LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112917\
Data File : BF101007.D
Acq On : 30 Nov 2017 5:42
Operator : SJ/JU
Sample : I6579-07
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HAR-3-E(0-1)

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-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	5.081	505	509	522	rBV	136677	175650	14.04%	1.405%
2	5.475	572	576	579	rBV	1251355	1210049	96.72%	9.679%
3	6.487	743	748	751	rBV	1184989	1213356	96.98%	9.706%
4	6.628	767	772	775	rBV	1325750	1251125	100.00%	10.008%
5	6.851	807	810	814	rBV	388890	318769	25.48%	2.550%
6	7.010	833	837	840	rBV	1186040	966521	77.25%	7.731%
7	7.416	901	906	909	rBV	759049	707123	56.52%	5.656%
8	8.134	1024	1028	1031	rBV	467467	373725	29.87%	2.989%
9	8.686	1119	1122	1126	rBV	55133	44902	3.59%	0.359%
10	9.210	1206	1211	1214	rBV	1495886	1222818	97.74%	9.782%
11	9.598	1275	1277	1282	rVB	36215	27248	2.18%	0.218%
12	9.892	1323	1327	1330	rBV	363092	329729	26.35%	2.638%
13	10.598	1444	1447	1451	rBV	167872	146650	11.72%	1.173%
14	10.680	1457	1461	1464	rBV	681532	562587	44.97%	4.500%
15	11.380	1576	1580	1582	rBV	324141	297804	23.80%	2.382%
16	11.398	1582	1583	1587	rVB	138937	107882	8.62%	0.863%
17	11.451	1590	1592	1595	rVB	27933	21945	1.75%	0.176%
18	11.880	1661	1665	1666	rBV	18177	18820	1.50%	0.151%
19	11.904	1666	1669	1673	rVB2	26358	35637	2.85%	0.285%
20	11.992	1680	1684	1686	rBV2	29359	32601	2.61%	0.261%
21	12.427	1752	1758	1760	rBV	15705	15639	1.25%	0.125%
22	12.516	1770	1773	1778	rVB4	15187	16330	1.31%	0.131%
23	12.592	1782	1786	1789	rBV	294790	234960	18.78%	1.879%
24	12.822	1819	1825	1829	rBV	278140	273259	21.84%	2.186%
25	12.869	1831	1833	1838	rVB3	13971	15088	1.21%	0.121%
26	12.963	1845	1849	1852	rBV	1160008	967607	77.34%	7.740%
27	13.045	1856	1863	1866	rBV2	18739	34204	2.73%	0.274%
28	13.127	1874	1877	1878	rBV3	15557	17081	1.37%	0.137%
29	13.145	1878	1880	1884	rVB2	29884	29829	2.38%	0.239%
30	13.251	1894	1898	1901	rBV2	27601	36306	2.90%	0.290%
31	13.345	1910	1914	1917	rBV	21132	20975	1.68%	0.168%
32	13.380	1917	1920	1924	rVB2	19765	19464	1.56%	0.156%
33	13.657	1965	1967	1971	rVB	27131	23946	1.91%	0.192%
34	13.769	1981	1986	1988	rBV2	21626	27983	2.24%	0.224%

LSC Area Percent Report

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Operator : SJ/JU
Sample : I6579-07
Misc :
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Instrument : BNA_F
ClientSampleId : HAR-3-E(0-1)

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

35	13.798	1988	1991	1993	rVB	18290	14591	1.17%	0.117%
36	13.851	1993	2000	2001	rBV4	41593	60042	4.80%	0.480%
37	14.021	2021	2029	2031	rBV2	445671	515487	41.20%	4.123%
38	14.045	2031	2033	2040	rVB	130278	121891	9.74%	0.975%
39	14.127	2044	2047	2051	rBV	20380	16764	1.34%	0.134%
40	14.174	2051	2055	2057	rBV5	9331	14550	1.16%	0.116%
41	14.245	2064	2067	2070	rVB2	14503	17050	1.36%	0.136%
42	14.410	2090	2095	2098	rBV	27496	32164	2.57%	0.257%
43	14.486	2105	2108	2110	rBV4	12732	16762	1.34%	0.134%
44	14.904	2175	2179	2181	rBV3	13090	21340	1.71%	0.171%
45	15.063	2202	2206	2209	rBV	110860	153644	12.28%	1.229%
46	15.168	2222	2224	2228	rVB	17884	19620	1.57%	0.157%
47	15.368	2254	2258	2264	rVB	69353	86534	6.92%	0.692%
48	15.433	2264	2269	2274	rBV	89810	125972	10.07%	1.008%
49	15.498	2275	2280	2283	rBV	243295	302640	24.19%	2.421%
50	15.927	2351	2353	2358	rVB5	15443	20046	1.60%	0.160%
51	15.992	2360	2364	2368	rBV6	9055	20495	1.64%	0.164%
52	16.627	2469	2472	2478	rVB8	17106	28764	2.30%	0.230%
53	16.968	2526	2530	2538	rVB2	32043	56025	4.48%	0.448%
54	17.421	2601	2607	2613	rBV2	28704	59297	4.74%	0.474%

Sum of corrected areas: 12501290

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Misc :
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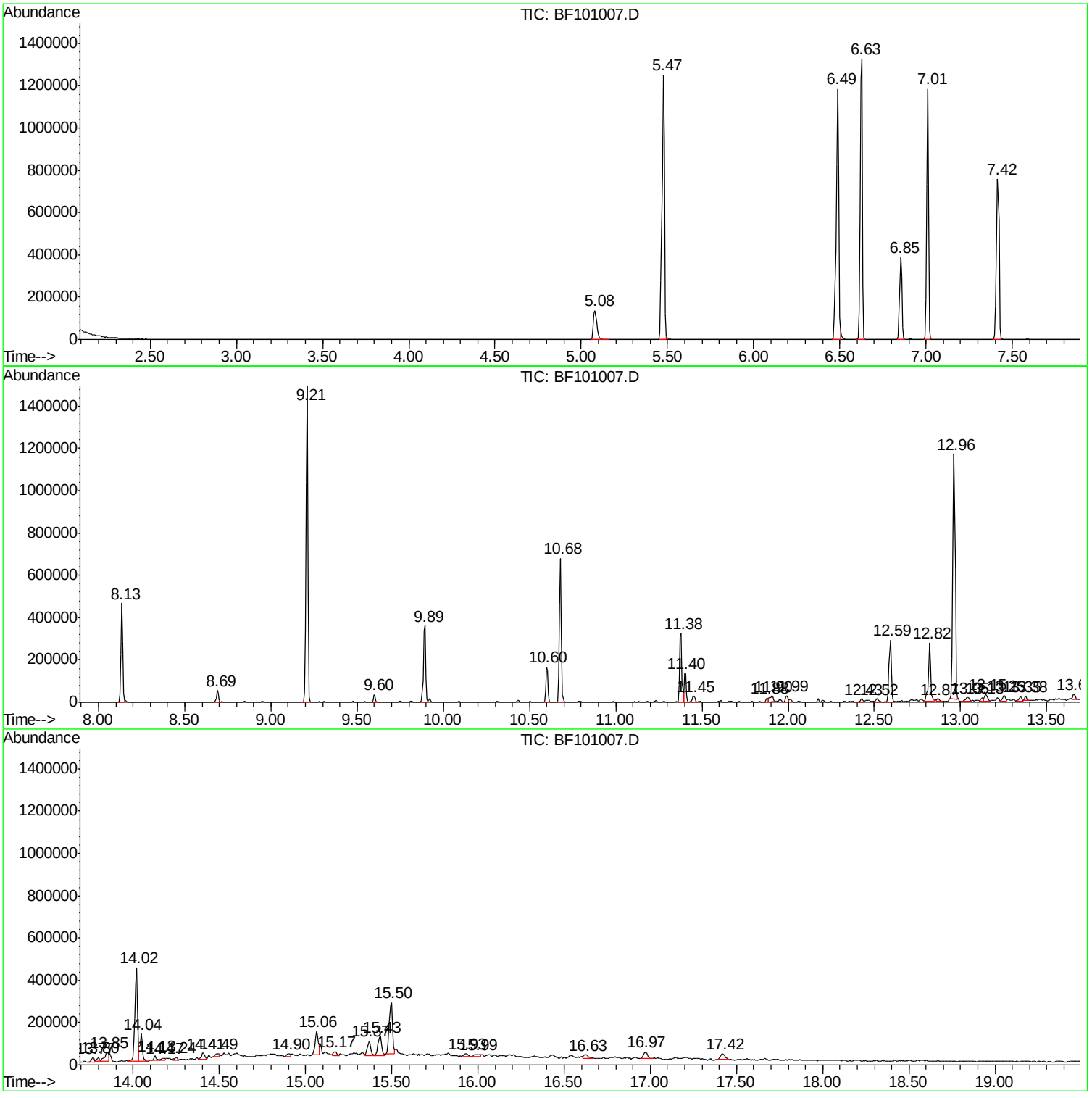
Instrument :
BNA_F
ClientSampleId :
HAR-3-E(0-1)

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

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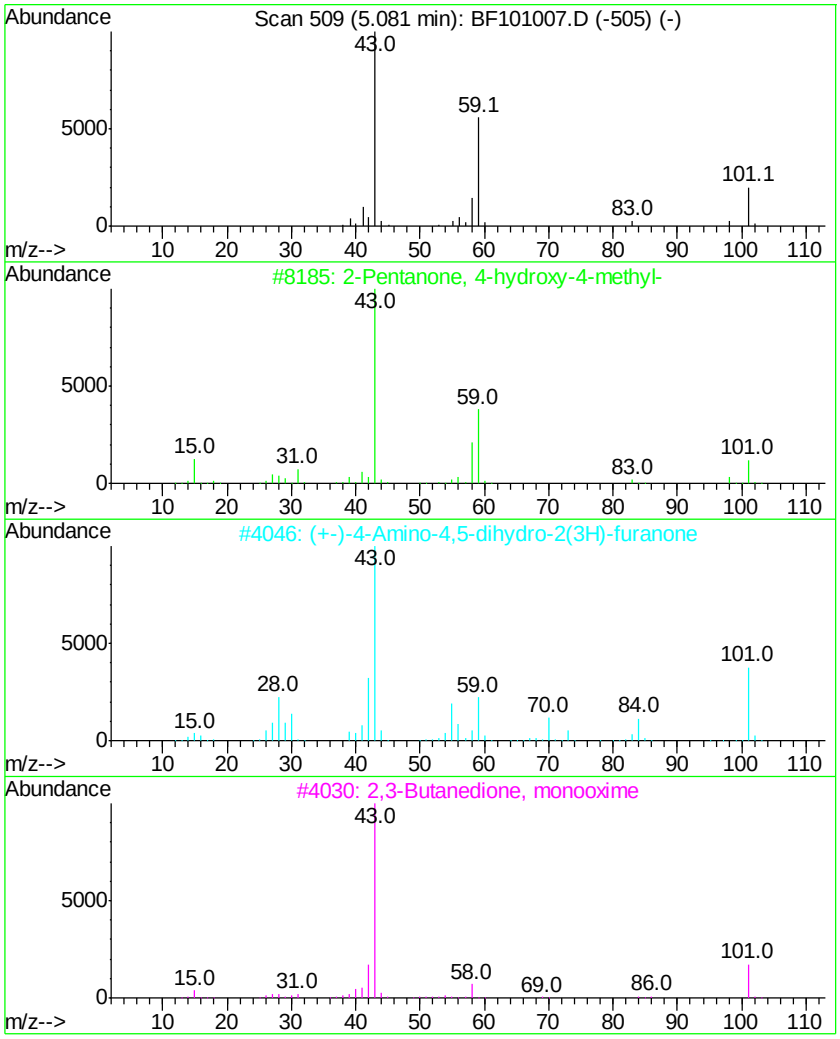
TIC Integration Parameters: LSCINT.P

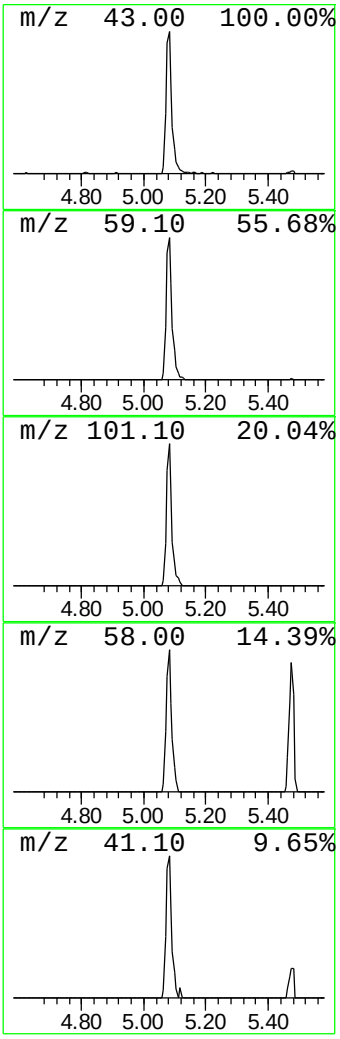
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	11.02 ng	175650	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Operator : SJ/JU
Sample : I6579-07
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HAR-3-E(0-1)

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

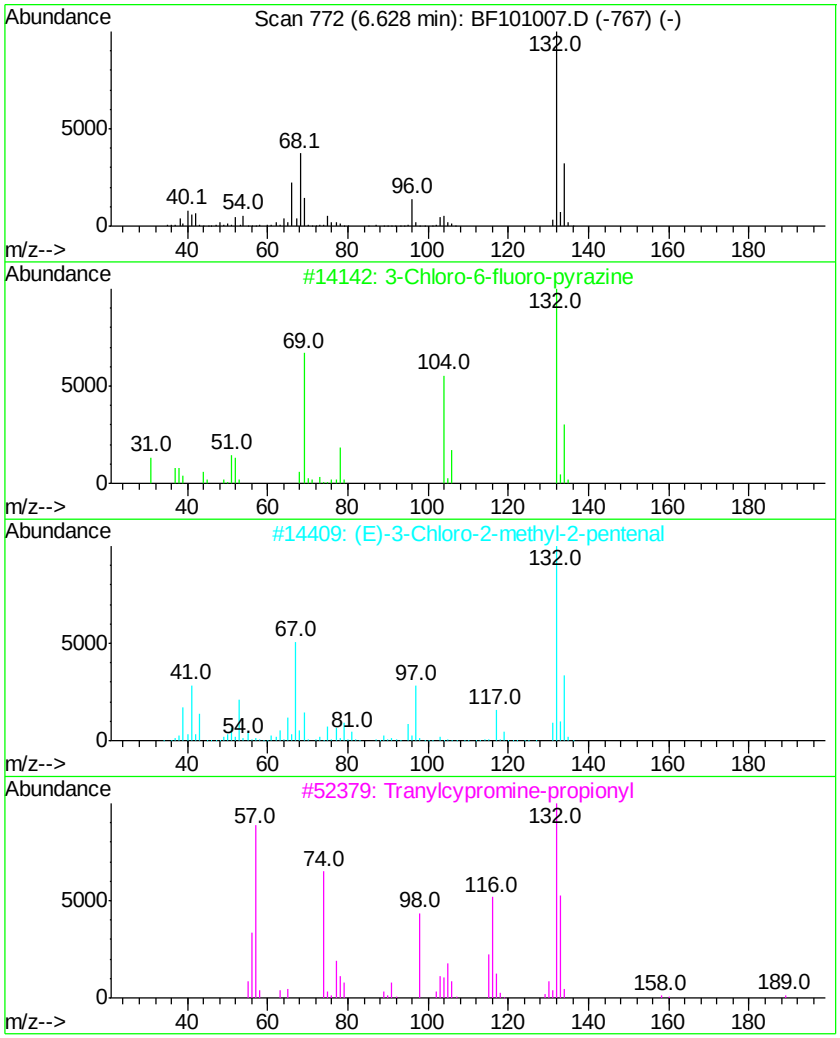
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

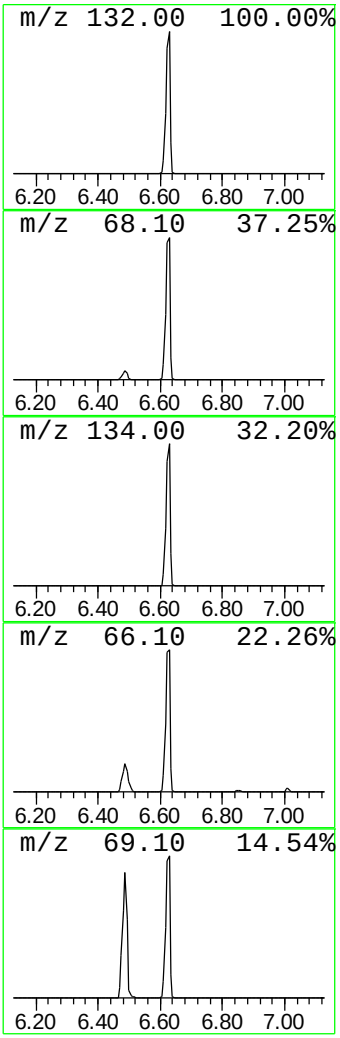
****

Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	78.50 ng	1251130	1,4-Dichlorobenzene-d4	6.85

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	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





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Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HAR-3-E(0-1)

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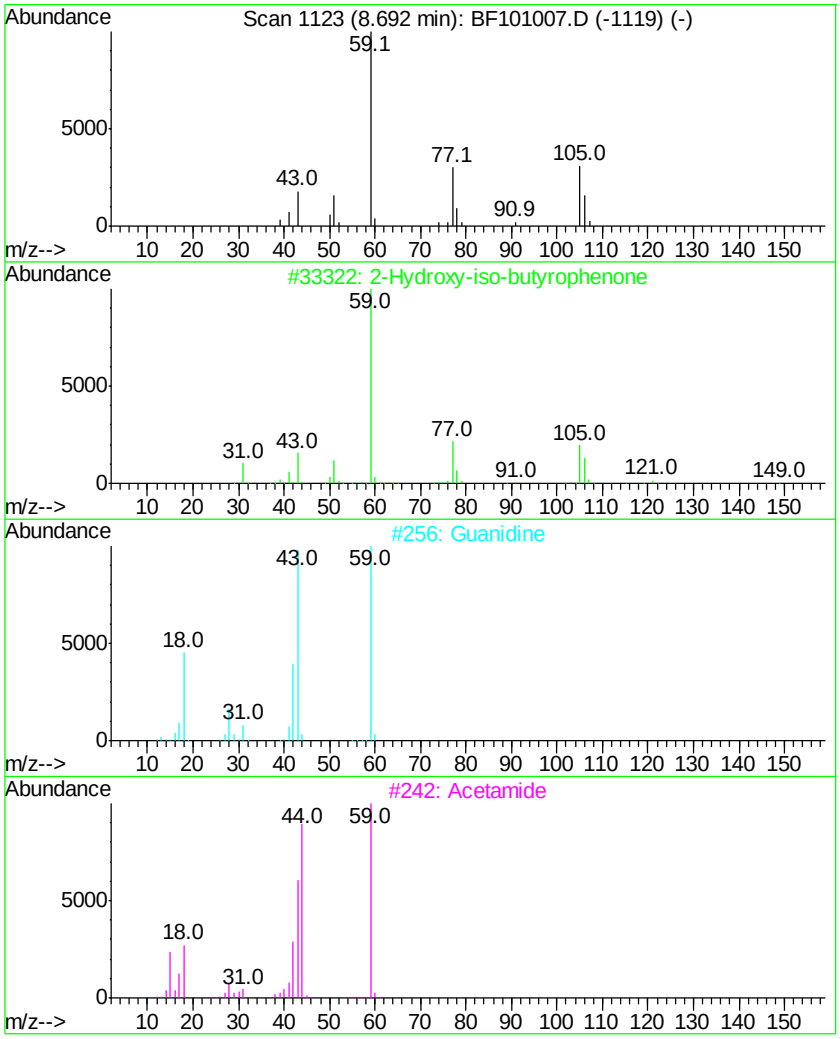
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

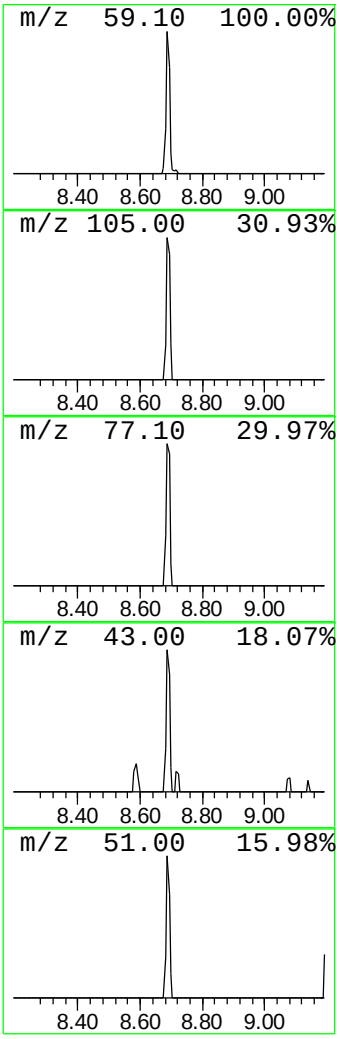
****

Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.69	2.40 ng	44902	Naphthalene-d8	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	90
2	Guanidine	59	CH5N3	000113-00-8	5
3	Acetamide	59	C2H5NO	000060-35-5	5
4	Propylamine	59	C3H9N	000107-10-8	4
5	Ethane, 1,1-dimethoxy-	90	C4H10O2	000534-15-6	4





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Instrument : BNA_F
ClientSampleId : HAR-3-E(0-1)

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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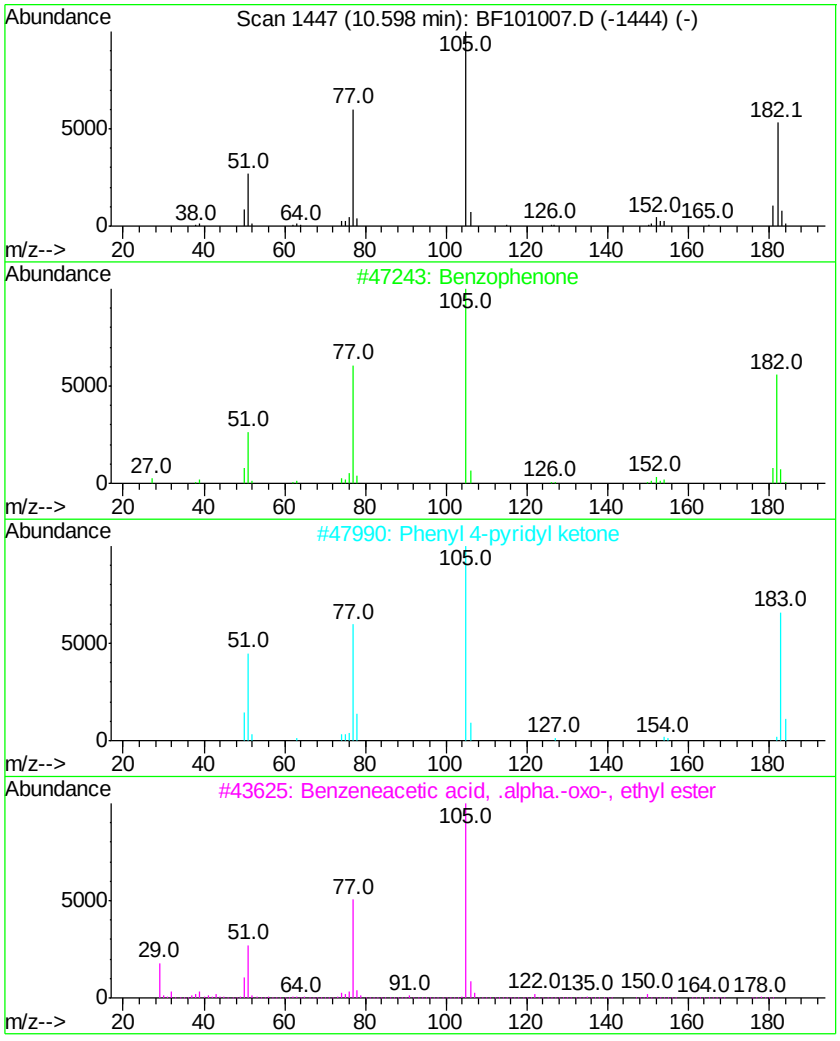
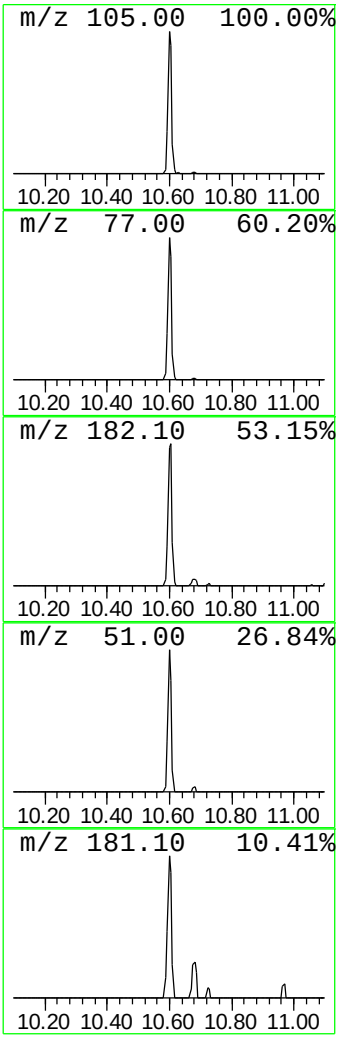
****

Peak Number 5 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.60	8.90 ng	146650	Acenaphthene-d10	9.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	53
3	Benzeneacetic acid, .alpha.-oxo-...	178	C10H10O3	001603-79-8	47
4	1,2,4-Triazine-3,5(2H,4H)-dione,...	249	C10H7N3O3S	024168-34-1	47
5	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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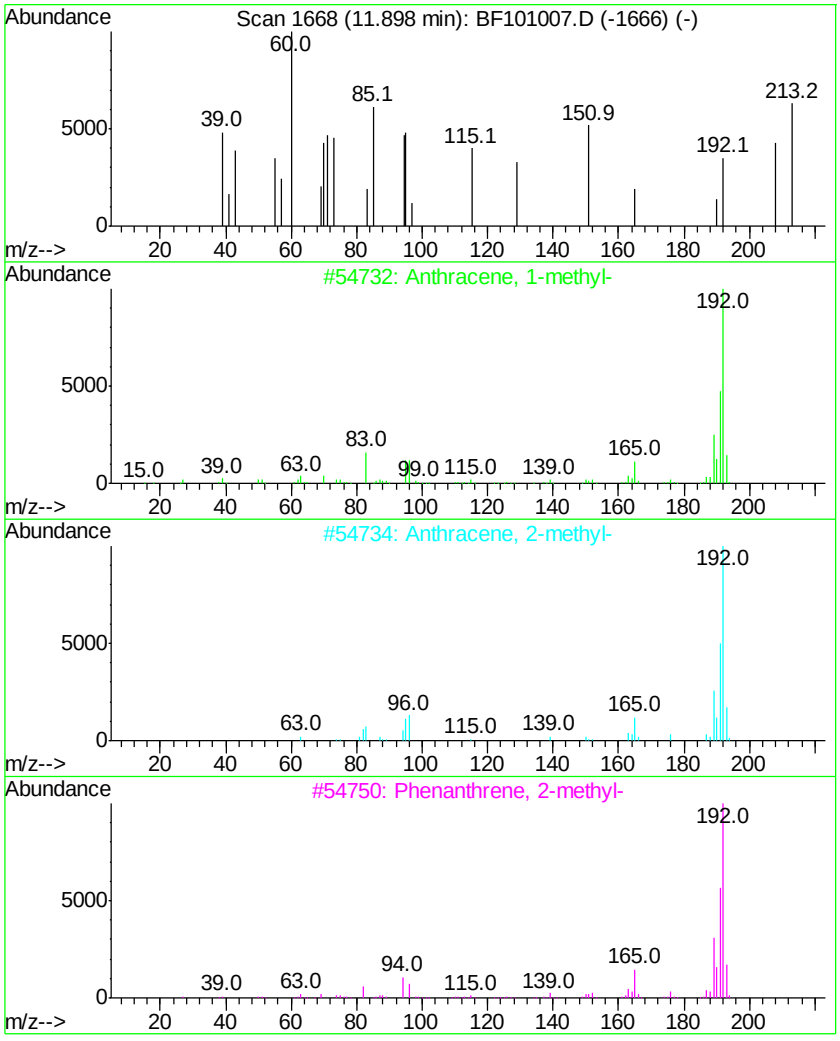
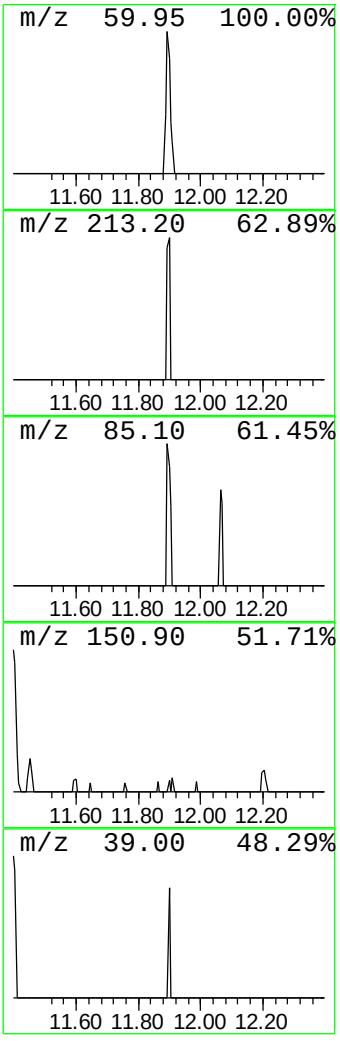
Peak Number 6 Anthracene, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	2.39 ng	35637	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	53
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	53
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	53
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	53
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	50





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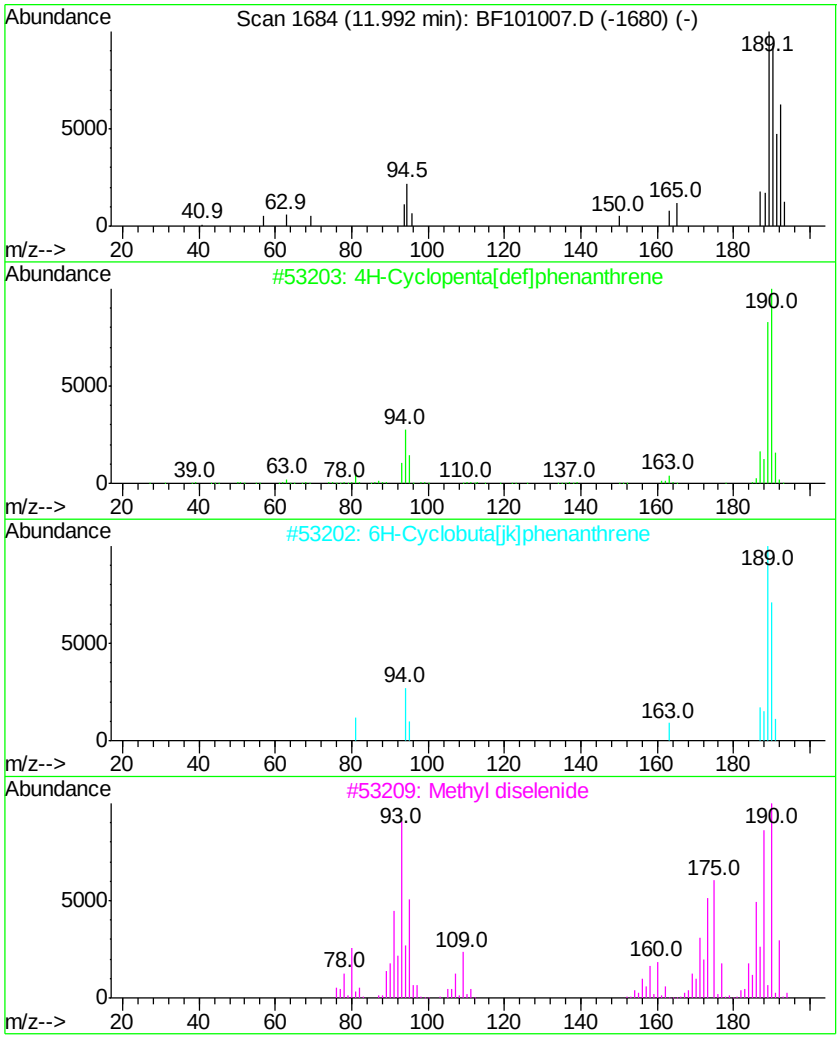
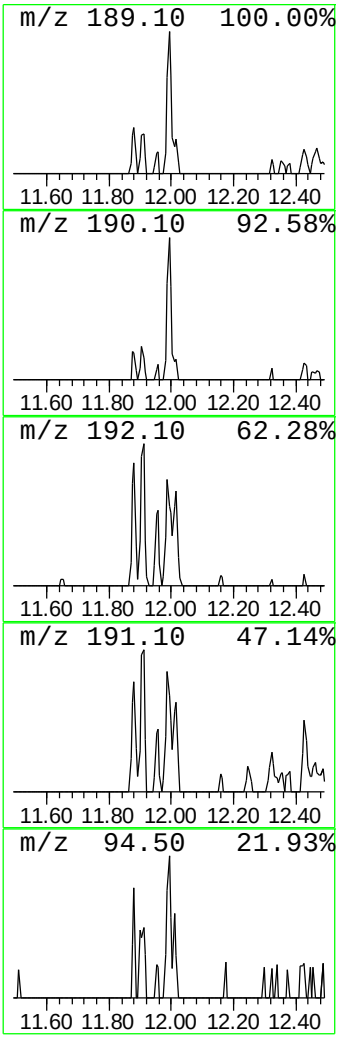
Peak Number 7 4H-Cyclopenta[def]phenanthrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	2.19 ng	32601	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	58
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	53
3	Methyl diselenide	190	C2H6Se2	007101-31-7	41
4	5-Thiazolecarboxamide, 4-amino-2...	189	C5H7N3OS2	1000338-08-9	27
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	27





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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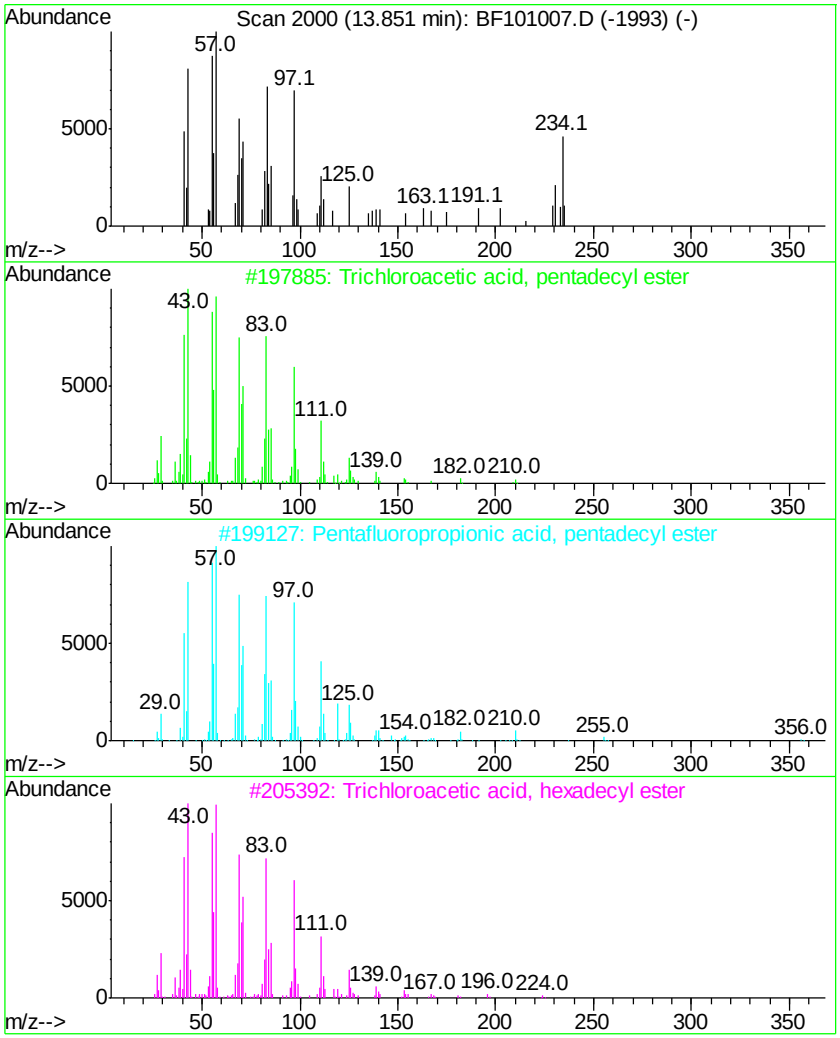
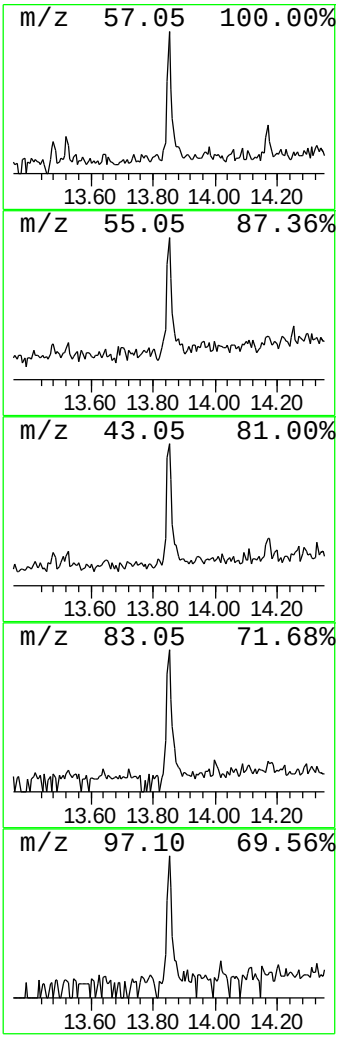
Peak Number 8 Trichloroacetic acid, penta... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	2.33 ng	60042	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	60
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	60
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	60
4	1-Docosene	308	C22H44	001599-67-3	55
5	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	55





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Misc :
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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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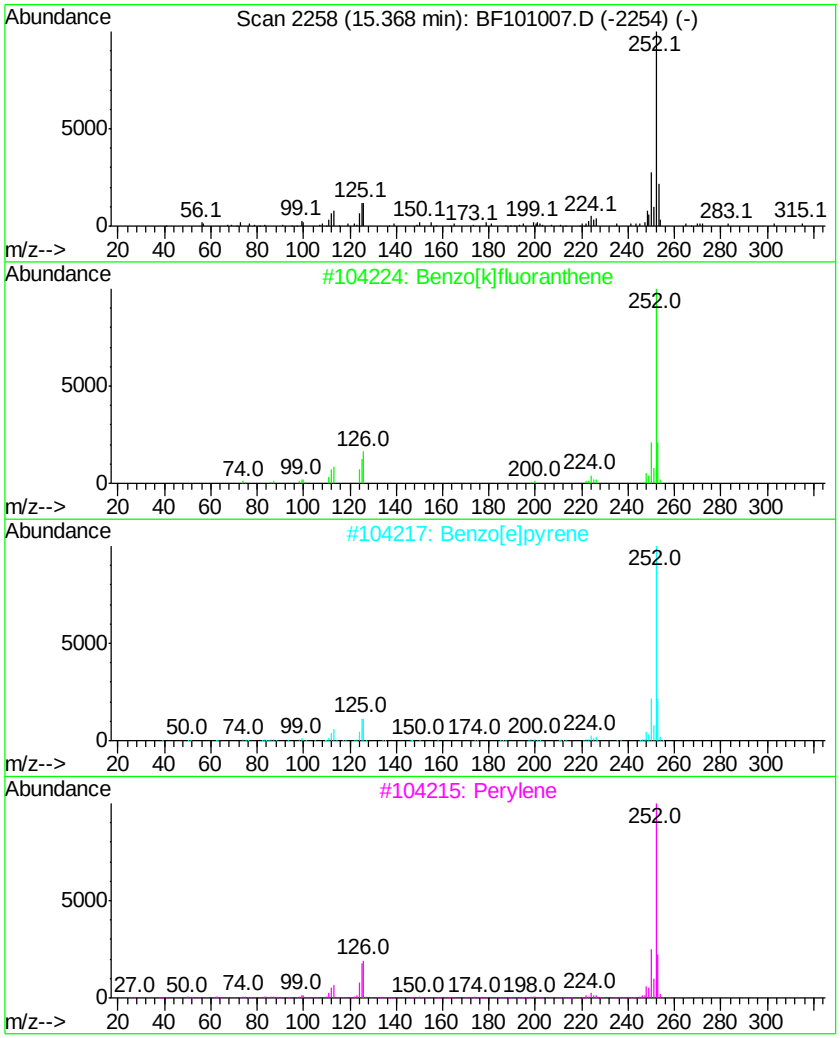
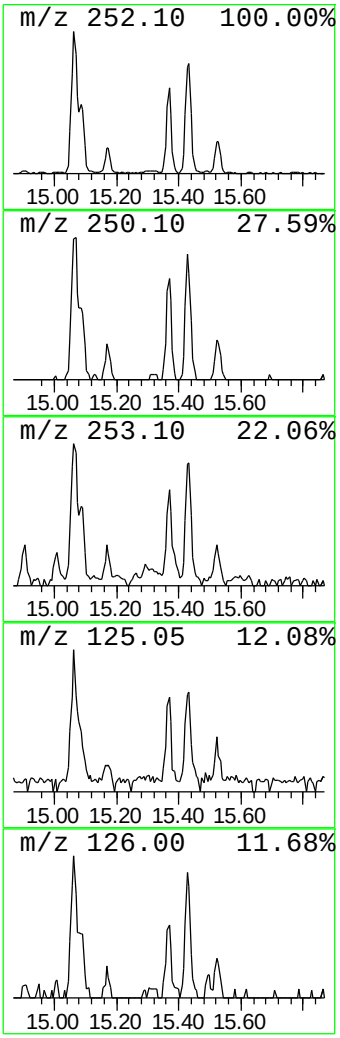
Peak Number 9 Benzo[k]fluoranthene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.37	5.72 ng	86534	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[k]fluoranthene	252	C20H12	000207-08-9	98
2	Benzo[e]pyrene	252	C20H12	000192-97-2	95
3	Perylene	252	C20H12	000198-55-0	94
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93
5	Benzo[a]pyrene	252	C20H12	000050-32-8	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112917\
Data File : BF101007.D
Acq On : 30 Nov 2017 5:42
Operator : SJ/JU
Sample : I6579-07
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HAR-3-E(0-1)

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.08	11.0	ng	175650	1	6.85	318769	20.0
unknown6.63	6.63	78.5	ng	1251130	1	6.85	318769	20.0
2-Hydroxy-iso-but...	8.69	2.4	ng	44902	2	8.13	373725	20.0
Benzophenone	10.60	8.9	ng	146650	3	9.89	329729	20.0
Anthracene, 1-met...	11.90	2.4	ng	35637	4	11.38	297804	20.0
4H-Cyclopenta[def...	11.99	2.2	ng	32601	4	11.38	297804	20.0
Trichloroacetic a...	13.85	2.3	ng	60042	5	14.02	515487	20.0
Benzo[k]fluoranthene	15.37	5.7	ng	86534	6	15.50	302640	20.0