LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042718\
Data File : BF104895.D
Acq On : 27 Apr 2018 21:32
Operator : JU/SJ
Sample : J2566-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

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	494	498	508	rVB	91044	124765	4.58%	0.446%
2	5.428	563	568	583	rBV	2382571	2621937	96.30%	9.367%
3	6.451	737	742	759	rBV	2325740	2625829	96.45%	9.381%
4	6.575	759	763	766	rBV	2818960	2672520	98.16%	9.547%
5	6.798	798	801	805	rBV	725397	574802	21.11%	2.053%
6	6.957	824	828	831	rBV	2418302	2081916	76.47%	7.438%
7	7.369	893	898	901	rBV	1700427	1582602	58.13%	5.654%
8	7.463	911	914	921	rVB	19238	27983	1.03%	0.100%
9	8.080	1016	1019	1037	rVB	725180	794074	29.17%	2.837%
10	9.157	1198	1202	1206	rBV	2737787	2722592	100.00%	9.726%
11	9.551	1266	1269	1277	rVB	217146	206089	7.57%	0.736%
12	9.763	1302	1305	1309	rVB	58008	45245	1.66%	0.162%
13	9.839	1314	1318	1321	rVV2	903855	757474	27.82%	2.706%
14	9.869	1321	1323	1327	rVB	89816	84019	3.09%	0.300%
15	10.045	1350	1353	1357	rVB2	30837	30365	1.12%	0.108%
16	10.263	1387	1390	1393	rVB2	81765	72870	2.68%	0.260%
17	10.392	1408	1412	1416	rVB	63023	56620	2.08%	0.202%
18	10.633	1449	1453	1464	rBV	1528819	1646156	60.46%	5.881%
19	10.733	1467	1470	1480	rVB	73275	99145	3.64%	0.354%
20	10.939	1500	1505	1508	rBV4	22827	36192	1.33%	0.129%
21	11.180	1543	1546	1549	rBV3	52379	56331	2.07%	0.201%
22	11.227	1552	1554	1558	rVB	37889	34506	1.27%	0.123%
23	11.333	1568	1572	1574	rBV	749966	708664	26.03%	2.532%
24	11.357	1574	1576	1581	rVV	591521	472072	17.34%	1.686%
25	11.410	1581	1585	1587	rVV	119310	111152	4.08%	0.397%
26	11.568	1607	1612	1617	rBV2	55145	68990	2.53%	0.246%
27	11.610	1617	1619	1625	rVB2	33856	32042	1.18%	0.114%
28	11.851	1654	1660	1668	rBV2	299607	429752	15.78%	1.535%
29	11.945	1673	1676	1679	rVV	124783	136996	5.03%	0.489%
30	11.968	1679	1680	1686	rVB	49349	34806	1.28%	0.124%
31	12.021	1686	1689	1691	rBV	34622	33829	1.24%	0.121%
32	12.127	1705	1707	1710	rBV	49716	42849	1.57%	0.153%
33	12.163	1710	1713	1718	rVB	30228	36090	1.33%	0.129%
34	12.380	1748	1750	1753	rBV	35999	37872	1.39%	0.135%

LSC Area Percent Report

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Data File : BF104895.D
Acq On : 27 Apr 2018 21:32
Operator : JU/SJ
Sample : J2566-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

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	12.421	1753	1757	1759	rVV4	29661	37393	1.37%	0.134%
36	12.474	1763	1766	1770	rBV3	29097	39391	1.45%	0.141%
37	12.551	1775	1779	1784	rBV	815253	743145	27.30%	2.655%
38	12.639	1791	1794	1797	rBV2	41281	40959	1.50%	0.146%
39	12.780	1811	1818	1824	rBV	699423	777120	28.54%	2.776%
40	12.827	1824	1826	1830	rVB2	34195	34189	1.26%	0.122%
41	12.921	1835	1842	1845	rBV	2394052	2174168	79.86%	7.767%
42	12.992	1851	1854	1858	rBV2	37800	64004	2.35%	0.229%
43	13.080	1867	1869	1871	rBV3	34244	37819	1.39%	0.135%
44	13.110	1871	1874	1876	rVB	113485	105438	3.87%	0.377%
45	13.174	1882	1885	1887	rBV2	100598	82007	3.01%	0.293%
46	13.210	1888	1891	1894	rBV2	57968	67807	2.49%	0.242%
47	13.333	1910	1912	1919	rBV2	38258	62433	2.29%	0.223%
48	13.621	1959	1961	1965	rVB	35801	28839	1.06%	0.103%
49	13.727	1977	1979	1981	rBV	50447	44043	1.62%	0.157%
50	13.757	1981	1984	1986	rBV	45751	41011	1.51%	0.147%
51	13.804	1989	1992	1995	rVV3	264433	248678	9.13%	0.888%
52	13.980	2017	2022	2025	rBV2	720794	918457	33.73%	3.281%
53	14.004	2025	2026	2033	rVB	280219	245555	9.02%	0.877%
54	14.086	2038	2040	2043	rVB	64616	47004	1.73%	0.168%
55	15.027	2196	2200	2202	rBV	187831	269945	9.92%	0.964%
56	15.327	2248	2251	2257	rVB	109712	137448	5.05%	0.491%
57	15.386	2258	2261	2267	rBV	168657	203134	7.46%	0.726%
58	15.451	2268	2272	2276	rBV	353638	442824	16.26%	1.582%

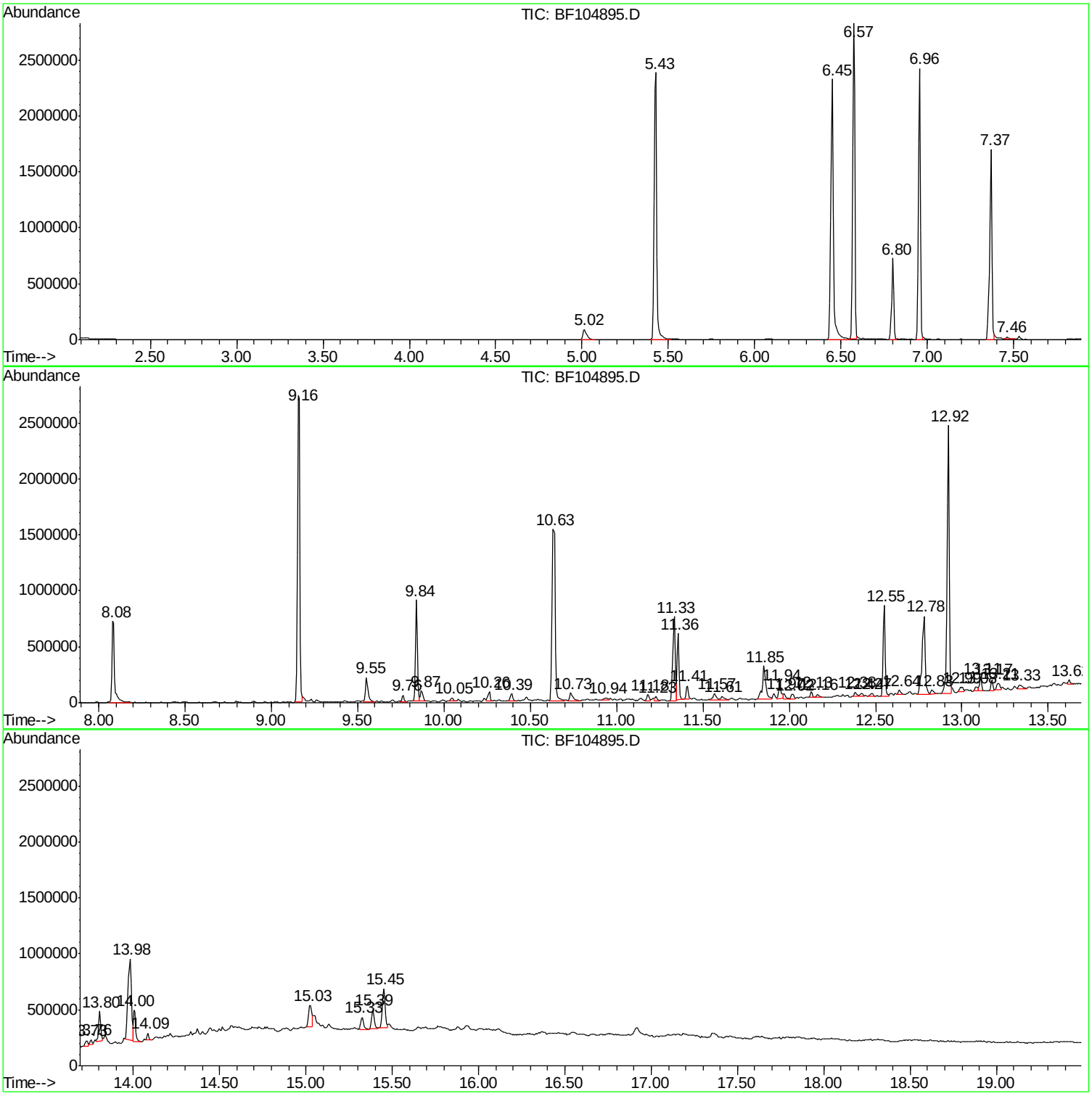
Sum of corrected areas: 27991957

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042718\
Data File : BF104895.D
Acq On : 27 Apr 2018 21:32
Operator : JU/SJ
Sample : J2566-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042718\
Data File : BF104895.D
Acq On : 27 Apr 2018 21:32
Operator : JU/SJ
Sample : J2566-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

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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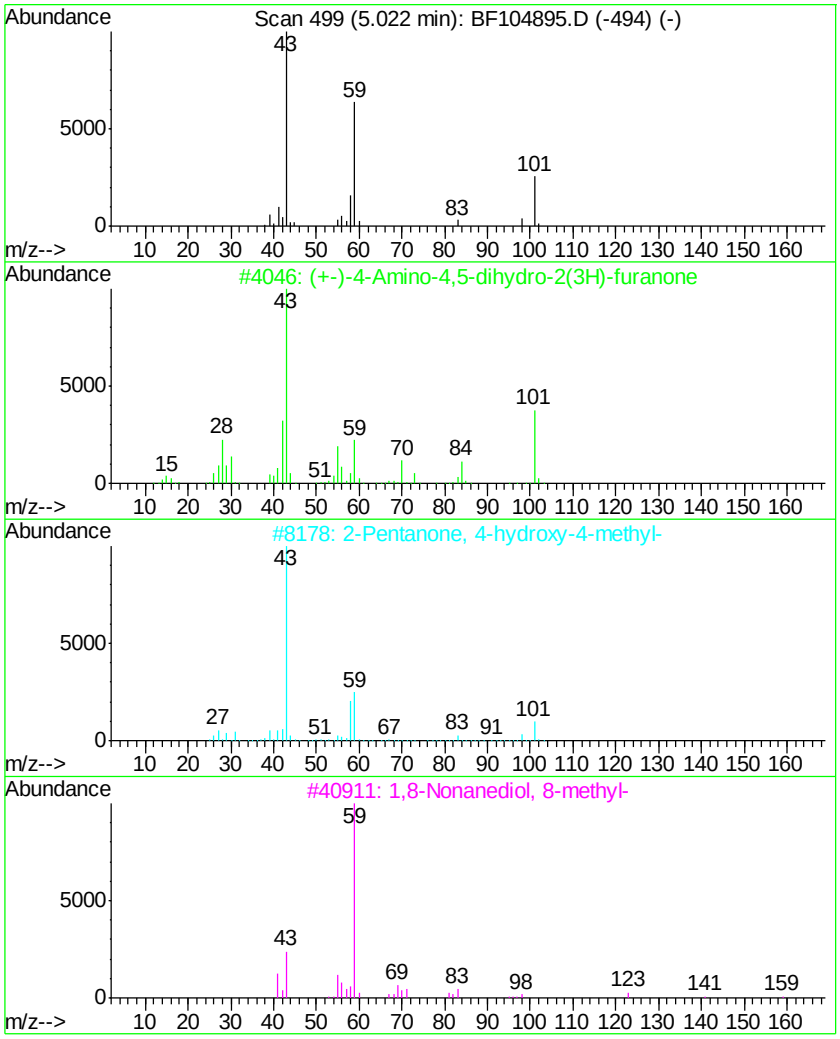
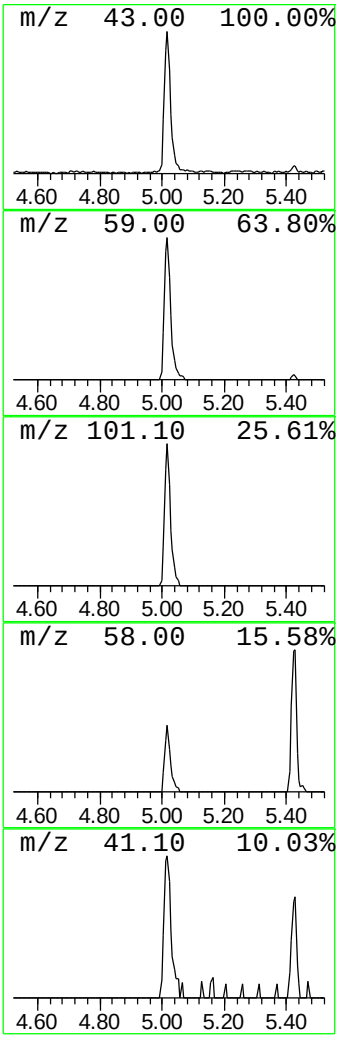
Peak Number 1 unknown5.02 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	4.34 ng	124765	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	47
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
3	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	Acetone	58	C3H6O	000067-64-1	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042718\
Data File : BF104895.D
Acq On : 27 Apr 2018 21:32
Operator : JU/SJ
Sample : J2566-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

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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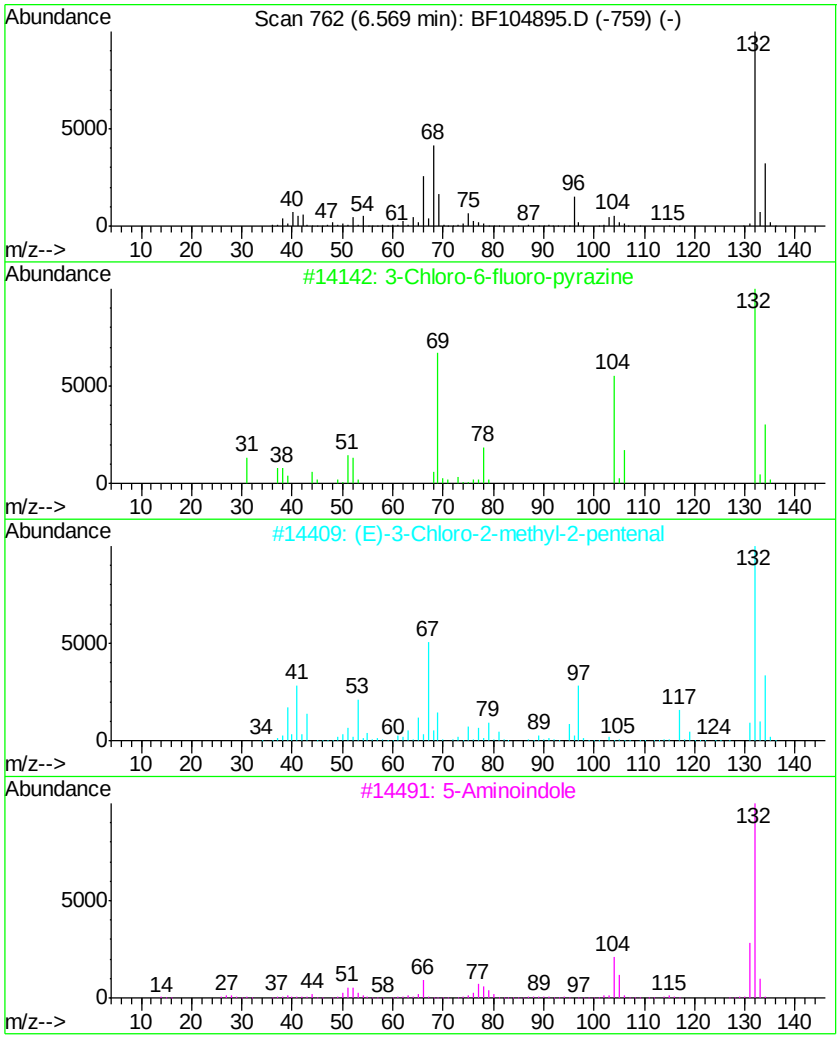
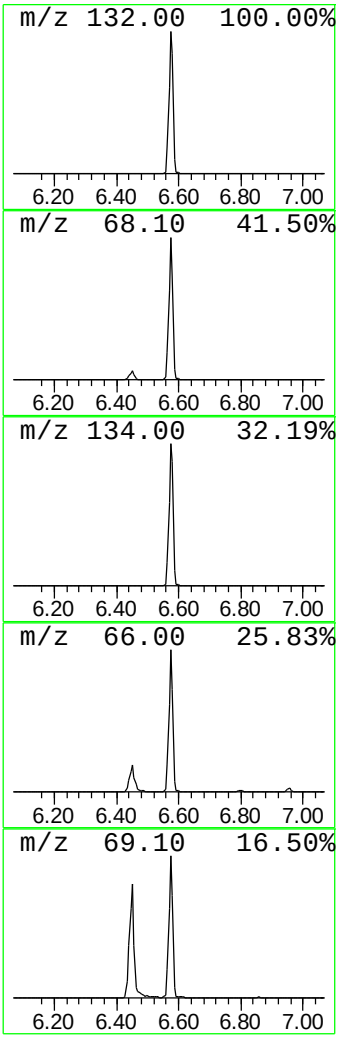
Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	92.99 ng	2672520	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	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042718\
Data File : BF104895.D
Acq On : 27 Apr 2018 21:32
Operator : JU/SJ
Sample : J2566-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

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

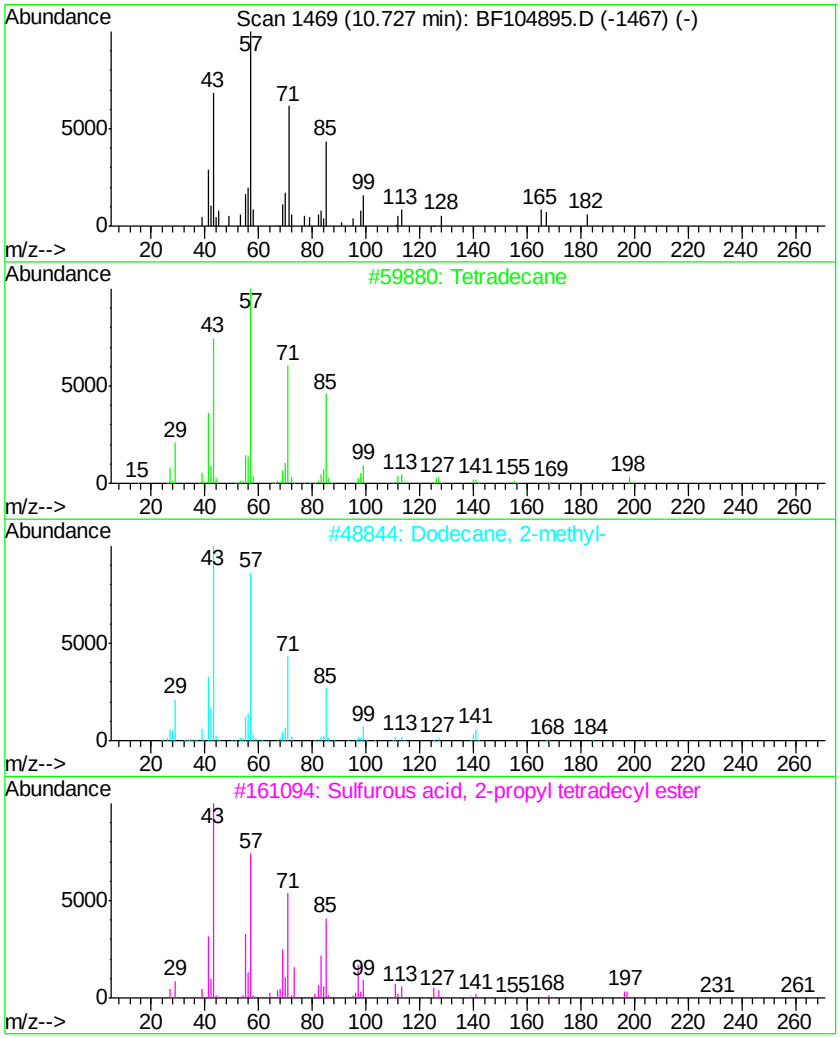
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

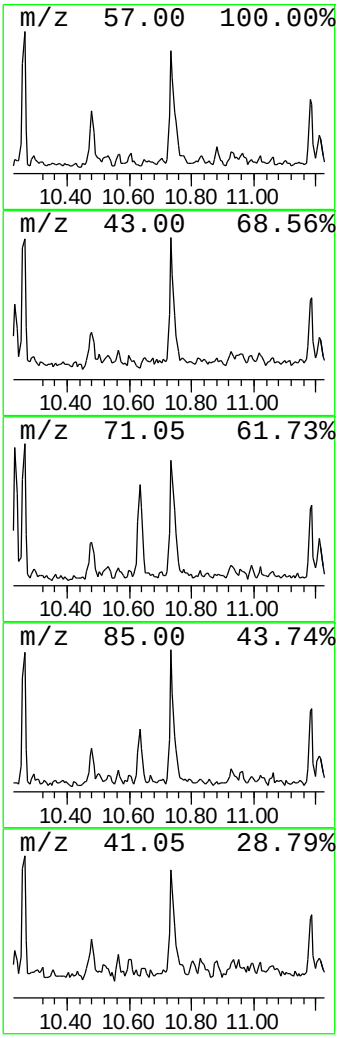
****

Peak Number 4 Tetradecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.73	2.80 ng	99145	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	86
2	Dodecane, 2-methyl-	184	C13H28	001560-97-0	78
3	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	78
4	Tritetracontane	605	C43H88	007098-21-7	78
5	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	72





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042718\
Data File : BF104895.D
Acq On : 27 Apr 2018 21:32
Operator : JU/SJ
Sample : J2566-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

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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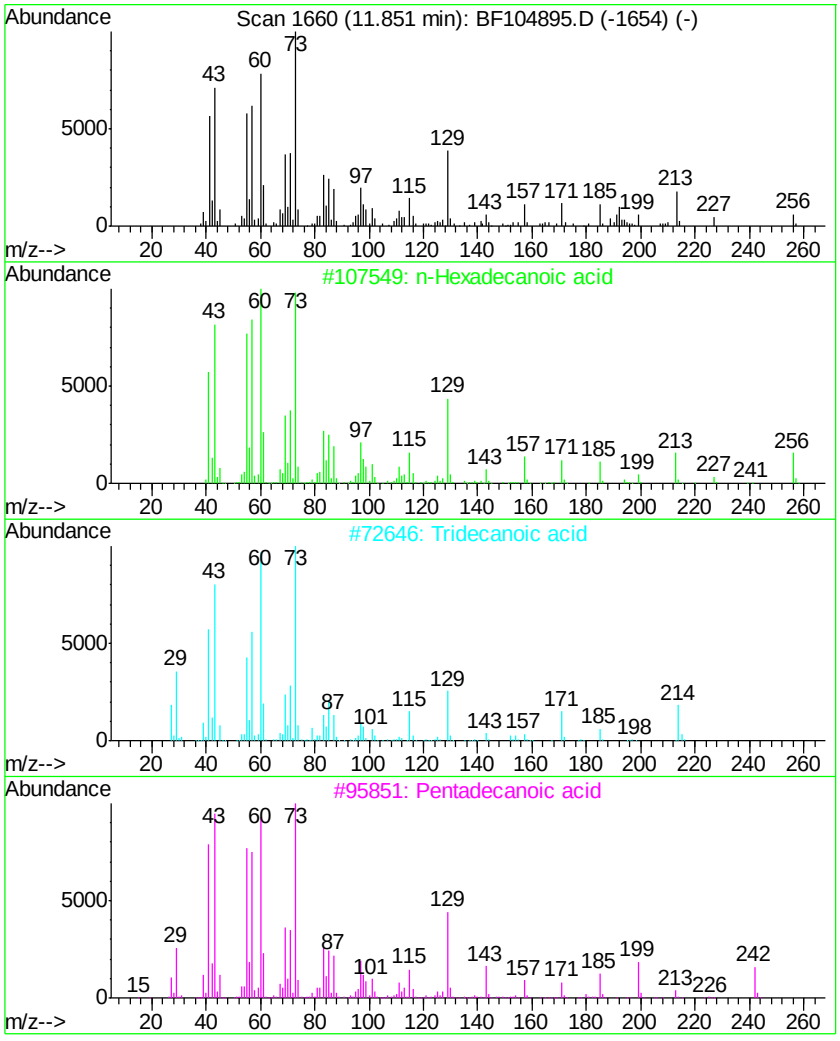
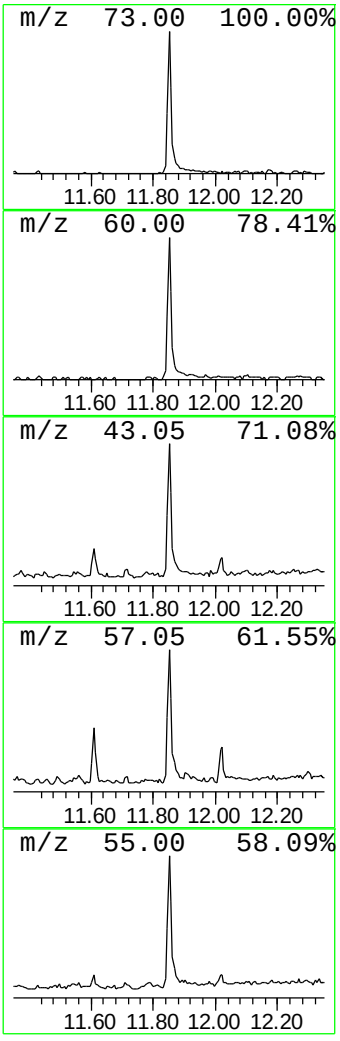
Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	12.13 ng	429752	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





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Sample : J2566-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

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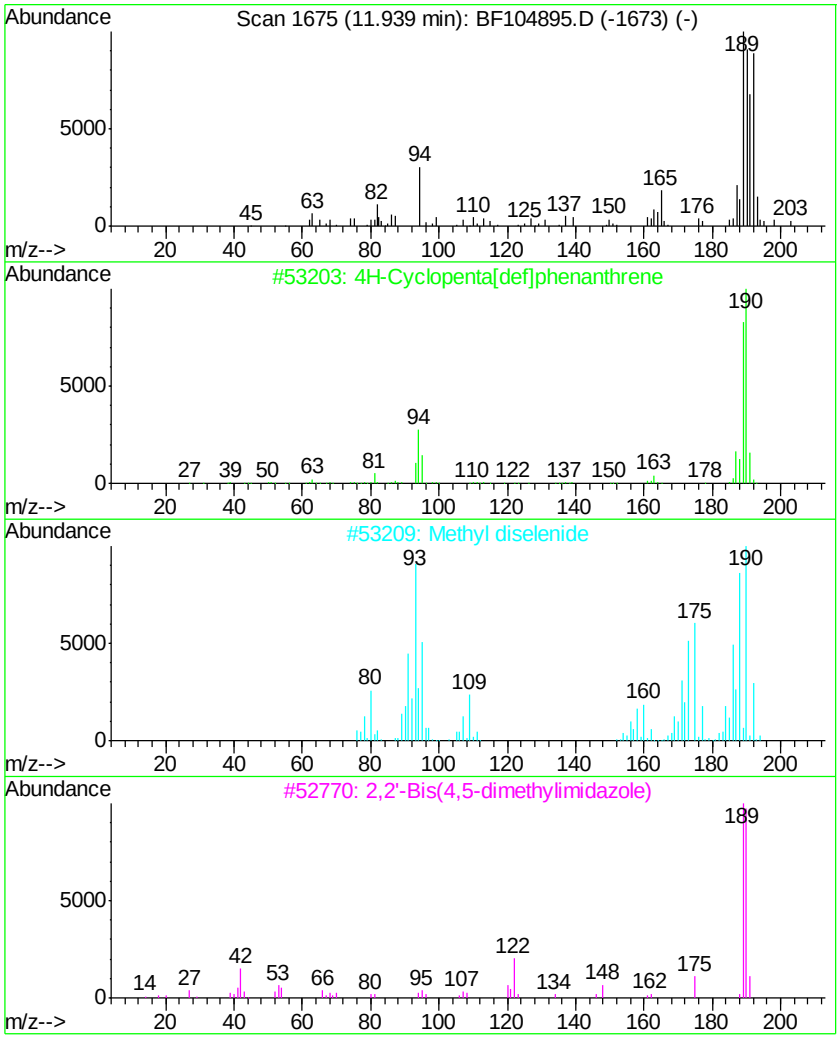
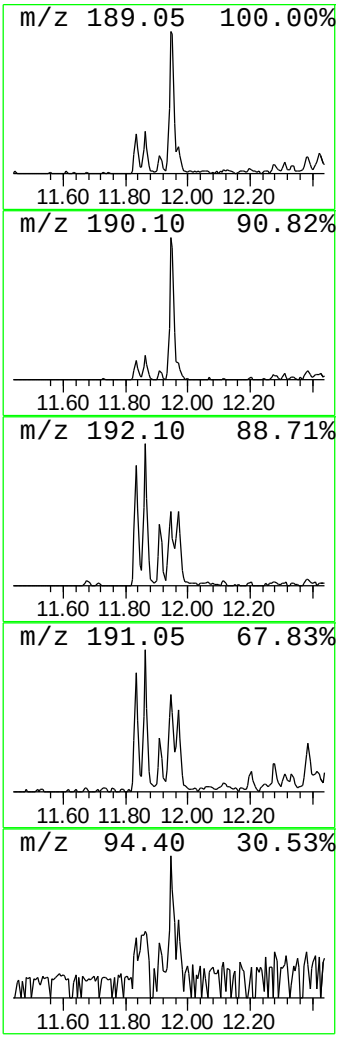
Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	3.87 ng	136996	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	81
2	Methyl diselenide	190	C2H6Se2	007101-31-7	43
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	28
4	6,7-Methylenedioxy-4(3H)-quinazo...	190	C9H6N2O3	028310-11-4	28
5	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	25





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Operator : JU/SJ
Sample : J2566-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

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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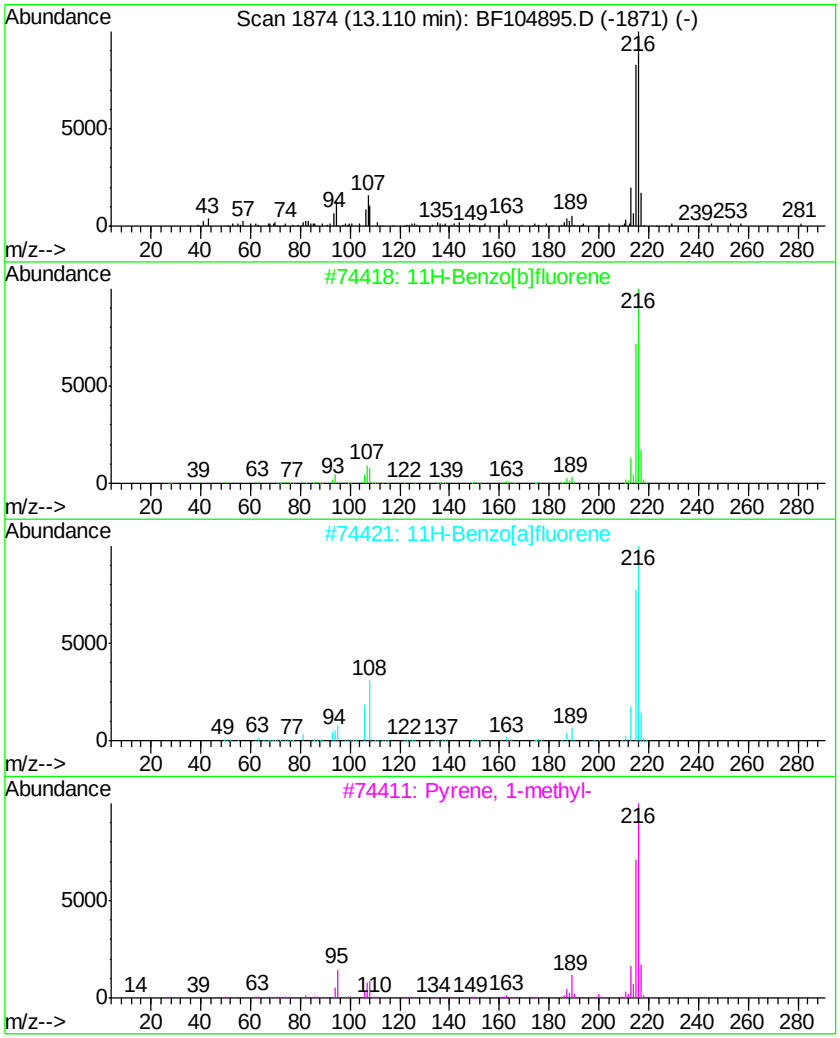
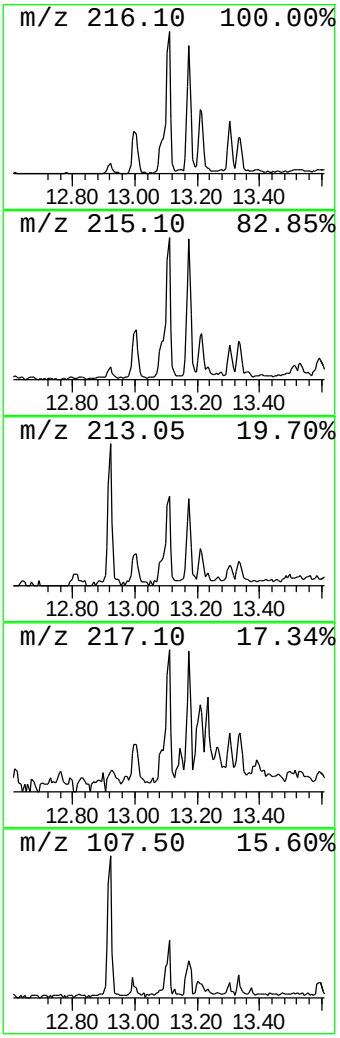
Peak Number 7 11H-Benzo[b]fluorene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.11	2.30 ng	105438	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	93
2	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
3	Pyrene, 1-methyl-	216	C17H12	002381-21-7	86
4	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	72
5	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	68





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Data File : BF104895.D
Acq On : 27 Apr 2018 21:32
Operator : JU/SJ
Sample : J2566-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

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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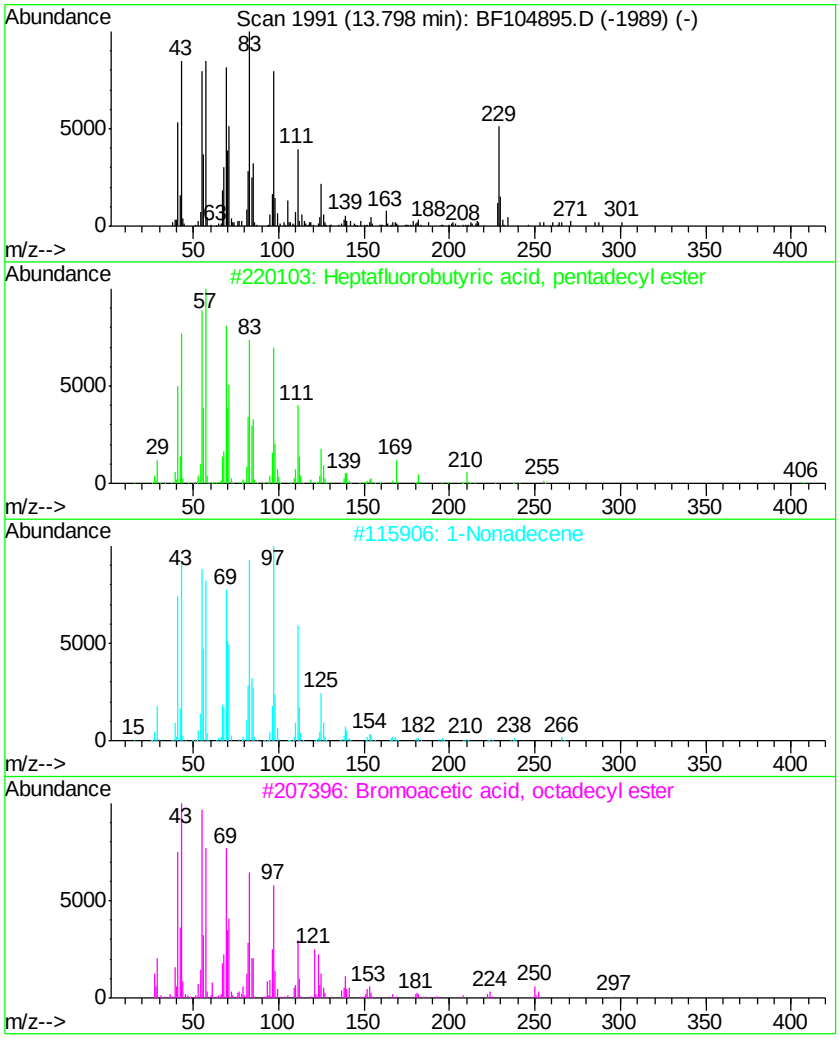
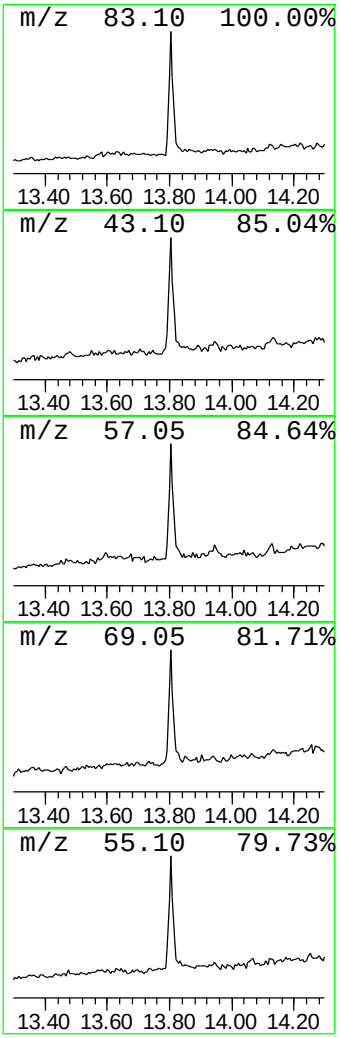
Peak Number 8 Heptafluorobutyric acid, pe... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	5.42 ng	248678	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042718\
Data File : BF104895.D
Acq On : 27 Apr 2018 21:32
Operator : JU/SJ
Sample : J2566-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

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

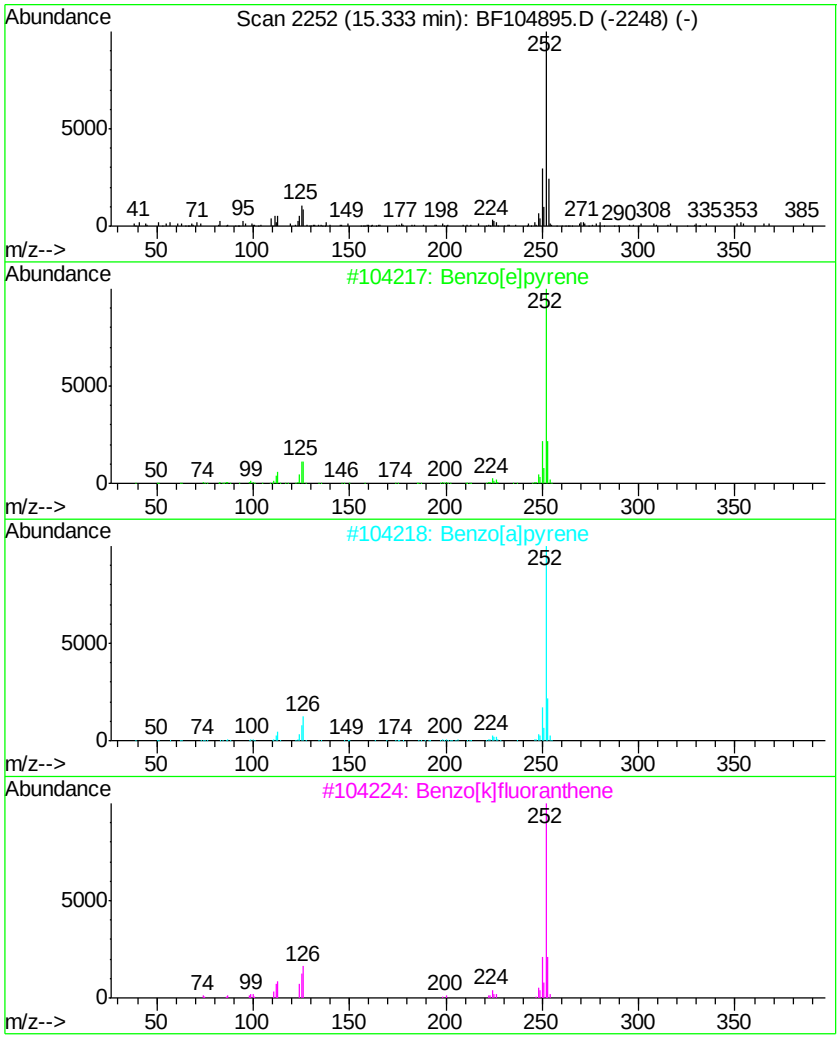
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

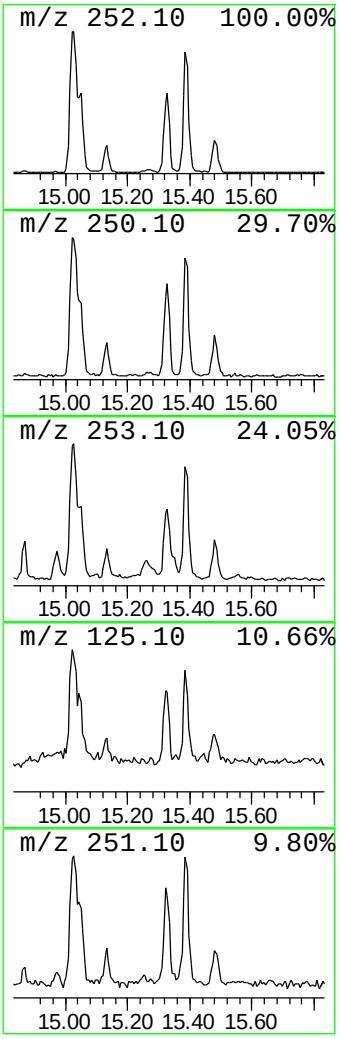
****

Peak Number 9 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.33	6.21 ng	137448	Perylene-d12	15.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[a]pyrene	252	C20H12	000050-32-8	96
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93
5	Perylene	252	C20H12	000198-55-0	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042718\
Data File : BF104895.D
Acq On : 27 Apr 2018 21:32
Operator : JU/SJ
Sample : J2566-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

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
unknown5.02	5.02	4.3	ng	124765	1	6.80	574802	20.0
unknown6.57	6.57	93.0	ng	2672520	1	6.80	574802	20.0
Tetradecane	10.73	2.8	ng	99145	4	11.33	708664	20.0
n-Hexadecanoic acid	11.85	12.1	ng	429752	4	11.33	708664	20.0
4H-Cyclopenta[def...	11.94	3.9	ng	136996	4	11.33	708664	20.0
11H-Benzo[b]fluorene	13.11	2.3	ng	105438	5	13.98	918457	20.0
Heptafluorobutyri...	13.80	5.4	ng	248678	5	13.98	918457	20.0
Benzo[e]pyrene	15.33	6.2	ng	137448	6	15.45	442824	20.0