LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102271.D
Acq On : 20 Jan 2018 17:41
Operator : SJ/JU
Sample : J1228-26
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-5

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-BF010918.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	4.928	478	483	493	rVB	179220	259401	7.32%	0.748%
2	5.334	547	552	555	rBV	3241800	3419460	96.53%	9.859%
3	6.363	721	727	737	rVB	3082558	3527015	99.57%	10.169%
4	6.492	744	749	752	rBV	3607532	3425166	96.69%	9.876%
5	6.716	784	787	791	rBV	1032447	914304	25.81%	2.636%
6	6.875	810	814	817	rBV	2971940	2632051	74.30%	7.589%
7	7.287	878	884	887	rBV	2124811	2158938	60.95%	6.225%
8	7.998	1001	1005	1009	rBV	1288636	1202412	33.94%	3.467%
9	8.557	1096	1100	1104	rBV	56196	47676	1.35%	0.137%
10	9.081	1183	1189	1192	rBV	3885544	3542263	100.00%	10.213%
11	9.475	1251	1256	1259	rBV	327563	299037	8.44%	0.862%
12	9.616	1275	1280	1287	rBV	188053	159730	4.51%	0.461%
13	9.686	1287	1292	1294	rVB	62620	48216	1.36%	0.139%
14	9.757	1299	1304	1307	rBV	1226136	1192557	33.67%	3.438%
15	10.186	1374	1377	1378	rBV2	44815	38314	1.08%	0.110%
16	10.404	1409	1414	1420	rBV4	31308	46769	1.32%	0.135%
17	10.469	1420	1425	1432	rVB	117550	119827	3.38%	0.345%
18	10.545	1432	1438	1441	rBV	1855539	1742170	49.18%	5.023%
19	10.657	1454	1457	1461	rBV3	47009	58495	1.65%	0.169%
20	11.239	1552	1556	1558	rBV	1138724	987460	27.88%	2.847%
21	11.257	1558	1559	1565	rVV	70596	69002	1.95%	0.199%
22	11.310	1565	1568	1571	rVB	71007	59005	1.67%	0.170%
23	11.739	1638	1641	1643	rBV	69920	61551	1.74%	0.177%
24	11.763	1643	1645	1649	rVB	72741	70484	1.99%	0.203%
25	11.845	1656	1659	1662	rBV2	94428	105232	2.97%	0.303%
26	11.869	1662	1663	1667	rVB	52456	43399	1.23%	0.125%
27	12.180	1711	1716	1719	rBV2	49548	63517	1.79%	0.183%
28	12.210	1719	1721	1724	rVV	74785	69670	1.97%	0.201%
29	12.239	1724	1726	1728	rVB	56452	43312	1.22%	0.125%
30	12.286	1728	1734	1737	rBV	194608	203828	5.75%	0.588%
31	12.322	1737	1740	1742	rVV2	83682	97087	2.74%	0.280%
32	12.369	1746	1748	1753	rBV2	62869	78101	2.20%	0.225%
33	12.445	1758	1761	1765	rVV	223369	198829	5.61%	0.573%
34	12.539	1775	1777	1780	rVB	67254	55557	1.57%	0.160%

LSC Area Percent Report

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Data File : BF102271.D
Acq On : 20 Jan 2018 17:41
Operator : SJ/JU
Sample : J1228-26
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-5

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-BF010918.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.616	1786	1790	1794	rBV4	32232	52324	1.48%	0.151%
36	12.674	1796	1800	1802	rVV	391524	335814	9.48%	0.968%
37	12.698	1802	1804	1807	rVV	123140	113288	3.20%	0.327%
38	12.733	1807	1810	1813	rVB	146148	145373	4.10%	0.419%
39	12.827	1821	1826	1829	rBV	2464392	2420921	68.34%	6.980%
40	12.892	1834	1837	1844	rBV4	94435	154504	4.36%	0.445%
41	12.986	1849	1853	1854	rBV2	73504	95736	2.70%	0.276%
42	13.110	1870	1874	1877	rVB	141941	123711	3.49%	0.357%
43	13.174	1882	1885	1887	rBV3	34473	39764	1.12%	0.115%
44	13.198	1887	1889	1892	rVV	129958	106245	3.00%	0.306%
45	13.227	1892	1894	1897	rVB	110556	96323	2.72%	0.278%
46	13.269	1897	1901	1904	rBV2	53612	55628	1.57%	0.160%
47	13.510	1939	1942	1947	rVB	96113	108708	3.07%	0.313%
48	13.568	1950	1952	1956	rVB	75565	71872	2.03%	0.207%
49	13.610	1956	1959	1961	rBV2	92130	109152	3.08%	0.315%
50	13.674	1968	1970	1974	rBV2	31602	57551	1.62%	0.166%
51	13.716	1974	1977	1981	rVB2	162347	178666	5.04%	0.515%
52	13.874	1998	2004	2007	rBV2	1038480	1151441	32.51%	3.320%
53	13.898	2007	2008	2010	rVB	181456	99160	2.80%	0.286%
54	13.957	2016	2018	2023	rVB4	47167	44974	1.27%	0.130%
55	14.186	2055	2057	2060	rBV3	33609	39445	1.11%	0.114%
56	14.221	2061	2063	2065	rVV2	55023	51482	1.45%	0.148%
57	14.257	2065	2069	2072	rVV	142632	176414	4.98%	0.509%
58	14.292	2072	2075	2079	rVB	86414	78252	2.21%	0.226%
59	14.380	2088	2090	2092	rVB2	58994	49762	1.40%	0.143%
60	14.621	2129	2131	2136	rVB2	114714	136159	3.84%	0.393%
61	14.886	2173	2176	2180	rBV2	139645	224303	6.33%	0.647%
62	14.992	2191	2194	2197	rBV	51961	59564	1.68%	0.172%
63	15.174	2222	2225	2230	rVB	124983	143859	4.06%	0.415%
64	15.233	2231	2235	2240	rBV	160040	190491	5.38%	0.549%
65	15.298	2241	2246	2249	rBV	577302	704221	19.88%	2.030%
66	16.674	2476	2480	2486	rVB2	51976	99970	2.82%	0.288%
67	17.092	2546	2551	2558	rVB2	61860	127827	3.61%	0.369%

Sum of corrected areas: 34682739

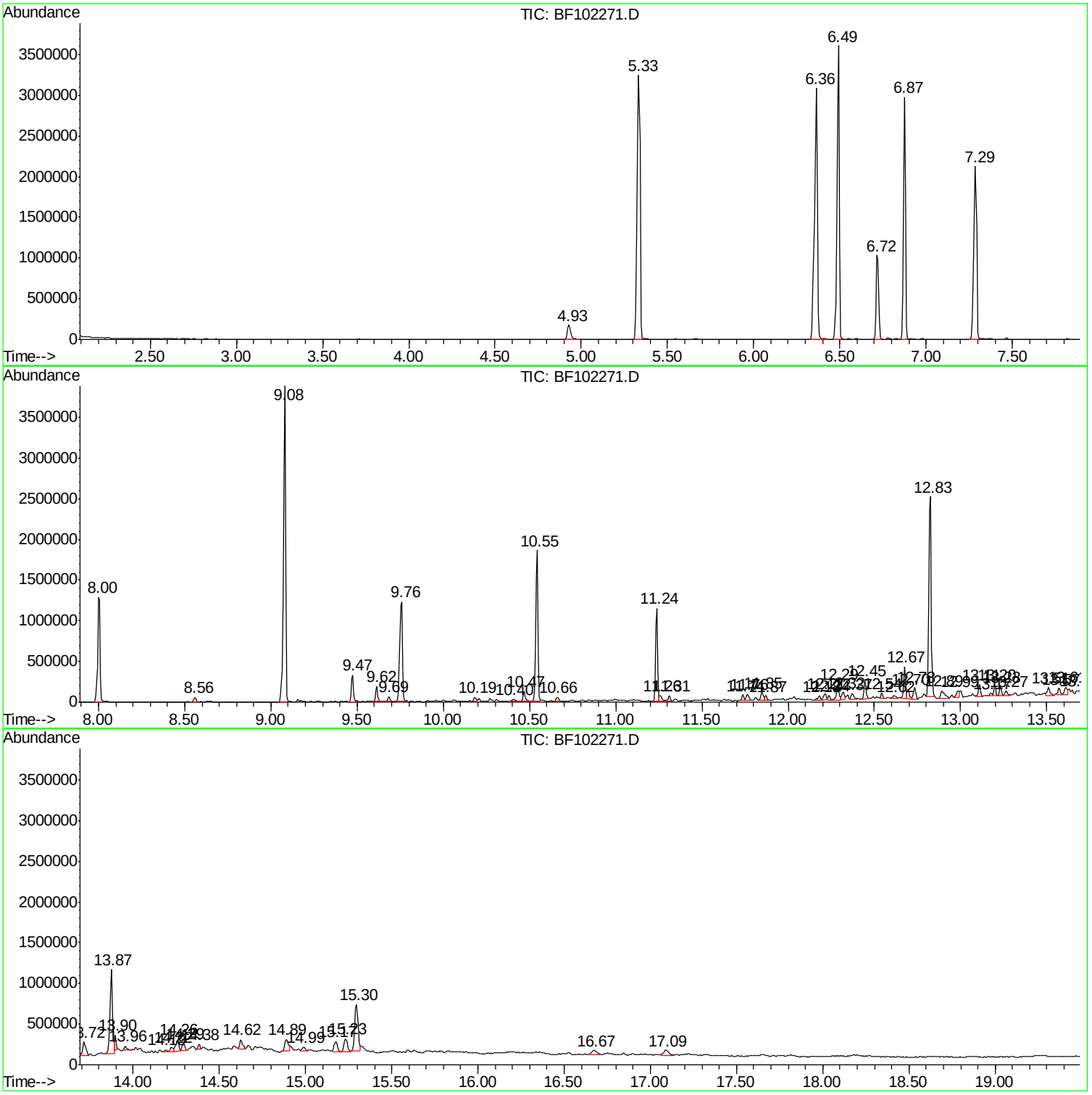
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102271.D
Acq On : 20 Jan 2018 17:41
Operator : SJ/JU
Sample : J1228-26
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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\BF012018\
Data File : BF102271.D
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

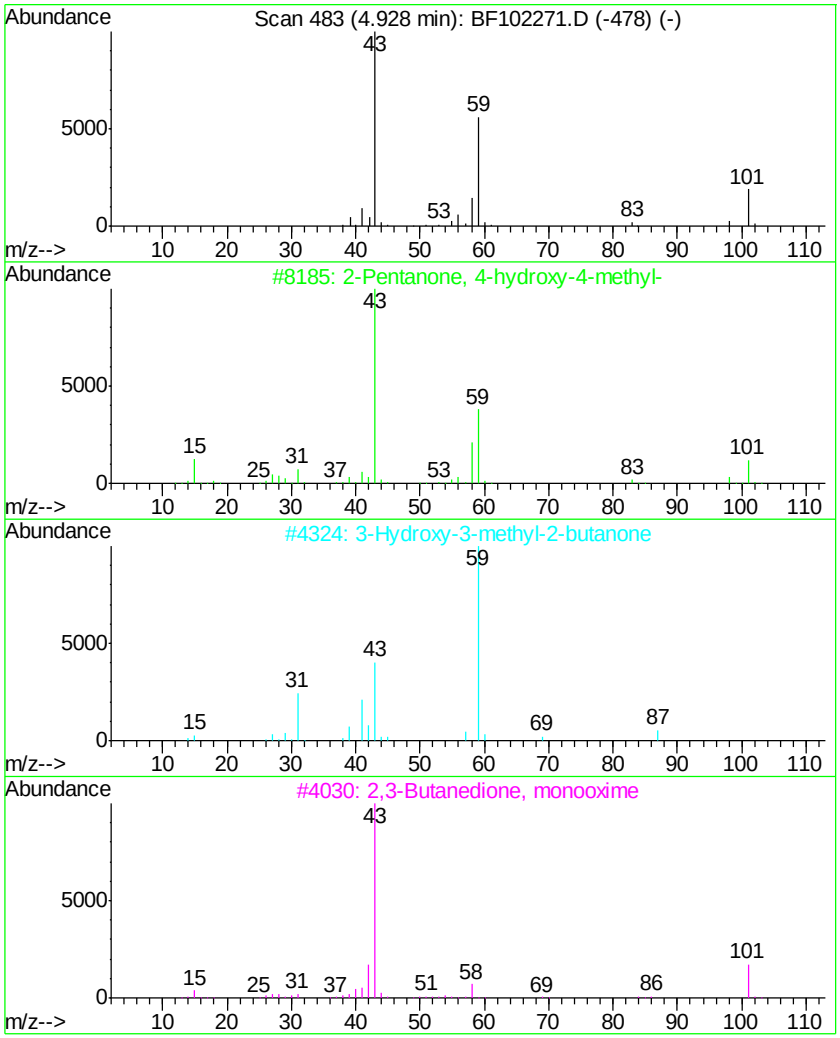
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

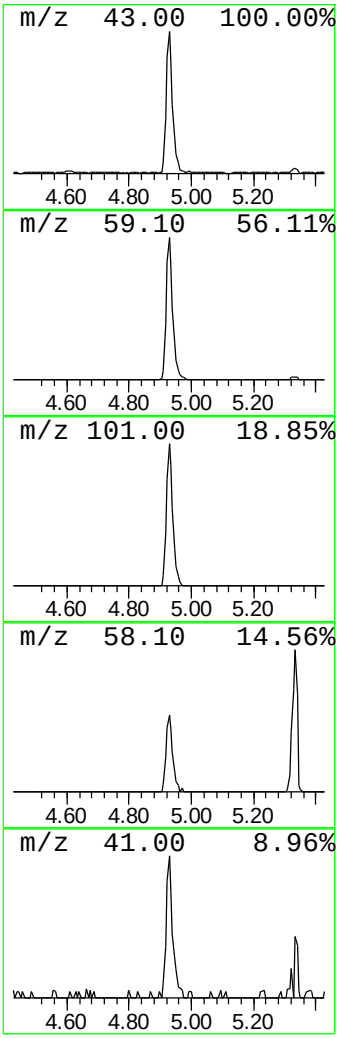
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	5.67 ng	259401	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	1,2-Butanediol	90	C4H10O2	000584-03-2	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102271.D
Acq On : 20 Jan 2018 17:41
Operator : SJ/JU
Sample : J1228-26
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

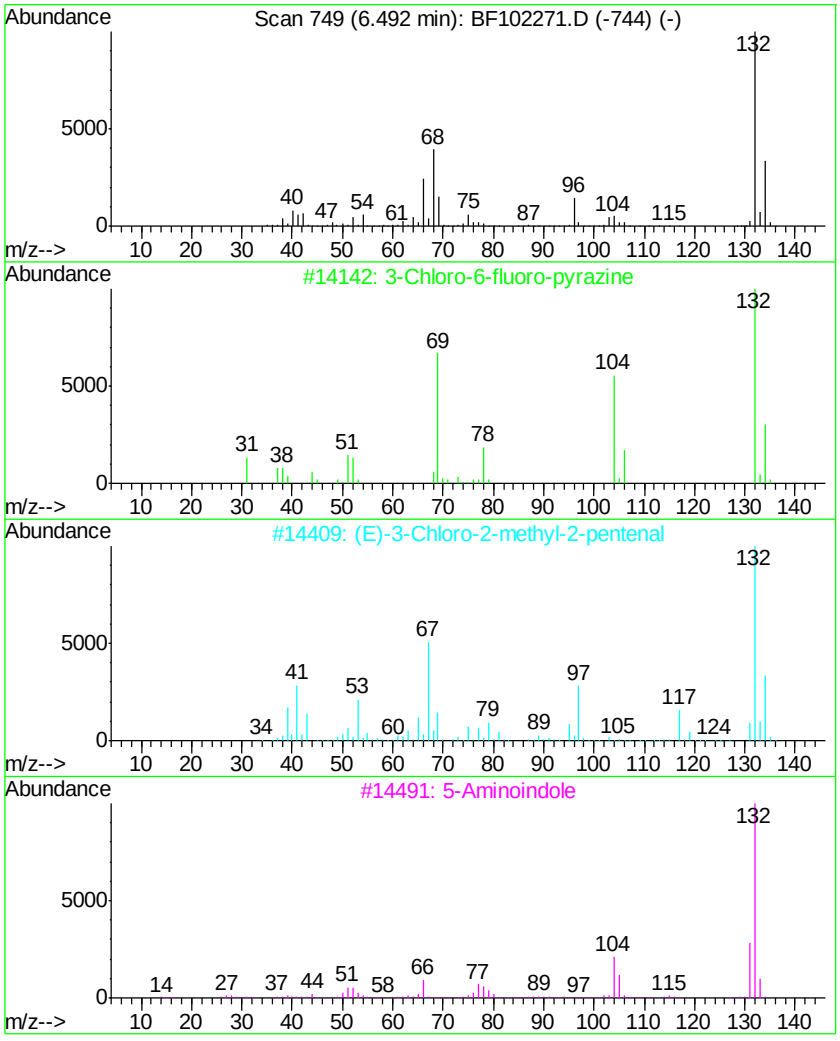
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

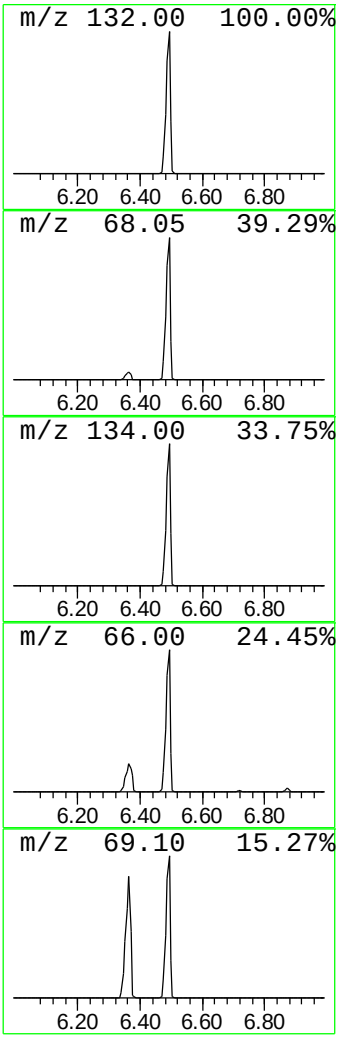
****

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	74.92 ng	3425170	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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Acq On : 20 Jan 2018 17:41
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Sample : J1228-26
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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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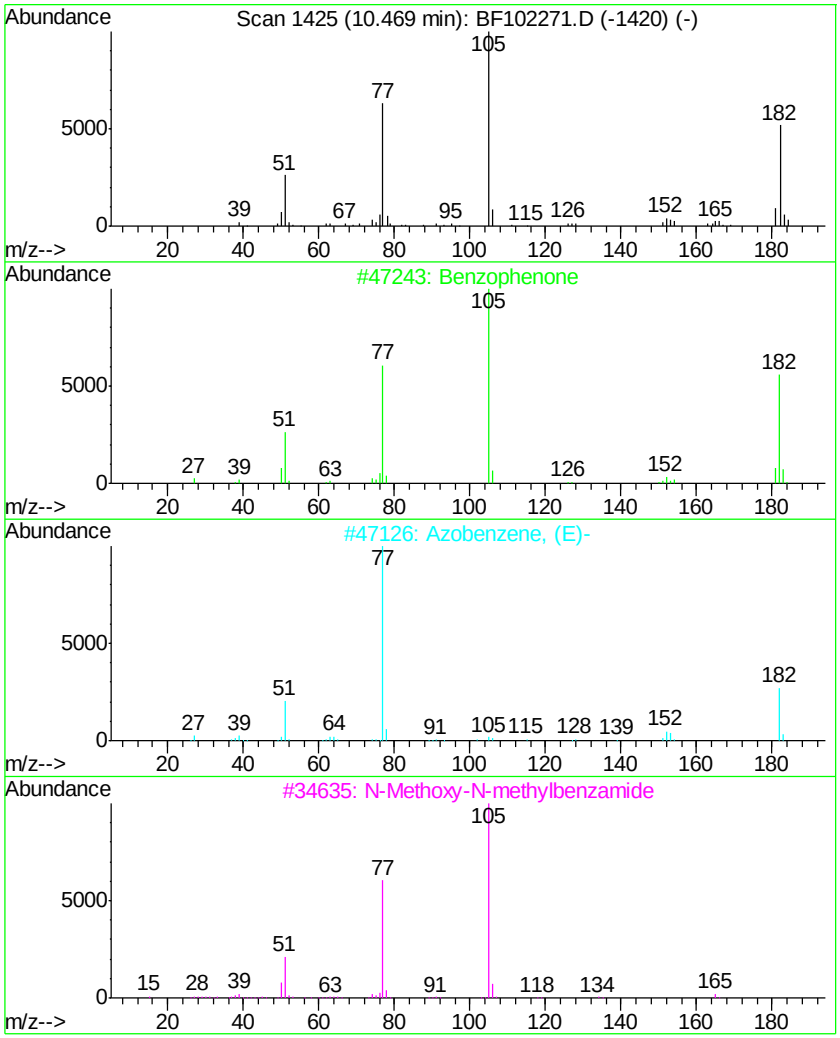
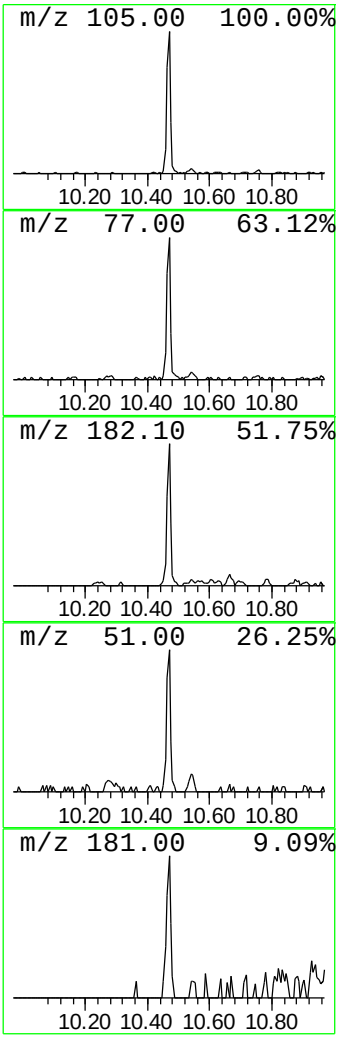
Peak Number 4 Benzophenone Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.47	2.01 ng	119827	Acenaphthene-d10	9.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Azobenzene, (E)-	182	C12H10N2	017082-12-1	59
3	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	46
4	1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	43
5	Phenylglyoxal	134	C8H6O2	001074-12-0	43





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102271.D
Acq On : 20 Jan 2018 17:41
Operator : SJ/JU
Sample : J1228-26
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

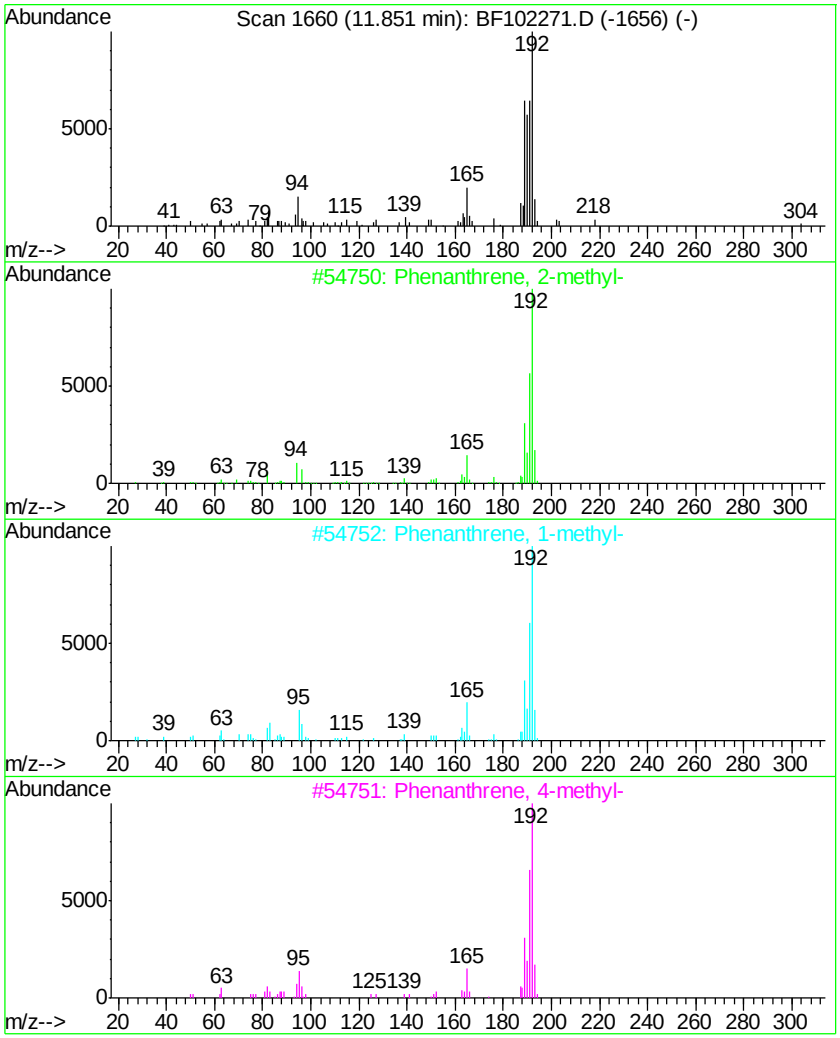
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

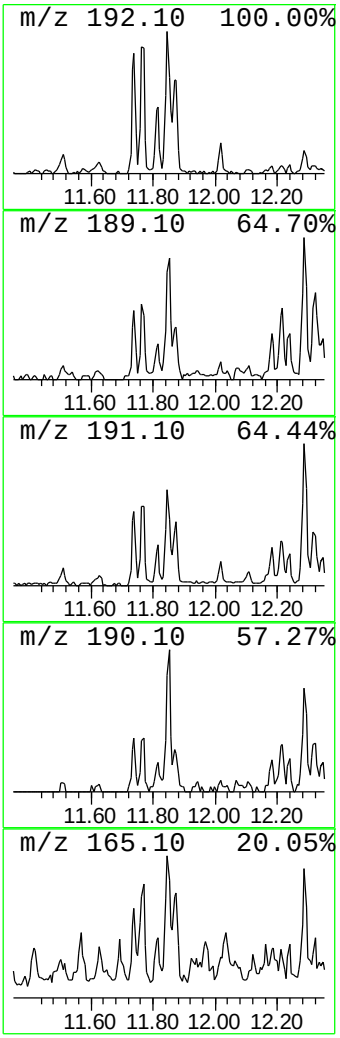
****

Peak Number 5 Phenanthrene, 2-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	2.13 ng	105232	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	94
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	94
3	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	93
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	86
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	81





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102271.D
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Sample : J1228-26
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

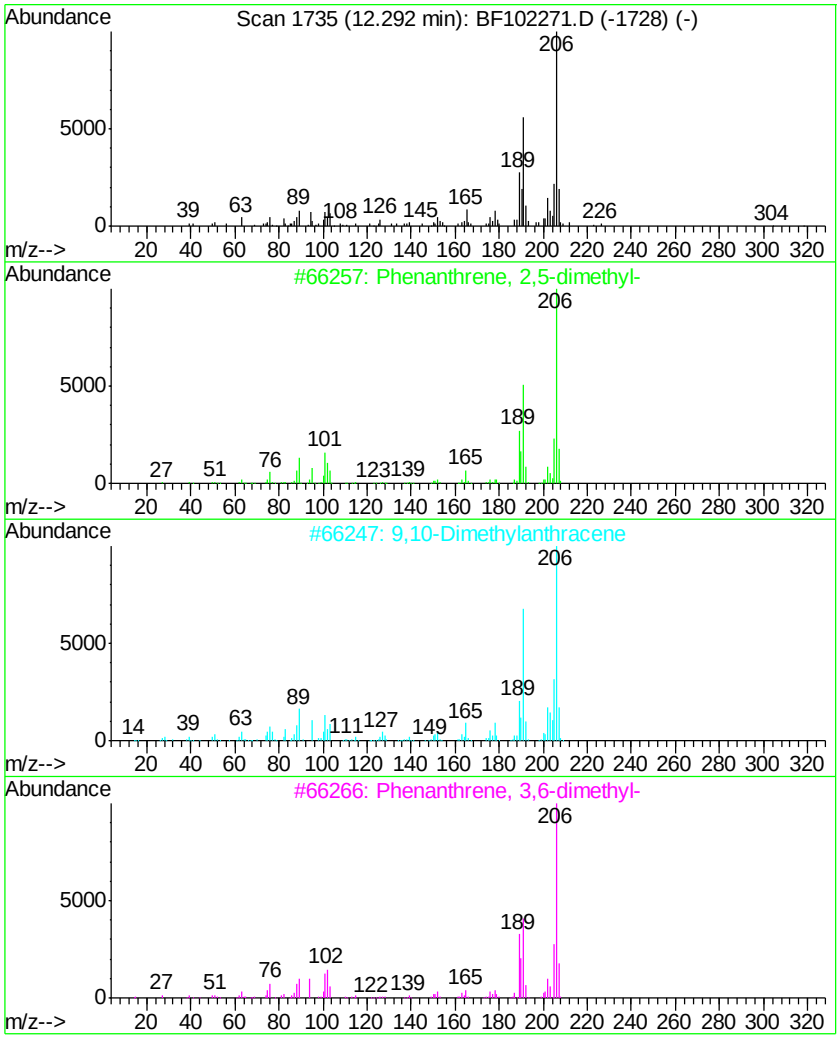
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

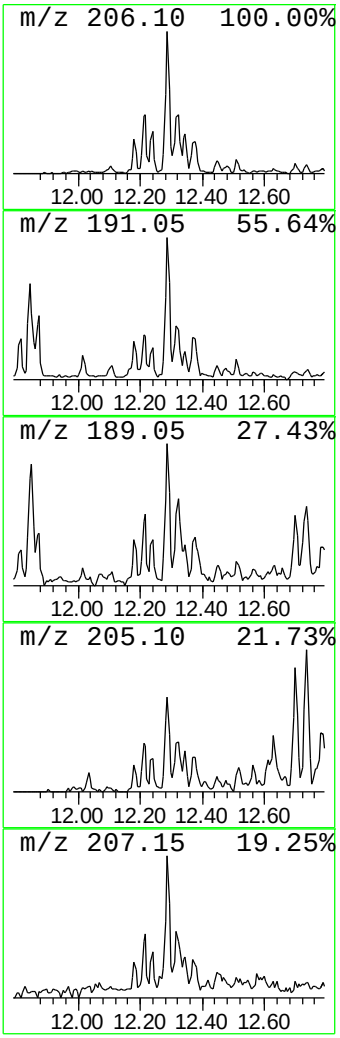
****

Peak Number 6 Phenanthrene, 2,5-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.29	4.13 ng	203828	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	98
2	9,10-Dimethylanthracene	206	C16H14	000781-43-1	97
3	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	93
4	Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	93
5	Anthracene, 1,4-dimethyl-	206	C16H14	000781-92-0	93





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Sample : J1228-26
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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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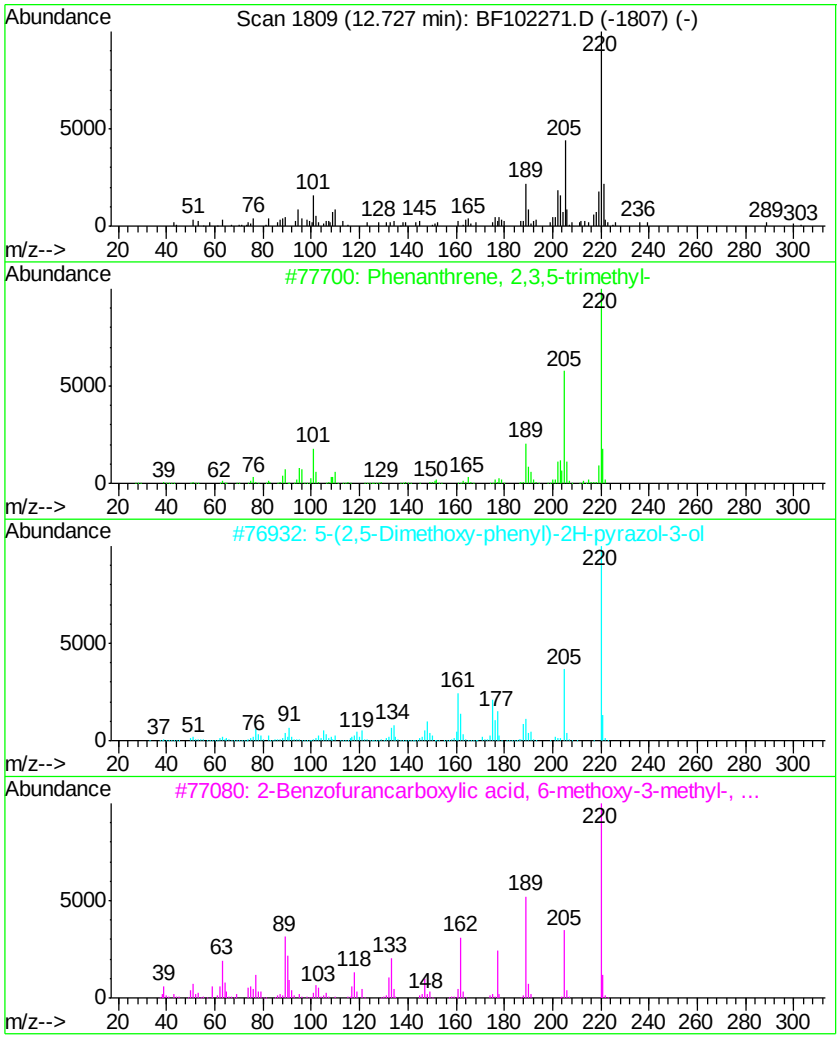
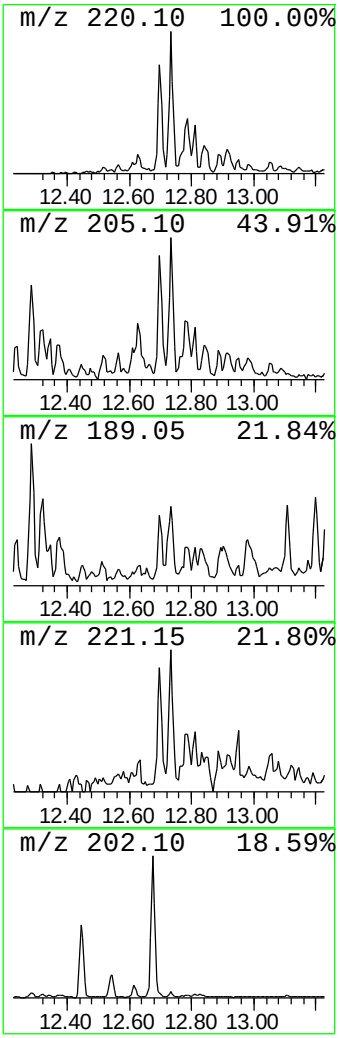
Peak Number 7 Phenanthrene, 2,3,5-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	2.53 ng	145373	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,3,5-trimethyl-	220	C17H16	003674-73-5	94
2	5-(2,5-Dimethoxy-phenyl)-2H-pyra...	220	C11H12N2O3	1000278-26-9	64
3	2-Benzofurancarboxylic acid, 6-m...	220	C12H12O4	1000349-99-8	58
4	7-Nitro-6-methoxy-2,3-dimethylin...	220	C11H12N2O3	068289-71-4	58
5	Benzo[b]dihydropyran, 6-hydroxy-...	220	C14H20O2	050442-70-1	53





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102271.D
Acq On : 20 Jan 2018 17:41
Operator : SJ/JU
Sample : J1228-26
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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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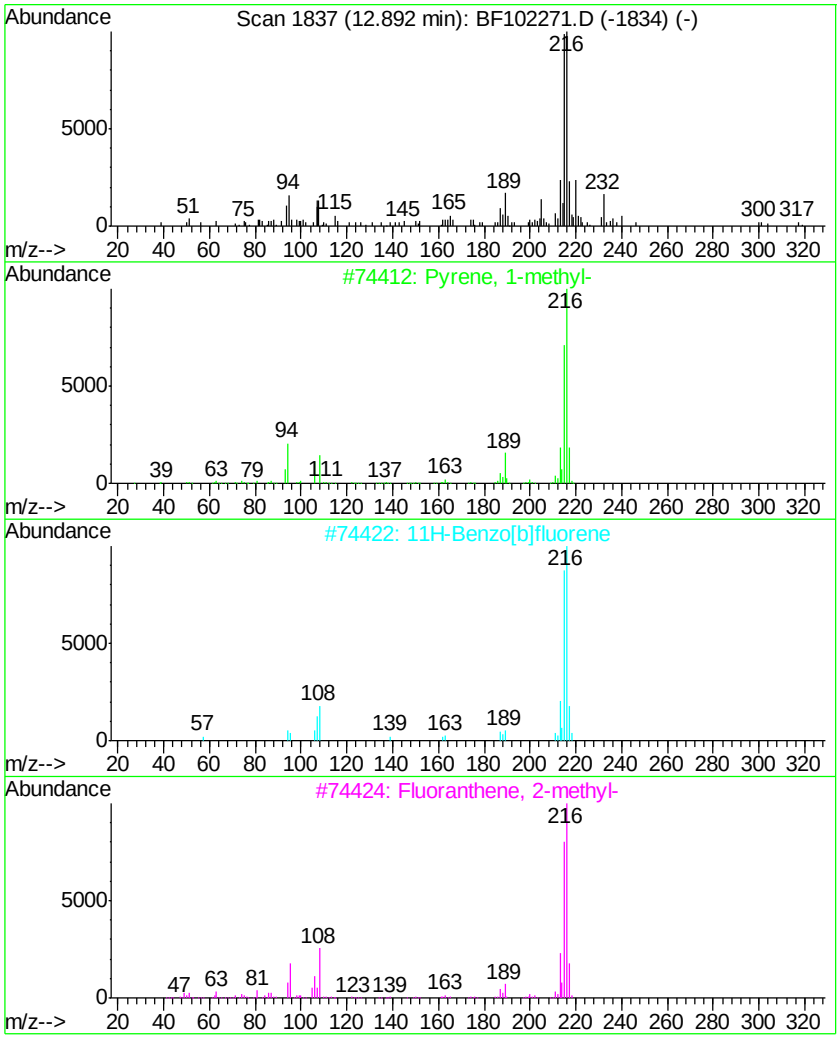
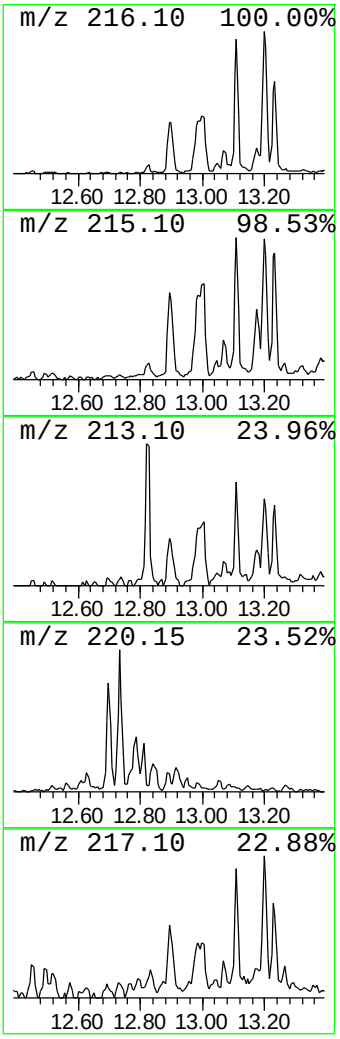
Peak Number 8 Pyrene, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.89	2.68 ng	154504	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	98
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	86
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	70
4	Pyrene, 2-methyl-	216	C17H12	003442-78-2	64
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	62





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Data File : BF102271.D
Acq On : 20 Jan 2018 17:41
Operator : SJ/JU
Sample : J1228-26
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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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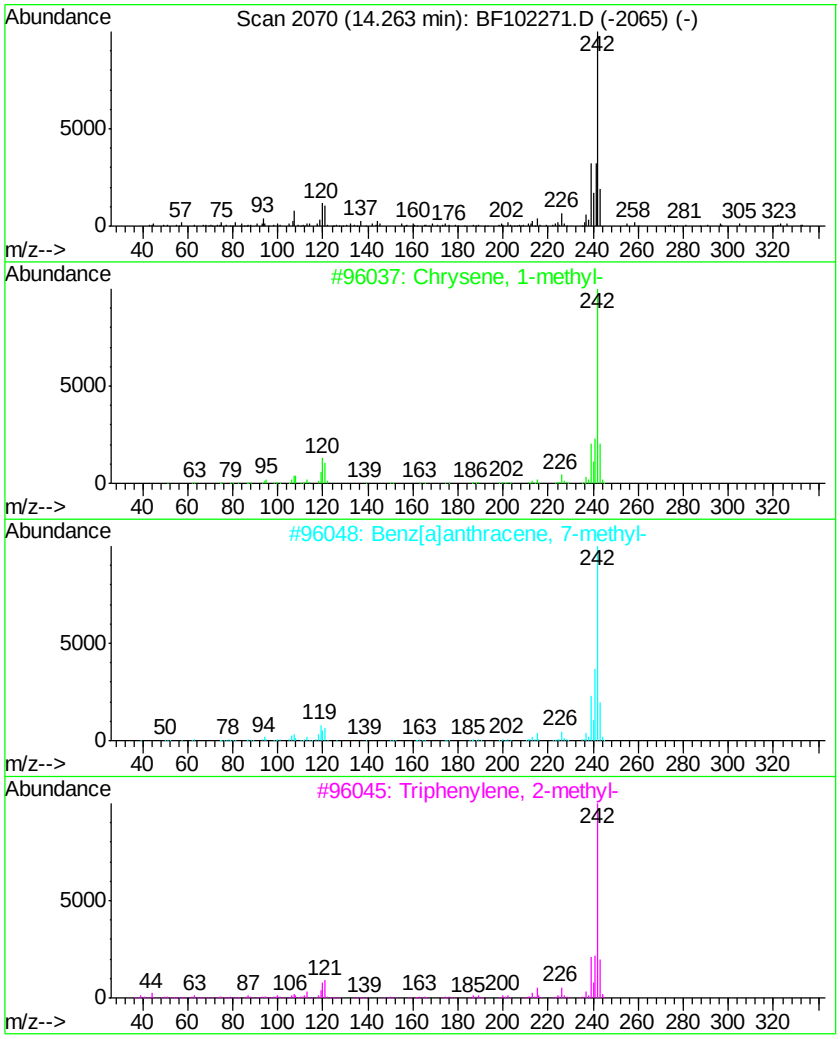
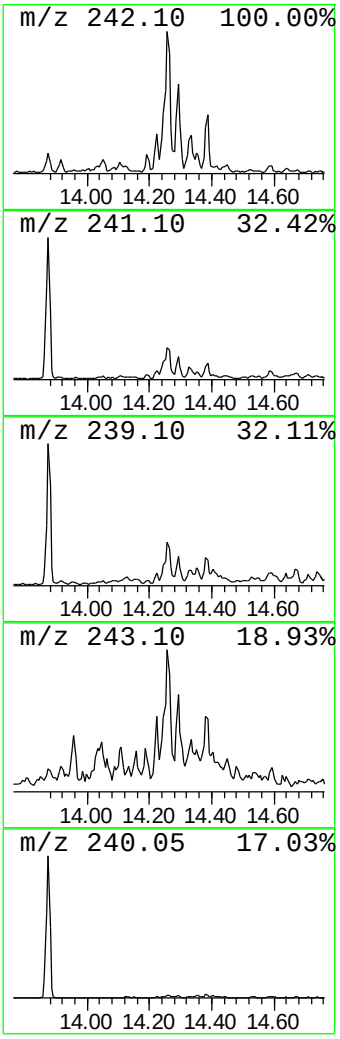
Peak Number 11 Chrysene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.26	3.06 ng	176414	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Chrysene, 1-methyl-	242	C19H14	003351-28-8	94
2	Benz[a]anthracene, 7-methyl-	242	C19H14	002541-69-7	93
3	Triphenylene, 2-methyl-	242	C19H14	001705-84-6	90
4	Benz[a]anthracene, 1-methyl-	242	C19H14	002498-77-3	89
5	Benz[a]anthracene, 8-methyl-	242	C19H14	002381-31-9	89





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102271.D
Acq On : 20 Jan 2018 17:41
Operator : SJ/JU
Sample : J1228-26
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
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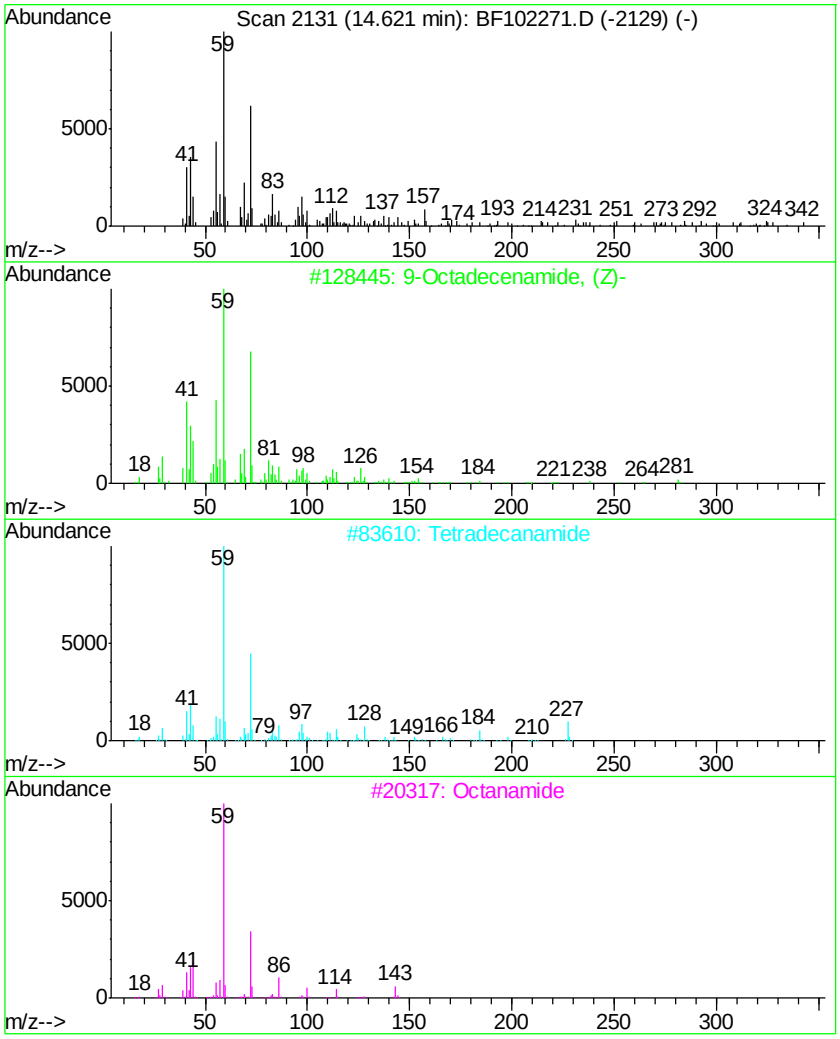
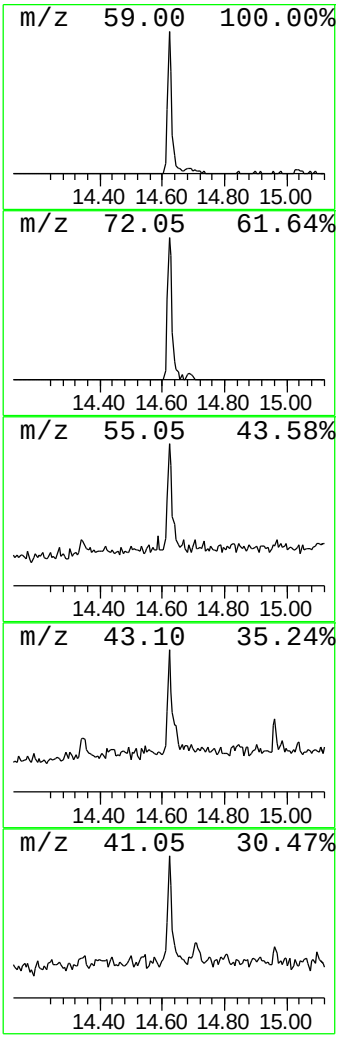
Peak Number 12 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	3.87 ng	136159	Perylene-d12	15.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	Tetradecanamide	227	C14H29NO	000638-58-4	72
3	Octanamide	143	C8H17NO	000629-01-6	64
4	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	59
5	Octadecanamide	283	C18H37NO	000124-26-5	53





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102271.D
Acq On : 20 Jan 2018 17:41
Operator : SJ/JU
Sample : J1228-26
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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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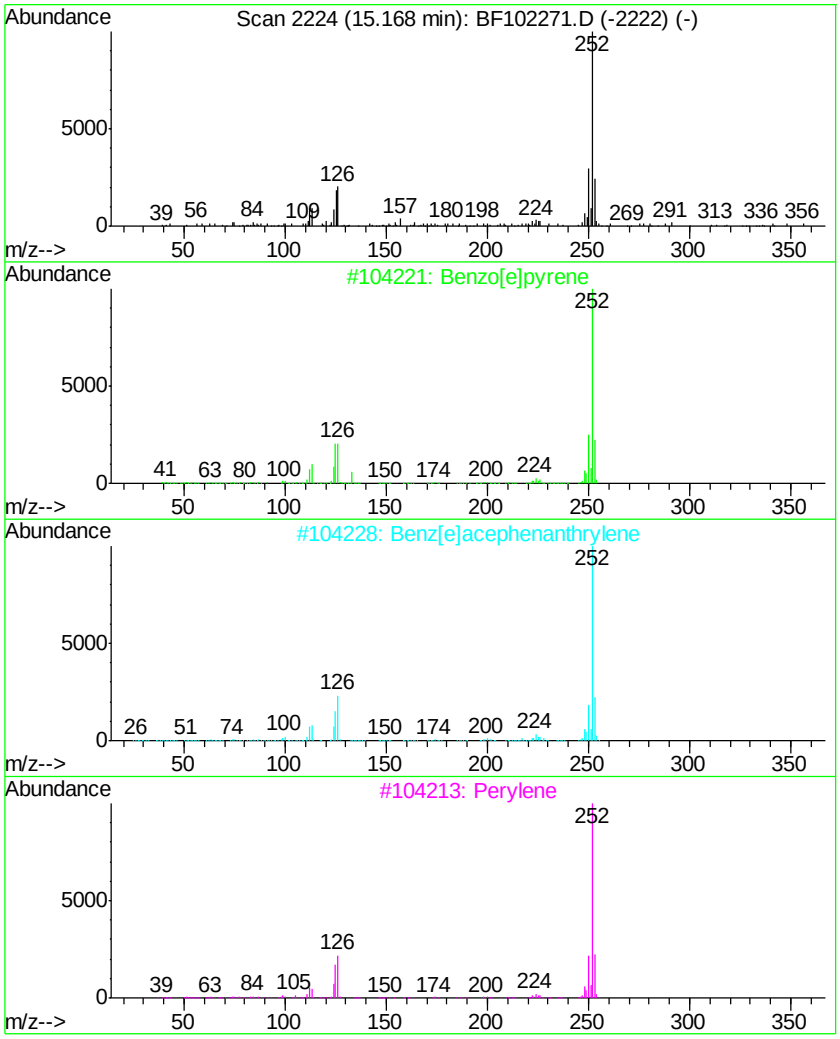
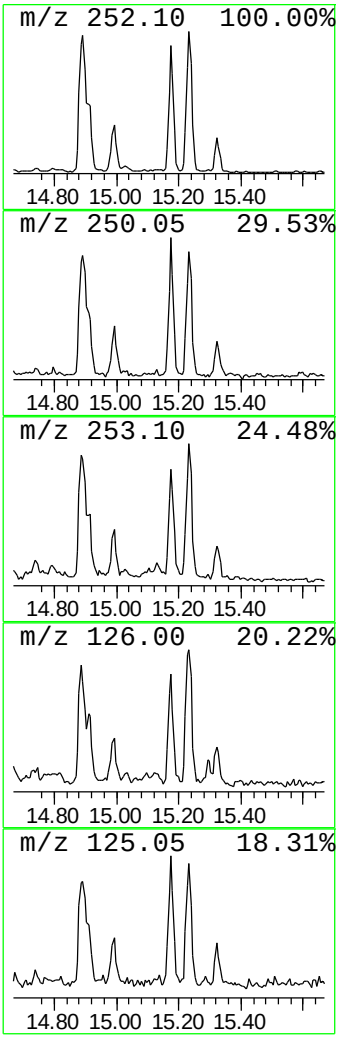
Peak Number 13 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	4.09 ng	143859	Perylene-d12	15.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	93
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93
3	Perylene	252	C20H12	000198-55-0	90
4	Benzo[a]pyrene	252	C20H12	000050-32-8	90
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012018\
Data File : BF102271.D
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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.93	5.7	ng	259401	1	6.72	914304	20.0
unknown6.49	6.49	74.9	ng	3425170	1	6.72	914304	20.0
Benzophenone	10.47	2.0	ng	119827	3	9.75	1192560	20.0
Phenanthrene, 2-m...	11.85	2.1	ng	105232	4	11.24	987460	20.0
Phenanthrene, 2,5...	12.29	4.1	ng	203828	4	11.24	987460	20.0
Phenanthrene, 2,3...	12.73	2.5	ng	145373	5	13.87	1151440	20.0
Pyrene, 1-methyl-	12.89	2.7	ng	154504	5	13.87	1151440	20.0
Chrysene, 1-methyl-	14.26	3.1	ng	176414	5	13.87	1151440	20.0
9-Octadecenamide,...	14.62	3.9	ng	136159	6	15.30	704221	20.0
Benzo[e]pyrene	15.17	4.1	ng	143859	6	15.30	704221	20.0