LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
Data File : BF098561.D
Acq On : 15 Sep 2017 11:23
Operator : SJ/JU
Sample : I5161-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-14-0-14.25

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-BF091117.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	3.546	242	248	256	rBV	136806	223323	6.45%	0.582%
2	4.822	462	465	478	rBV	328721	483441	13.96%	1.259%
3	5.257	534	539	558	rBV	3036465	3362884	97.10%	8.760%
4	6.304	712	717	732	rBV	3140474	3463363	100.00%	9.021%
5	6.422	732	737	743	rVB	3319729	3459477	99.89%	9.011%
6	6.640	771	774	782	rVB	894400	838650	24.21%	2.185%
7	6.798	797	801	812	rBV	2883633	2566619	74.11%	6.686%
8	7.216	867	872	875	rBV	2216858	2135641	61.66%	5.563%
9	7.928	988	993	996	rBV	1355297	1147657	33.14%	2.989%
10	9.004	1171	1176	1179	rBV	3473097	3235832	93.43%	8.429%
11	9.404	1240	1244	1247	rVB	444928	361781	10.45%	0.942%
12	9.539	1263	1267	1272	rBV	48312	43286	1.25%	0.113%
13	9.680	1285	1291	1294	rBV	1402237	1236207	35.69%	3.220%
14	9.710	1294	1296	1301	rVB	85664	70530	2.04%	0.184%
15	9.886	1322	1326	1328	rBV	37877	37632	1.09%	0.098%
16	10.228	1381	1384	1388	rVB	81173	75639	2.18%	0.197%
17	10.392	1408	1412	1415	rVB2	45649	50175	1.45%	0.131%
18	10.469	1419	1425	1436	rBV	1898559	1856173	53.59%	4.835%
19	10.598	1442	1447	1453	rVB2	54285	84887	2.45%	0.221%
20	10.775	1472	1477	1479	rBV4	30643	40143	1.16%	0.105%
21	10.904	1493	1499	1501	rBV6	18577	34873	1.01%	0.091%
22	11.057	1523	1525	1532	rVB2	64719	66378	1.92%	0.173%
23	11.163	1539	1543	1545	rBV	1371022	1204224	34.77%	3.137%
24	11.186	1545	1547	1550	rVV	917579	697496	20.14%	1.817%
25	11.239	1550	1556	1559	rVB	164394	178028	5.14%	0.464%
26	11.398	1578	1583	1588	rBV2	86259	110446	3.19%	0.288%
27	11.663	1625	1628	1630	rBV	100360	84072	2.43%	0.219%
28	11.692	1630	1633	1636	rVB	148034	122116	3.53%	0.318%
29	11.774	1643	1647	1649	rBV	207652	187405	5.41%	0.488%
30	11.798	1649	1651	1653	rVB	65586	49931	1.44%	0.130%
31	11.957	1676	1678	1681	rBV	81445	65829	1.90%	0.171%
32	11.992	1681	1684	1689	rVB	94434	80246	2.32%	0.209%
33	12.139	1706	1709	1711	rBV	42954	37359	1.08%	0.097%
34	12.210	1718	1721	1724	rBV	69433	81347	2.35%	0.212%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
Data File : BF098561.D
Acq On : 15 Sep 2017 11:23
Operator : SJ/JU
Sample : I5161-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-14-0-14.25

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-BF091117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.251	1726	1728	1730	rVV3	61483	56014	1.62%	0.146%
36	12.304	1733	1737	1741	rBV3	51428	65557	1.89%	0.171%
37	12.374	1745	1749	1753	rBV	1280350	1118116	32.28%	2.912%
38	12.521	1771	1774	1777	rVB2	35168	38892	1.12%	0.101%
39	12.598	1782	1787	1790	rVV	913072	1031883	29.79%	2.688%
40	12.651	1794	1796	1802	rVB2	57832	68394	1.97%	0.178%
41	12.745	1808	1812	1819	rVB	2296795	2301125	66.44%	5.994%
42	12.821	1821	1825	1829	rVV2	63790	101958	2.94%	0.266%
43	12.910	1837	1840	1841	rBV2	55313	65055	1.88%	0.169%
44	12.927	1841	1843	1847	rVB	157173	154448	4.46%	0.402%
45	12.998	1852	1855	1857	rVB	135123	111933	3.23%	0.292%
46	13.033	1857	1861	1864	rBV2	97526	115784	3.34%	0.302%
47	13.127	1874	1877	1879	rVB	50098	44241	1.28%	0.115%
48	13.157	1879	1882	1885	rBV	51282	54774	1.58%	0.143%
49	13.310	1906	1908	1909	rBV2	39075	34810	1.01%	0.091%
50	13.445	1929	1931	1935	rVB	61711	50721	1.46%	0.132%
51	13.551	1946	1949	1951	rBV	68105	72203	2.08%	0.188%
52	13.574	1951	1953	1955	rVB	71988	52884	1.53%	0.138%
53	13.598	1955	1957	1959	rBV	56232	57619	1.66%	0.150%
54	13.645	1962	1965	1970	rVB2	248815	287113	8.29%	0.748%
55	13.798	1984	1991	1994	rBV2	1058177	1435424	41.45%	3.739%
56	13.821	1994	1995	1999	rVB	383505	306058	8.84%	0.797%
57	13.904	2006	2009	2011	rVB	73122	64749	1.87%	0.169%
58	14.186	2055	2057	2059	rVB	83580	62700	1.81%	0.163%
59	14.280	2069	2073	2075	rBV3	89557	105295	3.04%	0.274%
60	14.810	2159	2163	2166	rBV	409966	583133	16.84%	1.519%
61	14.904	2177	2179	2185	rVB2	80281	97362	2.81%	0.254%
62	15.086	2207	2210	2215	rVB	247632	277885	8.02%	0.724%
63	15.145	2216	2220	2225	rBV	342929	401463	11.59%	1.046%
64	15.204	2225	2230	2233	rBV	659711	820280	23.68%	2.137%
65	15.604	2296	2298	2302	rVB2	56324	57719	1.67%	0.150%
66	16.539	2452	2457	2462	rBV	164617	284380	8.21%	0.741%
67	16.939	2520	2525	2535	rBV	115781	237313	6.85%	0.618%

Sum of corrected areas: 38390375

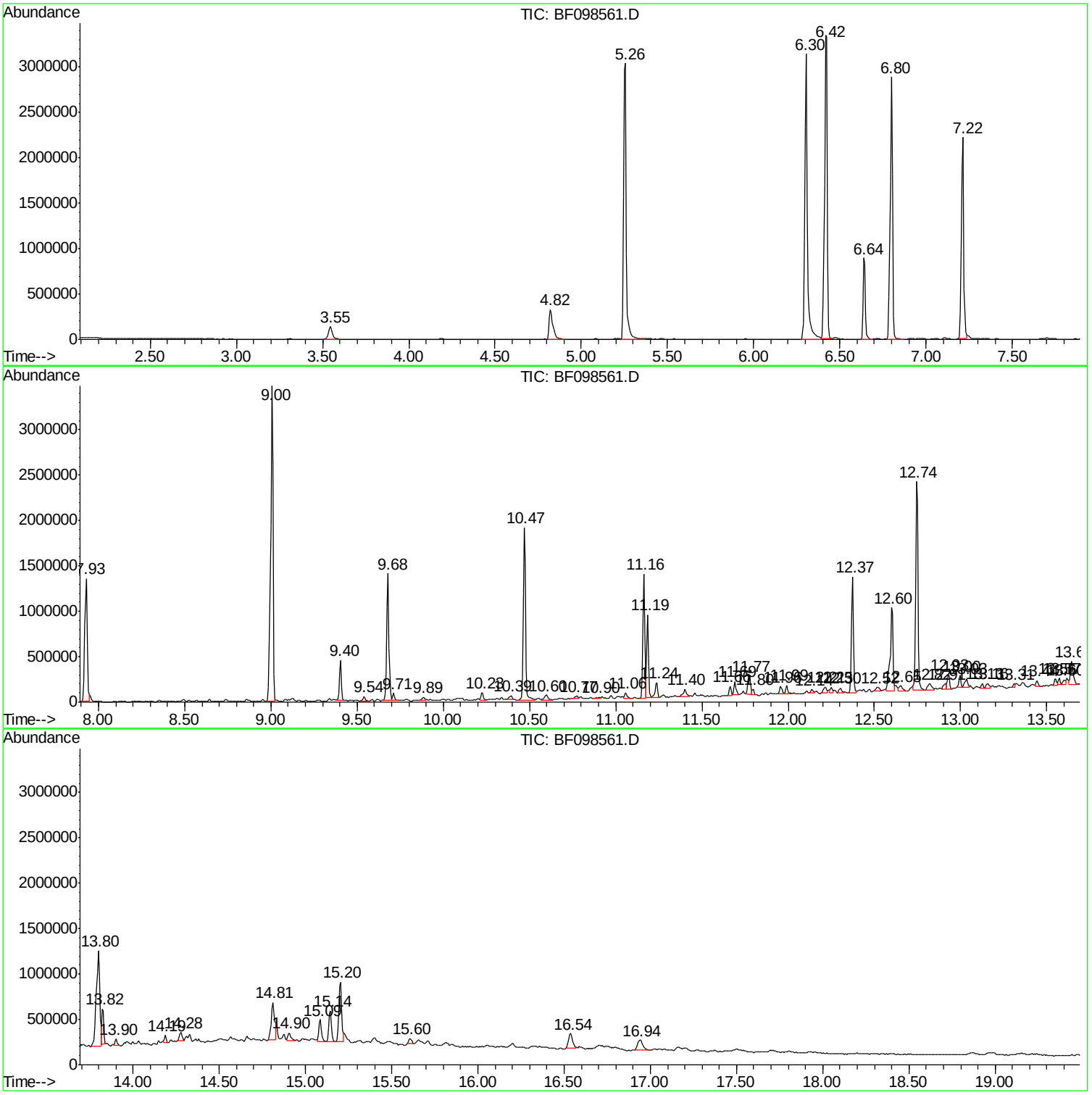
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
Data File : BF098561.D
Acq On : 15 Sep 2017 11:23
Operator : SJ/JU
Sample : I5161-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-14-0-14.25

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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\BF091517\
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

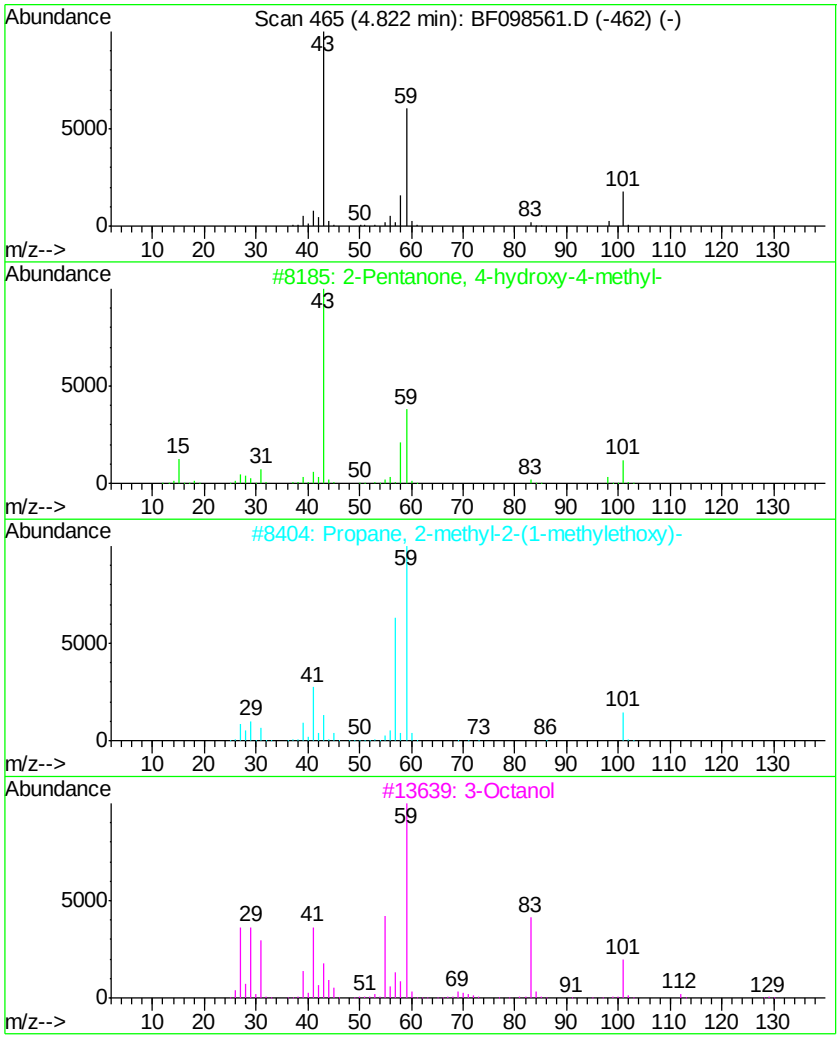
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

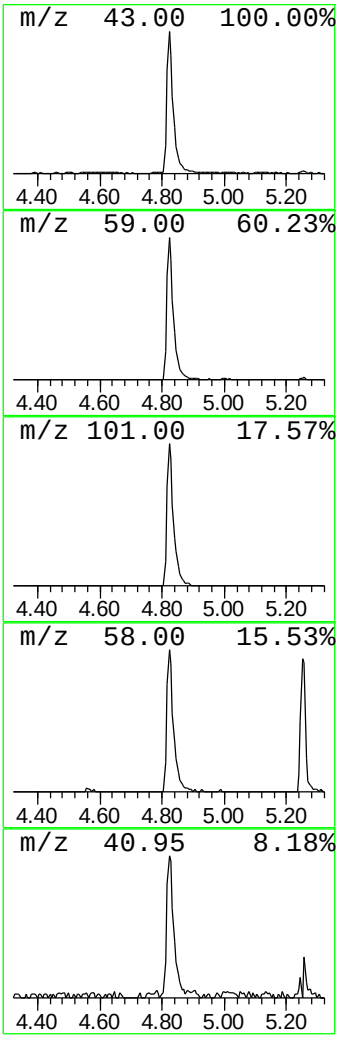
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.82	11.53 ng	483441	1,4-Dichlorobenzene-d4	6.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3	3-Octanol	130	C8H18O	000589-98-0	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
Data File : BF098561.D
Acq On : 15 Sep 2017 11:23
Operator : SJ/JU
Sample : I5161-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-14-0-14.25

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

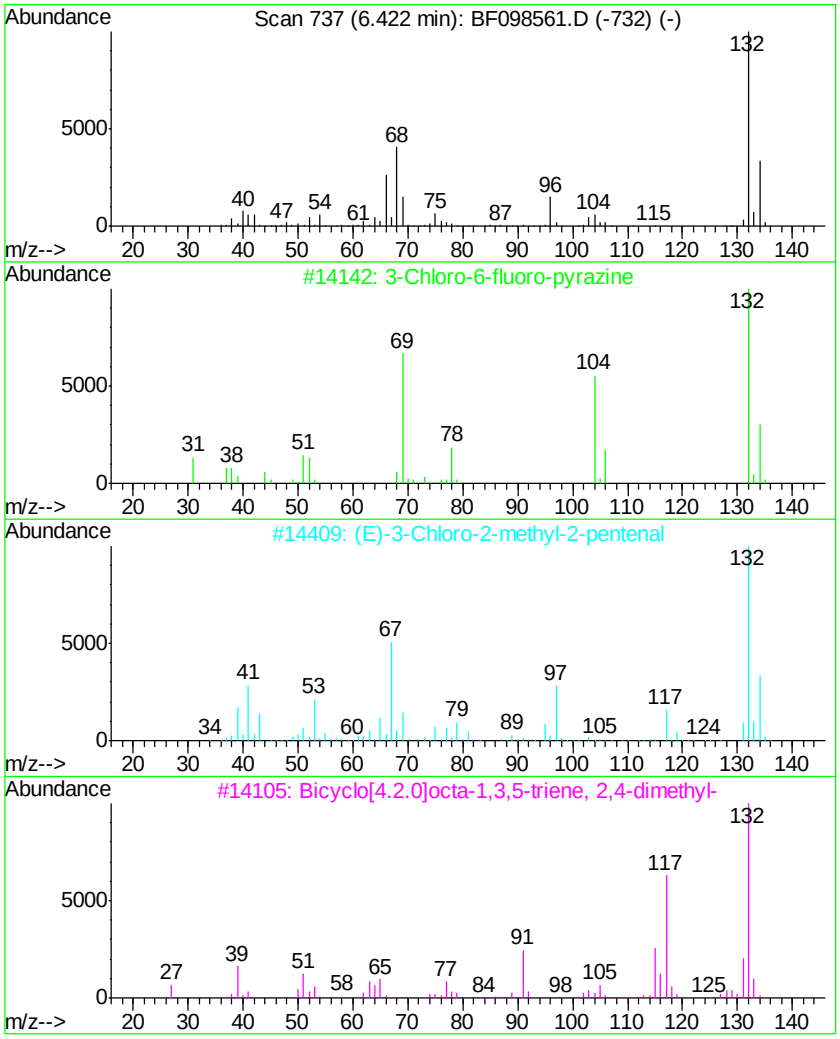
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

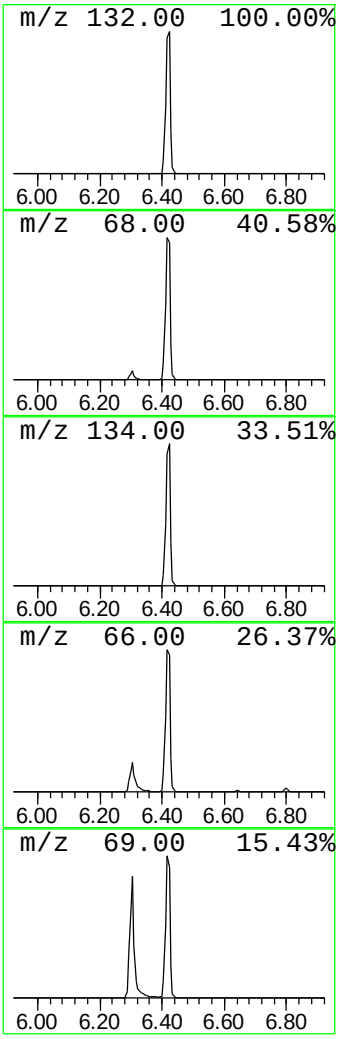
****

Peak Number 3 unknown6.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.42	82.50 ng	3459480	1,4-Dichlorobenzene-d4	6.64

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	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
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Sample : I5161-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-14-0-14.25

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
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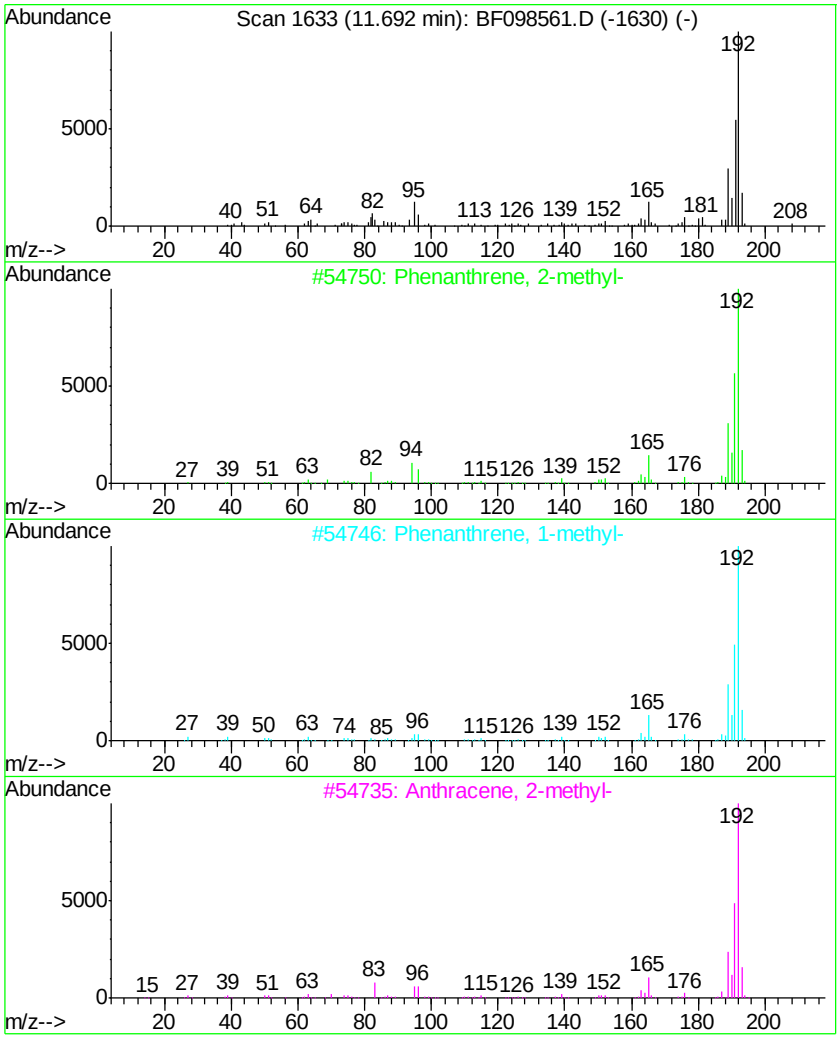
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

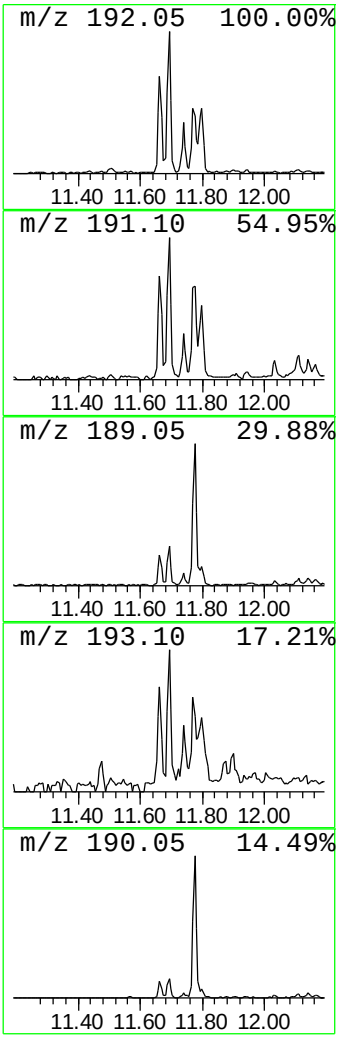
****

Peak Number 5 Phenanthrene, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.69	2.03 ng	122116	Phenanthrene-d10	11.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	97
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	97
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	97
4	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	96
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	96





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
Data File : BF098561.D
Acq On : 15 Sep 2017 11:23
Operator : SJ/JU
Sample : I5161-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-14-0-14.25

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

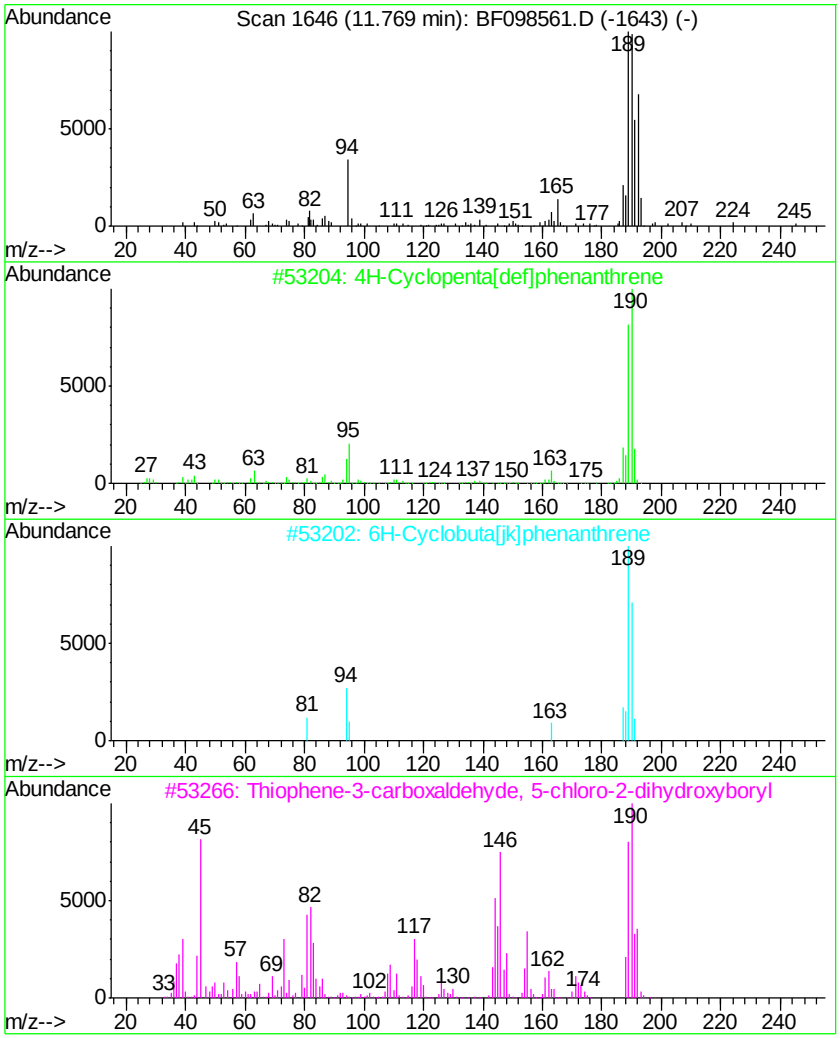
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

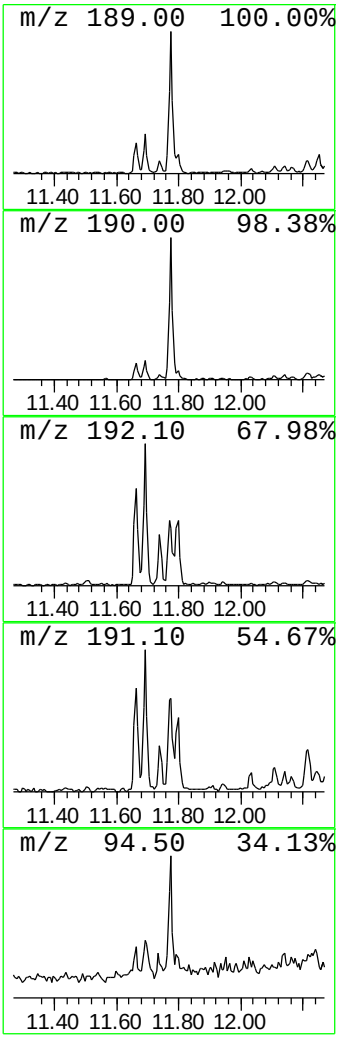
****

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	3.11 ng	187405	Phenanthrene-d10	11.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	90
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	64
3	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	64
4	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	53
5	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	40





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
Data File : BF098561.D
Acq On : 15 Sep 2017 11:23
Operator : SJ/JU
Sample : I5161-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-14-0-14.25

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

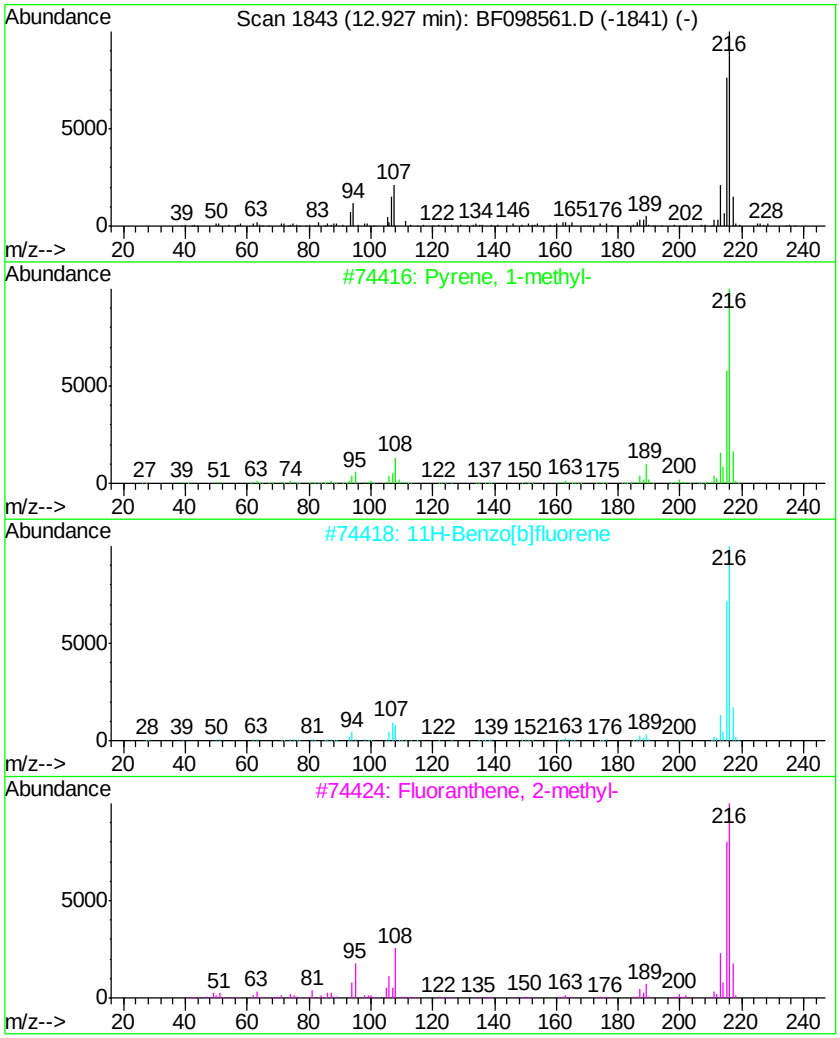
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

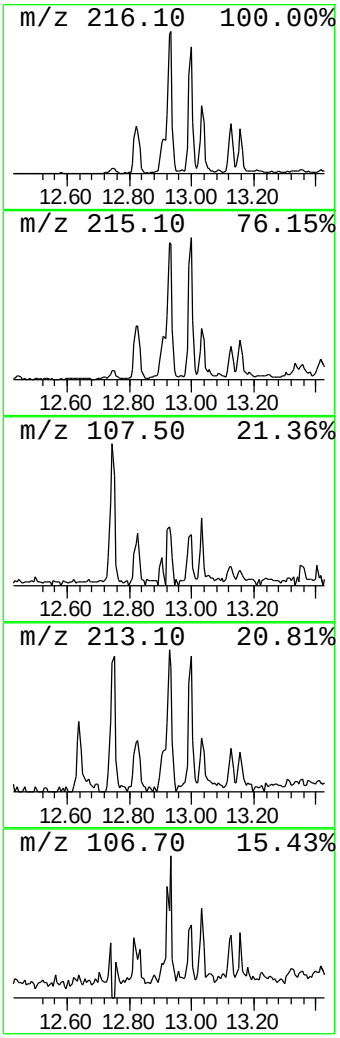
****

Peak Number 7 Pyrene, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.93	2.15 ng	154448	Chrysene-d12	13.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	90
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	87
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	87
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	81
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	74





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
Data File : BF098561.D
Acq On : 15 Sep 2017 11:23
Operator : SJ/JU
Sample : I5161-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-14-0-14.25

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

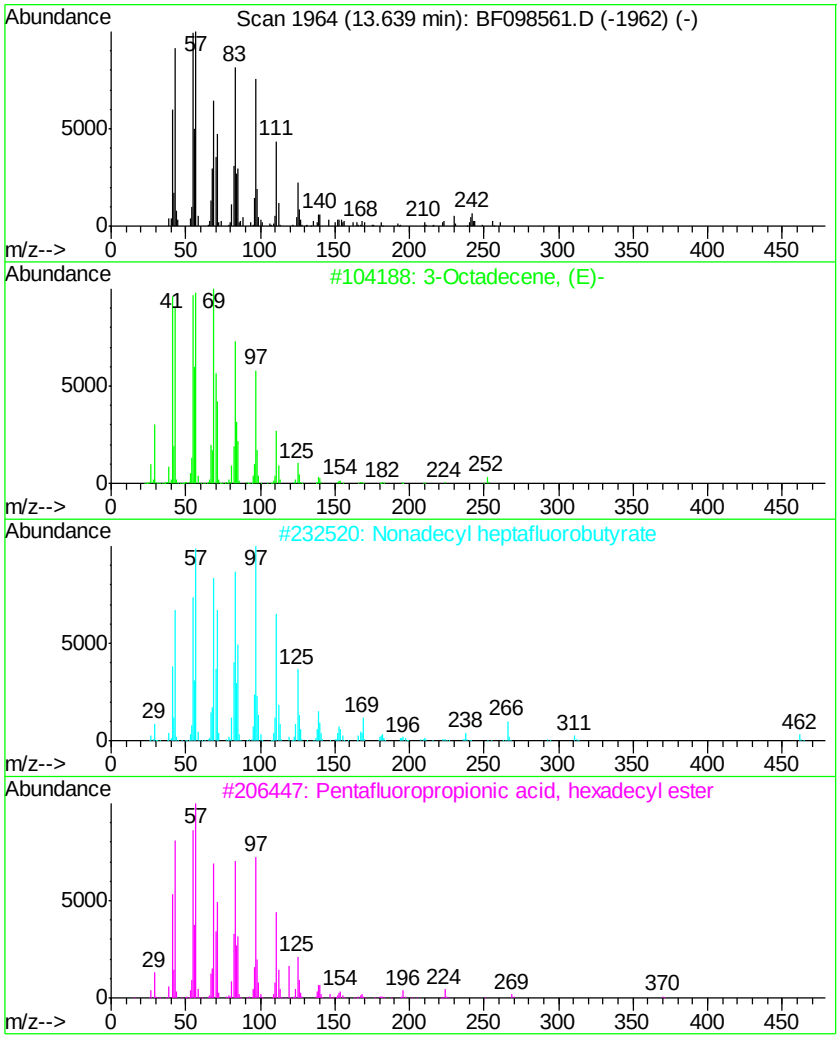
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

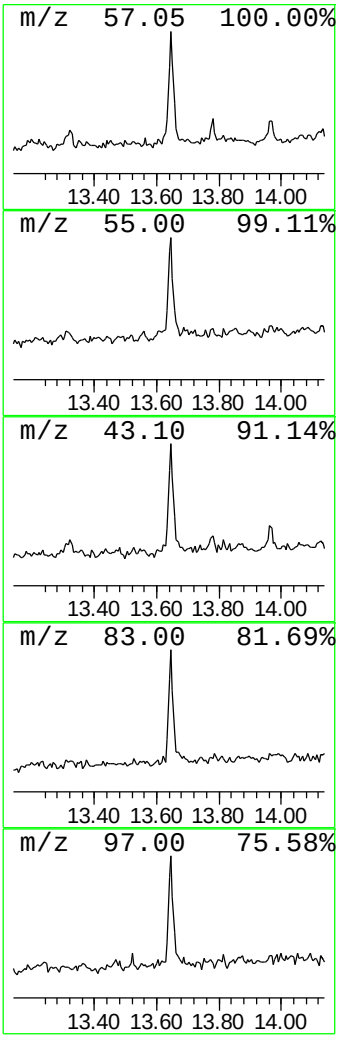
****

Peak Number 8 3-Octadecene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.64	4.00 ng	287113	Chrysene-d12	13.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octadecene, (E)-	252	C18H36	007206-19-1	91
2	Nonadecyl heptafluorobutyrate	480	C23H39F7O2	1000351-83-9	90
3	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	90
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	90
5	Z-5-Nonadecene	266	C19H38	1000131-11-8	89





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
Data File : BF098561.D
Acq On : 15 Sep 2017 11:23
Operator : SJ/JU
Sample : I5161-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-14-0-14.25

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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...	4.82	11.5	ng	483441	1	6.64	838650	20.0
unknown6.42	6.42	82.5	ng	3459480	1	6.64	838650	20.0
Phenanthrene, 2-m...	11.69	2.0	ng	122116	4	11.16	1204220	20.0
4H-Cyclopenta[def...	11.77	3.1	ng	187405	4	11.16	1204220	20.0
Pyrene, 1-methyl-	12.93	2.1	ng	154448	5	13.80	1435420	20.0
3-Octadecene, (E)-	13.64	4.0	ng	287113	5	13.80	1435420	20.0