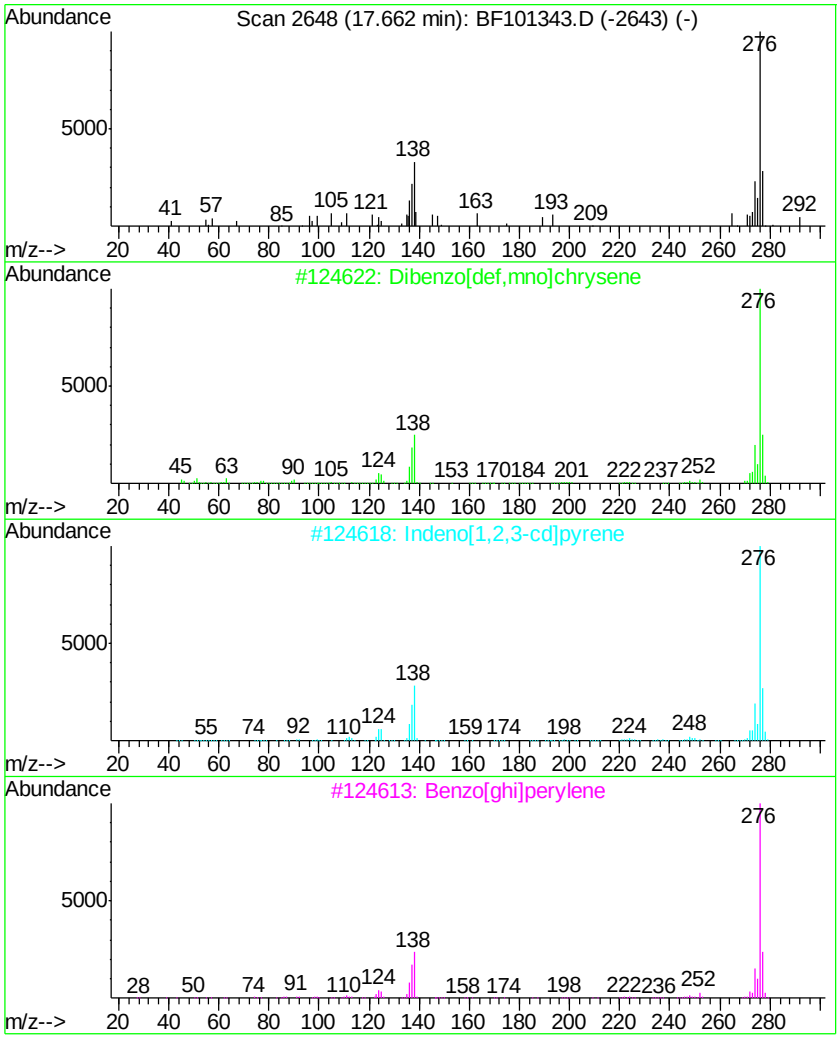
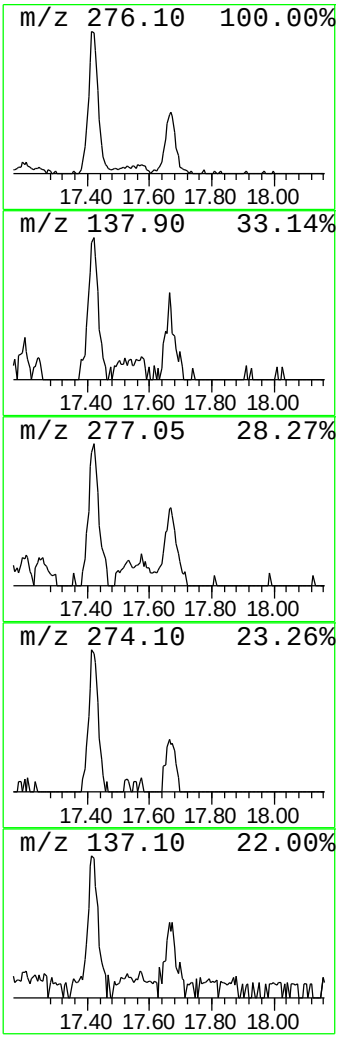
Peak Number 9 Dibenzo[def,mno]chrysene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.66	4.28 ng	47904	Perylene-d12	15.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	87
2	Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	87
3	Benzo[ghi]perylene	276	C22H12	000191-24-2	81
4	Indeno[1,2,3-cd]fluoranthene	276	C22H12	000193-43-1	74
5	2-Naphthalenol, 1-[(2,4-dimethyl...	276	C18H16N2O	003118-97-6	37





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121217\
Data File : BF101343.D
Acq On : 12 Dec 2017 21:20
Operator : SJ/JU
Sample : I6822-10 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-9(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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
unknown6.59	6.59	21.3	ng	250987	1	6.82	235807	20.0
Benzaldehyde, 3,5...	11.97	2.3	ng	29797	4	11.36	260615	20.0
Benz[a]anthracene...	14.39	2.2	ng	56203	5	14.00	508322	20.0
7,12-Dihydrobenzo...	14.89	2.6	ng	29209	6	15.48	224077	20.0
Perylene	15.36	10.3	ng	115718	6	15.48	224077	20.0
Dibenzo[def,mno]c...	17.66	4.3	ng	47904	6	15.48	224077	20.0