LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112917\
Data File : BF100991.D
Acq On : 29 Nov 2017 21:11
Operator : SJ/JU
Sample : I6610-15
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-X(0-2)-20171127

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	5.081	506	509	518	rBV	73738	97125	5.01%	0.335%
2	5.475	572	576	580	rBV	1307870	1298473	67.00%	4.483%
3	6.492	744	749	758	rVB	1352536	1364238	70.39%	4.710%
4	6.628	768	772	775	rBV	1594171	1368672	70.62%	4.726%
5	6.851	807	810	814	rBV	422530	361695	18.66%	1.249%
6	7.010	833	837	840	rBV	1230154	1024002	52.83%	3.536%
7	7.422	902	907	910	rBV	810498	810297	41.81%	2.798%
8	8.133	1025	1028	1031	rBV	521785	457457	23.60%	1.579%
9	8.945	1163	1166	1169	rBV	38746	28220	1.46%	0.097%
10	9.210	1207	1211	1214	rBV	1627079	1314532	67.83%	4.539%
11	9.545	1263	1268	1271	rBV	42744	47006	2.43%	0.162%
12	9.604	1275	1278	1280	rBV	145643	118401	6.11%	0.409%
13	9.751	1298	1303	1306	rBV	74492	61131	3.15%	0.211%
14	9.810	1309	1313	1318	rVB	56560	50343	2.60%	0.174%
15	9.892	1323	1327	1330	rVV	516041	443315	22.87%	1.531%
16	9.921	1330	1332	1335	rVB	147338	107714	5.56%	0.372%
17	10.092	1356	1361	1365	rVV2	65258	66568	3.43%	0.230%
18	10.310	1396	1398	1402	rVB	62395	53506	2.76%	0.185%
19	10.439	1416	1420	1424	rVB	119367	103012	5.32%	0.356%
20	10.592	1444	1446	1453	rVB	34400	34417	1.78%	0.119%
21	10.680	1457	1461	1465	rVB	852999	745760	38.48%	2.575%
22	10.786	1476	1479	1487	rVB3	47478	65146	3.36%	0.225%
23	10.986	1506	1513	1516	rBV3	40419	54280	2.80%	0.187%
24	11.110	1529	1534	1536	rBV3	24430	30582	1.58%	0.106%
25	11.186	1544	1547	1550	rVB	49793	44868	2.32%	0.155%
26	11.233	1550	1555	1557	rVV2	43236	51355	2.65%	0.177%
27	11.274	1557	1562	1567	rVB	70970	67865	3.50%	0.234%
28	11.380	1576	1580	1582	rBV	467353	413941	21.36%	1.429%
29	11.410	1582	1585	1588	rVV	1062764	982422	50.69%	3.392%
30	11.457	1588	1593	1596	rVV	311673	253449	13.08%	0.875%
31	11.610	1612	1619	1623	rBV2	102858	113556	5.86%	0.392%
32	11.674	1626	1630	1633	rVV2	30595	37911	1.96%	0.131%
33	11.710	1633	1636	1640	rVB4	42467	42984	2.22%	0.148%
34	11.880	1660	1665	1667	rVV	194443	198783	10.26%	0.686%

LSC Area Percent Report

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Acq On : 29 Nov 2017 21:11
Operator : SJ/JU
Sample : I6610-15
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-X(0-2)-20171127

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

35	11.904	1667	1669	1673	rVV2	372311	384914	19.86%	1.329%
36	11.957	1676	1678	1681	rVV	103804	85645	4.42%	0.296%
37	11.992	1681	1684	1687	rVV	278822	331243	17.09%	1.144%
38	12.015	1687	1688	1692	rVB	138826	75815	3.91%	0.262%
39	12.063	1692	1696	1698	rBV3	23710	29225	1.51%	0.101%
40	12.174	1712	1715	1718	rVV	140265	116024	5.99%	0.401%
41	12.204	1718	1720	1725	rVB	109536	88459	4.56%	0.305%
42	12.321	1738	1740	1743	rVB	39244	34545	1.78%	0.119%
43	12.357	1743	1746	1748	rBV	37732	28639	1.48%	0.099%
44	12.380	1748	1750	1752	rVB	42292	30158	1.56%	0.104%
45	12.427	1752	1758	1761	rBV	101619	128233	6.62%	0.443%
46	12.468	1761	1765	1767	rVV4	63459	92956	4.80%	0.321%
47	12.521	1771	1774	1778	rVB	91298	101686	5.25%	0.351%
48	12.604	1783	1788	1791	rBV	1576452	1600021	82.56%	5.524%
49	12.657	1795	1797	1799	rVV	53494	40053	2.07%	0.138%
50	12.686	1799	1802	1805	rVV2	112279	99680	5.14%	0.344%
51	12.745	1805	1812	1815	rVV3	68875	114037	5.88%	0.394%
52	12.833	1820	1827	1831	rVV2	1442452	1733359	89.44%	5.985%
53	12.874	1831	1834	1838	rVB2	84474	98441	5.08%	0.340%
54	12.962	1838	1849	1852	rBV	1146905	1164035	60.06%	4.019%
55	13.039	1856	1862	1866	rBV3	133404	222301	11.47%	0.768%
56	13.074	1866	1868	1870	rVV	35959	30643	1.58%	0.106%
57	13.127	1873	1877	1878	rVV3	110729	123923	6.39%	0.428%
58	13.151	1878	1881	1884	rVV	264868	268595	13.86%	0.927%
59	13.186	1884	1887	1890	rVV2	27313	37272	1.92%	0.129%
60	13.221	1890	1893	1895	rVV2	186891	186725	9.63%	0.645%
61	13.257	1895	1899	1901	rVV2	197104	232951	12.02%	0.804%
62	13.280	1901	1903	1906	rVV3	62763	66290	3.42%	0.229%
63	13.310	1906	1908	1911	rVV2	45980	47722	2.46%	0.165%
64	13.351	1912	1915	1918	rVV3	106698	117518	6.06%	0.406%
65	13.380	1918	1920	1923	rVV	108246	107811	5.56%	0.372%
66	13.439	1926	1930	1932	rVV4	64835	76654	3.96%	0.265%
67	13.462	1932	1934	1937	rVB2	34727	32209	1.66%	0.111%
68	13.527	1942	1945	1948	rBV3	37837	58997	3.04%	0.204%
69	13.633	1960	1963	1965	rBV3	31014	34300	1.77%	0.118%
70	13.662	1965	1968	1972	rVB	131893	135260	6.98%	0.467%
71	13.768	1982	1986	1989	rBV2	148573	181680	9.37%	0.627%

LSC Area Percent Report

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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-X(0-2)-20171127

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-BF110817.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	13.798	1989	1991	1993	rVV	152170	131468	6.78%	0.454%
73	13.827	1993	1996	1997	rVV	116221	126256	6.51%	0.436%
74	13.851	1997	2000	2002	rVV2	176684	233158	12.03%	0.805%
75	13.868	2002	2003	2006	rVB	143797	93049	4.80%	0.321%
76	13.998	2020	2025	2027	rBV	1726280	1938114	100.00%	6.692%
77	14.021	2027	2029	2032	rVV2	903562	1064546	54.93%	3.676%
78	14.051	2032	2034	2041	rVB	710174	715025	36.89%	2.469%
79	14.109	2041	2044	2045	rBV3	32053	31005	1.60%	0.107%
80	14.133	2045	2048	2052	rVV	158905	164075	8.47%	0.567%
81	14.168	2052	2054	2057	rVV2	66446	81965	4.23%	0.283%
82	14.215	2060	2062	2064	rVV	77410	64969	3.35%	0.224%
83	14.251	2064	2068	2071	rVV2	85750	115411	5.95%	0.398%
84	14.280	2071	2073	2076	rVB2	36477	30878	1.59%	0.107%
85	14.368	2086	2088	2091	rBV2	36147	36213	1.87%	0.125%
86	14.409	2092	2095	2098	rVV	147347	132804	6.85%	0.459%
87	14.445	2098	2101	2104	rVV	72096	60858	3.14%	0.210%
88	14.486	2104	2108	2110	rVV4	57810	90596	4.67%	0.313%
89	14.533	2114	2116	2118	rVV	77065	76114	3.93%	0.263%
90	14.556	2118	2120	2123	rVB2	84144	70668	3.65%	0.244%
91	14.721	2146	2148	2150	rBV2	33603	27909	1.44%	0.096%
92	15.074	2203	2208	2211	rBV	484570	804064	41.49%	2.776%
93	15.174	2222	2225	2232	rVB	102821	130437	6.73%	0.450%
94	15.374	2255	2259	2265	rVB	276038	386249	19.93%	1.334%
95	15.439	2265	2270	2275	rBV	435598	528660	27.28%	1.825%
96	15.498	2276	2280	2283	rVV	231553	305573	15.77%	1.055%
97	15.533	2283	2286	2293	rVB	124101	174159	8.99%	0.601%
98	16.980	2526	2532	2540	rVB2	172236	339185	17.50%	1.171%
99	17.433	2603	2609	2620	rBV	122719	275942	14.24%	0.953%
100	17.668	2644	2649	2655	rBV	38950	82059	4.23%	0.283%

Sum of corrected areas: 28962454

LSC Report - Integrated Chromatogram

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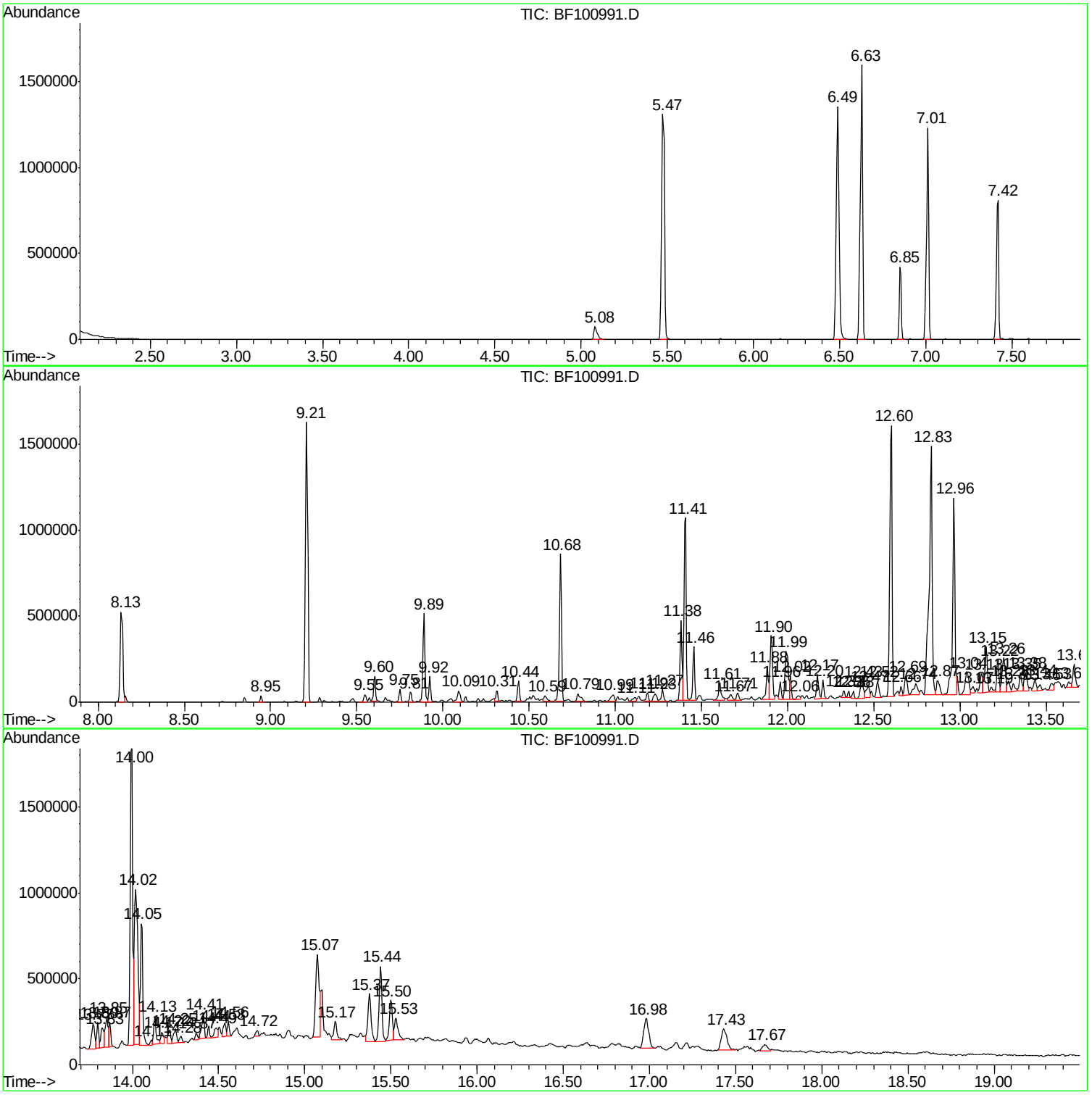
Data File : BF100991.D
Acq On : 29 Nov 2017 21:11
Operator : SJ/JU
Sample : I6610-15
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-X(0-2)-20171127

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\BF112917\
Data File : BF100991.D
Acq On : 29 Nov 2017 21:11
Operator : SJ/JU
Sample : I6610-15
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-X(0-2)-20171127

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

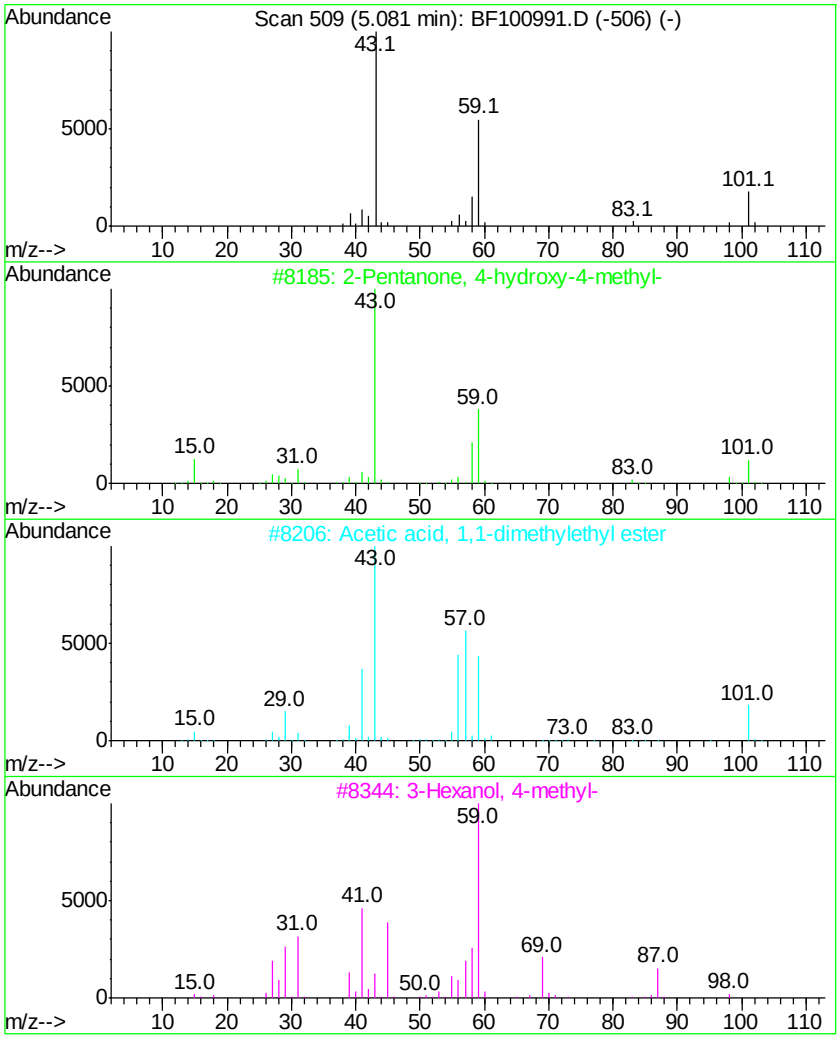
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

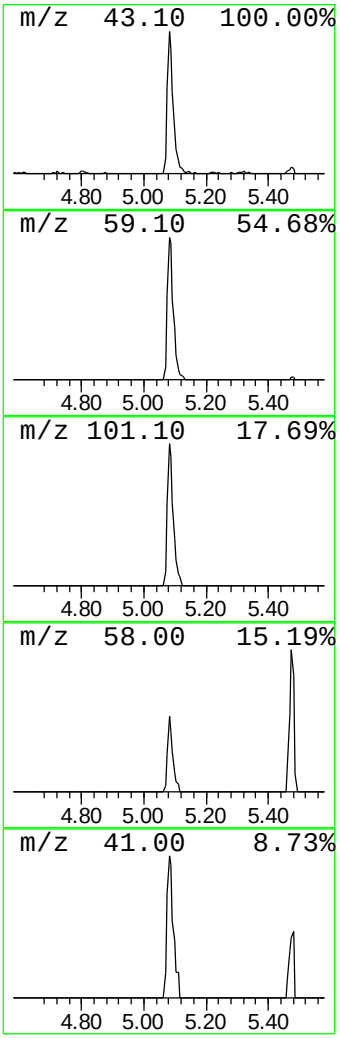
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	5.37 ng	97125	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	32
5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	23





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Sample : I6610-15
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Instrument :
BNA_F
ClientSampleId :
SB-X(0-2)-20171127

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

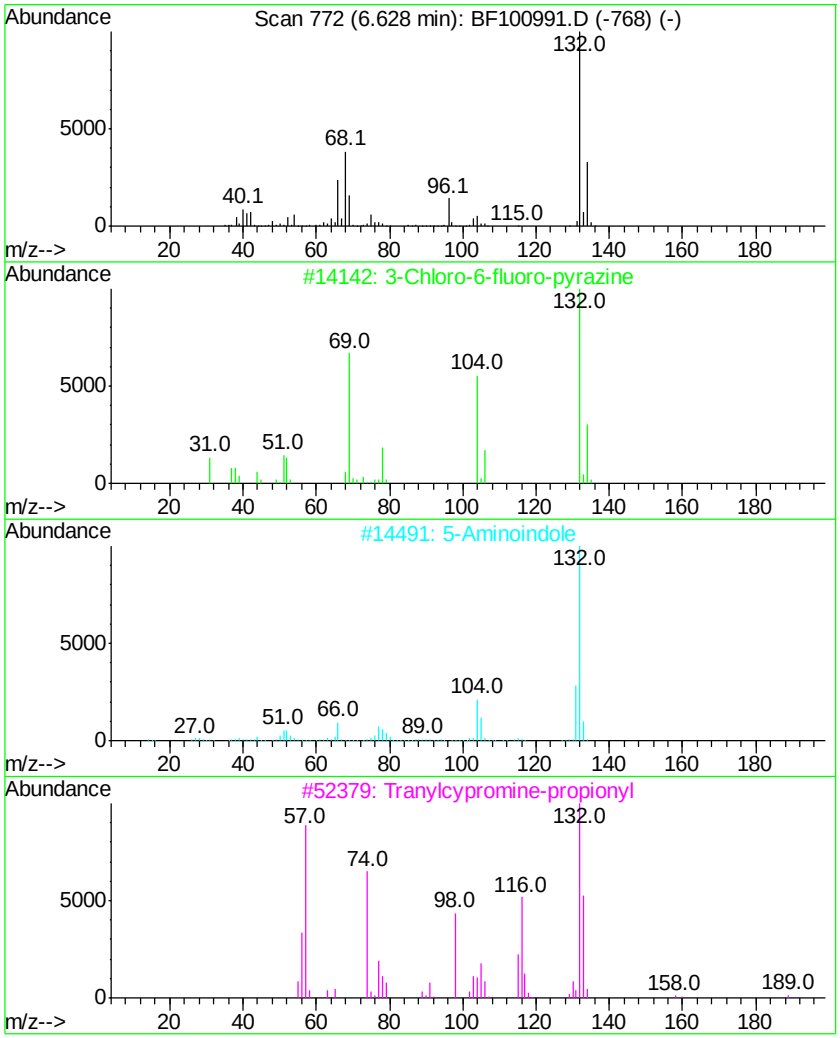
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

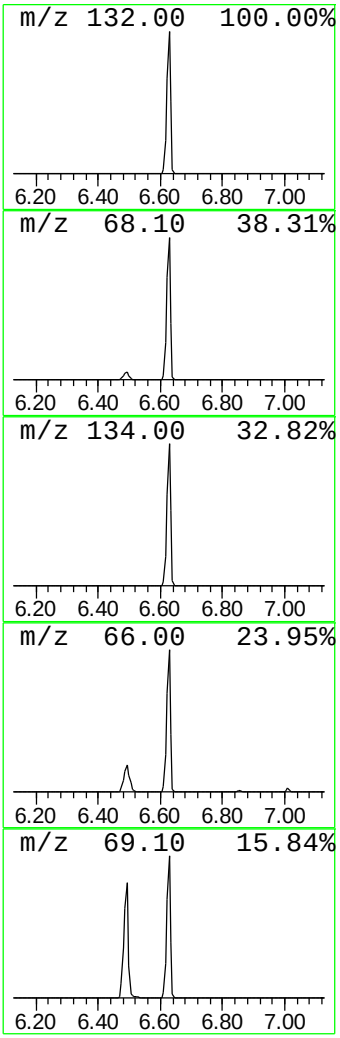
****

Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	75.68 ng	1368670	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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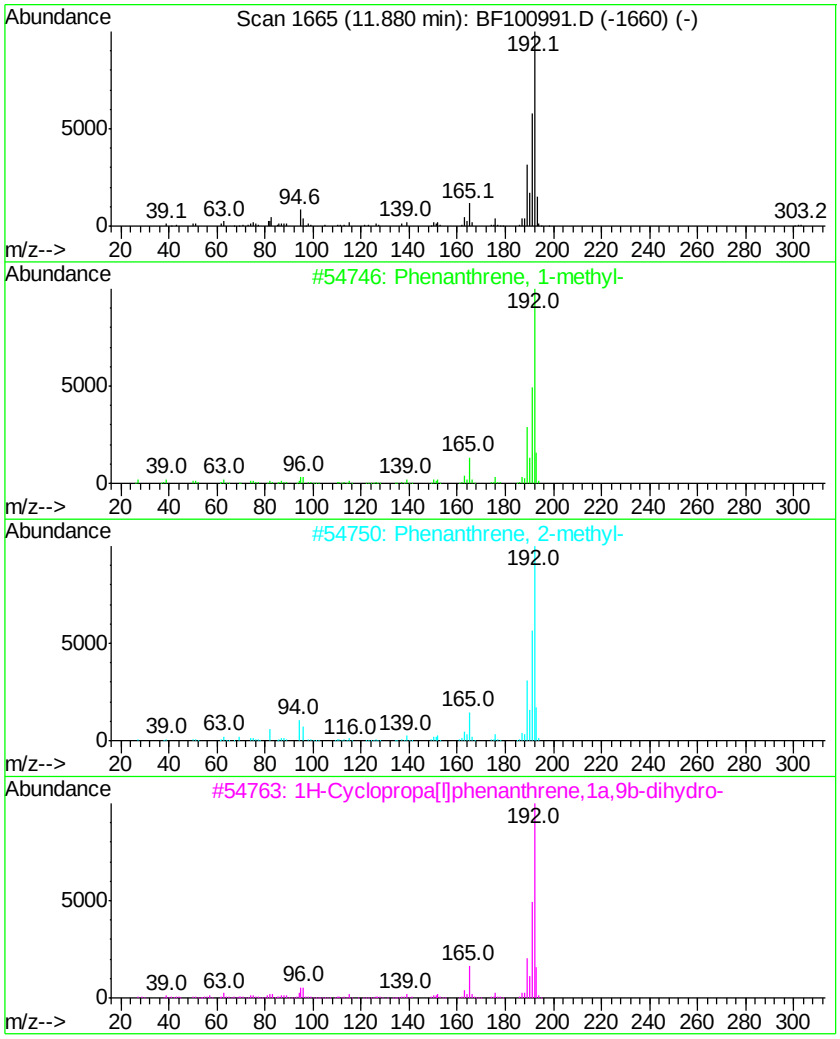
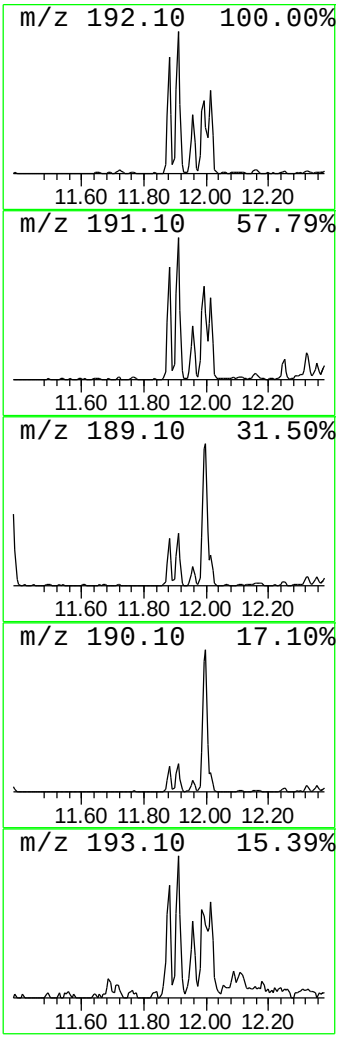
****

Peak Number 4 Phenanthrene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	9.60 ng	198783	Phenanthrene-d10	11.38

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	95
3	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	95
4	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	94
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	94





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Sample : I6610-15
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-X(0-2)-20171127

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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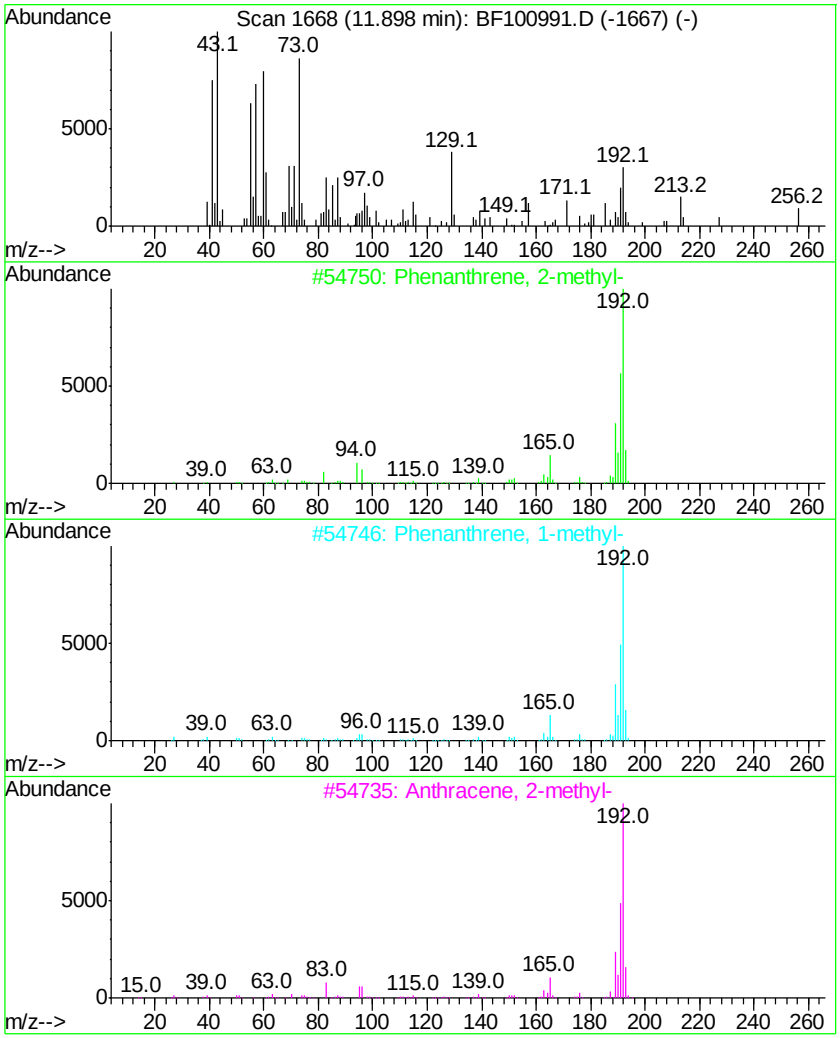
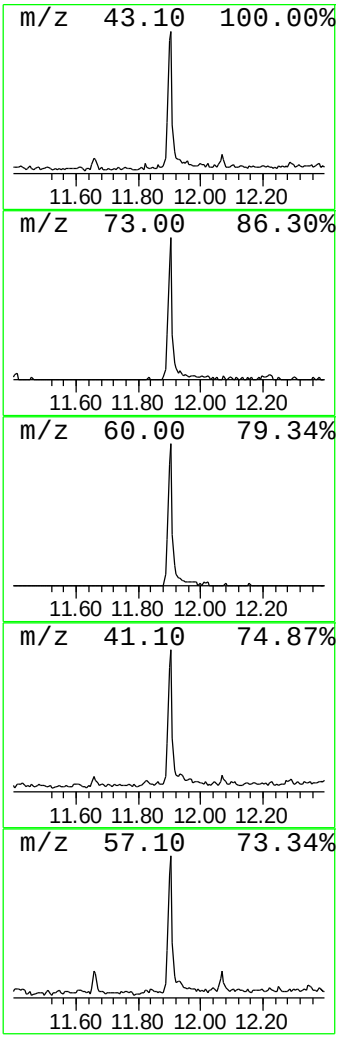
Peak Number 5 Phenanthrene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	18.60 ng	384914	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	98
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	97
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	97
4	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	96
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	95





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Data File : BF100991.D
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Operator : SJ/JU
Sample : I6610-15
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-X(0-2)-20171127

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

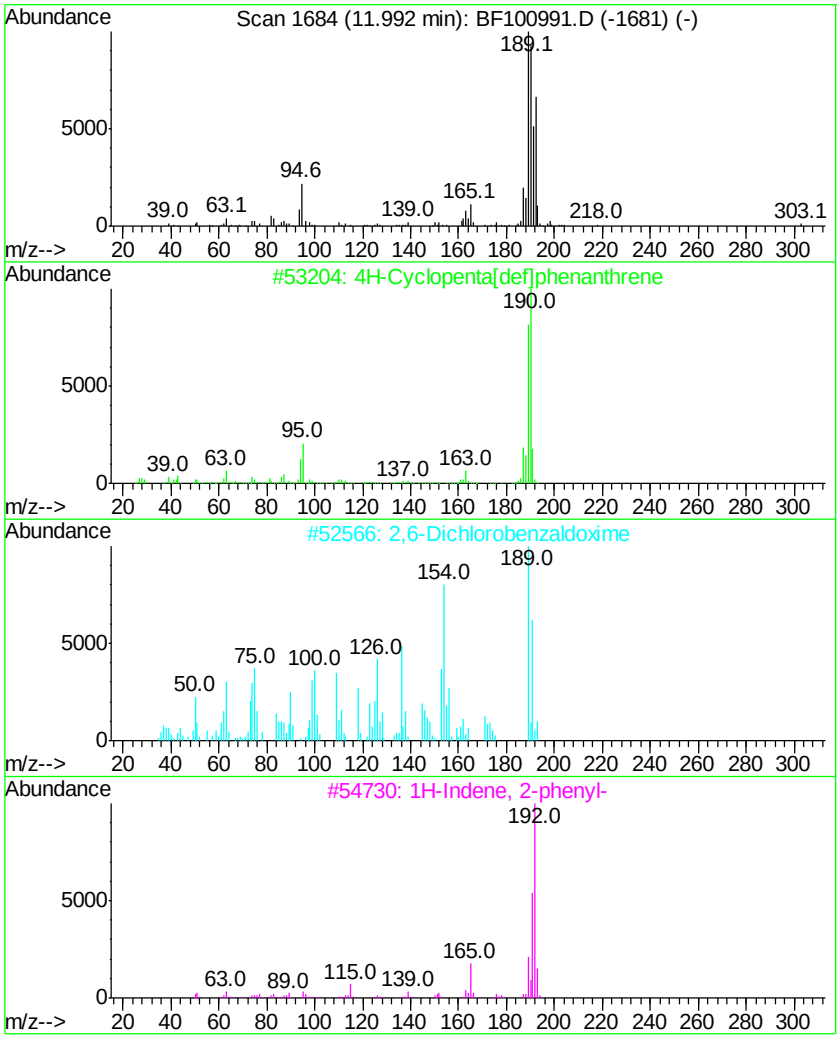
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

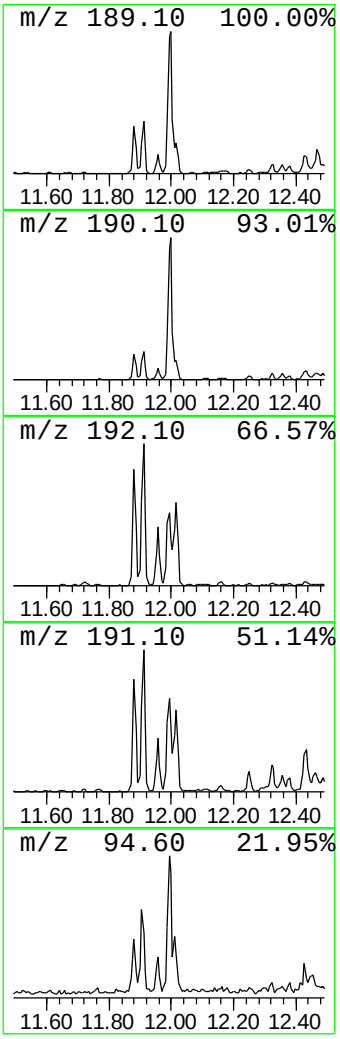
****

Peak Number 7 unknown11.99 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	16.00 ng	331243	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	49
2	2,6-Dichlorobenzaldoxime	189	C7H5Cl2NO	025185-95-9	42
3	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	38
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	30
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	30





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112917\
Data File : BF100991.D
Acq On : 29 Nov 2017 21:11
Operator : SJ/JU
Sample : I6610-15
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-X(0-2)-20171127

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

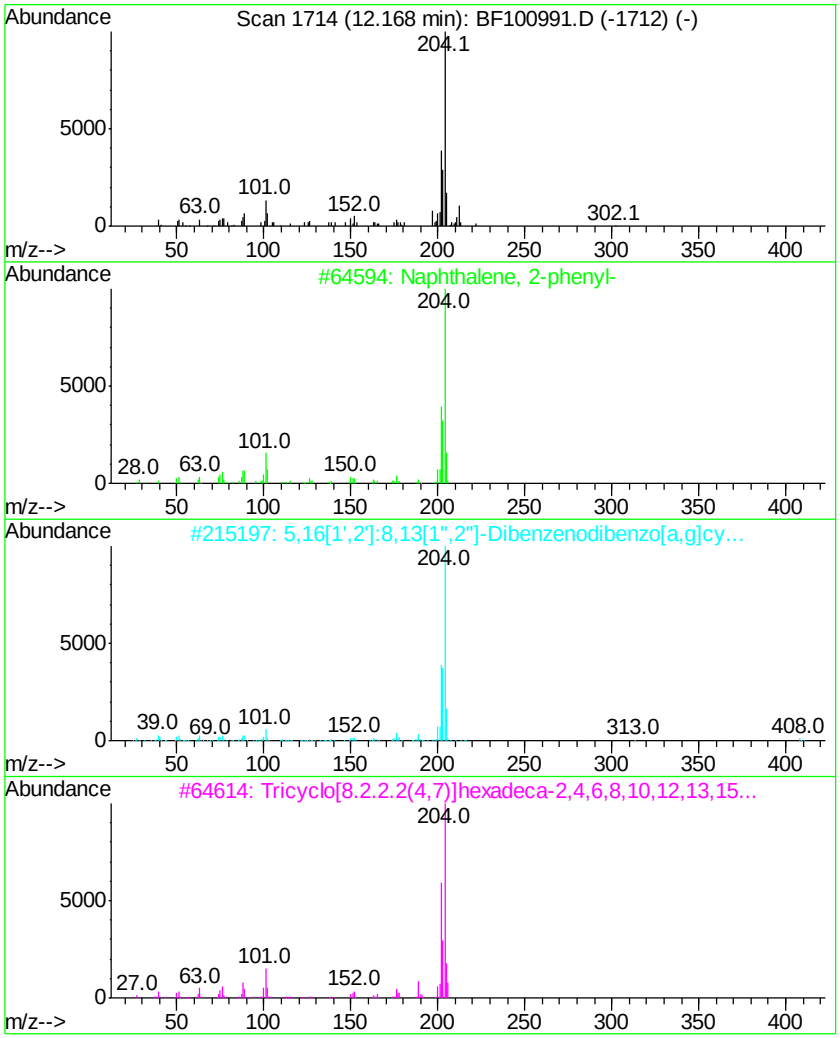
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

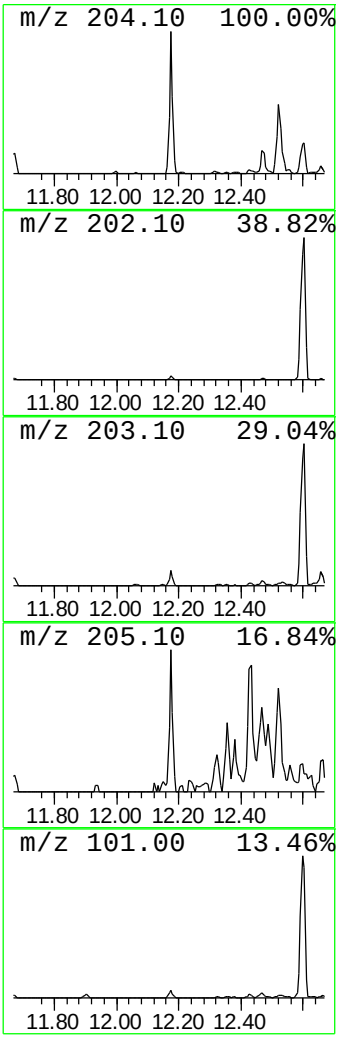
****

Peak Number 8 Naphthalene, 2-phenyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.17	5.61 ng	116024	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-phenyl-	204	C16H12	000612-94-2	93
2	5,16[1',2']:8,13[1'',2'']-Dibenz...	408	C32H24	005672-97-9	87
3	Tricyclo[8.2.2.2(4,7)]hexadeca-2...	204	C16H12	006572-60-7	64
4	9,10-Bis(bromomethyl)anthracene	362	C16H12Br2	034373-96-1	58
5	Naphthalene, 1-phenyl-	204	C16H12	000605-02-7	58





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Data File : BF100991.D
Acq On : 29 Nov 2017 21:11
Operator : SJ/JU
Sample : I6610-15
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-X(0-2)-20171127

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

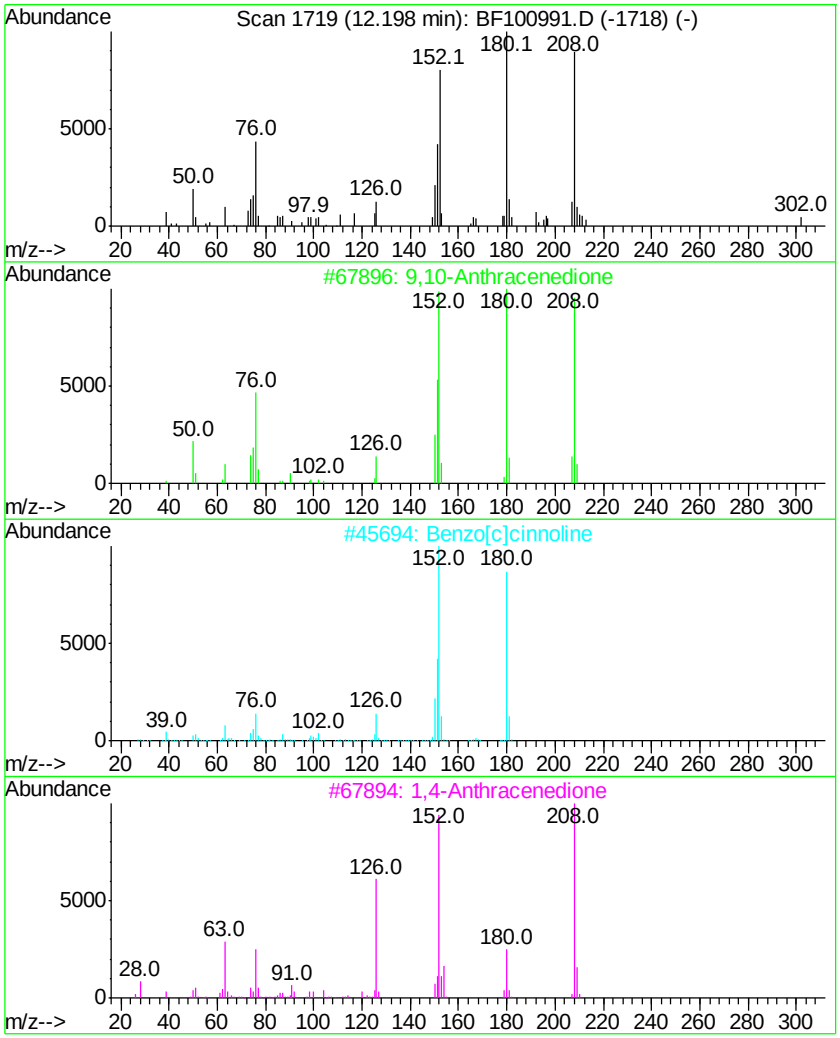
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

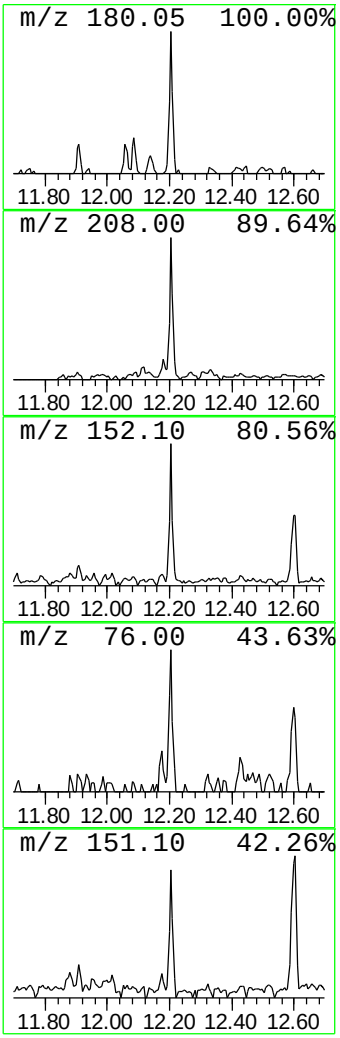
****

Peak Number 9 9,10-Anthracenedione Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.20	4.27 ng	88459	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Anthracenedione	208	C14H8O2	000084-65-1	98
2	Benzo[c]cinnoline	180	C12H8N2	000230-17-1	93
3	1,4-Anthracenedione	208	C14H8O2	000635-12-1	70
4	Benzo[h]cinnoline	180	C12H8N2	000230-31-9	64
5	1H-Phenalen-1-one	180	C13H8O	000548-39-0	64





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Operator : SJ/JU
Sample : I6610-15
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-X(0-2)-20171127

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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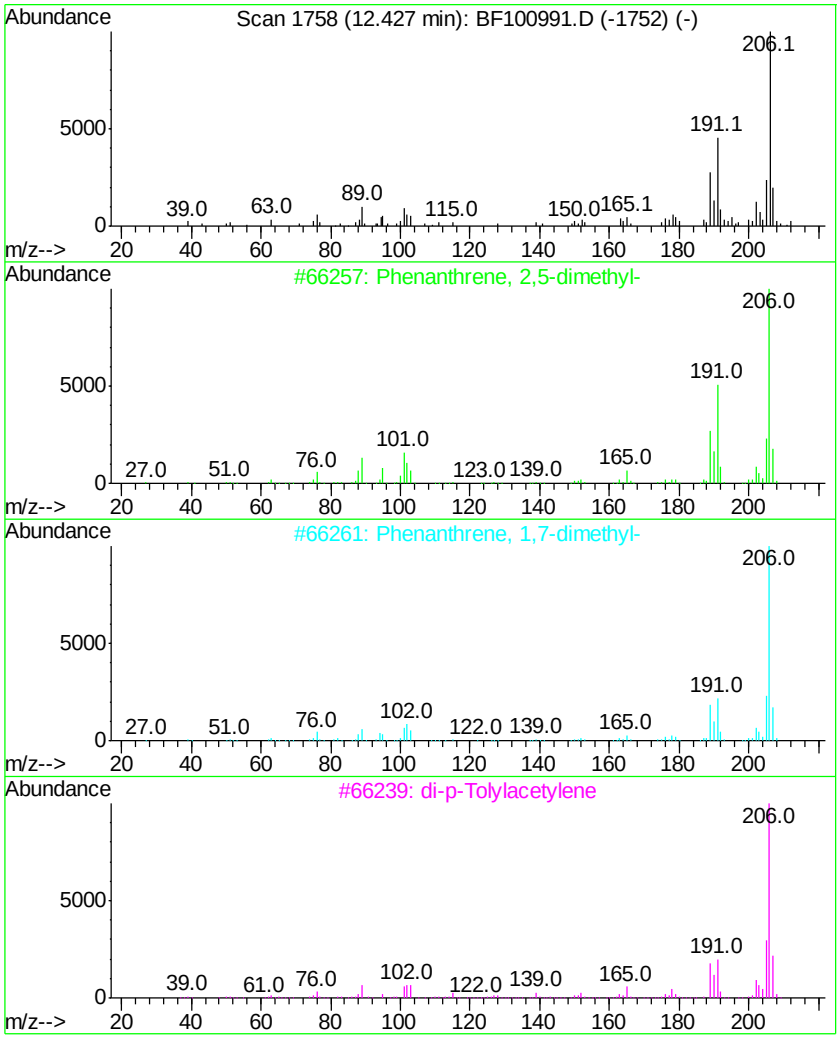
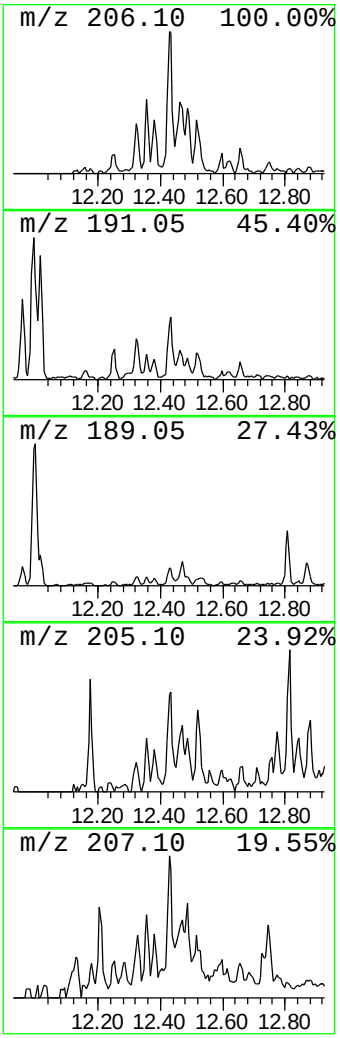
Peak Number 10 Phenanthrene, 2,5-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.43	6.20 ng	128233	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	97
2	Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	93
3	di-p-Tolylacetylene	206	C16H14	002789-88-0	93
4	9,10-Dimethylanthracene	206	C16H14	000781-43-1	93
5	Phenanthrene, 2,7-dimethyl-	206	C16H14	001576-69-8	93





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112917\
Data File : BF100991.D
Acq On : 29 Nov 2017 21:11
Operator : SJ/JU
Sample : I6610-15
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-X(0-2)-20171127

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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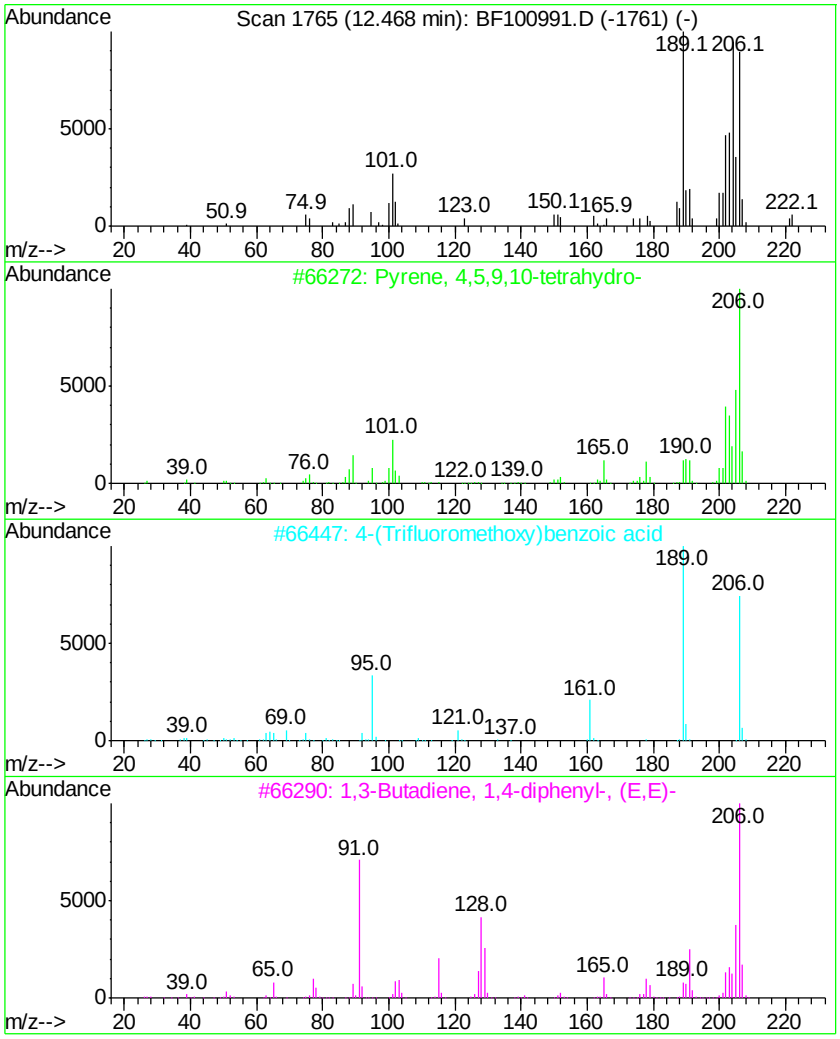
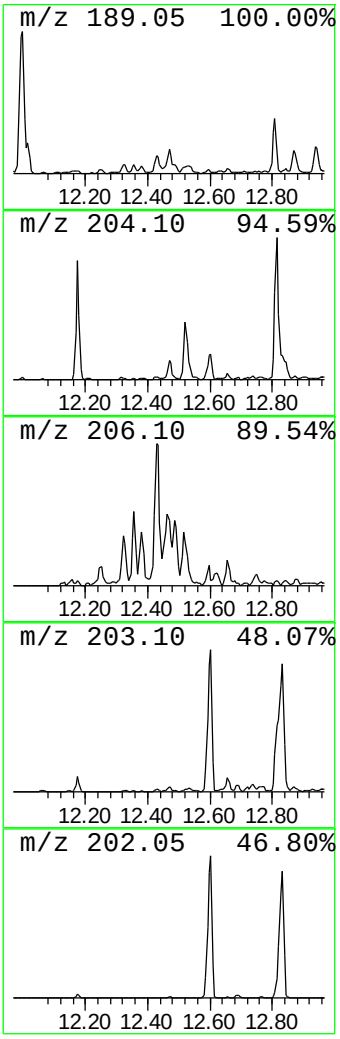
Peak Number 11 unknown12.47 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.47	4.49 ng	92956	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 4,5,9,10-tetrahydro-	206	C16H14	000781-17-9	38
2	4-(Trifluoromethoxy)benzoic acid	206	C8H5F3O3	000330-12-1	27
3	1,3-Butadiene, 1,4-diphenyl-, (E...	206	C16H14	000538-81-8	25
4	Benzene, 1,1'-(1-buten-3-yne-1,4...	204	C16H12	013141-45-2	25
5	Indeno[2,1-a]indene, 4b,5,9b,10-...	206	C16H14	005695-17-0	25





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Data File : BF100991.D
Acq On : 29 Nov 2017 21:11
Operator : SJ/JU
Sample : I6610-15
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-X(0-2)-20171127

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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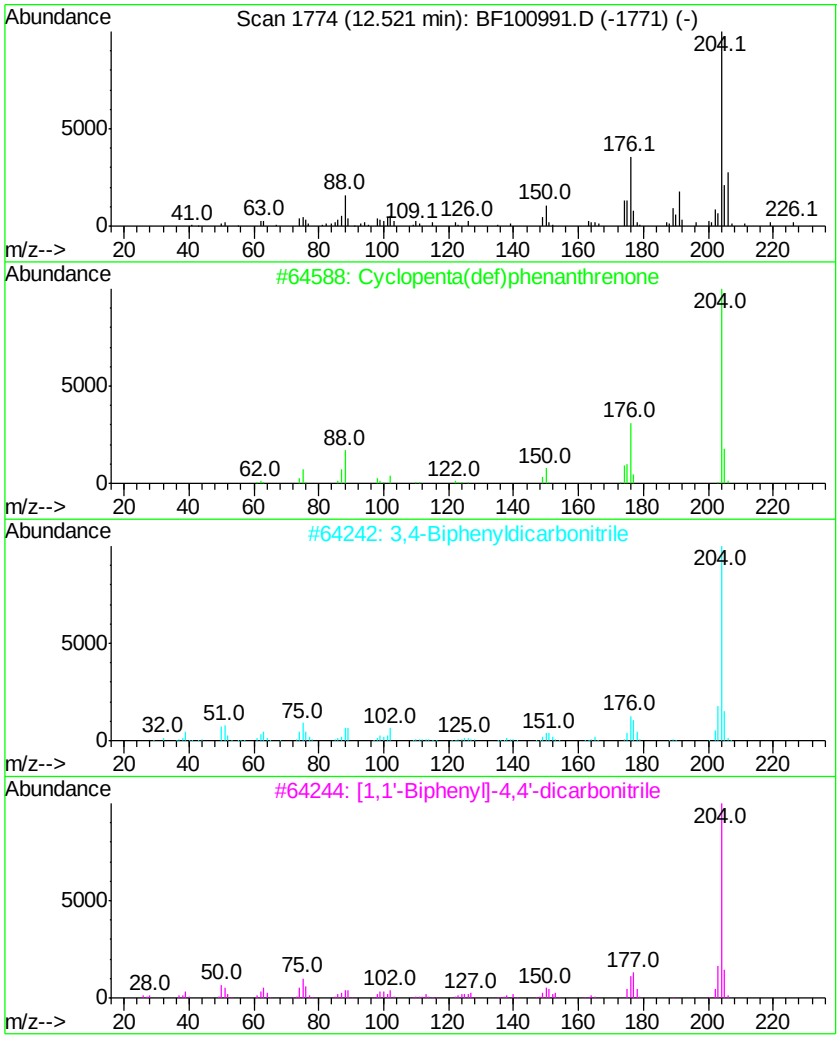
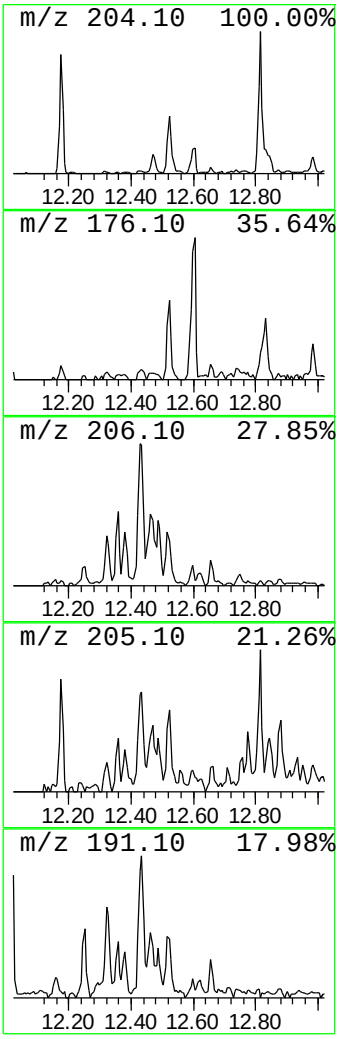
Peak Number 12 Cyclopenta(def)phenanthrenone Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.52	4.91 ng	101686	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenta(def)phenanthrenone	204	C15H8O	005737-13-3	89
2	3,4-Biphenyldicarbonitrile	204	C14H8N2	004128-63-6	53
3	[1,1'-Biphenyl]-4,4'-dicarbonitrile	204	C14H8N2	001591-30-6	50
4	Mannose, 6-deoxy-2,3,4,5-tetraki...	452	C18H44O5Si4	019127-15-2	50
5	[1,1'-Biphenyl]-2,2'-dicarbonitrile	204	C14H8N2	004341-02-0	50





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112917\
Data File : BF100991.D
Acq On : 29 Nov 2017 21:11
Operator : SJ/JU
Sample : I6610-15
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-X(0-2)-20171127

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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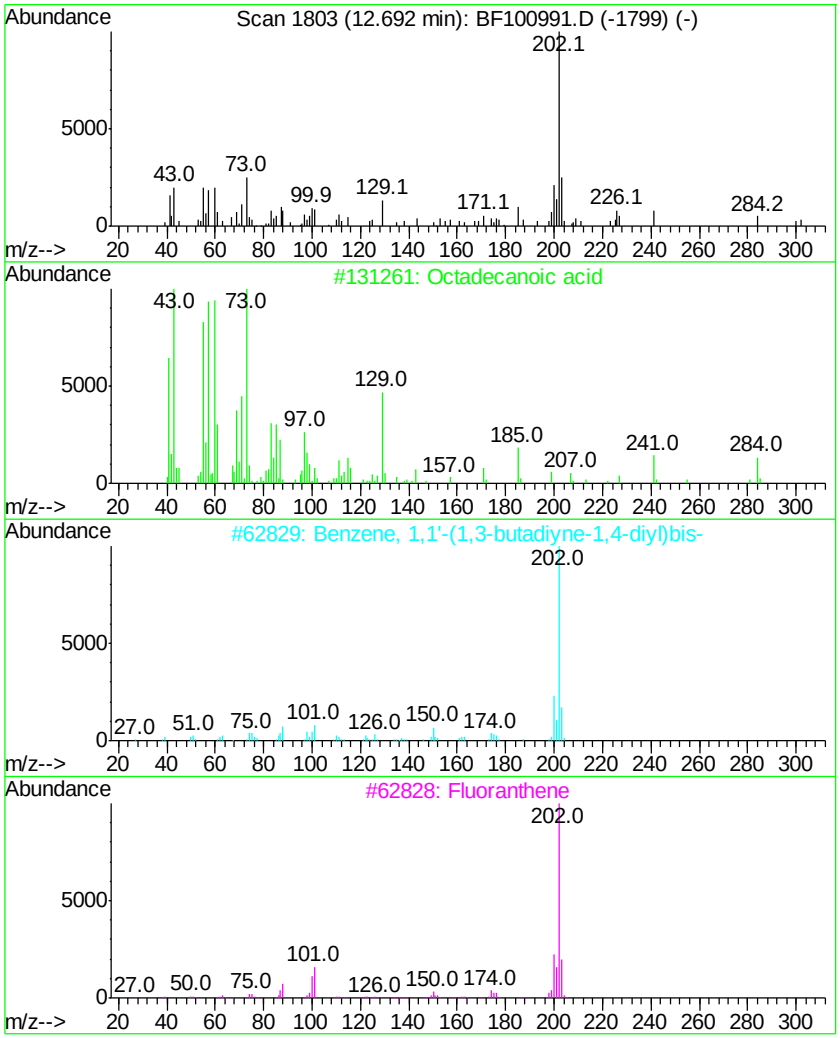
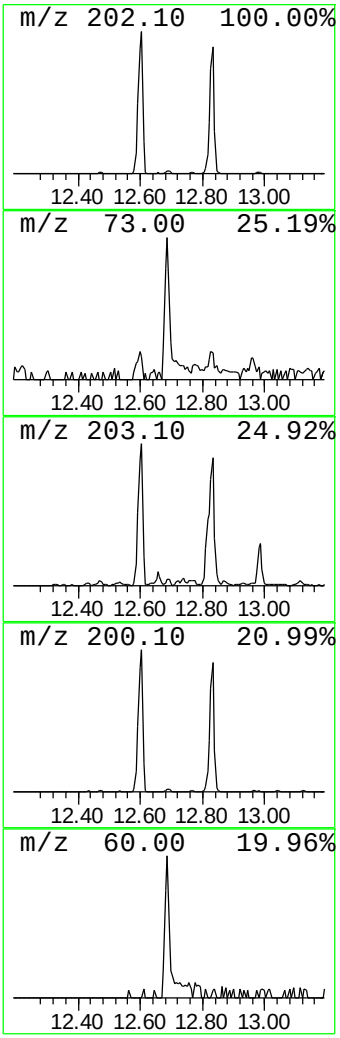
Peak Number 13 Octadecanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.69	4.82 ng	99680	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	92
2	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	46
3	Fluoranthene	202	C16H10	000206-44-0	46
4	Pyrene	202	C16H10	000129-00-0	43
5	Benzene, 2-methoxy-4-(2-propenyl...	202	C13H14O2	055956-27-9	43





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Acq On : 29 Nov 2017 21:11
Operator : SJ/JU
Sample : I6610-15
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-X(0-2)-20171127

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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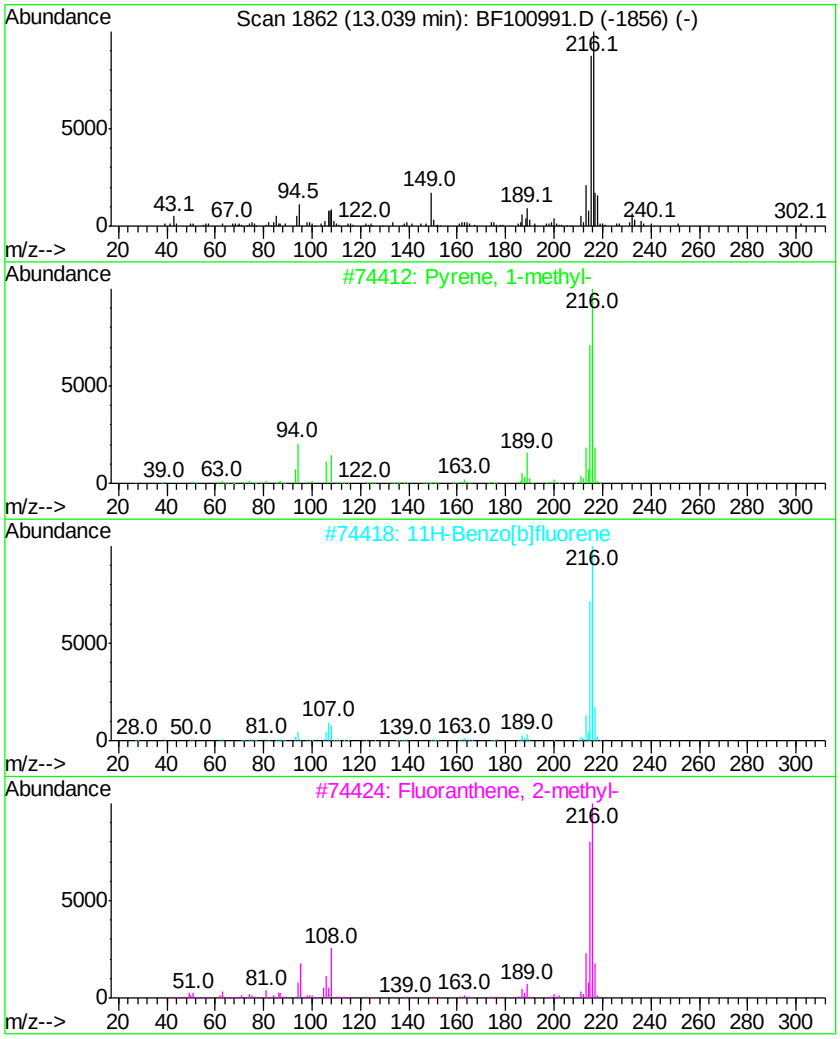
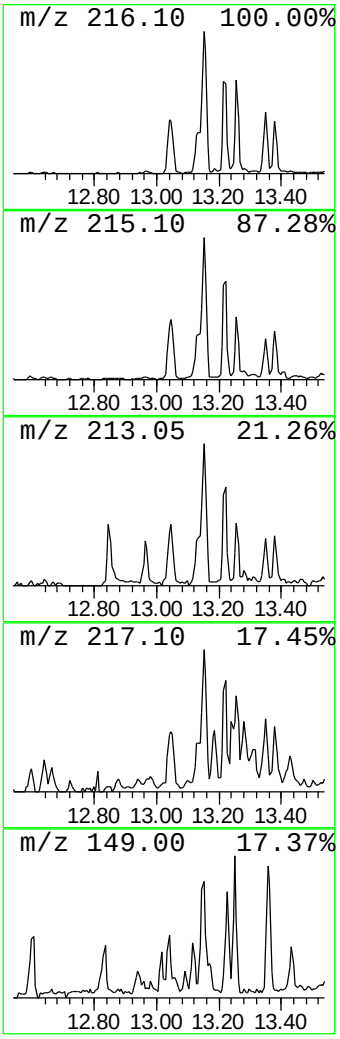
Peak Number 14 Pyrene, 1-methyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.04	4.18 ng	222301	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	93
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	90
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
5	Pyrene, 2-methyl-	216	C17H12	003442-78-2	86





Library Search Compound Report

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Acq On : 29 Nov 2017 21:11
Operator : SJ/JU
Sample : I6610-15
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-X(0-2)-20171127

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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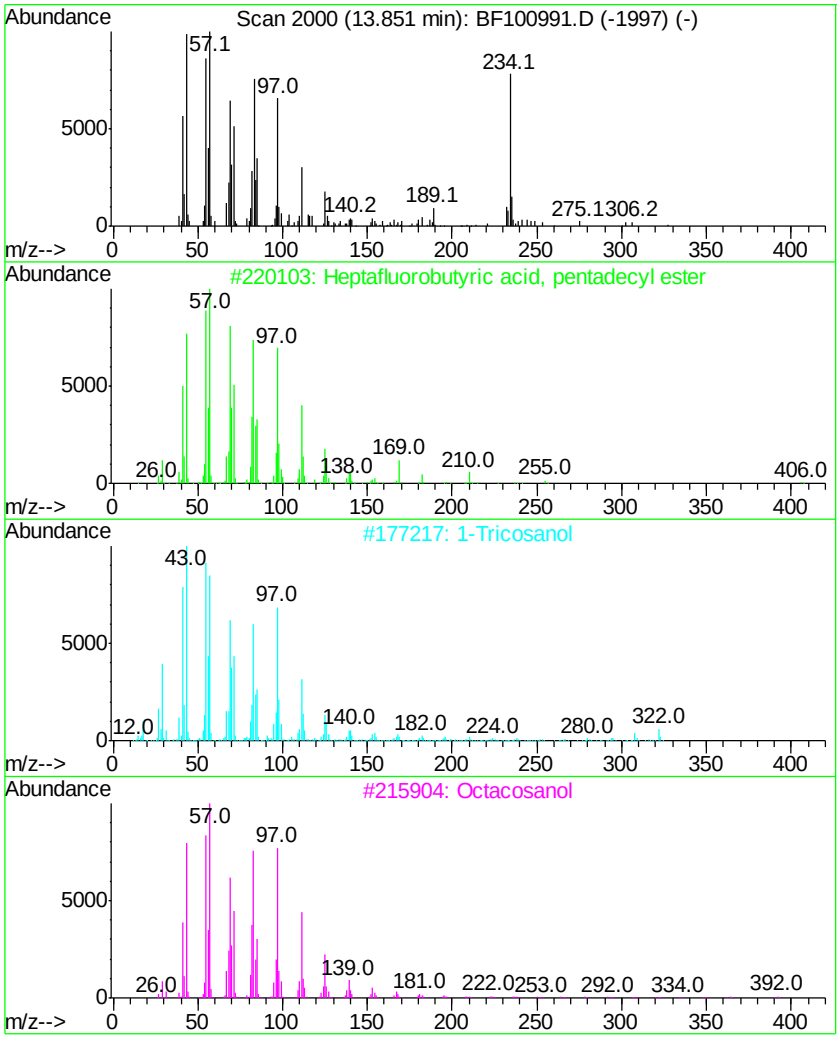
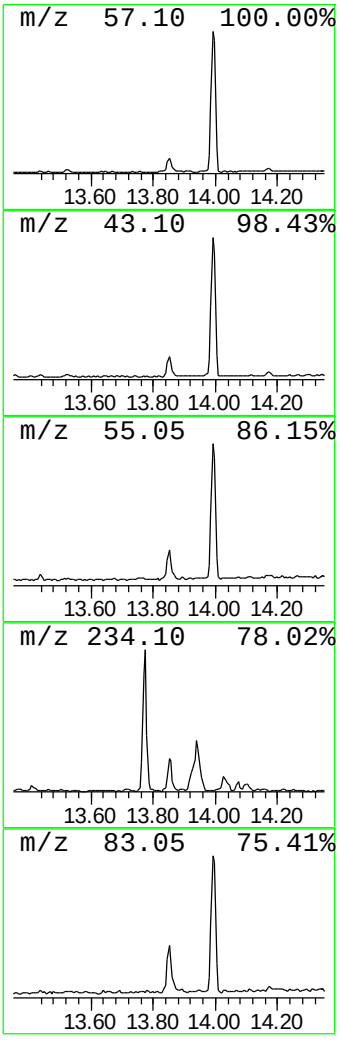
Peak Number 17 Heptafluorobutyric acid, pe... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	4.38 ng	233158	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	62
2	1-Tricosanol	340	C23H48O	003133-01-5	58
3	Octacosanol	410	C28H58O	000557-61-9	58
4	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	58
5	17-Pentatriacontene	491	C35H70	006971-40-0	58





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Acq On : 29 Nov 2017 21:11
Operator : SJ/JU
Sample : I6610-15
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-X(0-2)-20171127

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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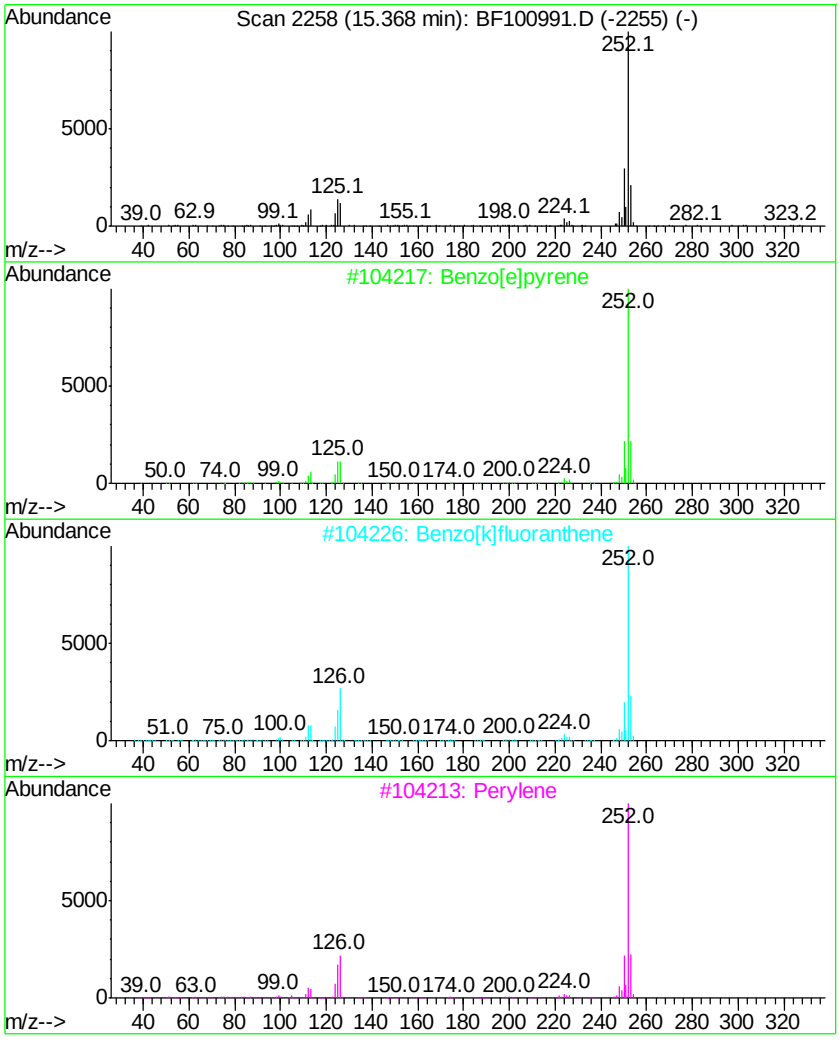
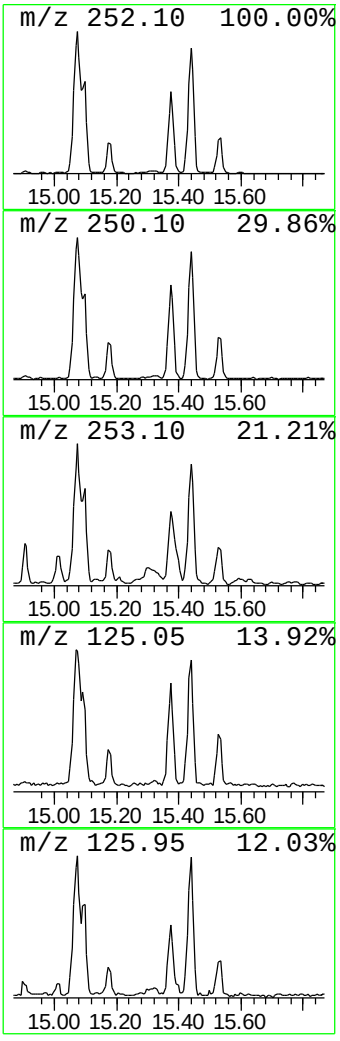
Peak Number 19 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.37	25.28 ng	386249	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
3	Perylene	252	C20H12	000198-55-0	93
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	90
5	Benzo[a]pyrene	252	C20H12	000050-32-8	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112917\
Data File : BF100991.D
Acq On : 29 Nov 2017 21:11
Operator : SJ/JU
Sample : I6610-15
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-X(0-2)-20171127

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.08	5.4	ng	97125	1	6.85	361695	20.0
unknown6.63	6.63	75.7	ng	1368670	1	6.85	361695	20.0
Phenanthrene, 1-m...	11.88	9.6	ng	198783	4	11.38	413941	20.0
Phenanthrene, 2-m...	11.90	18.6	ng	384914	4	11.38	413941	20.0
unknown11.99	11.99	16.0	ng	331243	4	11.38	413941	20.0
Naphthalene, 2-ph...	12.17	5.6	ng	116024	4	11.38	413941	20.0
9,10-Anthracenedione	12.20	4.3	ng	88459	4	11.38	413941	20.0
Phenanthrene, 2,5...	12.43	6.2	ng	128233	4	11.38	413941	20.0
unknown12.47	12.47	4.5	ng	92956	4	11.38	413941	20.0
Cyclopenta(def)ph...	12.52	4.9	ng	101686	4	11.38	413941	20.0
Octadecanoic acid	12.69	4.8	ng	99680	4	11.38	413941	20.0
Pyrene, 1-methyl-	13.04	4.2	ng	222301	5	14.03	1064550	20.0
Heptafluorobutyri...	13.85	4.4	ng	233158	5	14.03	1064550	20.0
Benzo[e]pyrene	15.37	25.3	ng	386249	6	15.50	305573	20.0