LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112217\
Data File : BF100844.D
Acq On : 23 Nov 2017 00:48
Operator : SJ/JU
Sample : I6548-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SAU-3-E(4-5)

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-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	5.092	506	511	521	rVB	97211	135335	7.86%	0.686%
2	5.487	573	578	581	rBV	1420570	1441048	83.69%	7.308%
3	6.492	744	749	760	rVB	1491400	1531852	88.96%	7.768%
4	6.628	768	772	776	rBV	1580733	1549328	89.98%	7.857%
5	6.857	808	811	815	rBV	592037	466267	27.08%	2.365%
6	6.916	818	821	824	rBV	42424	33535	1.95%	0.170%
7	7.016	834	838	841	rBV	1497153	1223718	71.07%	6.206%
8	7.422	902	907	910	rBV	1029692	979293	56.87%	4.966%
9	8.139	1025	1029	1032	rBV	760829	626148	36.36%	3.175%
10	9.216	1207	1212	1215	rBV	2005929	1721952	100.00%	8.733%
11	9.292	1221	1225	1227	rBV	26534	21582	1.25%	0.109%
12	9.486	1254	1258	1261	rBV2	38536	30257	1.76%	0.153%
13	9.610	1275	1279	1281	rBV	137664	122012	7.09%	0.619%
14	9.822	1308	1315	1317	rBV2	79265	75167	4.37%	0.381%
15	9.898	1324	1328	1331	rBV	812313	667195	38.75%	3.384%
16	9.927	1331	1333	1336	rVB	38498	27568	1.60%	0.140%
17	10.098	1360	1362	1366	rVB3	18838	20236	1.18%	0.103%
18	10.139	1366	1369	1373	rVB3	20146	19464	1.13%	0.099%
19	10.298	1392	1396	1397	rBV2	26628	25004	1.45%	0.127%
20	10.322	1397	1400	1403	rVB	88019	78645	4.57%	0.399%
21	10.439	1417	1420	1425	rVB2	28547	29833	1.73%	0.151%
22	10.539	1433	1437	1440	rBV2	20274	23854	1.39%	0.121%
23	10.686	1458	1462	1465	rBV	1155353	976200	56.69%	4.951%
24	10.792	1477	1480	1488	rVB	76110	84201	4.89%	0.427%
25	11.186	1544	1547	1552	rVV	25058	20216	1.17%	0.103%
26	11.239	1552	1556	1559	rVV3	42551	42112	2.45%	0.214%
27	11.280	1559	1563	1568	rVB2	22468	27888	1.62%	0.141%
28	11.386	1577	1581	1583	rBV	719236	698905	40.59%	3.544%
29	11.404	1583	1584	1588	rVV	416033	330010	19.16%	1.674%
30	11.457	1590	1593	1596	rVB	92555	69047	4.01%	0.350%
31	11.610	1613	1619	1626	rBV3	29589	49326	2.86%	0.250%
32	11.669	1626	1629	1634	rVB2	17541	25396	1.47%	0.129%
33	11.880	1660	1665	1667	rBV	65333	78317	4.55%	0.397%
34	11.904	1667	1669	1673	rVV2	124815	165463	9.61%	0.839%

LSC Area Percent Report

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Operator : SJ/JU
Sample : I6548-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SAU-3-E(4-5)

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

35	11.957	1676	1678	1681	rVV	34060	31423	1.82%	0.159%
36	11.998	1681	1685	1687	rVV2	88387	106459	6.18%	0.540%
37	12.016	1687	1688	1692	rVB	50517	36637	2.13%	0.186%
38	12.180	1713	1716	1718	rBV	44098	37824	2.20%	0.192%
39	12.204	1718	1720	1722	rVB	33450	24808	1.44%	0.126%
40	12.433	1754	1759	1762	rBV	39303	50558	2.94%	0.256%
41	12.468	1762	1765	1767	rVV3	27706	36254	2.11%	0.184%
42	12.521	1771	1774	1778	rVB2	35970	41554	2.41%	0.211%
43	12.598	1783	1787	1790	rBV	665179	569486	33.07%	2.888%
44	12.686	1799	1802	1805	rBV2	29001	23207	1.35%	0.118%
45	12.827	1820	1826	1829	rBV	585120	588726	34.19%	2.986%
46	12.874	1831	1834	1838	rVB2	29102	32476	1.89%	0.165%
47	12.968	1846	1850	1853	rVV	1407997	1220744	70.89%	6.191%
48	13.039	1857	1862	1867	rBV3	38634	64545	3.75%	0.327%
49	13.127	1874	1877	1878	rBV3	31362	31310	1.82%	0.159%
50	13.151	1878	1881	1884	rVB	59875	63740	3.70%	0.323%
51	13.215	1890	1892	1895	rVB	25974	21852	1.27%	0.111%
52	13.257	1895	1899	1902	rBV2	61098	64988	3.77%	0.330%
53	13.351	1911	1915	1917	rBV	31744	27781	1.61%	0.141%
54	13.380	1917	1920	1923	rVV2	30818	28446	1.65%	0.144%
55	13.533	1941	1946	1948	rBV5	15688	22838	1.33%	0.116%
56	13.657	1964	1967	1972	rVB	45633	48451	2.81%	0.246%
57	13.768	1982	1986	1989	rBV2	39282	51930	3.02%	0.263%
58	13.798	1989	1991	1993	rVV	46120	40663	2.36%	0.206%
59	13.821	1993	1995	1998	rVV	31439	47729	2.77%	0.242%
60	13.851	1998	2000	2009	rVB3	79501	127676	7.41%	0.647%
61	14.021	2024	2029	2032	rBV2	578881	707824	41.11%	3.590%
62	14.045	2032	2033	2039	rVB	226598	193213	11.22%	0.980%
63	14.127	2044	2047	2049	rBV	32941	25282	1.47%	0.128%
64	14.168	2051	2054	2058	rBV5	12288	22118	1.28%	0.112%
65	14.245	2063	2067	2070	rBV3	21946	33001	1.92%	0.167%
66	14.333	2079	2082	2087	rBV5	17151	30533	1.77%	0.155%
67	14.410	2091	2095	2098	rVB	47184	46860	2.72%	0.238%
68	14.439	2098	2100	2105	rBV2	28703	35373	2.05%	0.179%
69	14.715	2142	2147	2150	rBV4	21792	35666	2.07%	0.181%
70	15.062	2202	2206	2209	rBV	226326	327785	19.04%	1.662%
71	15.168	2221	2224	2228	rBV	39410	40190	2.33%	0.204%

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Instrument : BNA_F
ClientSampleId : SAU-3-E(4-5)

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
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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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72	15.268	2238	2241	2245	rBV5	10036	20477	1.19%	0.104%
73	15.368	2253	2258	2264	rVB	135880	173508	10.08%	0.880%
74	15.427	2264	2268	2274	rBV	186621	240152	13.95%	1.218%
75	15.498	2274	2280	2283	rBV	380860	507092	29.45%	2.572%
76	15.939	2351	2355	2358	rVB5	15872	20228	1.17%	0.103%
77	16.962	2524	2529	2539	rVB2	88986	172757	10.03%	0.876%
78	17.045	2539	2543	2549	rVB7	16011	30585	1.78%	0.155%
79	17.145	2557	2560	2564	rVB4	18628	23670	1.37%	0.120%
80	17.415	2599	2606	2612	rBV	69974	129856	7.54%	0.659%
81	17.650	2641	2646	2651	rBV3	19773	44116	2.56%	0.224%

Sum of corrected areas: 19718765

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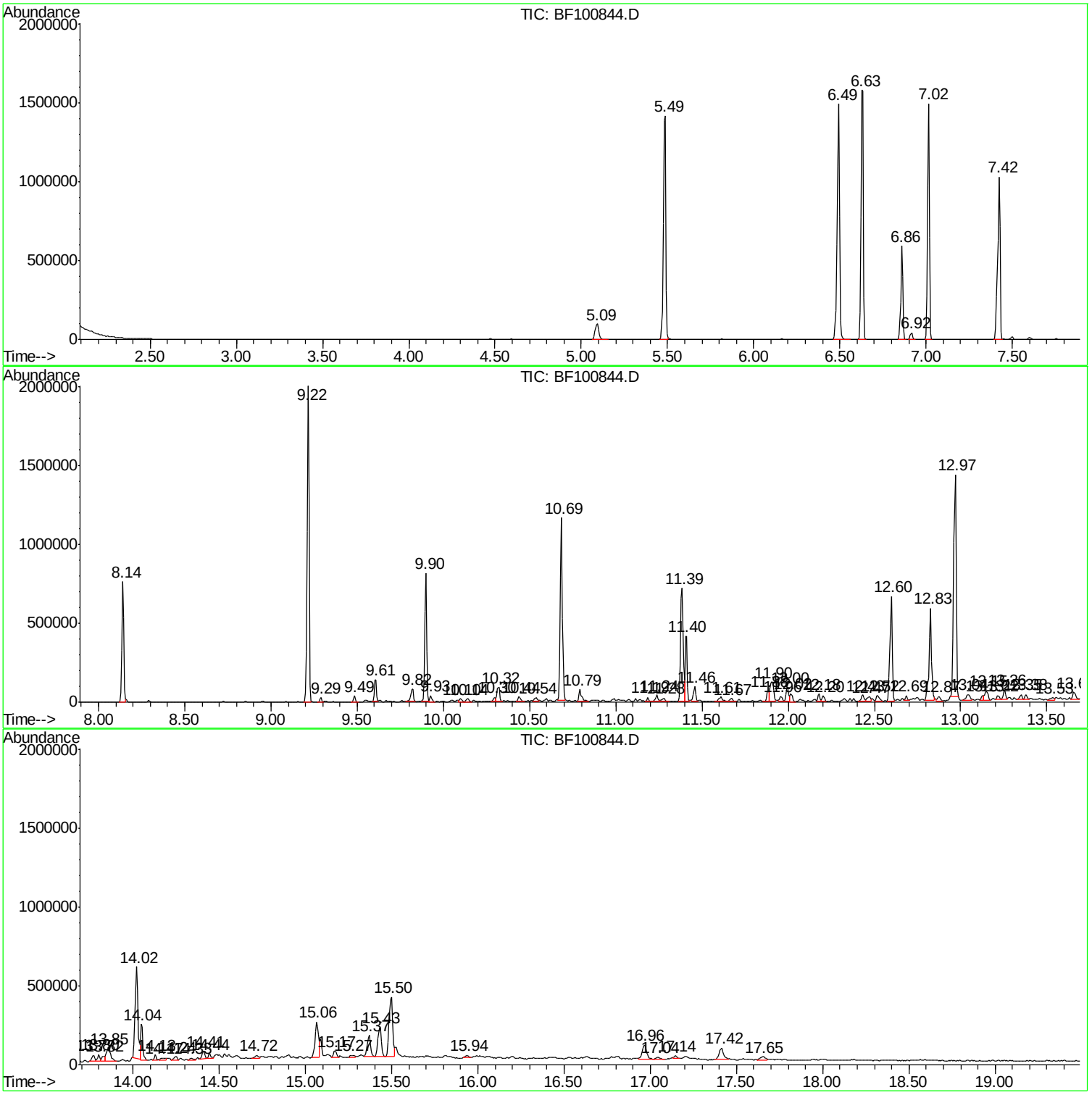
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAU-3-E(4-5)

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\BF112217\
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Operator : SJ/JU
Sample : I6548-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SAU-3-E(4-5)

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

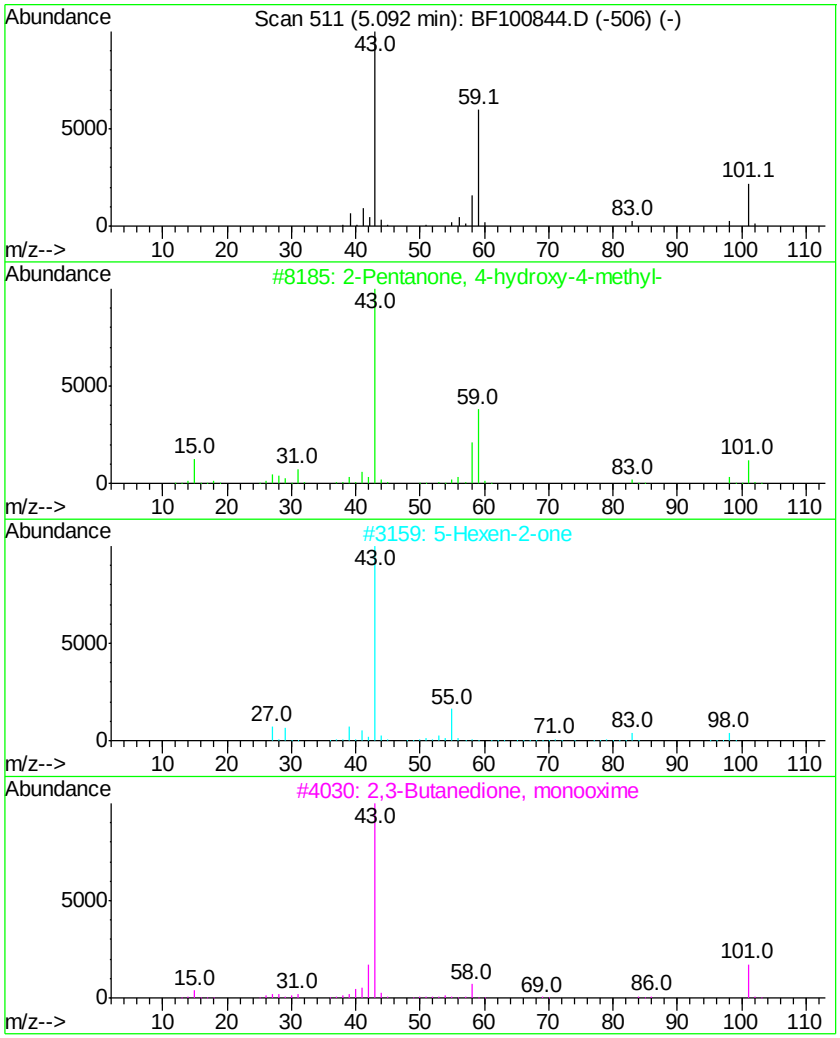
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

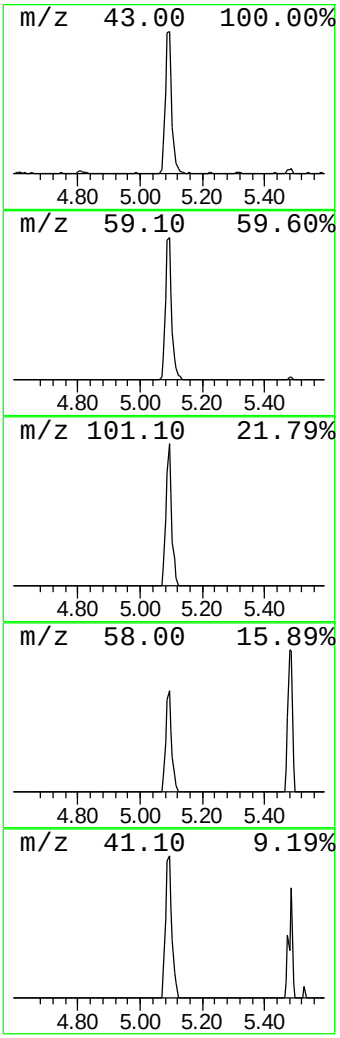
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	5.81 ng	135335	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	5-Hexen-2-one	98	C6H10O	000109-49-9	9
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9





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Instrument : BNA_F
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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
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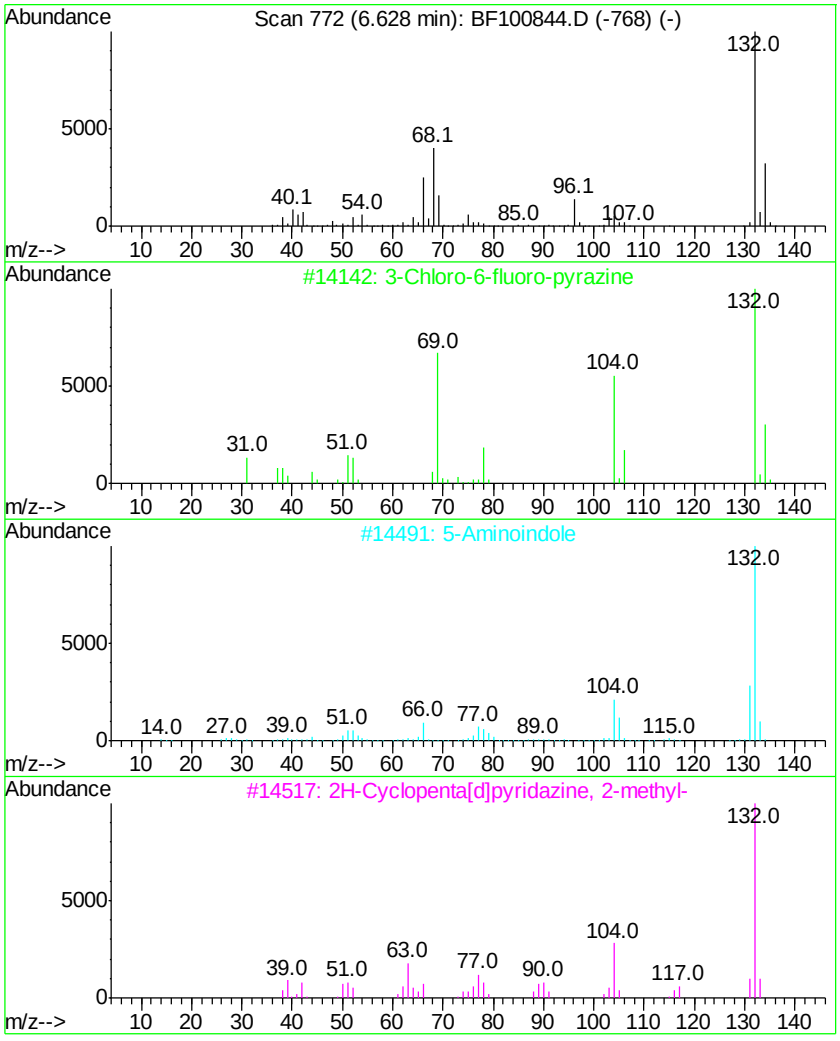
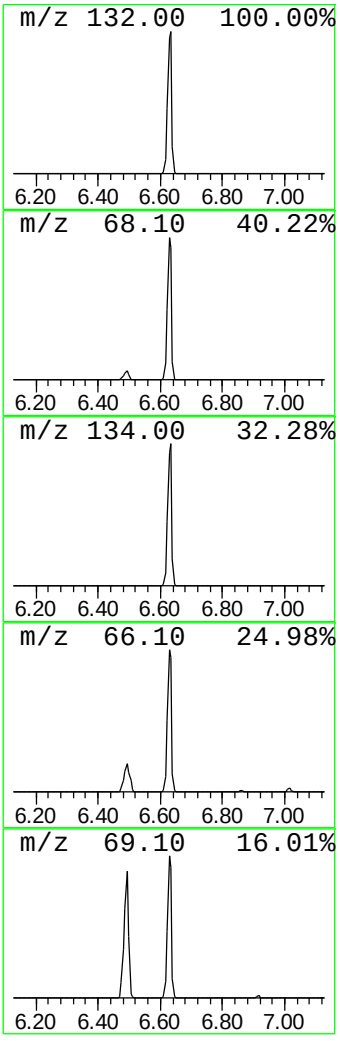
****

Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	66.46 ng	1549330	1,4-Dichlorobenzene-d4	6.86

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	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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TIC Library : C:\DATABASE\NIST11.L
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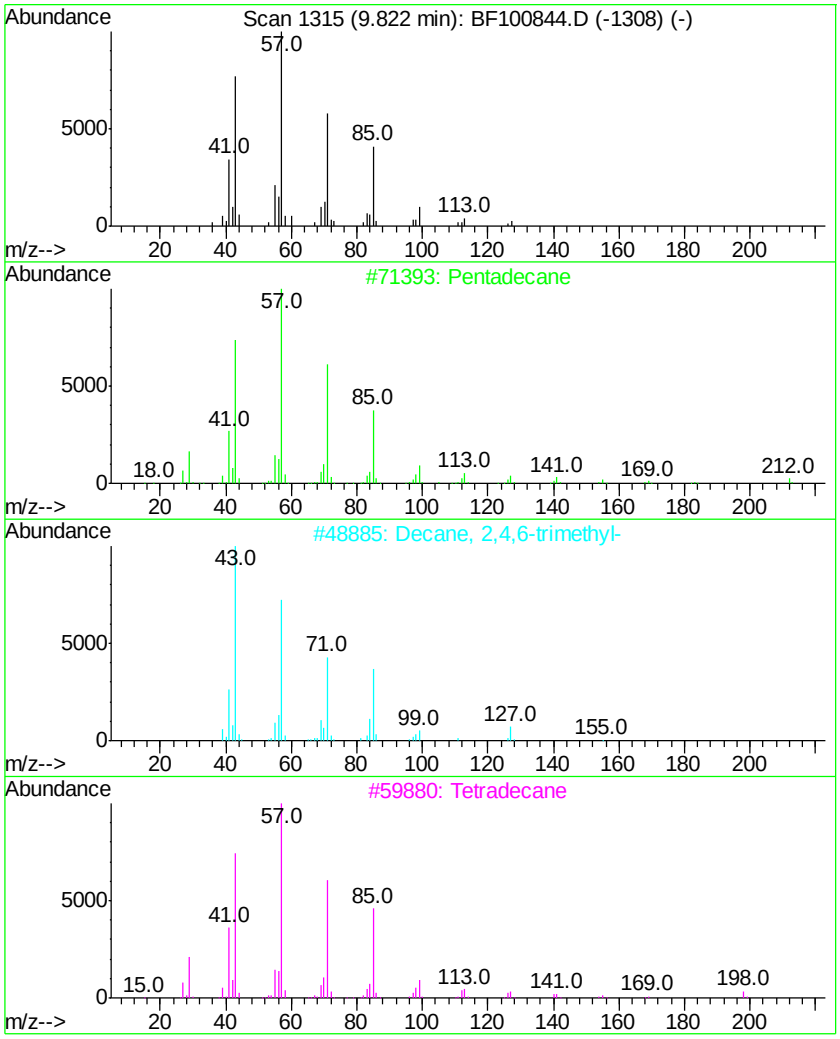
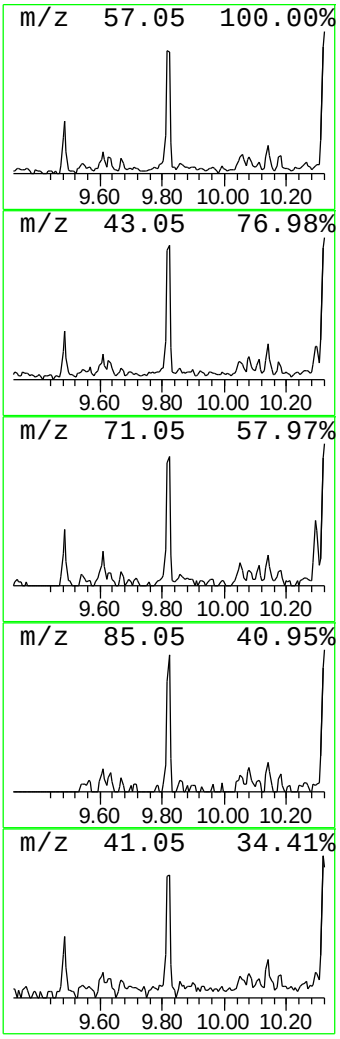
Peak Number 4 Pentadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.82	2.25 ng	75167	Acenaphthene-d10	9.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	86
2	Decane, 2,4,6-trimethyl-	184	C13H28	062108-27-4	78
3	Tetradecane	198	C14H30	000629-59-4	78
4	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	72
5	Hexadecane	226	C16H34	000544-76-3	72





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TIC Library : C:\DATABASE\NIST11.L
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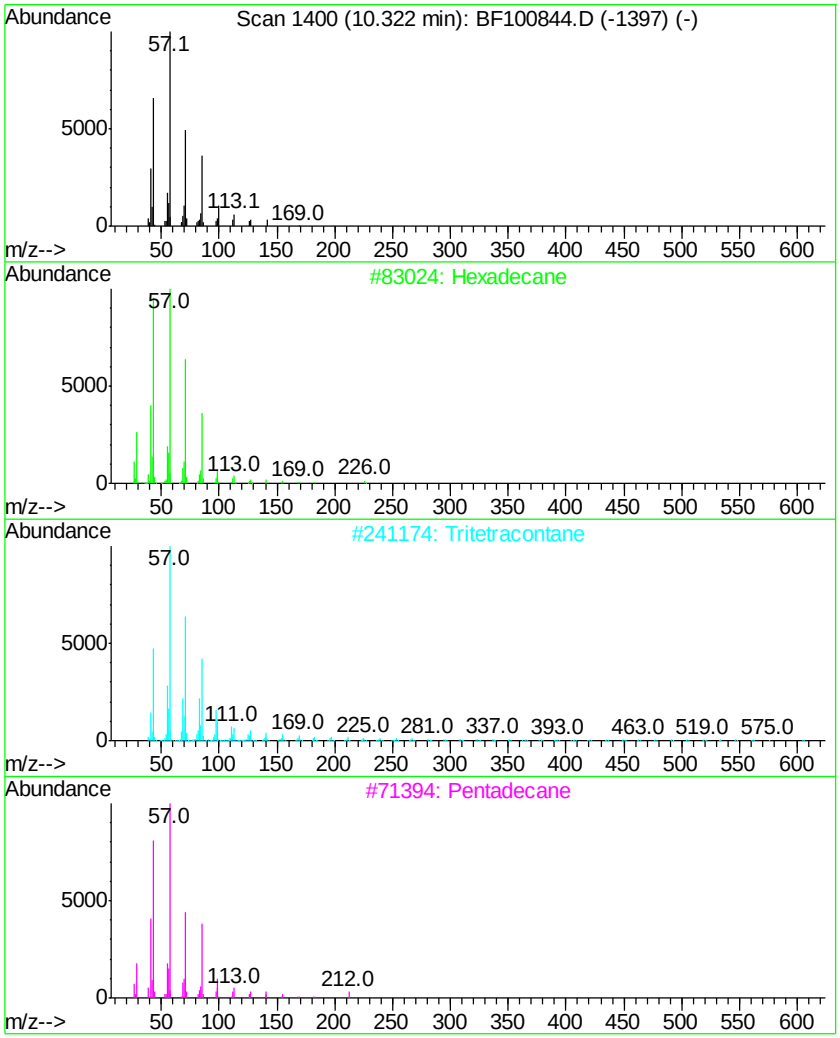
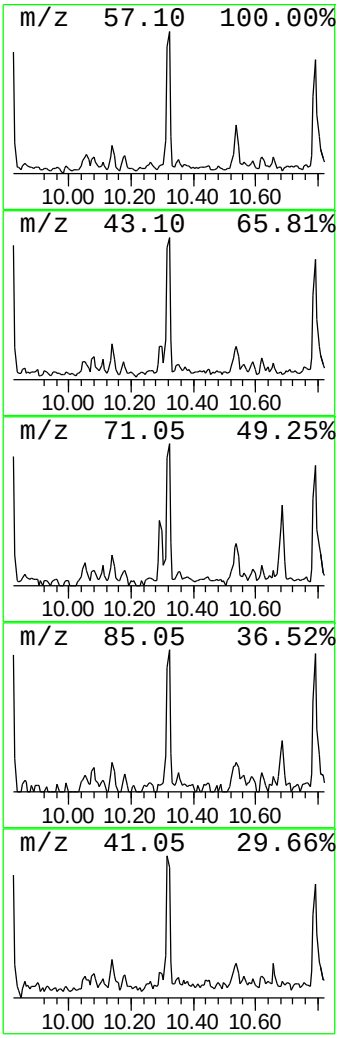
Peak Number 5 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.32	2.36 ng	78645	Acenaphthene-d10	9.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Tritetracontane	605	C43H88	007098-21-7	90
3	Pentadecane	212	C15H32	000629-62-9	90
4	Tetradecane	198	C14H30	000629-59-4	90
5	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	90





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

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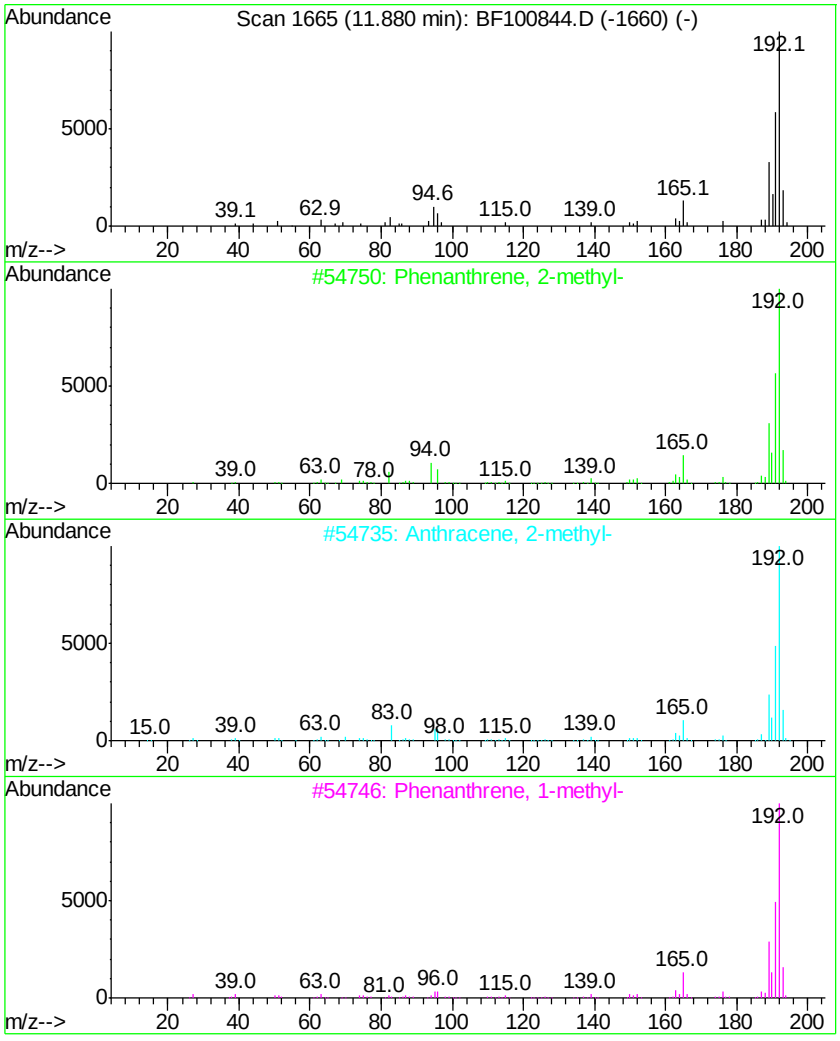
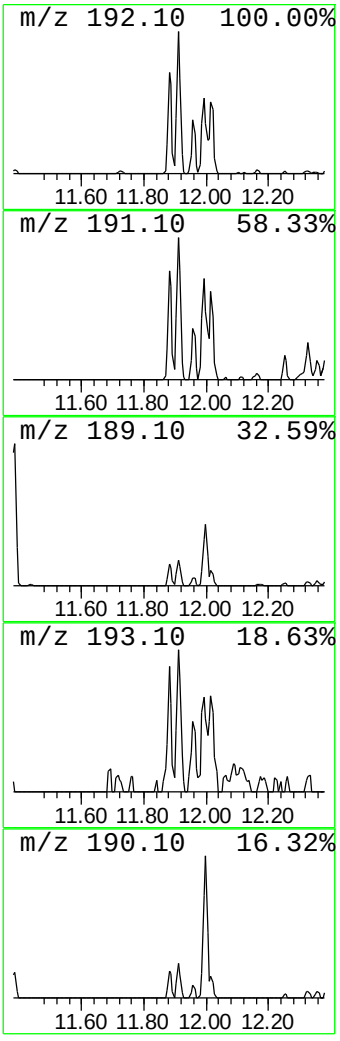
Peak Number 7 Phenanthrene, 2-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	2.24 ng	78317	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	97
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	96
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
4	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	95
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	94





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Data File : BF100844.D
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Operator : SJ/JU
Sample : I6548-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SAU-3-E(4-5)

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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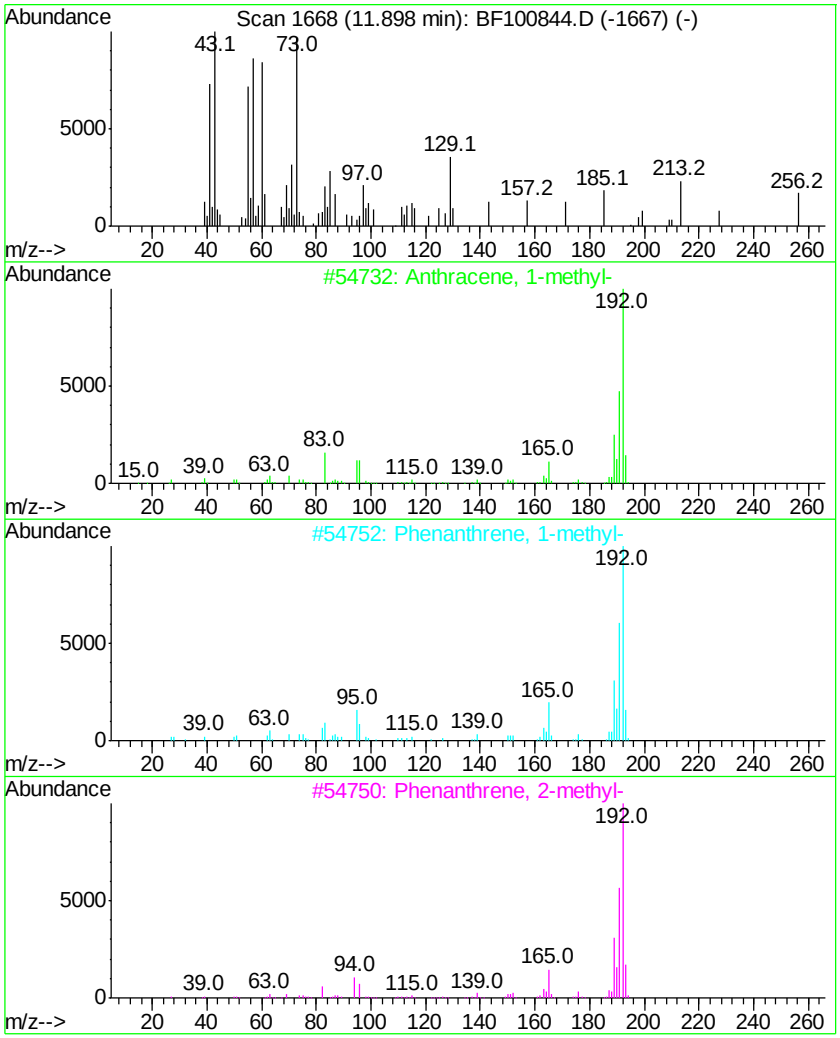
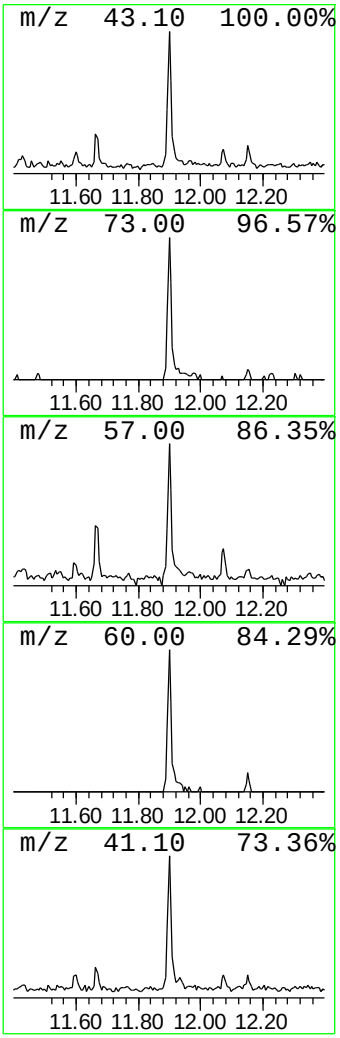
Peak Number 8 Anthracene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	4.73 ng	165463	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	91
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	91
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	89
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	87
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	60





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Data File : BF100844.D
Acq On : 23 Nov 2017 00:48
Operator : SJ/JU
Sample : I6548-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SAU-3-E(4-5)

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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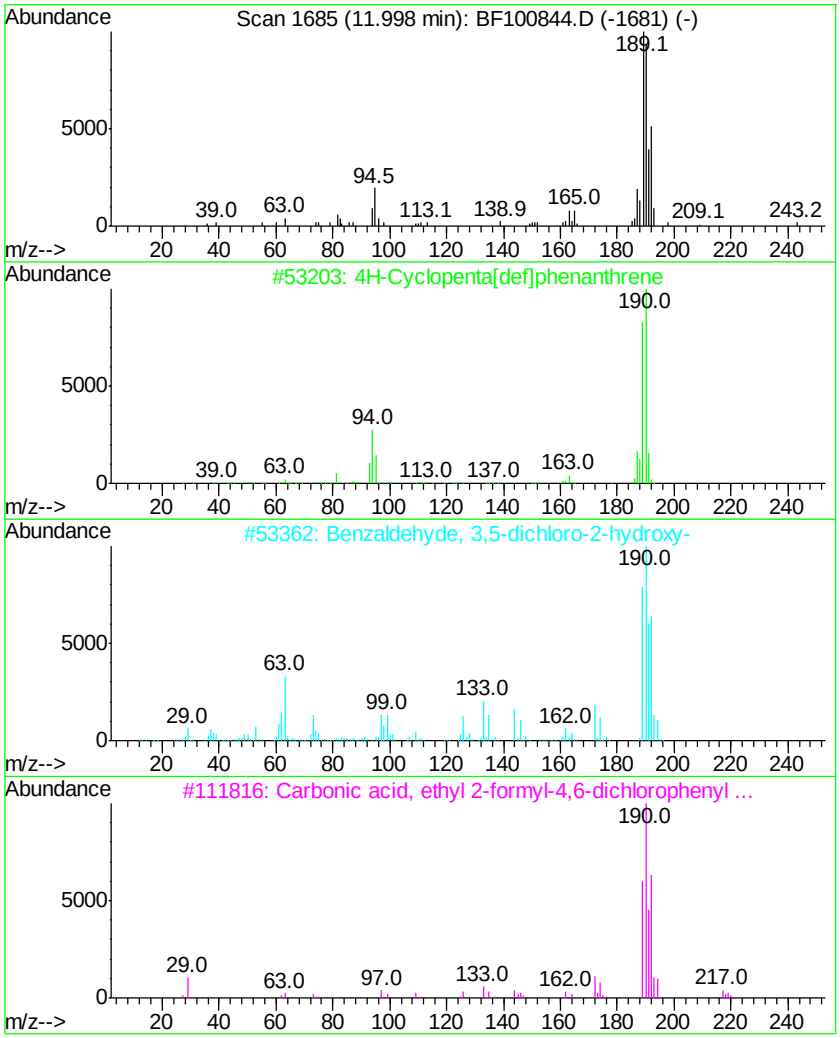
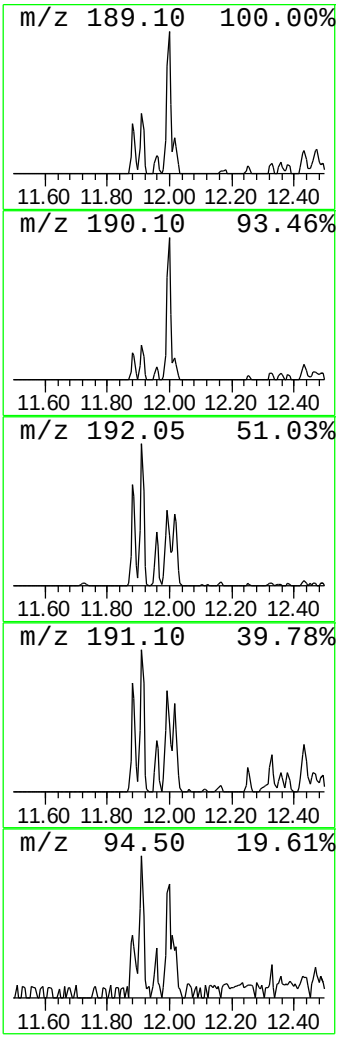
Peak Number 9 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.00	3.05 ng	106459	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	92
2	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	58
3	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	53
4	Methyl diselenide	190	C2H6Se2	007101-31-7	41
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	30





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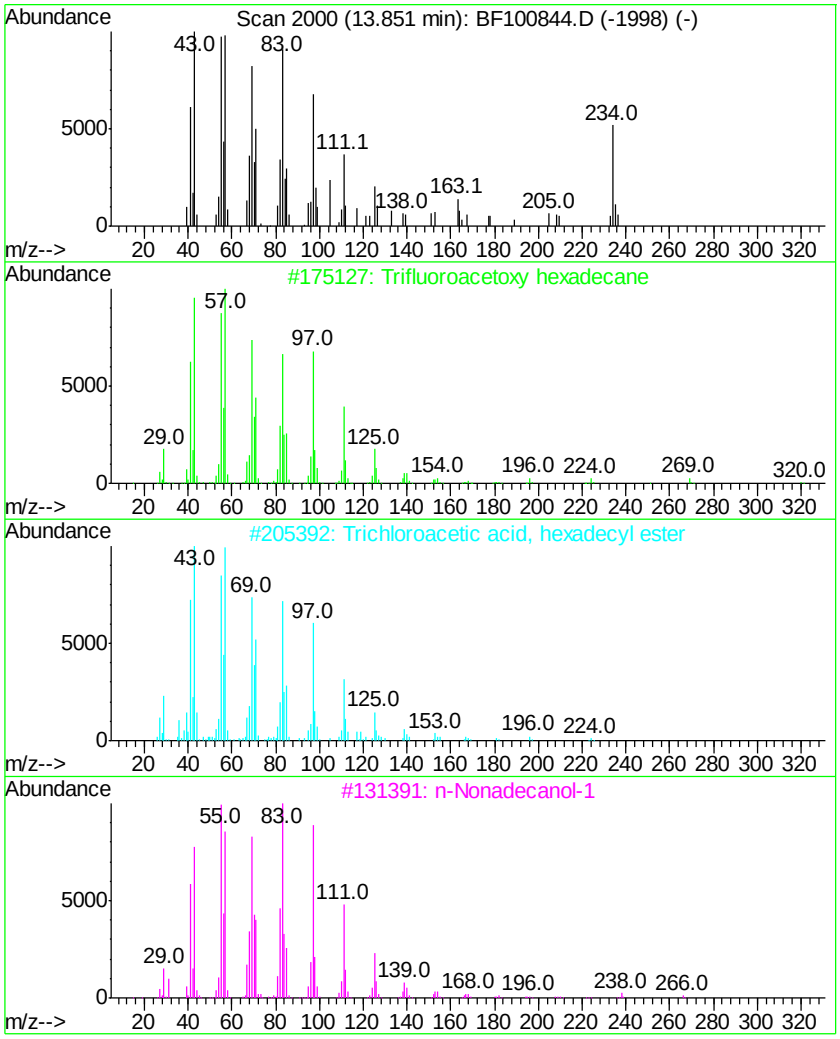
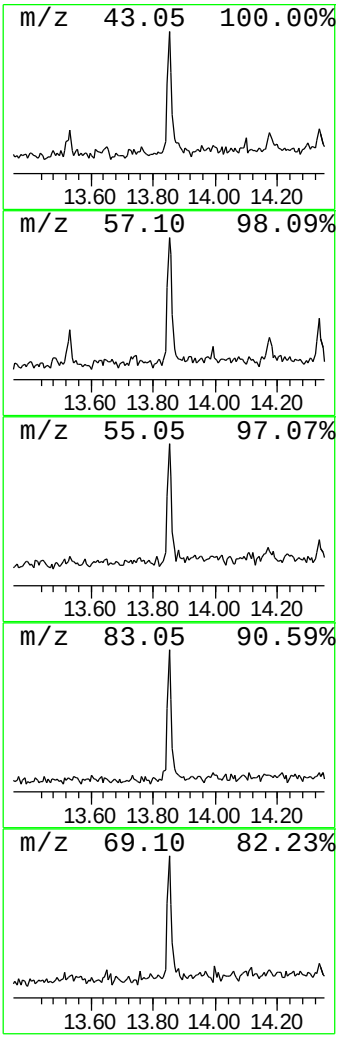
Peak Number 10 Trifluoroacetoxy hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	3.61 ng	127676	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	81
4	1-Heptacosanol	396	C27H56O	002004-39-9	81
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	81





Library Search Compound Report

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Acq On : 23 Nov 2017 00:48
Operator : SJ/JU
Sample : I6548-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SAU-3-E(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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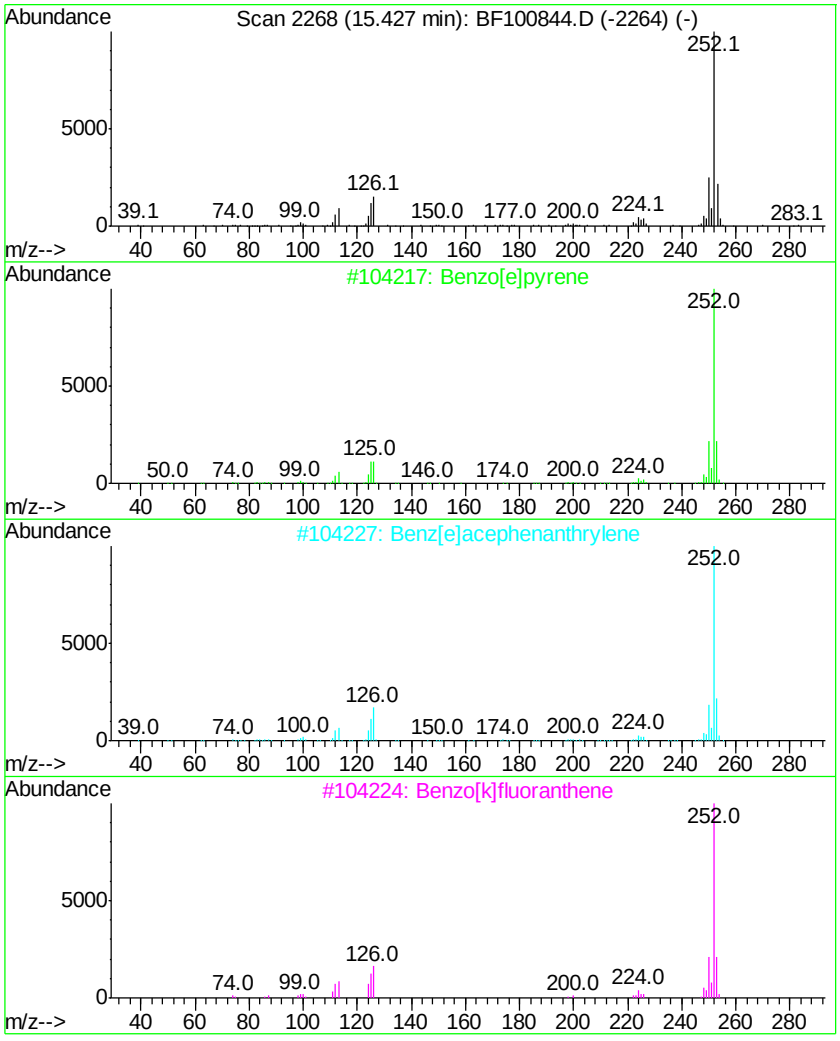
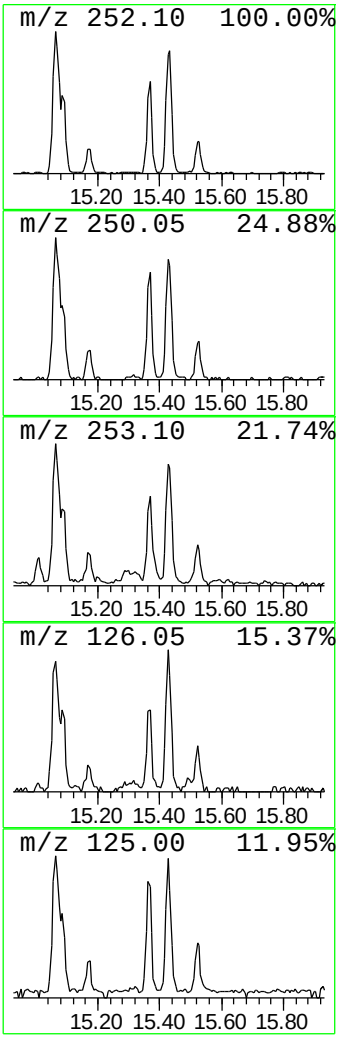
Peak Number 11 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.43	9.47 ng	240152	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	98
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
4	Benzo[a]pyrene	252	C20H12	000050-32-8	95
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	95





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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SAU-3-E(4-5)

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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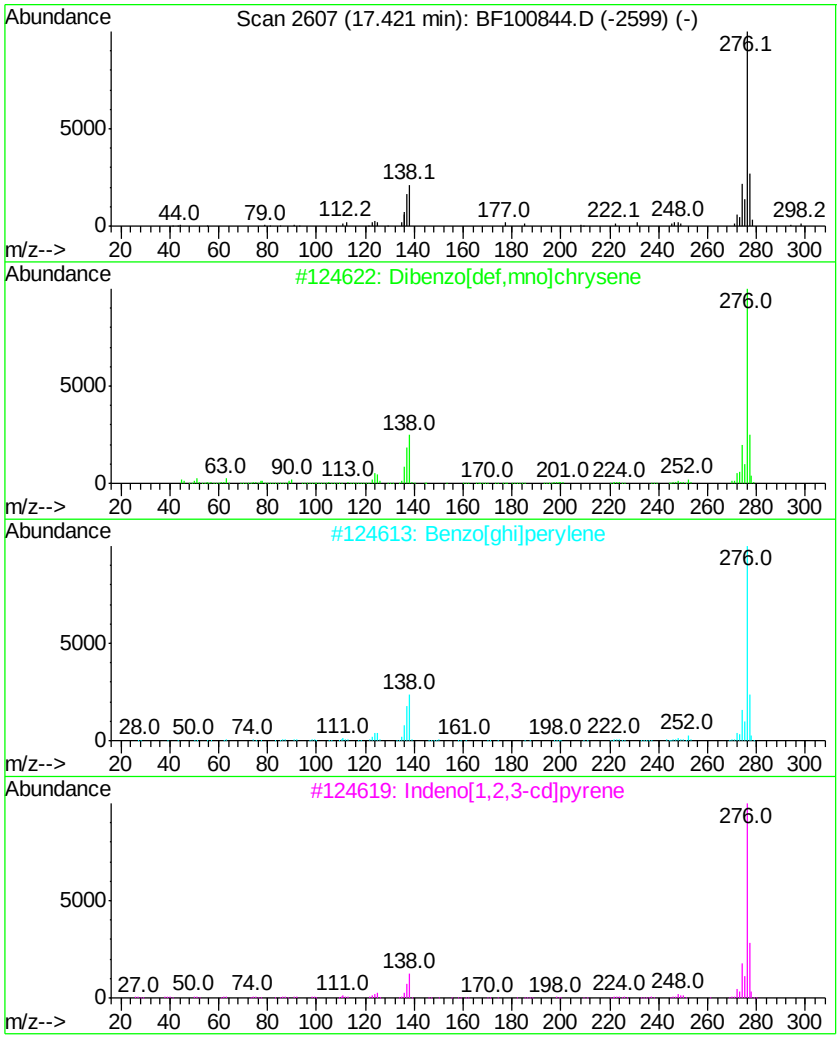
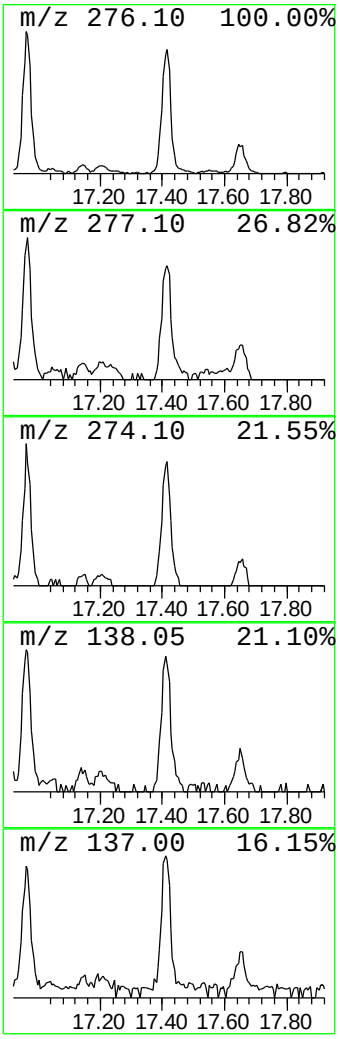
Peak Number 12 Dibenzo[def,mno]chrysene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.42	5.12 ng	129856	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	98
2	Benzo[ghi]perylene	276	C22H12	000191-24-2	98
3	Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	93
4	Indeno[1,2,3-cd]fluoranthene	276	C22H12	000193-43-1	91
5	Phenol, 2-(4-chlorophenyliminome...	276	C13H9ClN2O3	1000262-90-3	53





Tentatively Identified Compound (LSC) summary

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ClientSampleId : SAU-3-E(4-5)

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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...	5.09	5.8	ng	135335	1	6.86	466267	20.0
unknown6.63	6.63	66.5	ng	1549330	1	6.86	466267	20.0
Pentadecane	9.82	2.3	ng	75167	3	9.90	667195	20.0
Hexadecane	10.32	2.4	ng	78645	3	9.90	667195	20.0
Phenanthrene, 2-m...	11.88	2.2	ng	78317	4	11.39	698905	20.0
Anthracene, 1-met...	11.90	4.7	ng	165463	4	11.39	698905	20.0
4H-Cyclopenta[def...	12.00	3.0	ng	106459	4	11.39	698905	20.0
Trifluoroacetoxy ...	13.85	3.6	ng	127676	5	14.02	707824	20.0
Benzo[e]pyrene	15.43	9.5	ng	240152	6	15.50	507092	20.0
Dibenzo[def,mno]c...	17.42	5.1	ng	129856	6	15.50	507092	20.0