LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042518\
Data File : BF104791.D
Acq On : 25 Apr 2018 16:19
Operator : JU/SJ
Sample : J2505-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-2-COMP

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-BF040618.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	5.016	493	498	511	rVB	93064	128125	4.32%	0.400%
2	5.422	562	567	570	rBV	2715470	2672254	90.10%	8.333%
3	6.445	735	741	744	rBV	2531128	2733987	92.18%	8.526%
4	6.575	758	763	766	rBV	2959324	2913678	98.24%	9.086%
5	6.622	768	771	777	rVB	38737	36020	1.21%	0.112%
6	6.798	797	801	804	rBV	948317	752245	25.36%	2.346%
7	6.957	823	828	831	rBV	2443782	2190261	73.85%	6.830%
8	7.369	893	898	901	rBV	1878636	1773802	59.81%	5.531%
9	8.081	1012	1019	1025	rBV	1122353	1092565	36.84%	3.407%
10	9.163	1198	1203	1206	rBV	3184919	2965848	100.00%	9.249%
11	9.551	1266	1269	1277	rVB	397655	348853	11.76%	1.088%
12	9.763	1302	1305	1309	rVB	99674	75120	2.53%	0.234%
13	9.839	1314	1318	1321	rVV	1295047	1106674	37.31%	3.451%
14	9.869	1321	1323	1327	rVB	123409	108100	3.64%	0.337%
15	10.045	1350	1353	1357	rVB2	54683	49317	1.66%	0.154%
16	10.239	1382	1386	1387	rBV	30536	30804	1.04%	0.096%
17	10.263	1387	1390	1393	rVB2	130448	105555	3.56%	0.329%
18	10.386	1408	1411	1416	rVB	111662	98317	3.31%	0.307%
19	10.480	1424	1427	1430	rBV2	34767	38388	1.29%	0.120%
20	10.633	1449	1453	1462	rVB	1783270	1745217	58.84%	5.442%
21	10.733	1468	1470	1473	rBV	94738	107332	3.62%	0.335%
22	10.810	1480	1483	1485	rBV	43930	44642	1.51%	0.139%
23	10.839	1485	1488	1491	rVV2	46384	61337	2.07%	0.191%
24	10.875	1491	1494	1496	rVV	53049	53024	1.79%	0.165%
25	10.939	1500	1505	1507	rVV2	49434	75254	2.54%	0.235%
26	10.986	1511	1513	1517	rVV3	57480	70369	2.37%	0.219%
27	11.022	1517	1519	1522	rVV	70189	64630	2.18%	0.202%
28	11.063	1524	1526	1536	rVB3	49159	66888	2.26%	0.209%
29	11.186	1542	1547	1549	rBV2	83120	76897	2.59%	0.240%
30	11.227	1549	1554	1559	rVB2	45497	67717	2.28%	0.211%
31	11.333	1568	1572	1574	rBV	1048453	1015801	34.25%	3.168%
32	11.357	1574	1576	1579	rVV	877267	674334	22.74%	2.103%
33	11.404	1581	1584	1587	rVB	238699	210461	7.10%	0.656%
34	11.563	1607	1611	1617	rBV2	56807	69555	2.35%	0.217%

LSC Area Percent Report

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Operator : JU/SJ
Sample : J2505-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-2-COMP

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-BF040618.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.610	1617	1619	1626	rVB3	32270	38166	1.29%	0.119%
36	11.833	1653	1657	1659	rBV	75523	71701	2.42%	0.224%
37	11.863	1659	1662	1665	rVB	107530	97652	3.29%	0.305%
38	11.910	1665	1670	1673	rBV	53423	52225	1.76%	0.163%
39	11.945	1673	1676	1678	rVV	161574	156092	5.26%	0.487%
40	11.963	1678	1679	1683	rVB	45226	38538	1.30%	0.120%
41	12.127	1704	1707	1710	rBV	73917	60725	2.05%	0.189%
42	12.157	1710	1712	1718	rVV2	32220	38136	1.29%	0.119%
43	12.380	1746	1750	1752	rBV	43175	48370	1.63%	0.151%
44	12.404	1752	1754	1755	rVV	62535	55661	1.88%	0.174%
45	12.422	1755	1757	1759	rVV2	90176	77048	2.60%	0.240%
46	12.474	1762	1766	1769	rBV3	31432	38805	1.31%	0.121%
47	12.545	1774	1778	1782	rBV	1019637	954651	32.19%	2.977%
48	12.698	1800	1804	1807	rBV	36533	41963	1.41%	0.131%
49	12.774	1811	1817	1823	rBV	771860	936093	31.56%	2.919%
50	12.827	1823	1826	1830	rVB2	41908	49832	1.68%	0.155%
51	12.921	1834	1842	1845	rBV	2081252	2116238	71.35%	6.599%
52	12.998	1850	1855	1859	rBV4	42152	79752	2.69%	0.249%
53	13.080	1866	1869	1870	rBV2	40400	41981	1.42%	0.131%
54	13.104	1870	1873	1877	rVB	106505	104770	3.53%	0.327%
55	13.169	1881	1884	1887	rBV	80507	71535	2.41%	0.223%
56	13.210	1887	1891	1893	rBV2	63775	70684	2.38%	0.220%
57	13.333	1909	1912	1914	rBV	40634	40879	1.38%	0.127%
58	13.616	1957	1960	1964	rVB	39594	41178	1.39%	0.128%
59	13.727	1975	1979	1981	rBV	51395	57543	1.94%	0.179%
60	13.751	1981	1983	1986	rVV	55796	48397	1.63%	0.151%
61	13.804	1990	1992	2000	rVB2	104464	162054	5.46%	0.505%
62	13.980	2014	2022	2024	rBV2	777078	1031473	34.78%	3.217%
63	14.004	2024	2026	2033	rVB	323085	287217	9.68%	0.896%
64	14.086	2037	2040	2042	rVB	76527	65351	2.20%	0.204%
65	14.368	2086	2088	2091	rVB2	48669	41926	1.41%	0.131%
66	14.492	2107	2109	2111	rBV3	29939	30380	1.02%	0.095%
67	15.027	2196	2200	2203	rBV	201907	297614	10.03%	0.928%
68	15.133	2215	2218	2226	rBV	43482	69235	2.33%	0.216%
69	15.327	2248	2251	2257	rVB	115216	141556	4.77%	0.441%
70	15.386	2258	2261	2267	rVB	172564	207831	7.01%	0.648%
71	15.451	2268	2272	2276	rBV	452284	585383	19.74%	1.825%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
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Integrator: RTE
Smoothing : ON Filtering: 5
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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	16.909	2517	2520	2526	rVB2	56244	96170	3.24%	0.300%

Sum of corrected areas: 32068176

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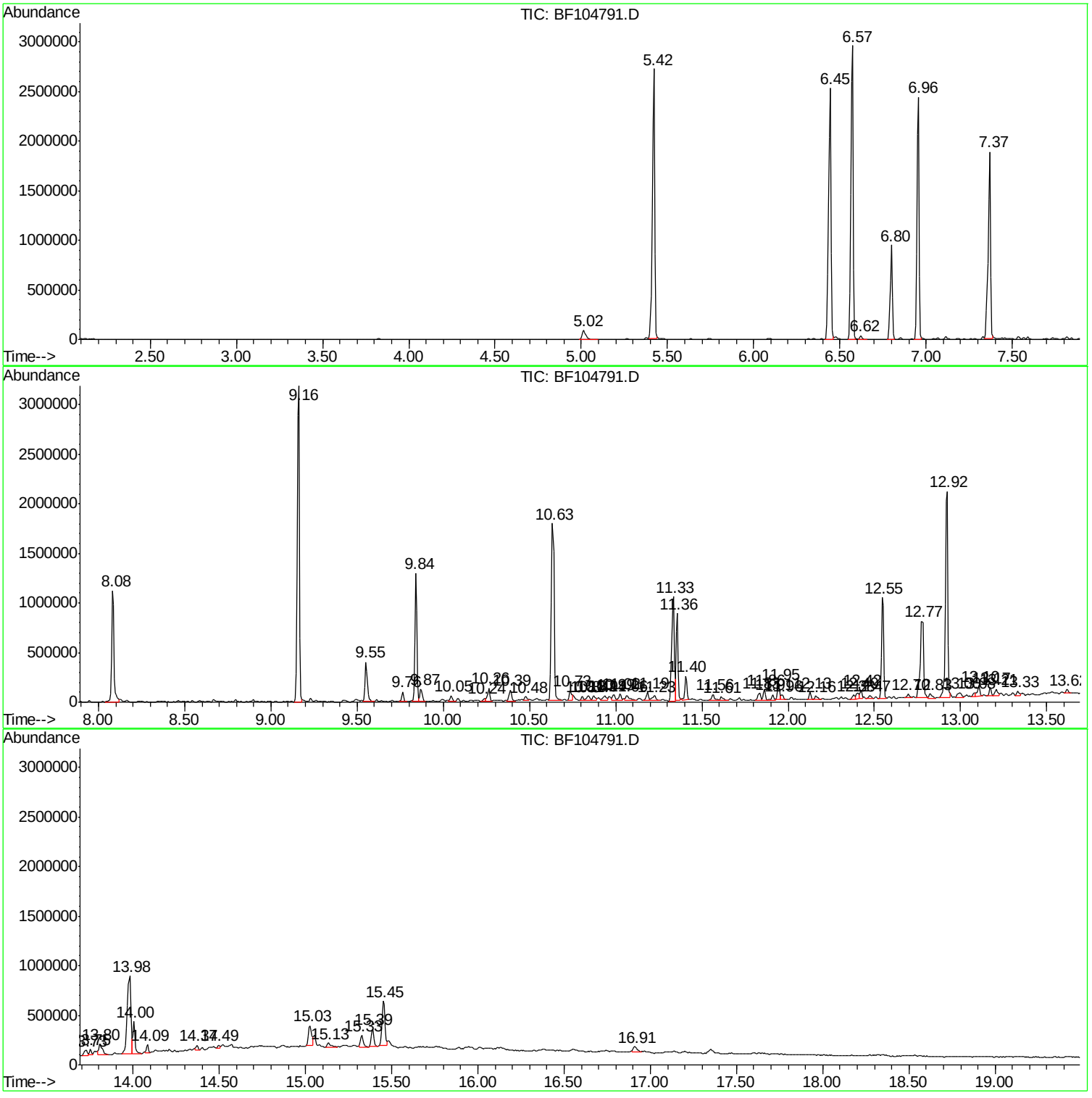
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Operator : JU/SJ
Sample : J2505-04
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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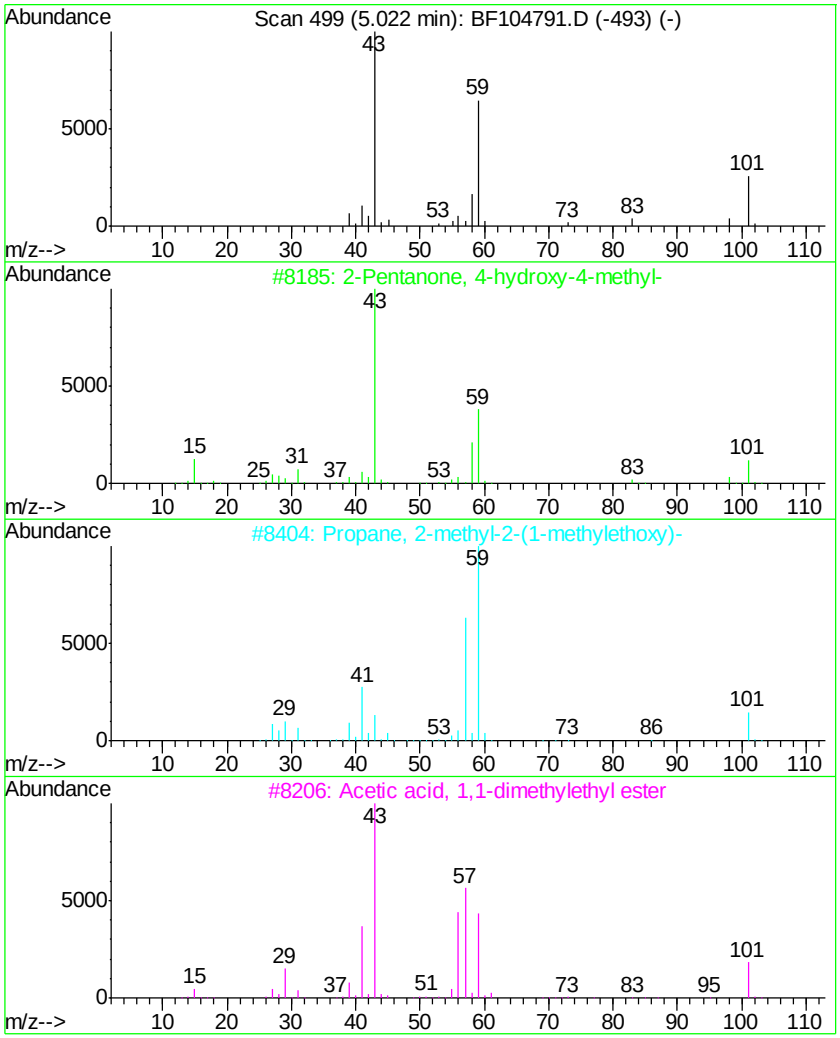
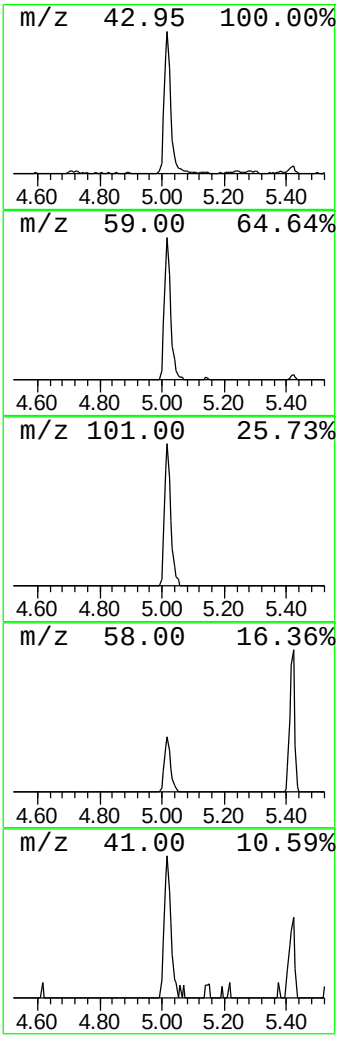
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	3.41 ng	128125	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	40
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
4	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
5	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25





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Sample : J2505-04
Misc :
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Instrument : BNA_F
ClientSampleId : S-2-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
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TIC Library : C:\DATABASE\NIST11.L
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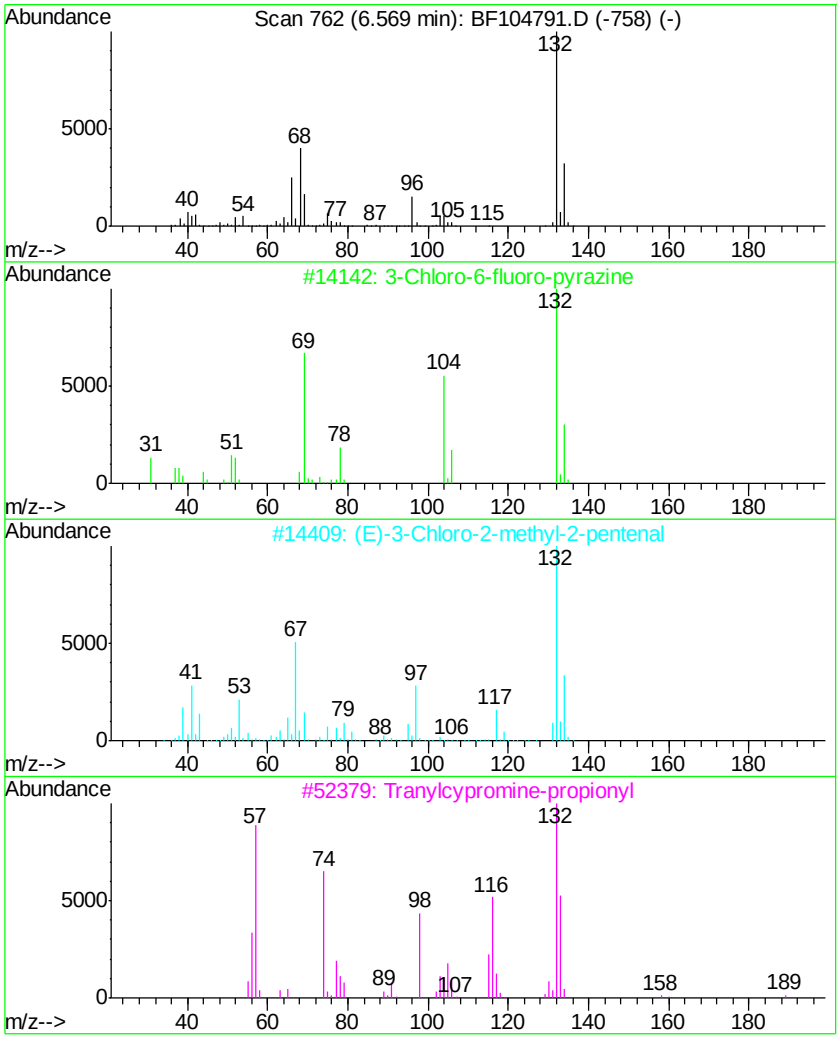
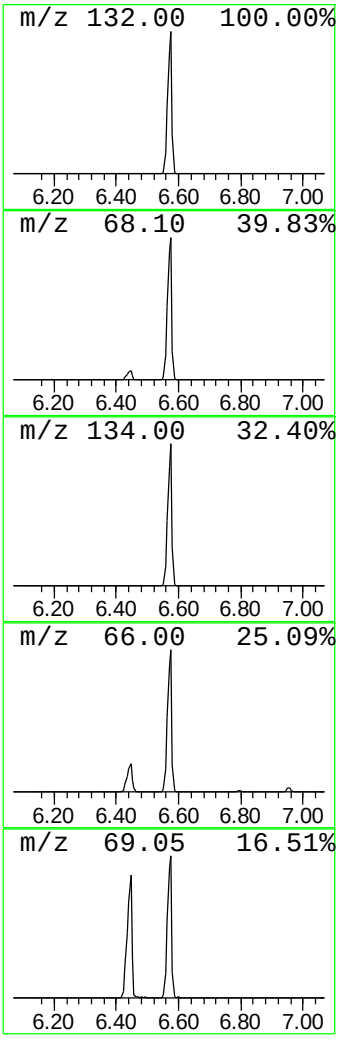
Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	77.47 ng	2913680	1,4-Dichlorobenzene-d4	6.80

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	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042518\
Data File : BF104791.D
Acq On : 25 Apr 2018 16:19
Operator : JU/SJ
Sample : J2505-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-2-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

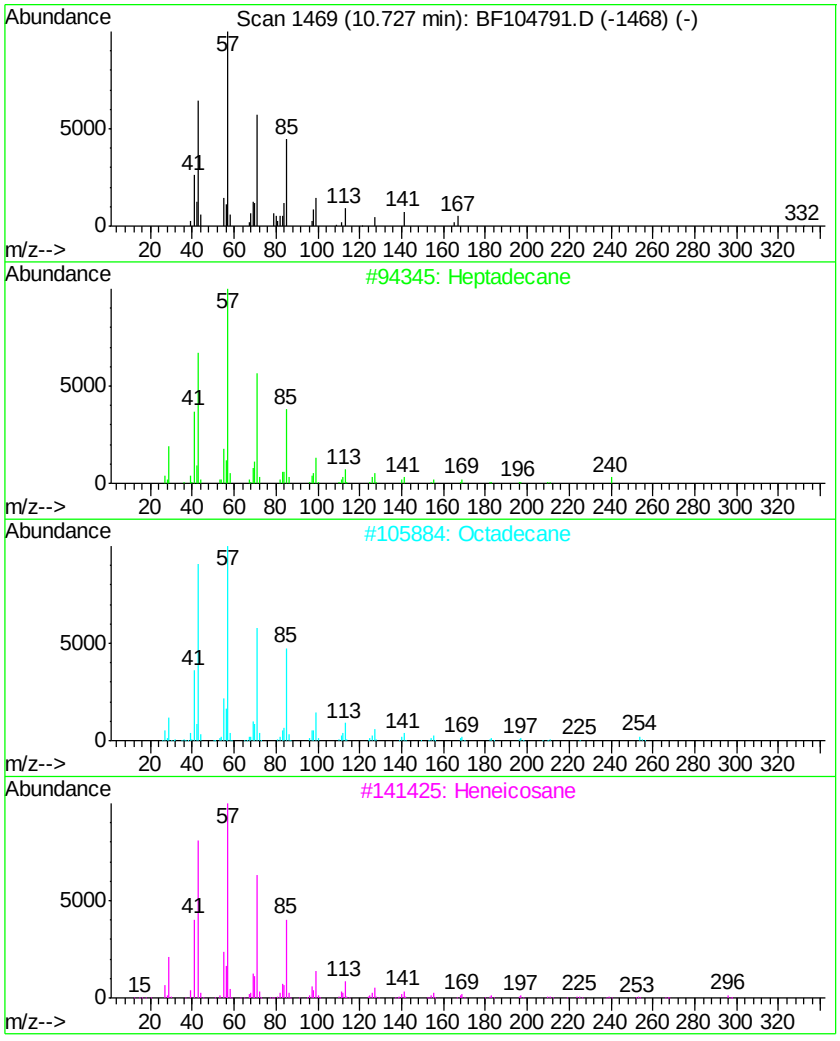
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

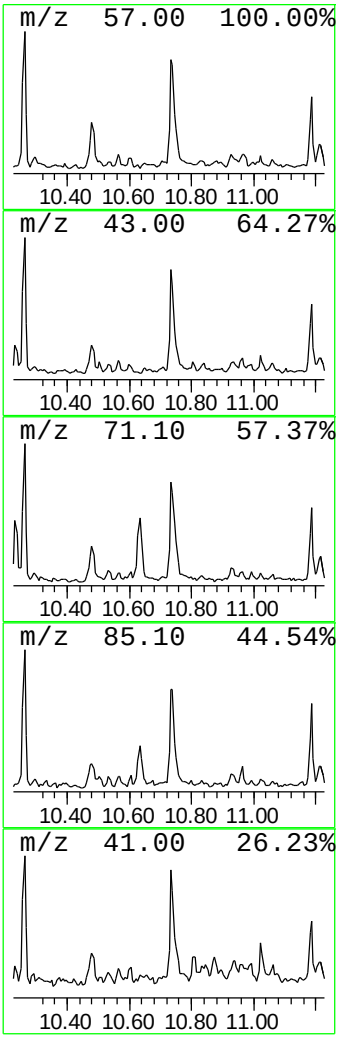
****

Peak Number 4 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.73	2.11 ng	107332	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Octadecane	254	C18H38	000593-45-3	91
3	Heneicosane	296	C21H44	000629-94-7	90
4	Eicosane	282	C20H42	000112-95-8	87
5	Pentadecane	212	C15H32	000629-62-9	87





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Instrument : BNA_F
ClientSampleId : S-2-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

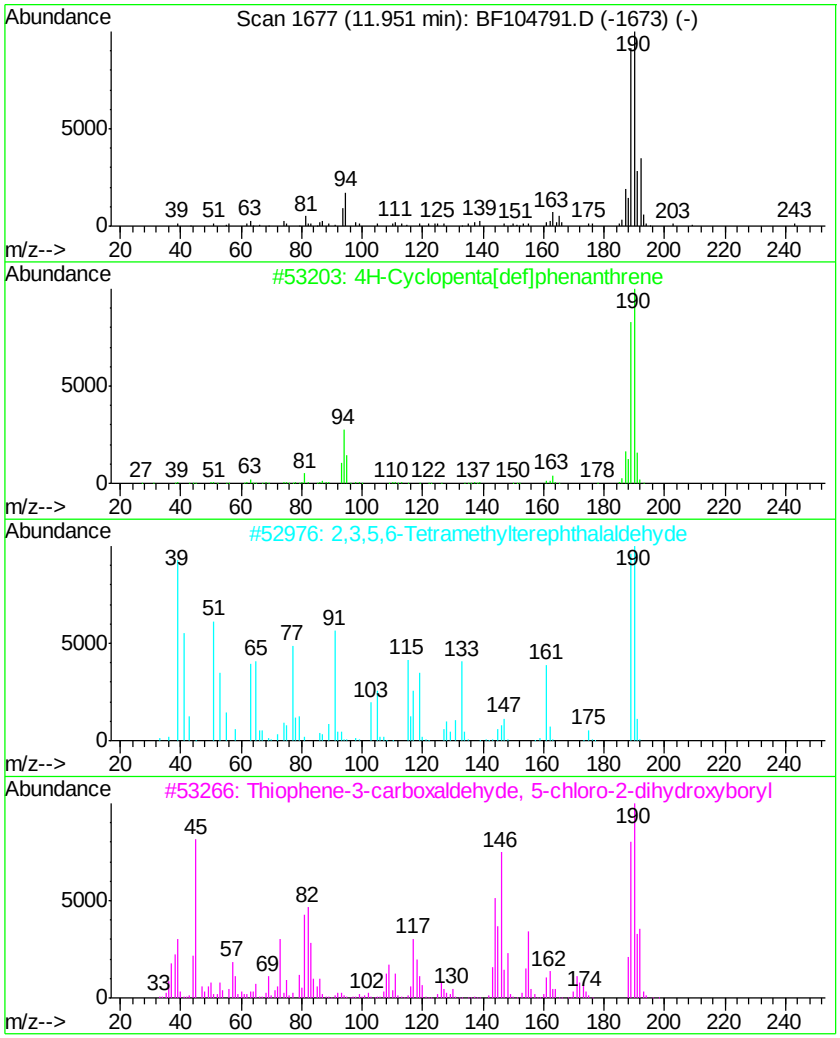
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

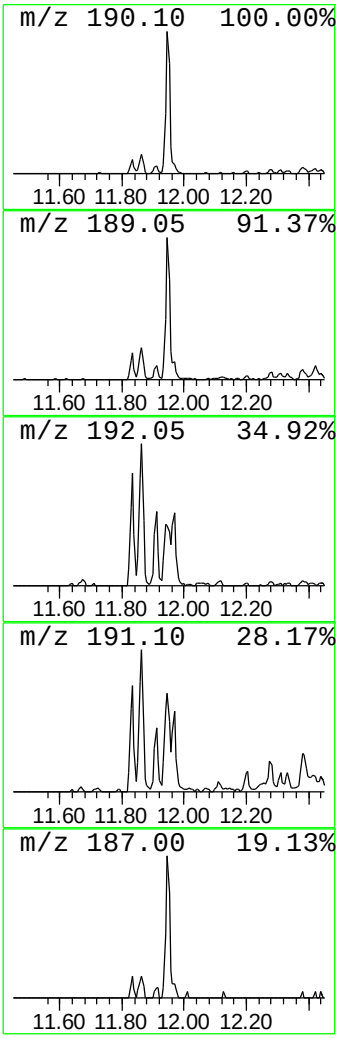
****

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	3.07 ng	156092	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	93
2	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	50
3	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	50
4	Methyl diselenide	190	C2H6Se2	007101-31-7	49
5	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	40





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Sample : J2505-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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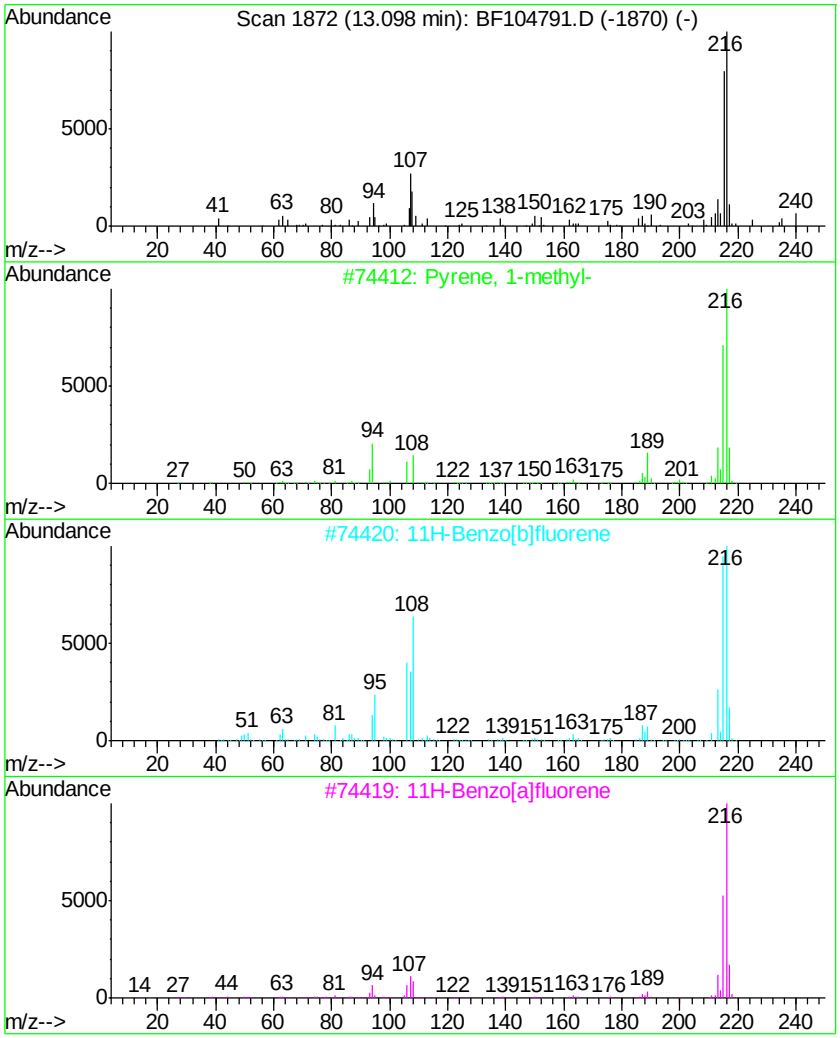
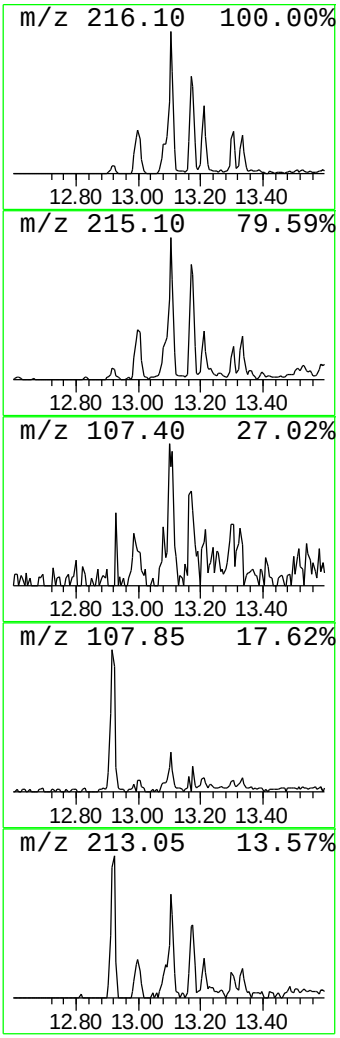
Peak Number 6 Pyrene, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.10	2.03 ng	104770	Chrysene-d12	13.98

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	91
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	90
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	81
5	1,3,5-Triazine-2,4,6-triamine, N...	216	C10H12N6	046731-79-7	59





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Operator : JU/SJ
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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-2-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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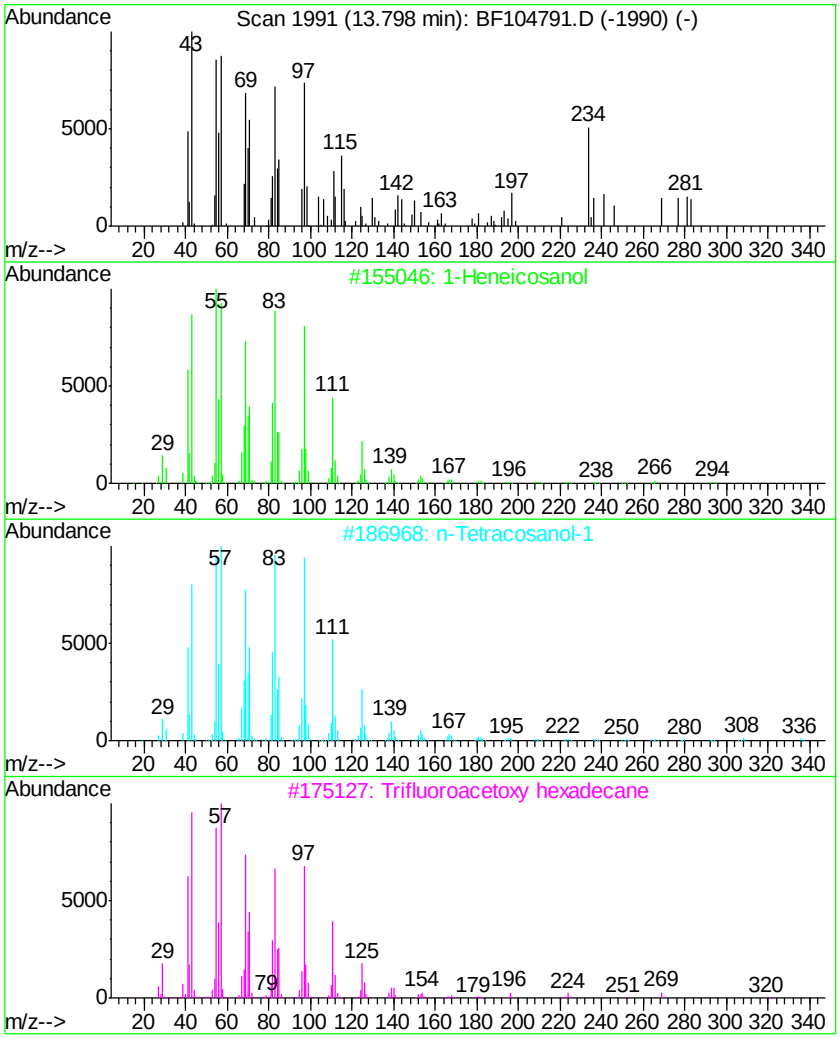
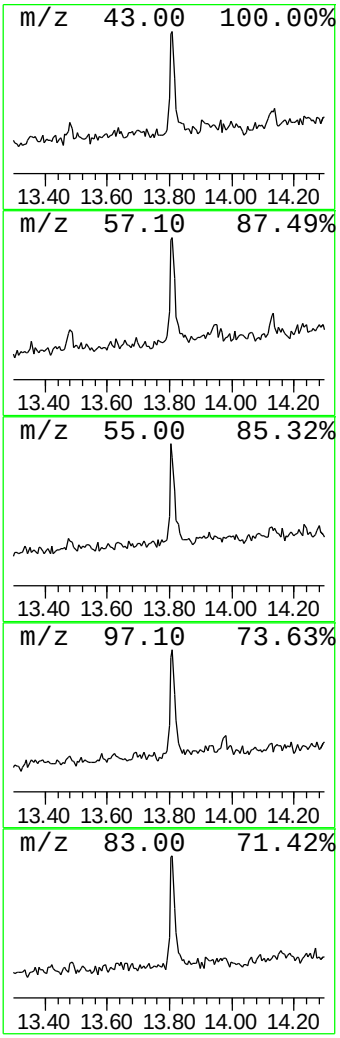
Peak Number 7 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	3.14 ng	162054	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	91
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	87
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	87





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Misc :
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Instrument : BNA_F
ClientSampleId : S-2-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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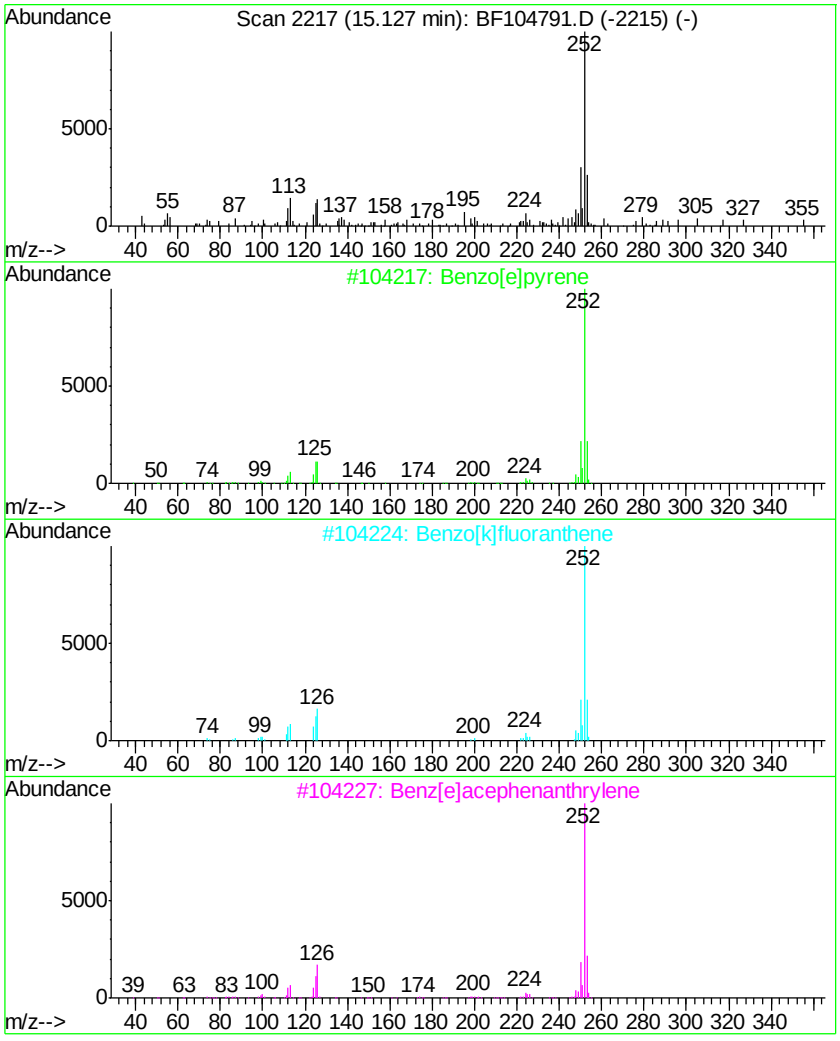
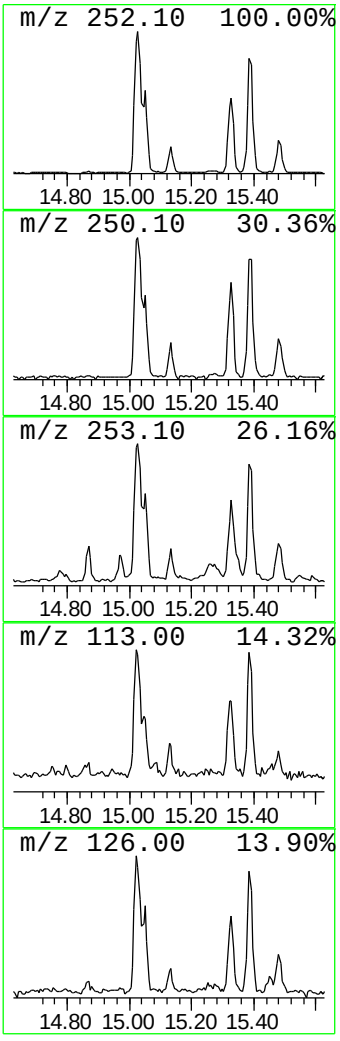
Peak Number 8 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.13	2.37 ng	69235	Perylene-d12	15.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	97
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93
4	Benzo[a]pyrene	252	C20H12	000050-32-8	81
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042518\
Data File : BF104791.D
Acq On : 25 Apr 2018 16:19
Operator : JU/SJ
Sample : J2505-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-2-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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...	5.02	3.4	ng	128125	1	6.80	752245	20.0
unknown6.57	6.57	77.5	ng	2913680	1	6.80	752245	20.0
Heptadecane	10.73	2.1	ng	107332	4	11.33	1015800	20.0
4H-Cyclopenta[def...	11.95	3.1	ng	156092	4	11.33	1015800	20.0
Pyrene, 1-methyl-	13.10	2.0	ng	104770	5	13.98	1031470	20.0
1-Heneicosanol	13.80	3.1	ng	162054	5	13.98	1031470	20.0
Benzo[e]pyrene	15.13	2.4	ng	69235	6	15.45	585383	20.0