LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121217\
Data File : BF101347.D
Acq On : 12 Dec 2017 23:08
Operator : SJ/JU
Sample : I6822-08
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2(13-15)

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-BF113017.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	5.045	500	503	513	rBV	53315	82928	7.02%	0.692%
2	5.445	567	571	590	rBV	1119623	1124196	95.16%	9.380%
3	6.463	739	744	762	rBV	1074573	1181416	100.00%	9.857%
4	6.598	762	767	770	rBV	1298913	1177938	99.71%	9.828%
5	6.822	802	805	812	rBB	317857	251017	21.25%	2.094%
6	6.981	828	832	835	rBV	910599	831195	70.36%	6.935%
7	7.392	897	902	905	rBV	718742	669420	56.66%	5.585%
8	8.104	1019	1023	1026	rBV	387425	320340	27.11%	2.673%
9	9.180	1201	1206	1209	rBV	1279724	1053924	89.21%	8.793%
10	9.574	1269	1273	1279	rVB	123900	104374	8.83%	0.871%
11	9.863	1318	1322	1325	rBV	384206	335106	28.36%	2.796%
12	9.892	1325	1327	1332	rVB	44660	33748	2.86%	0.282%
13	10.069	1354	1357	1360	rBV	23746	20768	1.76%	0.173%
14	10.280	1390	1393	1396	rVB	17601	14581	1.23%	0.122%
15	10.410	1411	1415	1420	rVB	43571	33925	2.87%	0.283%
16	10.657	1453	1457	1462	rBV	790606	695680	58.89%	5.804%
17	10.751	1470	1473	1478	rBV	20088	18814	1.59%	0.157%
18	11.204	1547	1550	1553	rBV2	20773	23819	2.02%	0.199%
19	11.251	1555	1558	1561	rVB	15270	13224	1.12%	0.110%
20	11.351	1572	1575	1578	rBV	347831	346264	29.31%	2.889%
21	11.380	1578	1580	1583	rVV	301094	237087	20.07%	1.978%
22	11.427	1583	1588	1591	rVV	48829	44671	3.78%	0.373%
23	11.586	1611	1615	1619	rBV2	32358	41190	3.49%	0.344%
24	11.857	1658	1661	1662	rBV	27302	22984	1.95%	0.192%
25	11.886	1663	1666	1668	rVB	33947	34162	2.89%	0.285%
26	11.968	1677	1680	1683	rBV2	39494	49259	4.17%	0.411%
27	12.151	1709	1711	1715	rVB2	24228	20381	1.73%	0.170%
28	12.186	1715	1717	1734	rVB5	39644	94805	8.02%	0.791%
29	12.574	1779	1783	1786	rBV	280254	225342	19.07%	1.880%
30	12.786	1815	1819	1820	rBV2	50807	56538	4.79%	0.472%
31	12.804	1820	1822	1827	rVV	219662	182545	15.45%	1.523%
32	12.851	1827	1830	1834	rVB2	15698	16128	1.37%	0.135%
33	12.939	1839	1845	1848	rVV	997826	857965	72.62%	7.158%
34	12.968	1848	1850	1854	rVB2	13066	12794	1.08%	0.107%

LSC Area Percent Report

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Acq On : 12 Dec 2017 23:08
Operator : SJ/JU
Sample : I6822-08
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2(13-15)

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-BF113017.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.021	1854	1859	1863	rBV4	16636	31224	2.64%	0.261%
36	13.133	1869	1878	1885	rVB	39091	51692	4.38%	0.431%
37	13.198	1885	1889	1892	rVB	28011	23692	2.01%	0.198%
38	13.233	1892	1895	1898	rBV2	15804	19662	1.66%	0.164%
39	13.362	1914	1917	1922	rVB3	10152	12503	1.06%	0.104%
40	13.498	1936	1940	1943	rBV4	7810	13127	1.11%	0.110%
41	13.780	1985	1988	1990	rVB2	17436	14338	1.21%	0.120%
42	13.821	1990	1995	2004	rVB4	106315	155893	13.20%	1.301%
43	14.004	2017	2026	2029	rBV2	371726	418818	35.45%	3.494%
44	14.033	2029	2031	2034	rVB	87822	73845	6.25%	0.616%
45	14.109	2042	2044	2048	rBV	22002	20961	1.77%	0.175%
46	14.239	2064	2066	2071	rVB2	17116	17470	1.48%	0.146%
47	14.392	2088	2092	2095	rVB	23921	22560	1.91%	0.188%
48	14.427	2095	2098	2100	rBV	12762	14074	1.19%	0.117%
49	14.462	2100	2104	2107	rBV6	14404	26032	2.20%	0.217%
50	14.521	2111	2114	2115	rBV3	12791	12539	1.06%	0.105%
51	14.539	2115	2117	2120	rVB3	16476	16153	1.37%	0.135%
52	15.051	2200	2204	2207	rBV	84836	118230	10.01%	0.986%
53	15.162	2219	2223	2226	rBV	26136	29034	2.46%	0.242%
54	15.356	2252	2256	2260	rBV	47538	58937	4.99%	0.492%
55	15.421	2263	2267	2271	rVB	83951	101428	8.59%	0.846%
56	15.480	2272	2277	2281	rVV	187820	249085	21.08%	2.078%
57	15.515	2281	2283	2290	rVB2	30934	37586	3.18%	0.314%
58	16.427	2436	2438	2443	rVB4	12242	13832	1.17%	0.115%
59	16.974	2525	2531	2537	rVB3	42623	84696	7.17%	0.707%
60	17.139	2557	2559	2566	rVB6	14255	25710	2.18%	0.215%
61	17.421	2603	2607	2614	rVB2	27398	56698	4.80%	0.473%
62	17.668	2646	2649	2656	rVB8	18787	37006	3.13%	0.309%

Sum of corrected areas: 11985353

LSC Report - Integrated Chromatogram

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Data File : BF101347.D
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Sample : I6822-08
Misc :
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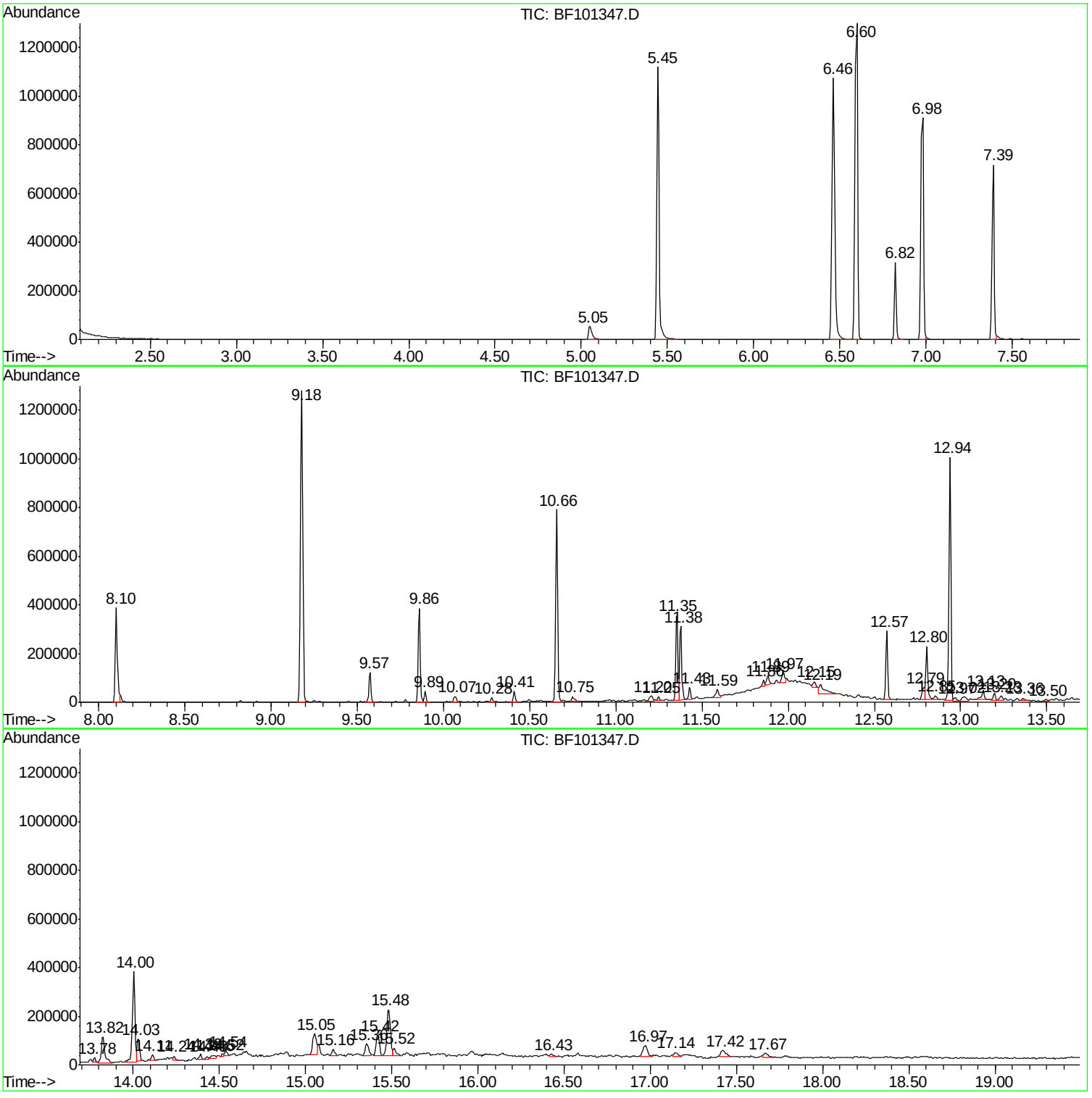
Instrument : BNA_F
ClientSampleId : SB-2(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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\BF121217\
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

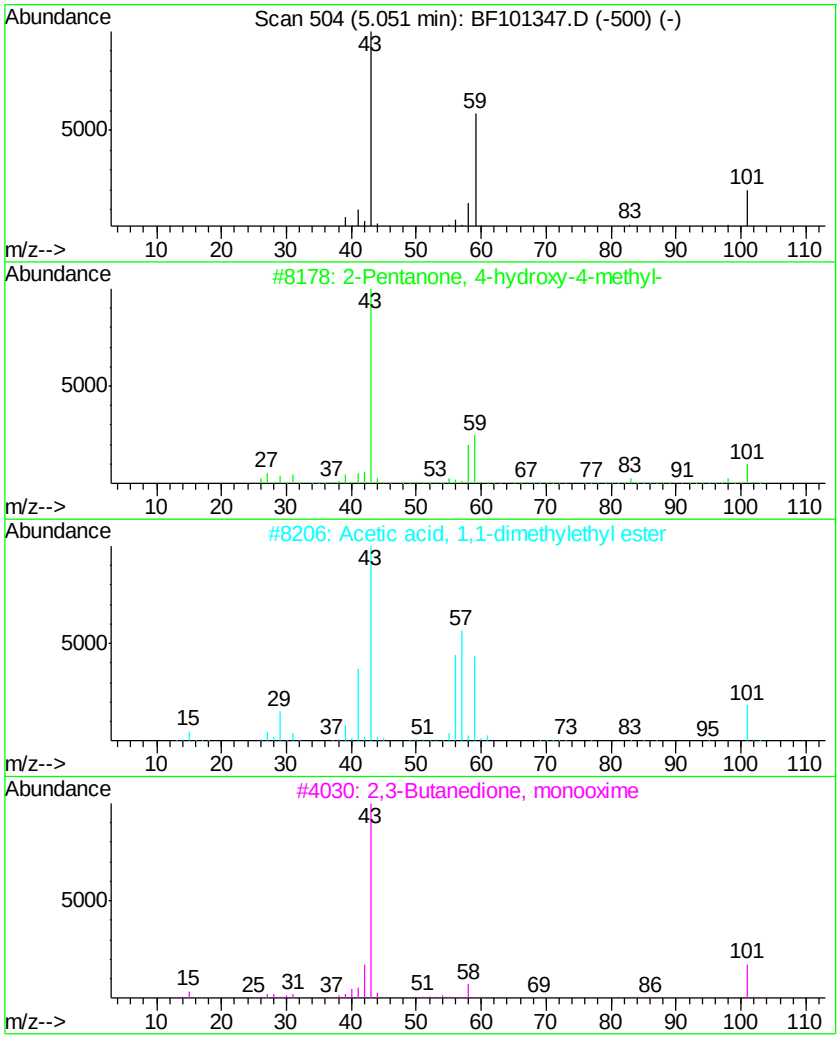
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

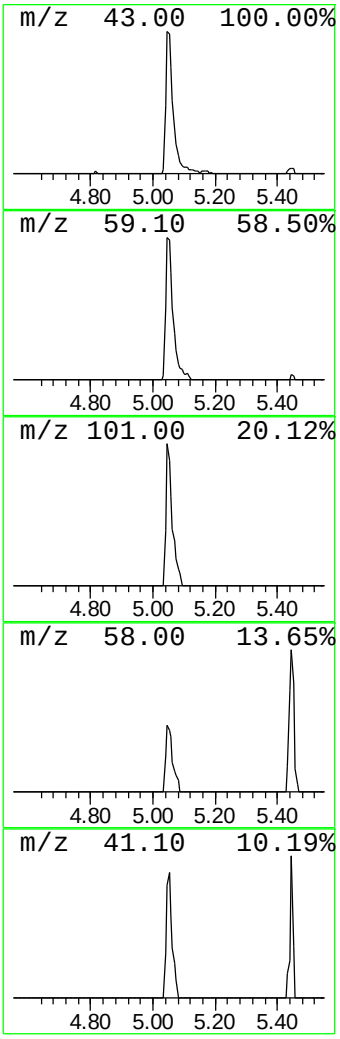
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	6.61 ng	82928	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121217\
Data File : BF101347.D
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Operator : SJ/JU
Sample : I6822-08
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

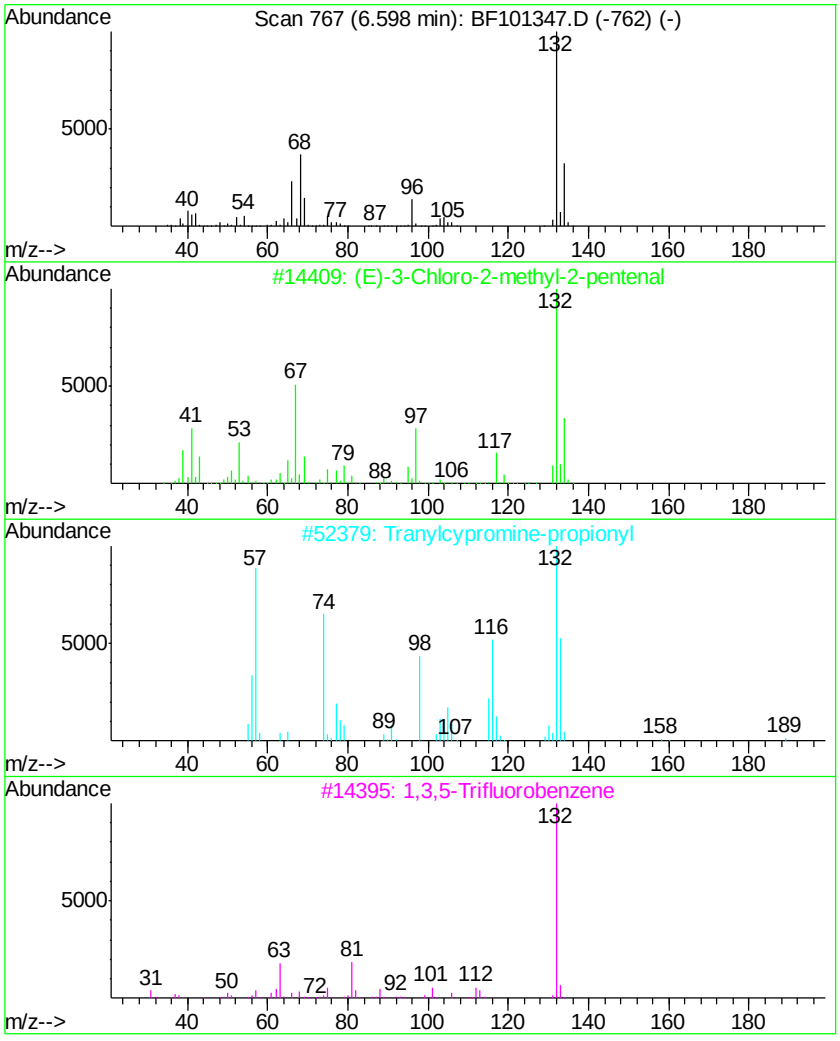
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

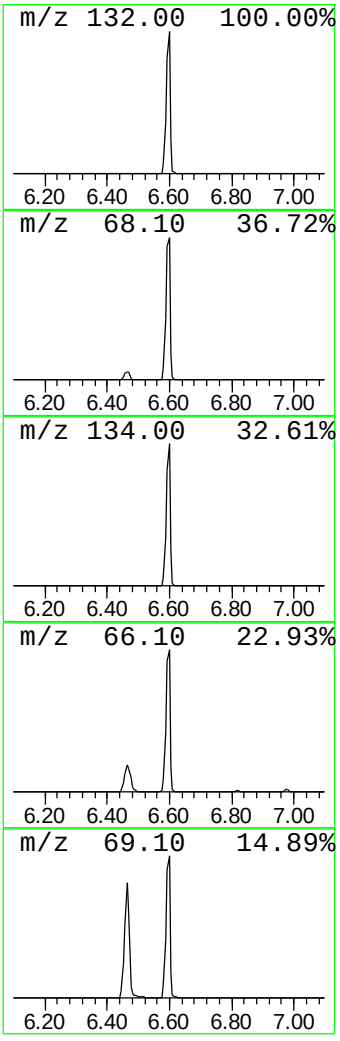
****

Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	93.85 ng	1177940	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Operator : SJ/JU
Sample : I6822-08
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
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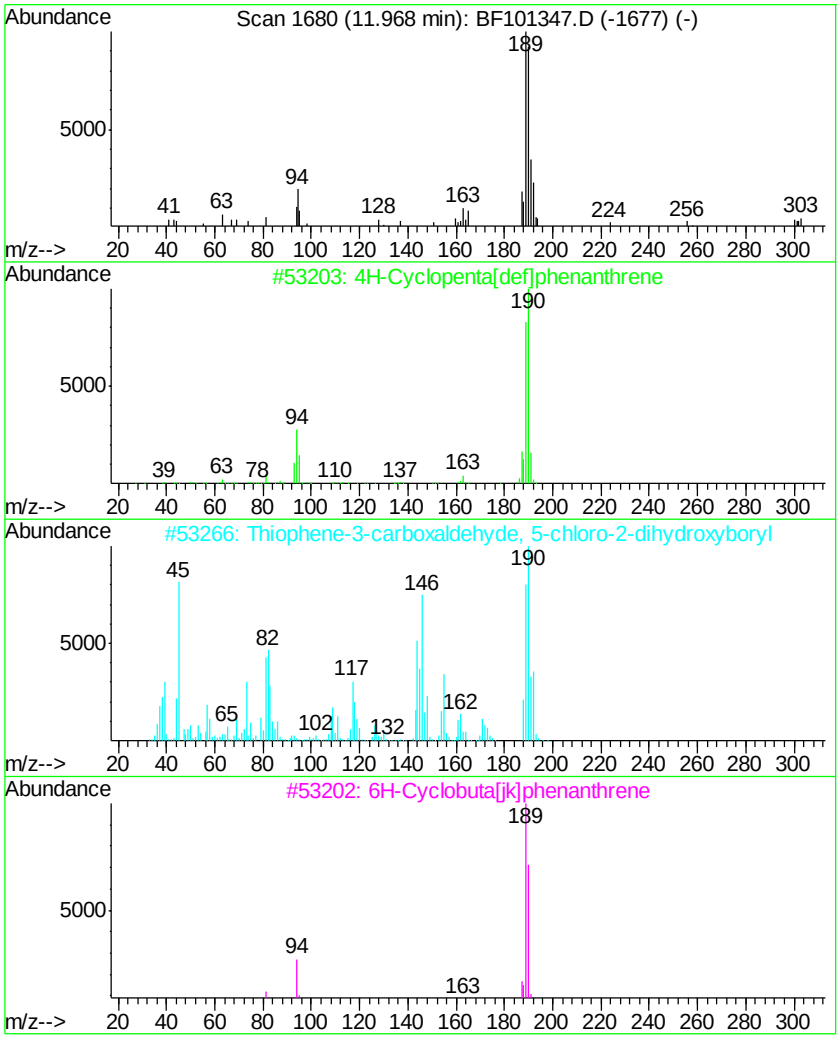
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

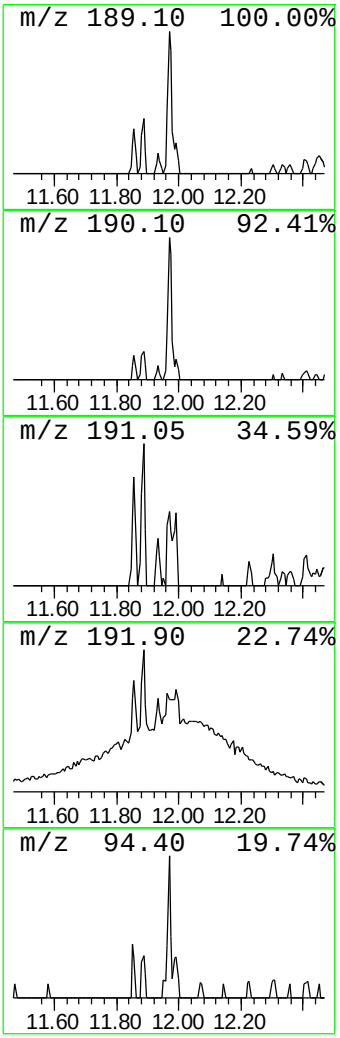
****

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.97	2.85 ng	49259	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	72
2	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	59
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	40
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	40
5	5-Thiazolecarboxamide, 4-amino-2...	189	C5H7N3OS2	1000338-08-9	27





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121217\
Data File : BF101347.D
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Sample : I6822-08
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

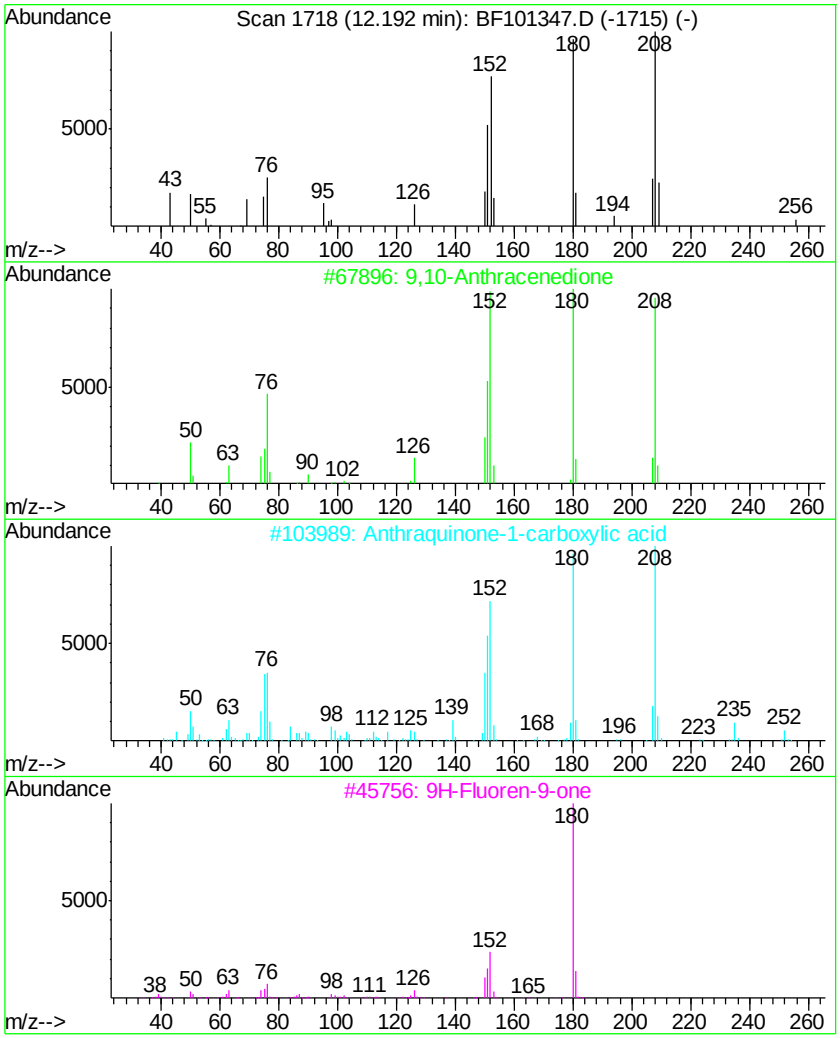
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

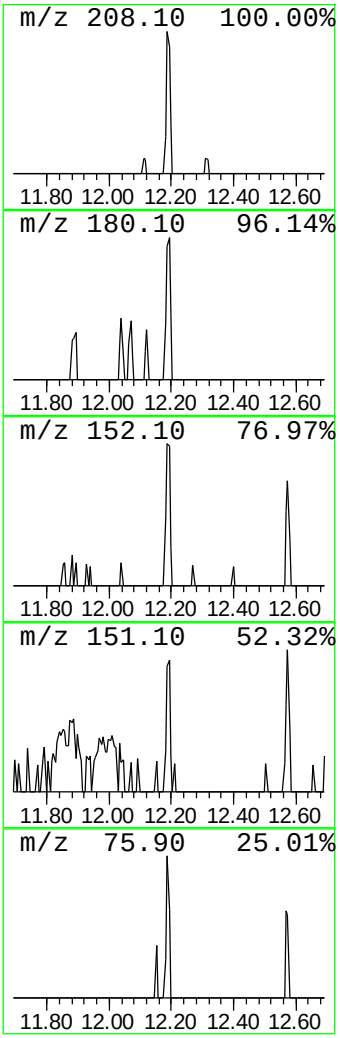
****

Peak Number 7 9,10-Anthracenedione Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.19	5.48 ng	94805	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Anthracenedione	208	C14H8O2	000084-65-1	87
2	Anthraquinone-1-carboxylic acid	252	C15H8O4	000602-69-7	72
3	9H-Fluoren-9-one	180	C13H8O	000486-25-9	46
4	Pyrene, 1,2,3,3a,4,5-hexahydro-	208	C16H16	005385-37-5	43
5	Naphthalene, 1,2,3,4-tetrahydro-...	208	C16H16	003018-20-0	43





Library Search Compound Report

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Sample : I6822-08
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ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

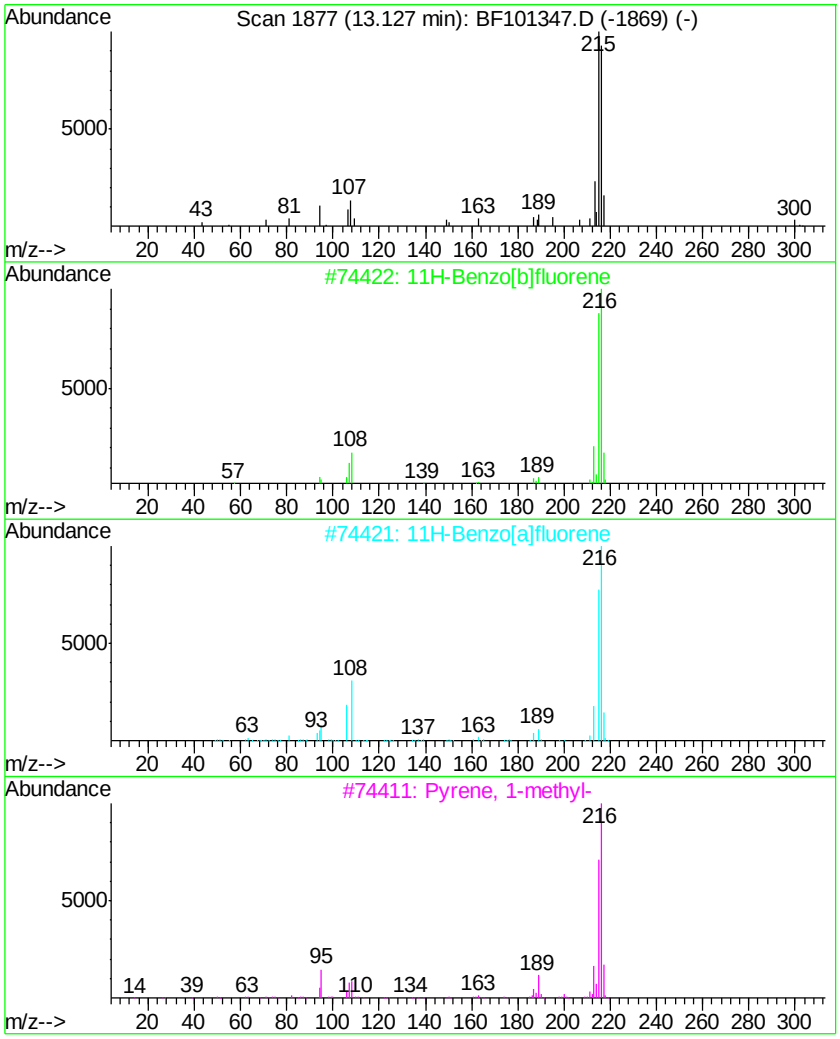
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

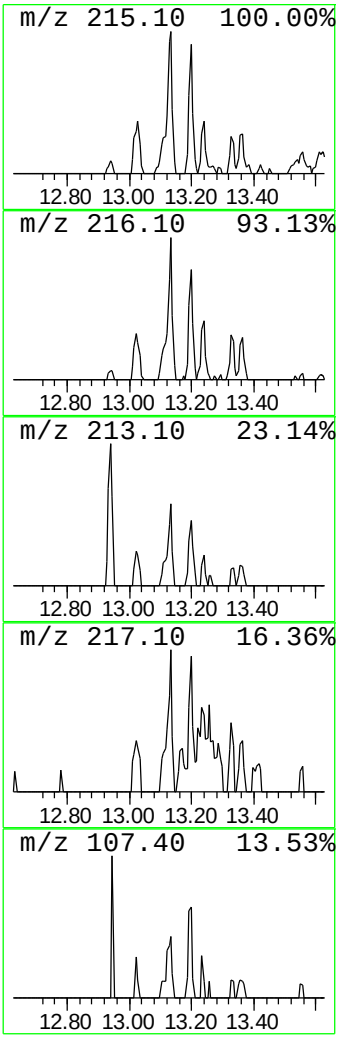
****

Peak Number 8 11H-Benzo[b]fluorene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.13	2.47 ng	51692	Chrysene-d12	14.00

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	90
3	Pyrene, 1-methyl-	216	C17H12	002381-21-7	90
4	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	87
5	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	87





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Instrument : BNA_F
ClientSampleId : SB-2(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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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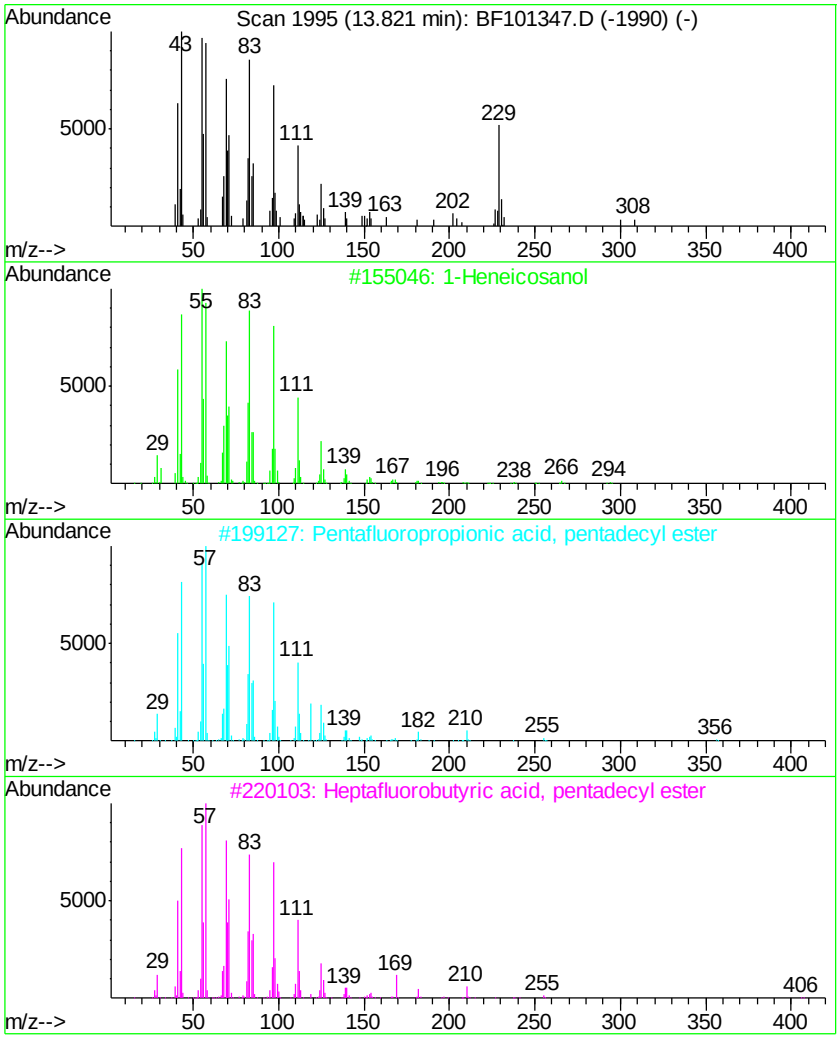
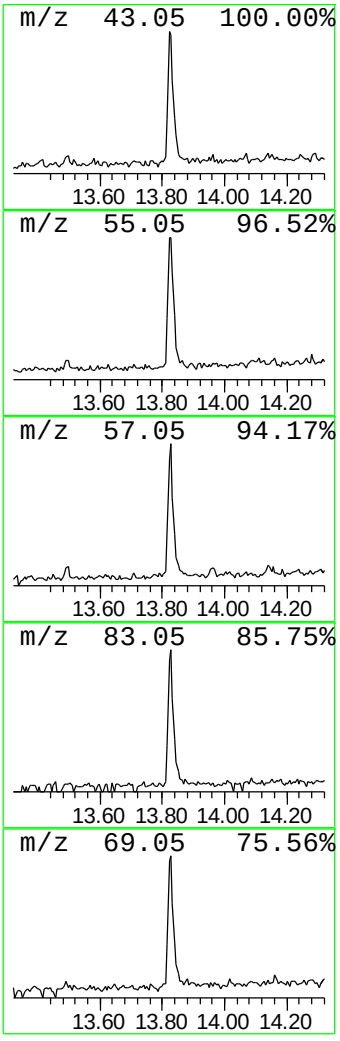
Peak Number 9 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	7.44 ng	155893	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
5	Behenic alcohol	326	C22H46O	000661-19-8	93





Library Search Compound Report

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Data File : BF101347.D
Acq On : 12 Dec 2017 23:08
Operator : SJ/JU
Sample : I6822-08
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

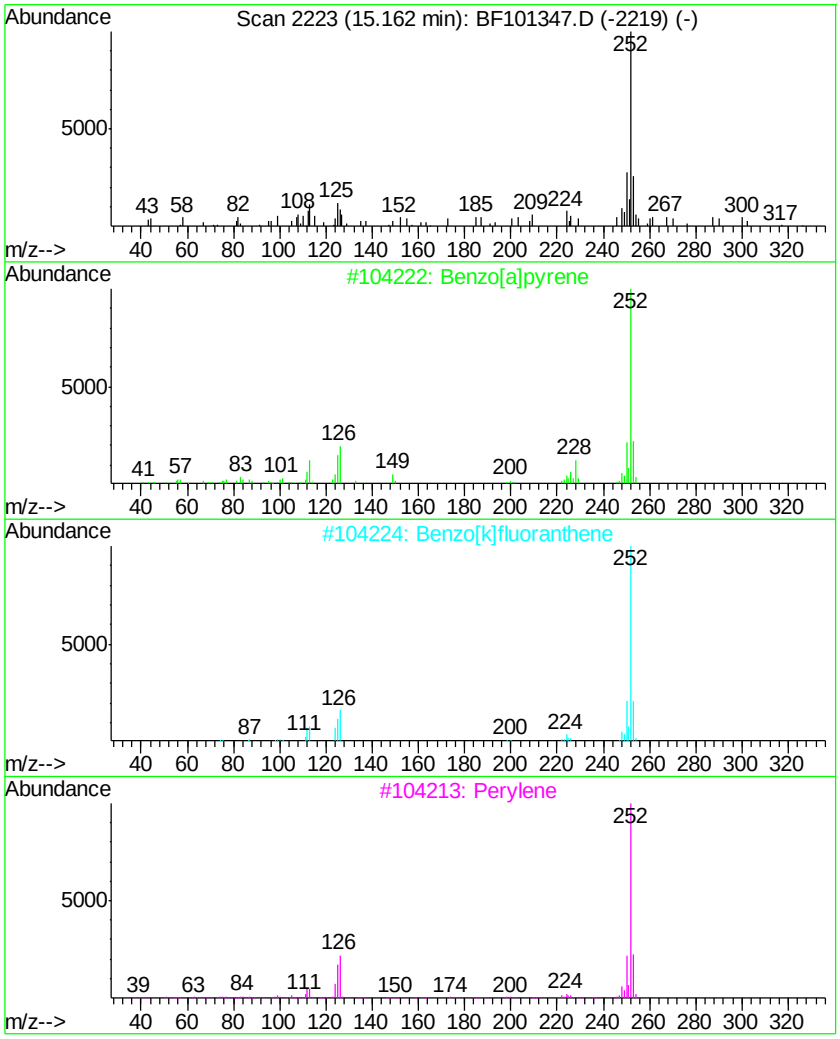
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

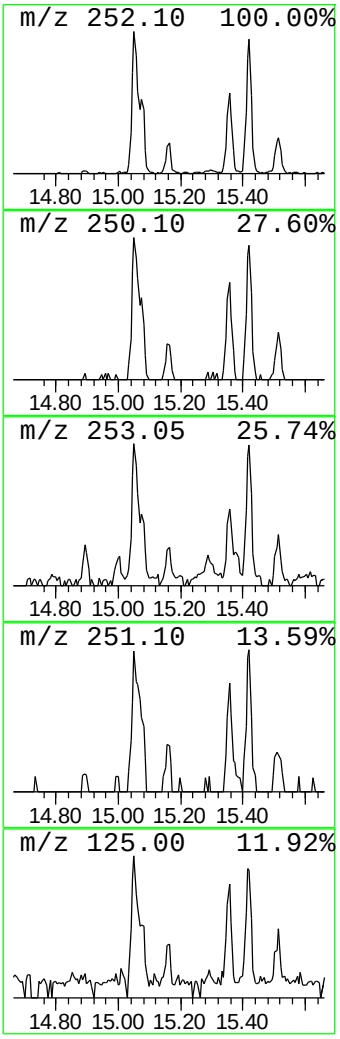
****

Peak Number 10 Benzo[a]pyrene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.16	2.33 ng	29034	Perylene-d12	15.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[a]pyrene	252	C20H12	000050-32-8	64
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	64
3	Perylene	252	C20H12	000198-55-0	58
4	Benzo[e]pyrene	252	C20H12	000192-97-2	58
5	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	58





Library Search Compound Report

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Data File : BF101347.D
Acq On : 12 Dec 2017 23:08
Operator : SJ/JU
Sample : I6822-08
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2(13-15)

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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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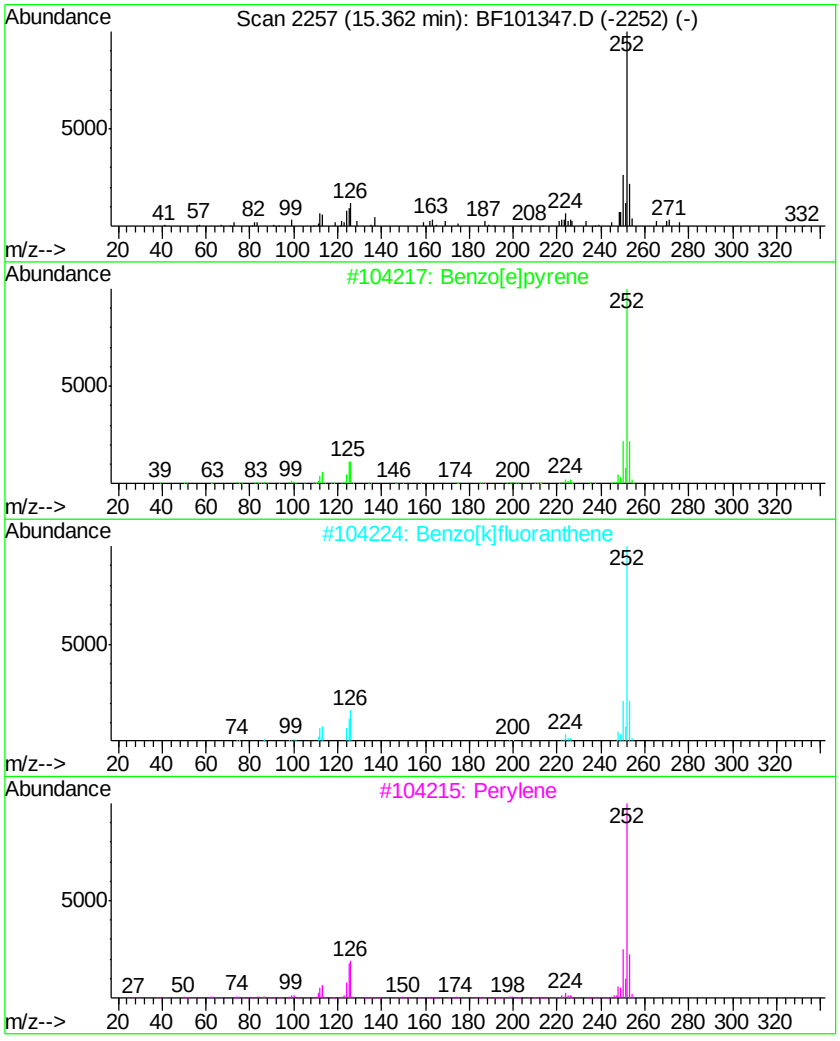
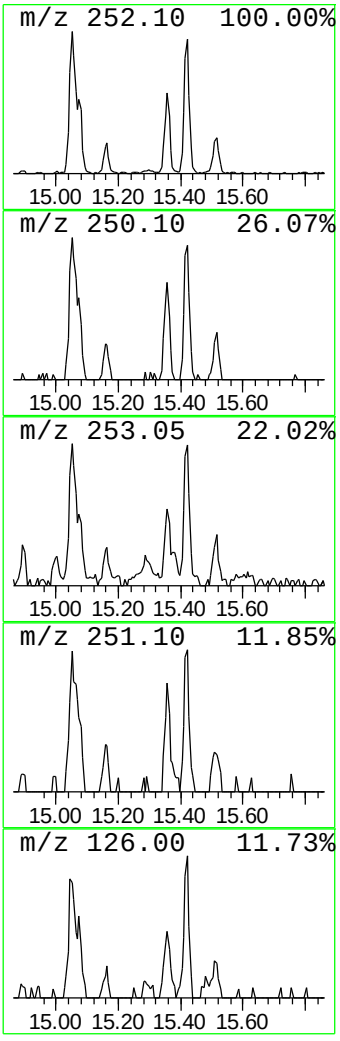
Peak Number 11 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.36	4.73 ng	58937	Perylene-d12	15.48

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





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121217\
Data File : BF101347.D
Acq On : 12 Dec 2017 23:08
Operator : SJ/JU
Sample : I6822-08
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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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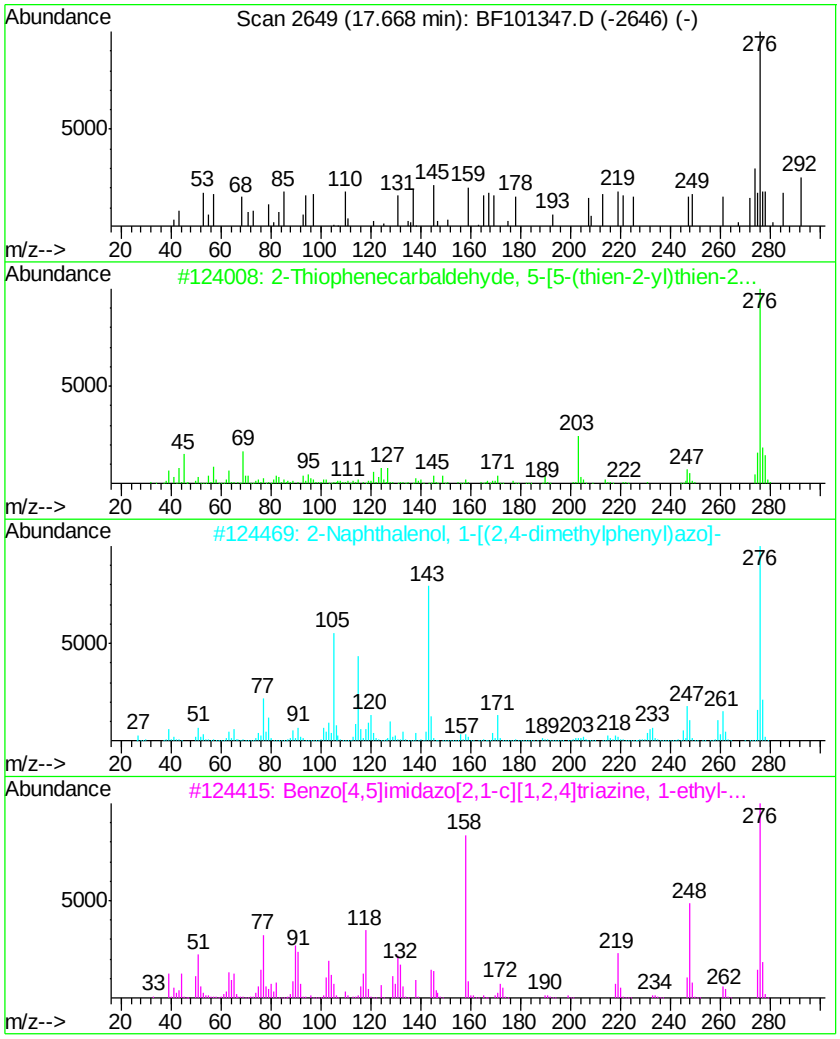
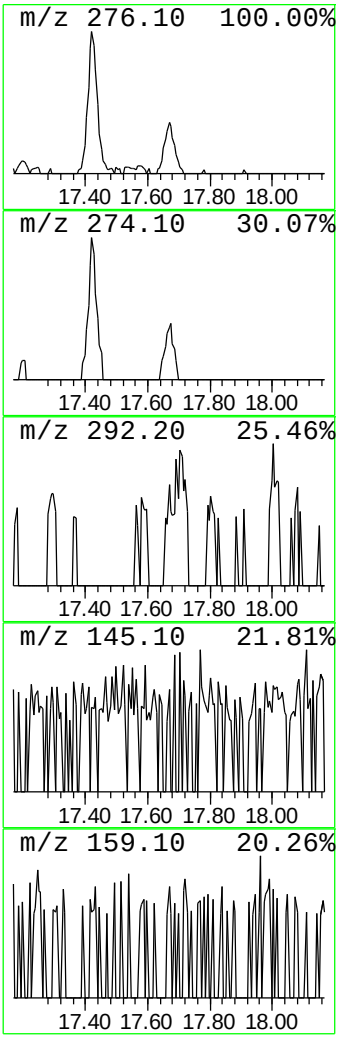
Peak Number 13 2-Thiophenecarbaldehyde, 5-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.67	2.97 ng	37006	Perylene-d12	15.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Thiophenecarbaldehyde, 5-[5-(t...	276	C13H8OS3	1000217-28-5	50
2	2-Naphthalenol, 1-[(2,4-dimethyl...	276	C18H16N2O	003118-97-6	49
3	Benzo[4,5]imidazo[2,1-c][1,2,4]t...	276	C17H16N4	1000302-82-6	49
4	1H-Cyclopenta[4,5]pyrido[1,2-a]b...	276	C17H16N4	329707-31-5	47
5	Ethyl 5[2,4-dimethoxyphenyl]pyra...	276	C14H16N2O4	1000211-63-5	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121217\
Data File : BF101347.D
Acq On : 12 Dec 2017 23:08
Operator : SJ/JU
Sample : I6822-08
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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...	5.05	6.6	ng	82928	1	6.82	251017	20.0
unknown6.60	6.60	93.8	ng	1177940	1	6.82	251017	20.0
4H-Cyclopenta[def...	11.97	2.9	ng	49259	4	11.35	346264	20.0
9,10-Anthracenedione	12.19	5.5	ng	94805	4	11.35	346264	20.0
11H-Benzo[b]fluorene	13.13	2.5	ng	51692	5	14.00	418818	20.0
1-Heneicosanol	13.82	7.4	ng	155893	5	14.00	418818	20.0
Benzo[a]pyrene	15.16	2.3	ng	29034	6	15.48	249085	20.0
Benzo[e]pyrene	15.36	4.7	ng	58937	6	15.48	249085	20.0
2-Thiophenecarbal...	17.67	3.0	ng	37006	6	15.48	249085	20.0