LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061017\
Data File : BF095856.D
Acq On : 10 Jun 2017 19:39
Operator : SJ/MA
Sample : I3583-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-2669

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-BF060517.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	4.569	504	507	526	rBV2	37298	104851	7.60%	0.638%
2	5.257	621	624	662	rBV	517331	1152699	83.56%	7.012%
3	6.922	904	907	920	rBV	652798	1107213	80.26%	6.736%
4	7.022	920	924	943	rVB	900101	1379513	100.00%	8.392%
5	7.369	979	983	996	rBV	253399	341046	24.72%	2.075%
6	7.604	1018	1023	1045	rBV	672029	922316	66.86%	5.611%
7	8.281	1134	1138	1161	rBV	456499	707180	51.26%	4.302%
8	9.398	1324	1328	1344	rBV	345532	477041	34.58%	2.902%
9	11.175	1625	1630	1651	rVB	1014217	1286738	93.27%	7.828%
10	11.874	1745	1749	1762	rBV	96244	144050	10.44%	0.876%
11	12.221	1803	1808	1813	rBV2	409871	531850	38.55%	3.235%
12	12.269	1813	1816	1822	rVB2	23677	36817	2.67%	0.224%
13	13.080	1946	1954	1959	rBV3	14828	20658	1.50%	0.126%
14	13.127	1959	1962	1969	rVB4	13193	21776	1.58%	0.132%
15	13.516	2024	2028	2042	rBV	462800	700254	50.76%	4.260%
16	13.845	2080	2084	2086	rBV3	13340	18930	1.37%	0.115%
17	14.615	2210	2215	2218	rBV2	414316	533410	38.67%	3.245%
18	14.651	2218	2221	2230	rVB	190799	261072	18.92%	1.588%
19	14.745	2233	2237	2249	rVB2	63662	98988	7.18%	0.602%
20	15.421	2345	2352	2356	rBV	46924	52610	3.81%	0.320%
21	15.468	2356	2360	2366	rVB	53999	62920	4.56%	0.383%
22	15.539	2368	2372	2374	rBV	18825	23709	1.72%	0.144%
23	15.568	2374	2377	2382	rVV3	67235	100652	7.30%	0.612%
24	15.621	2382	2386	2393	rVB3	30958	56171	4.07%	0.342%
25	15.874	2425	2429	2436	rBV	25283	32214	2.34%	0.196%
26	16.233	2485	2490	2493	rBV	28166	30787	2.23%	0.187%
27	16.274	2493	2497	2501	rVV4	14244	20492	1.49%	0.125%
28	16.357	2506	2511	2519	rVB4	26414	37814	2.74%	0.230%
29	16.433	2519	2524	2530	rBV	623354	699408	50.70%	4.255%
30	16.480	2530	2532	2539	rVB3	11331	14147	1.03%	0.086%
31	16.633	2553	2558	2562	rBV	15703	18800	1.36%	0.114%
32	16.733	2570	2575	2582	rBV	597701	704901	51.10%	4.288%
33	16.833	2587	2592	2595	rBV2	14687	22151	1.61%	0.135%
34	16.933	2606	2609	2613	rBV	30020	35757	2.59%	0.218%

LSC Area Percent Report

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Operator : SJ/MA
Sample : I3583-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-2669

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-BF060517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.986	2613	2618	2625	rVV	991163	1141890	82.77%	6.947%
36	17.068	2628	2632	2638	rVB	28283	43929	3.18%	0.267%
37	17.174	2645	2650	2652	rBV3	23736	33444	2.42%	0.203%
38	17.209	2652	2656	2662	rVB	69312	89617	6.50%	0.545%
39	17.298	2666	2671	2675	rBV	54674	62335	4.52%	0.379%
40	17.339	2675	2678	2687	rBV2	43958	81214	5.89%	0.494%
41	17.456	2693	2698	2702	rBV2	21513	27638	2.00%	0.168%
42	17.498	2702	2705	2711	rVV	17325	24594	1.78%	0.150%
43	17.780	2750	2753	2757	rVB3	10791	14528	1.05%	0.088%
44	17.903	2769	2774	2780	rVB2	22150	31630	2.29%	0.192%
45	18.009	2788	2792	2795	rBV	26607	32466	2.35%	0.198%
46	18.039	2795	2797	2800	rVV2	41038	46821	3.39%	0.285%
47	18.074	2800	2803	2807	rVV	26024	33010	2.39%	0.201%
48	18.115	2807	2810	2816	rVV	25112	28110	2.04%	0.171%
49	18.174	2818	2820	2827	rVV2	25133	32438	2.35%	0.197%
50	18.245	2827	2832	2840	rVV4	45480	83043	6.02%	0.505%
51	18.327	2840	2846	2850	rVV2	476645	723909	52.48%	4.404%
52	18.362	2850	2852	2864	rVV2	162821	259609	18.82%	1.579%
53	18.462	2864	2869	2876	rVV	37608	50862	3.69%	0.309%
54	18.562	2880	2886	2893	rVV4	13413	29995	2.17%	0.182%
55	18.621	2893	2896	2900	rVV3	23071	32029	2.32%	0.195%
56	18.668	2900	2904	2912	rVB4	17994	27663	2.01%	0.168%
57	18.845	2928	2934	2938	rBV3	30425	43522	3.15%	0.265%
58	18.886	2938	2941	2945	rVB2	23756	28394	2.06%	0.173%
59	18.956	2945	2953	2956	rBV4	24112	44672	3.24%	0.272%
60	19.450	3032	3037	3043	rBV4	14868	26283	1.91%	0.160%
61	19.597	3058	3062	3066	rVV	183682	265253	19.23%	1.614%
62	19.627	3066	3067	3074	rVB2	76466	86052	6.24%	0.523%
63	19.715	3079	3082	3086	rVB	32748	34201	2.48%	0.208%
64	19.833	3098	3102	3107	rVB6	15832	29284	2.12%	0.178%
65	19.892	3107	3112	3116	rBV	99223	119084	8.63%	0.724%
66	19.945	3116	3121	3126	rBV	154304	183372	13.29%	1.116%
67	19.997	3126	3130	3135	rBV	287215	376045	27.26%	2.288%
68	20.215	3163	3167	3173	rVB6	15244	25257	1.83%	0.154%
69	20.286	3173	3179	3183	rBV6	11136	19355	1.40%	0.118%
70	20.397	3191	3198	3201	rBV7	7815	19018	1.38%	0.116%
71	20.474	3208	3211	3216	rBV6	9451	16905	1.23%	0.103%

LSC Area Percent Report

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Acq On : 10 Jun 2017 19:39
Operator : SJ/MA
Sample : I3583-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-2669

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

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Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	20.903	3278	3284	3285	rBV5	10804	14739	1.07%	0.090%
73	21.027	3300	3305	3308	rBV3	14958	22984	1.67%	0.140%
74	21.180	3326	3331	3339	rBV	73355	130458	9.46%	0.794%
75	21.244	3339	3342	3349	rVB5	11956	17755	1.29%	0.108%
76	21.315	3350	3354	3358	rBV	19219	31078	2.25%	0.189%
77	21.356	3359	3361	3367	rVB4	12584	19326	1.40%	0.118%
78	21.515	3384	3388	3396	rBV2	51540	103495	7.50%	0.630%
79	21.727	3420	3424	3430	rVB3	16133	28342	2.05%	0.172%
80	23.227	3674	3679	3687	rVB4	12835	29966	2.17%	0.182%
81	23.391	3699	3707	3710	rBV3	14161	33584	2.43%	0.204%

Sum of corrected areas: 16438133

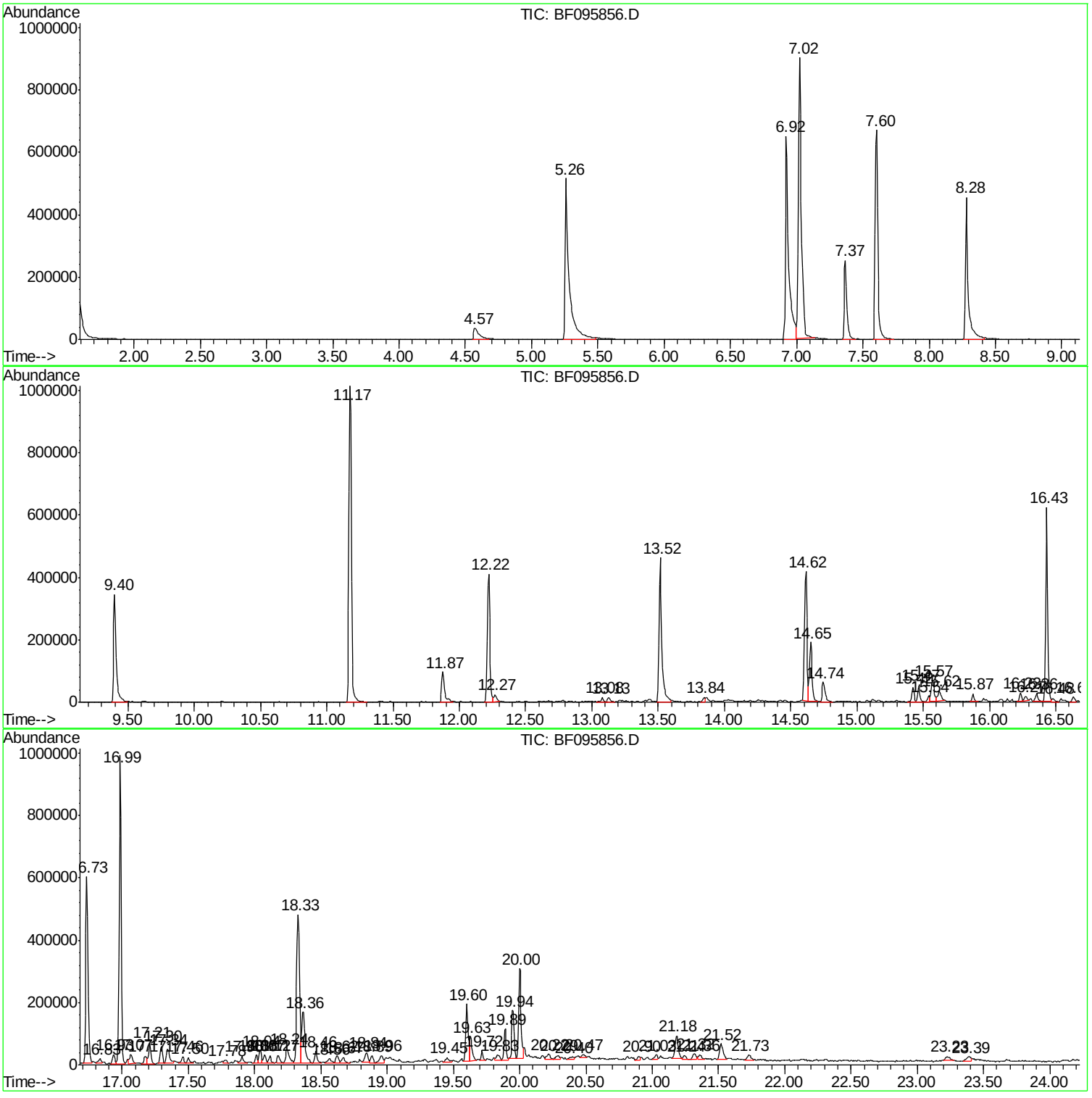
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061017\
Data File : BF095856.D
Acq On : 10 Jun 2017 19:39
Operator : SJ/MA
Sample : I3583-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-2669

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061017\
Data File : BF095856.D
Acq On : 10 Jun 2017 19:39
Operator : SJ/MA
Sample : I3583-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-2669

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

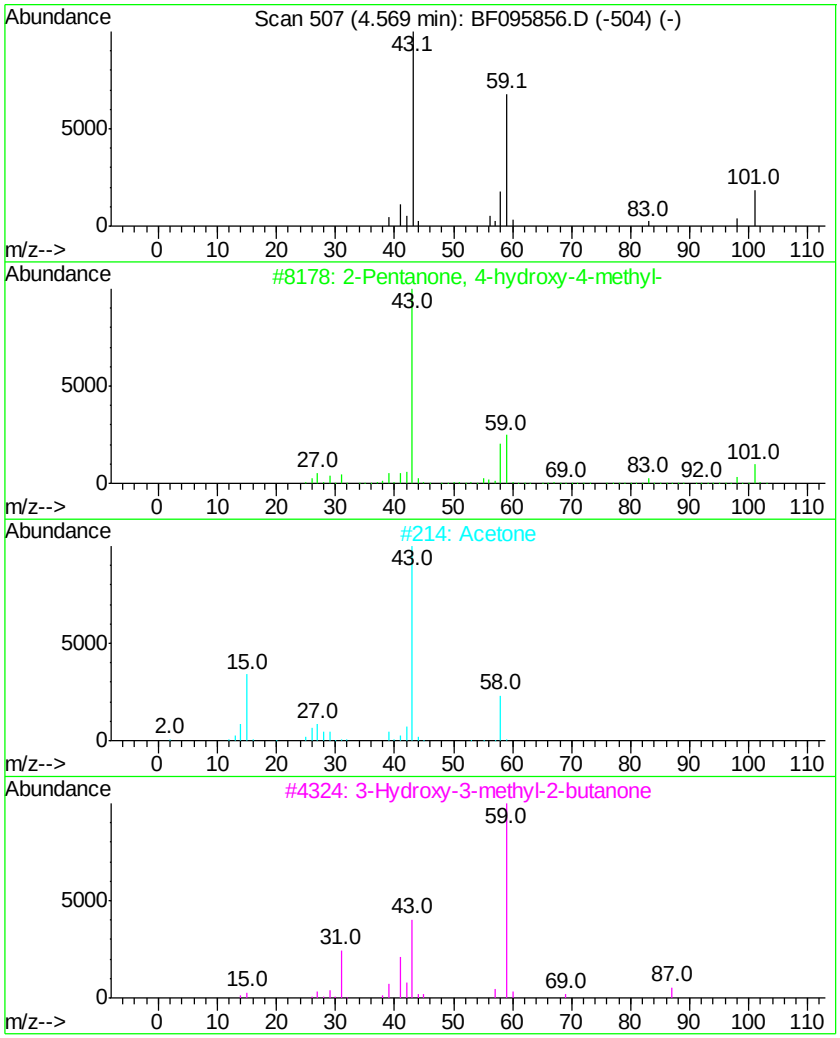
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

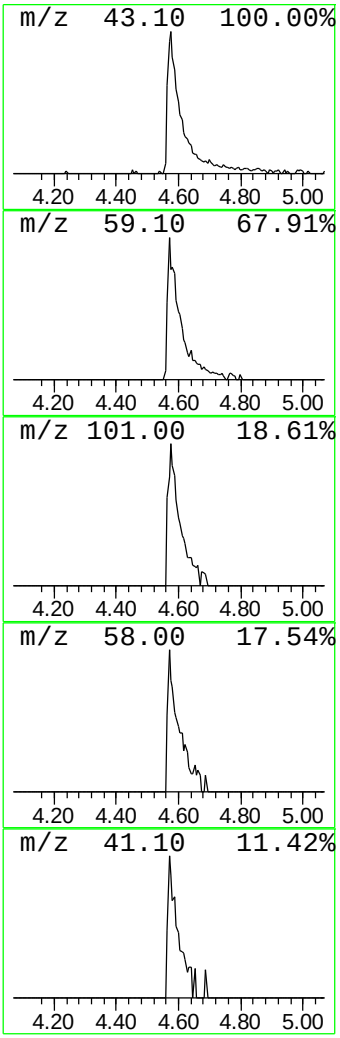
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.57	6.15 ng	104851	1,4-Dichlorobenzene-d4	7.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetone	58	C3H6O	000067-64-1	9
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9
4	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	9
5	3-Octanol	130	C8H18O	000589-98-0	9





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Sample : I3583-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-2669

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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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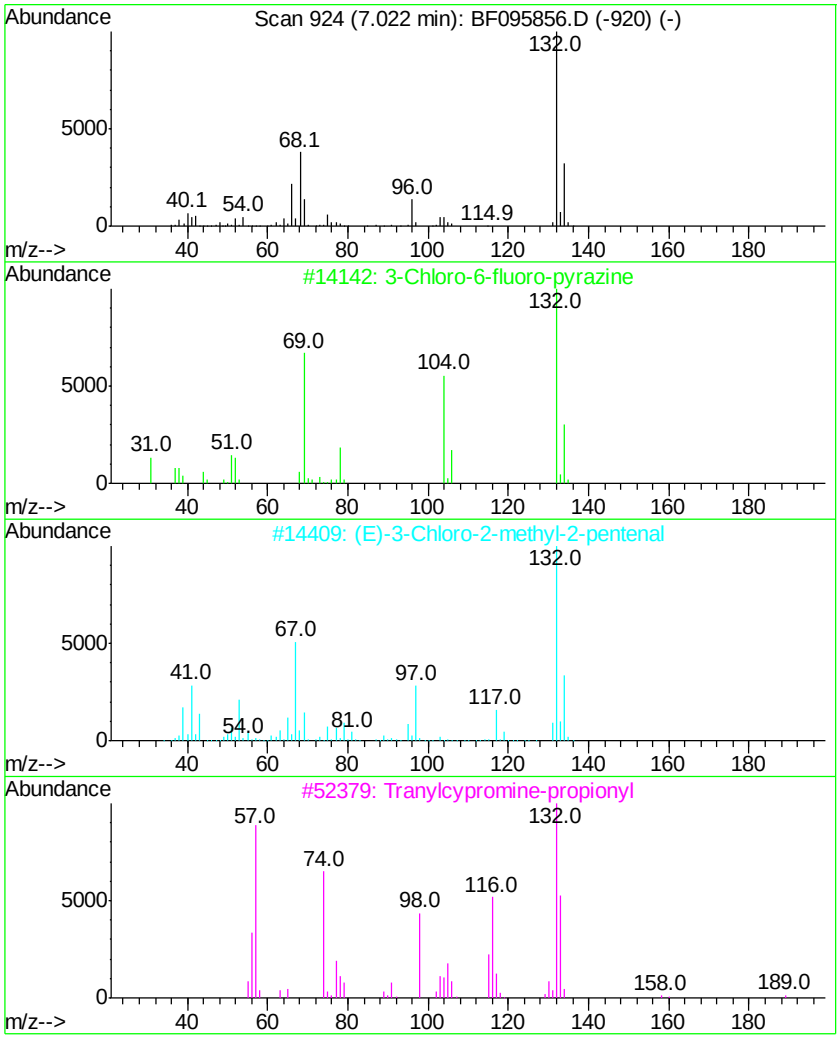
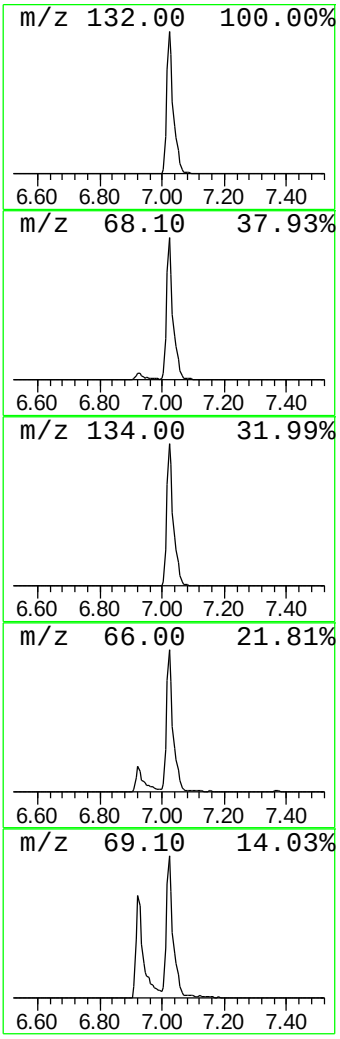
Peak Number 2 unknown7.02 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.02	80.90 ng	1379510	1,4-Dichlorobenzene-d4	7.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061017\
Data File : BF095856.D
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Operator : SJ/MA
Sample : I3583-01
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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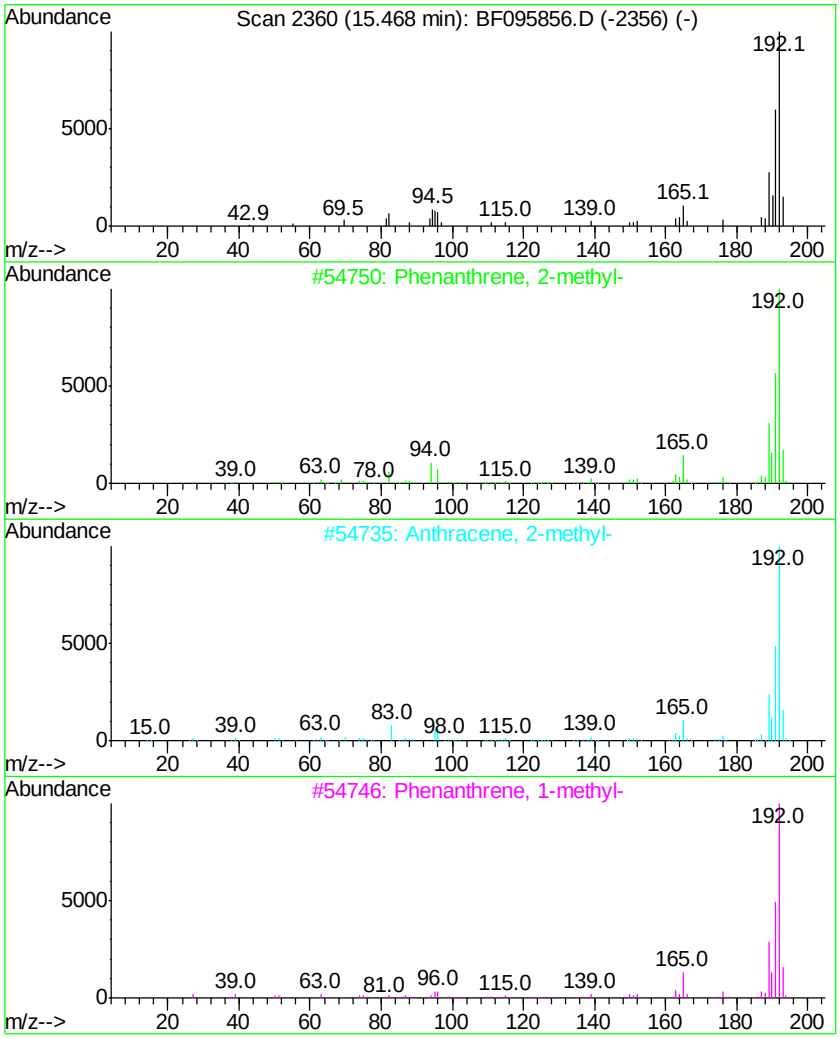
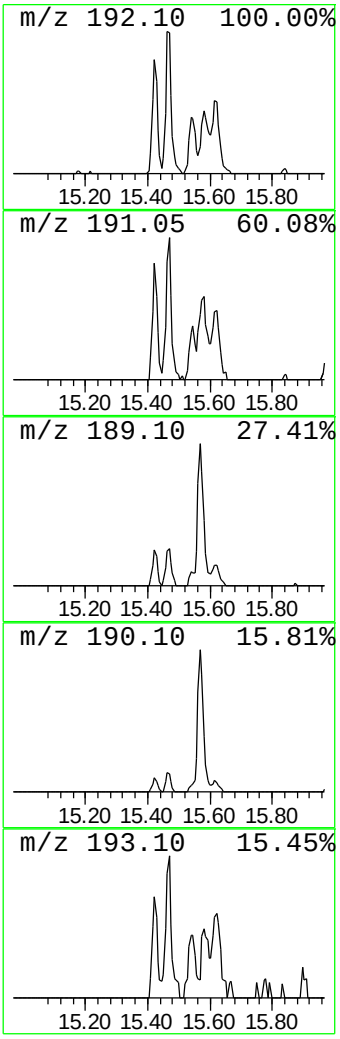
****

Peak Number 4 Phenanthrene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.47	2.36 ng	62920	Phenanthrene-d10	14.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	96
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	96
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	95
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	93
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	93





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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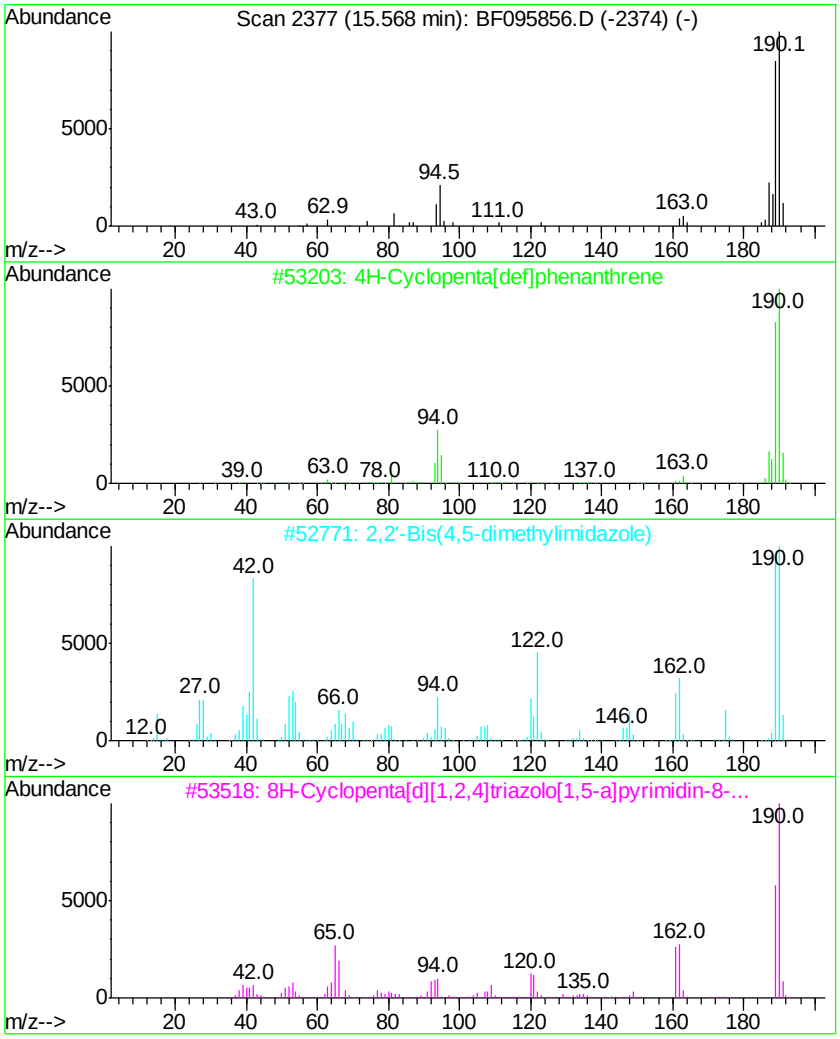
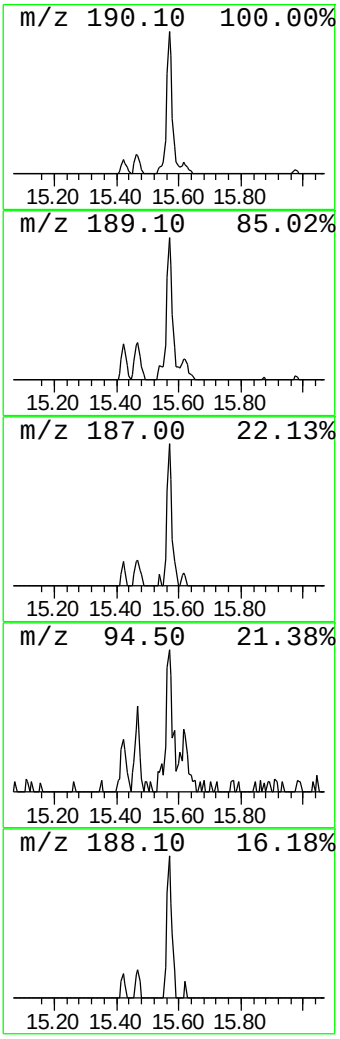
Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.57	3.77 ng	100652	Phenanthrene-d10	14.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	90
2	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	64
3	8H-Cyclopenta[d][1,2,4]triazolo[...	190	C9H10N4O	1000337-56-4	64
4	1H-Pyrazole-4-carboxaldehyde, 1-...	190	C10H7FN2O	1000338-05-6	58
5	6,7-Methylenedioxy-4(3H)-quinazo...	190	C9H6N2O3	028310-11-4	42





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ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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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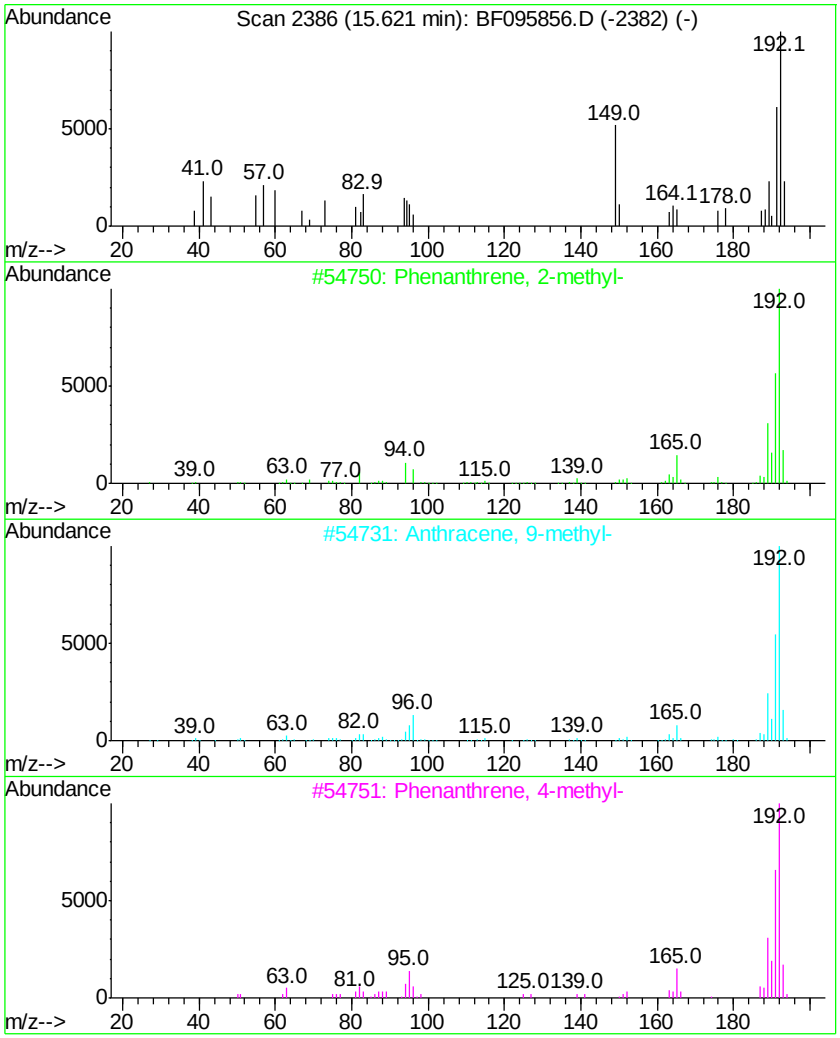
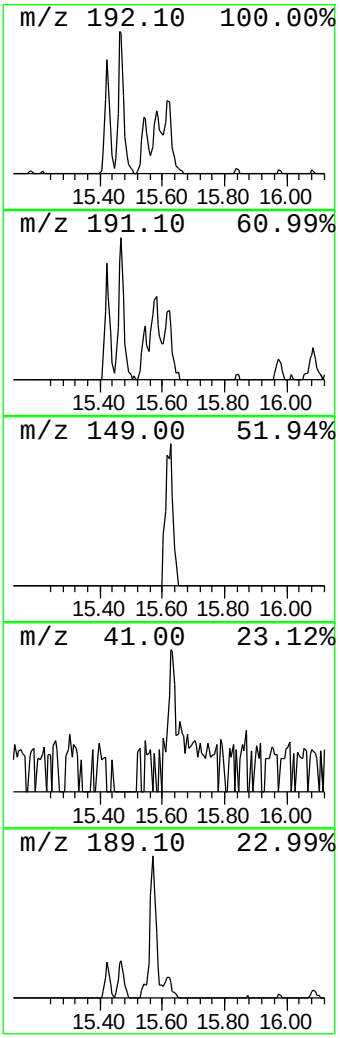
Peak Number 6 Anthracene, 9-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.62	2.11 ng	56171	Phenanthrene-d10	14.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	50
2	Anthracene, 9-methyl-	192	C15H12	000779-02-2	47
3	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	47
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	46
5	Naphtho[2,3-b]norbornadiene	192	C15H12	107426-38-0	43





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061017\
Data File : BF095856.D
Acq On : 10 Jun 2017 19:39
Operator : SJ/MA
Sample : I3583-01
Misc :
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Instrument : BNA_F
ClientSampleId : RO-2669

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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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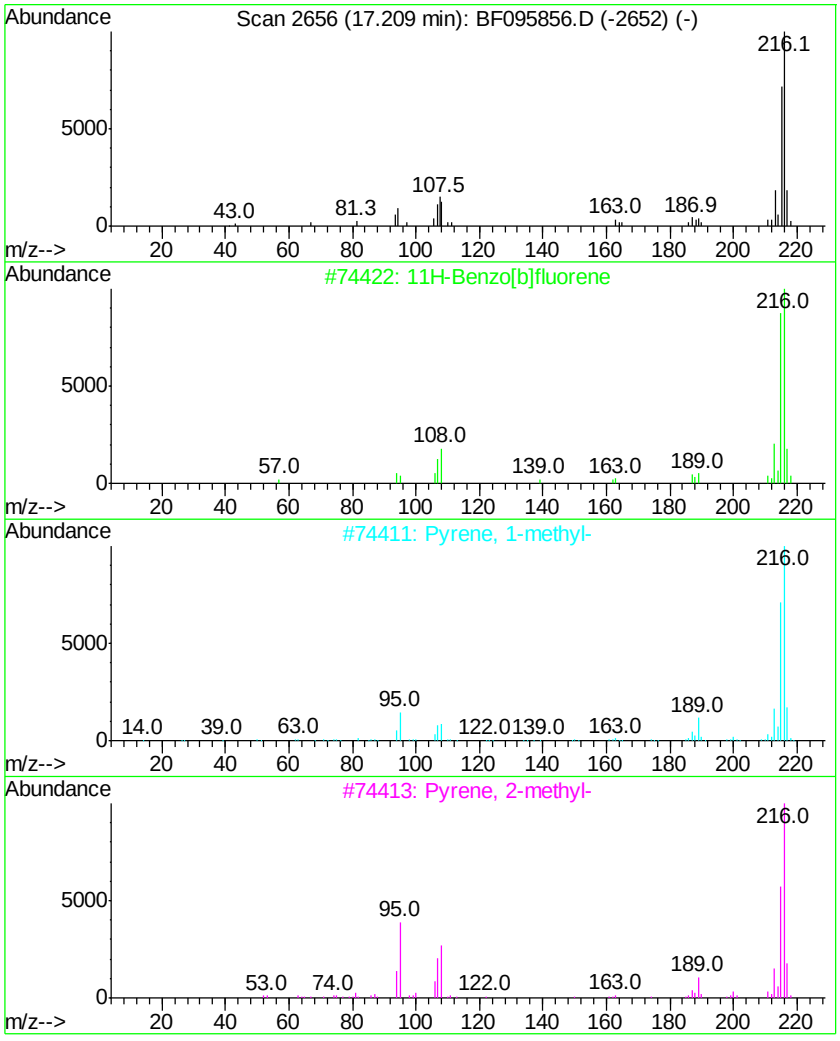
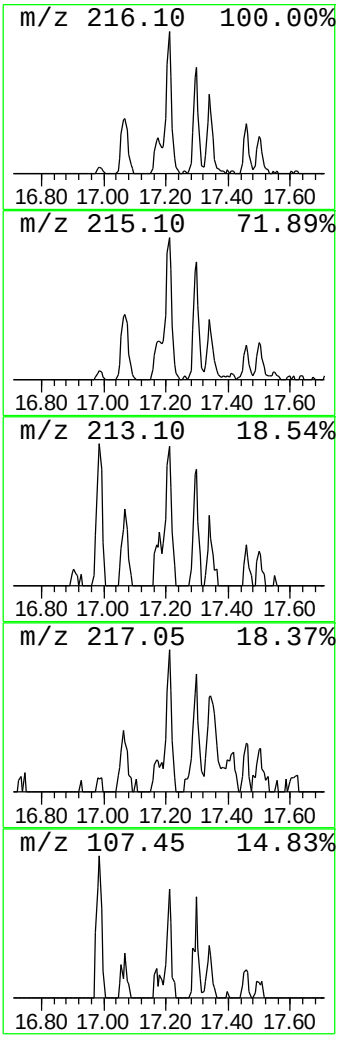
Peak Number 7 11H-Benzo[b]fluorene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.21	2.48 ng	89617	Chrysene-d12	18.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	95
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	93
3	Pyrene, 2-methyl-	216	C17H12	003442-78-2	93
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	90
5	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	90





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Data File : BF095856.D
Acq On : 10 Jun 2017 19:39
Operator : SJ/MA
Sample : I3583-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-2669

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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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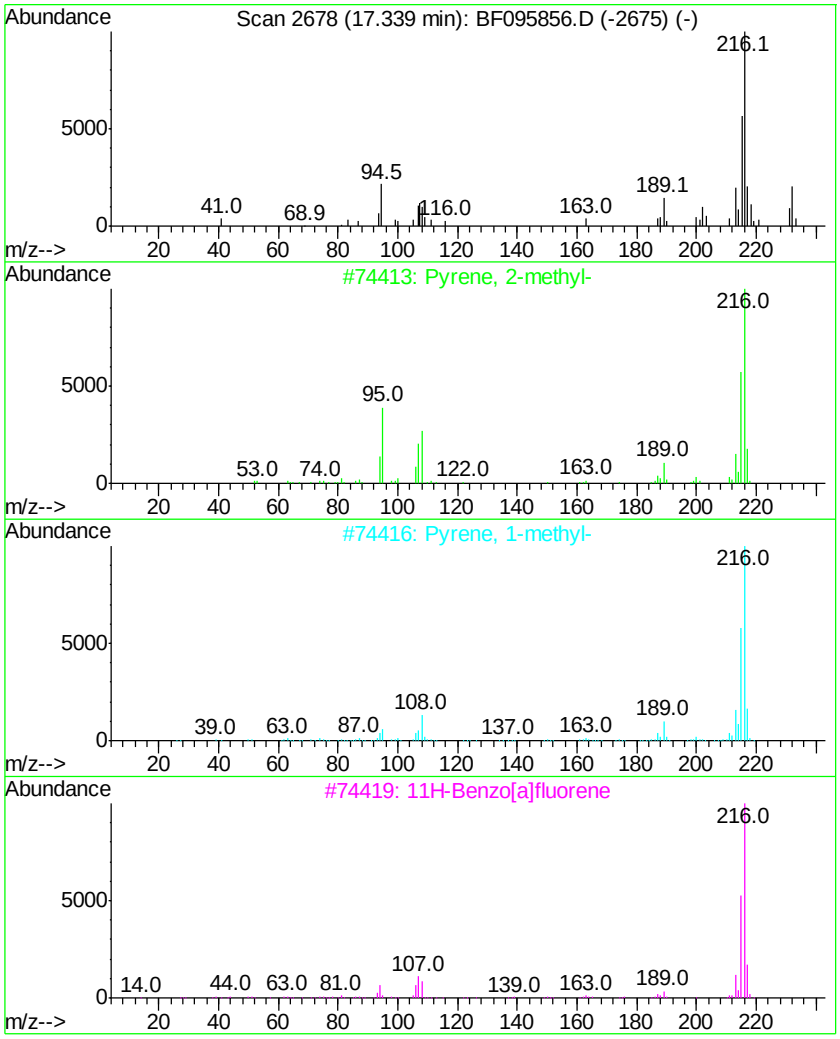
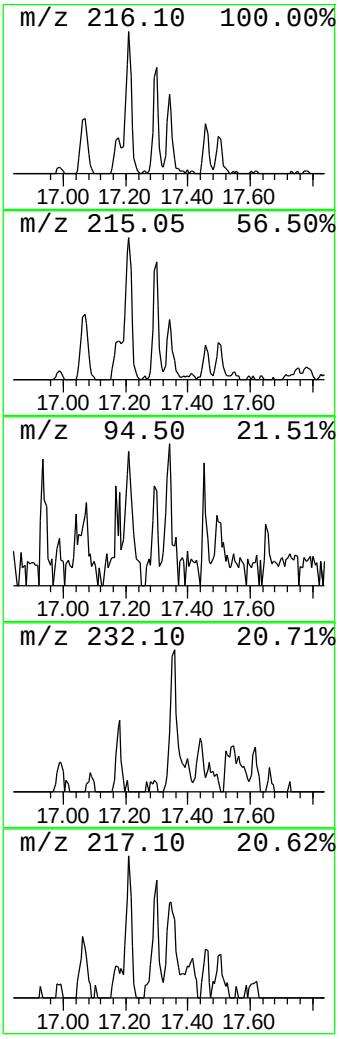
Peak Number 8 Pyrene, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.34	2.24 ng	81214	Chrysene-d12	18.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 2-methyl-	216	C17H12	003442-78-2	89
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	70
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	59
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	49
5	1,3-Dihydro-5,6-dimethyl-1-(2-pr...	216	C12H12N2S	080276-22-8	47





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061017\
Data File : BF095856.D
Acq On : 10 Jun 2017 19:39
Operator : SJ/MA
Sample : I3583-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-2669

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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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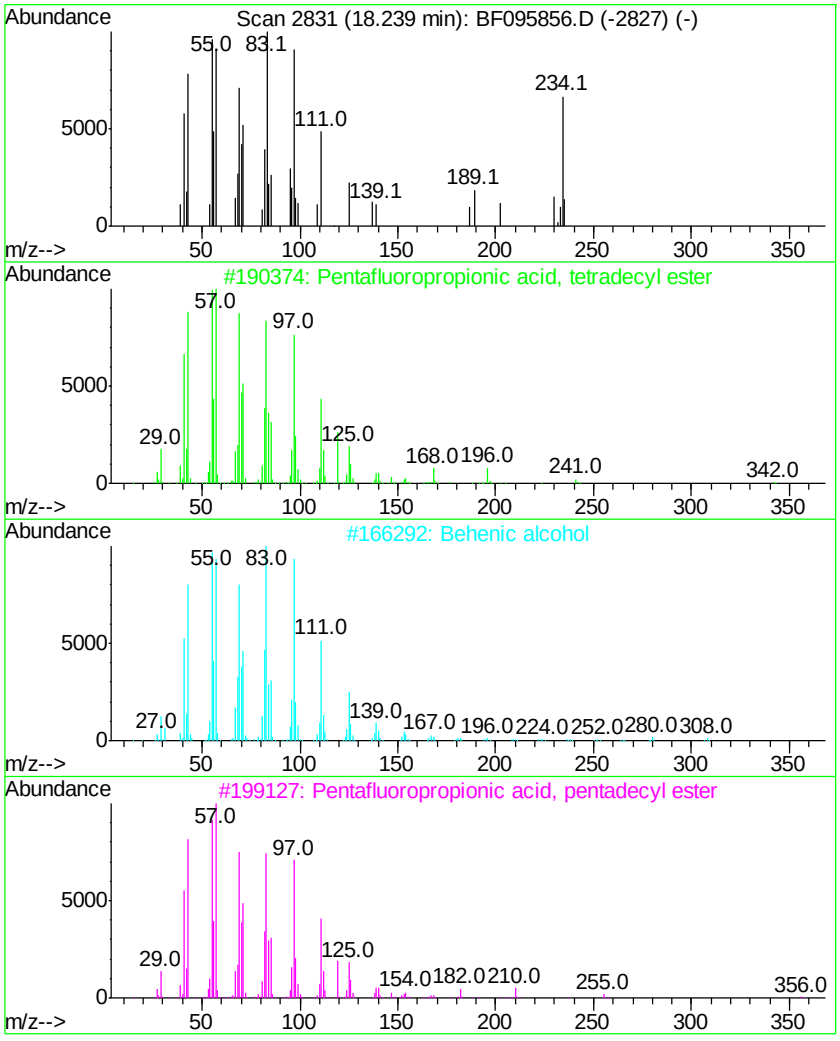
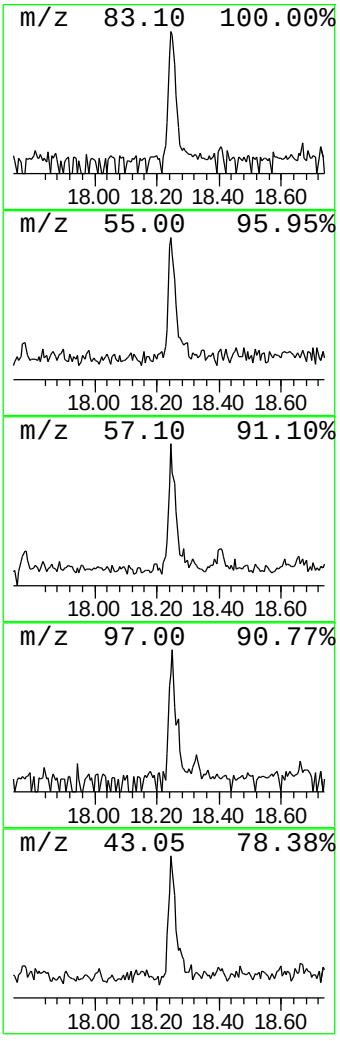
Peak Number 9 Pentafluoropropionic acid, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.24	2.29 ng	83043	Chrysene-d12	18.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	93
2	Behenic alcohol	326	C22H46O	000661-19-8	93
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	93





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061017\
Data File : BF095856.D
Acq On : 10 Jun 2017 19:39
Operator : SJ/MA
Sample : I3583-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-2669

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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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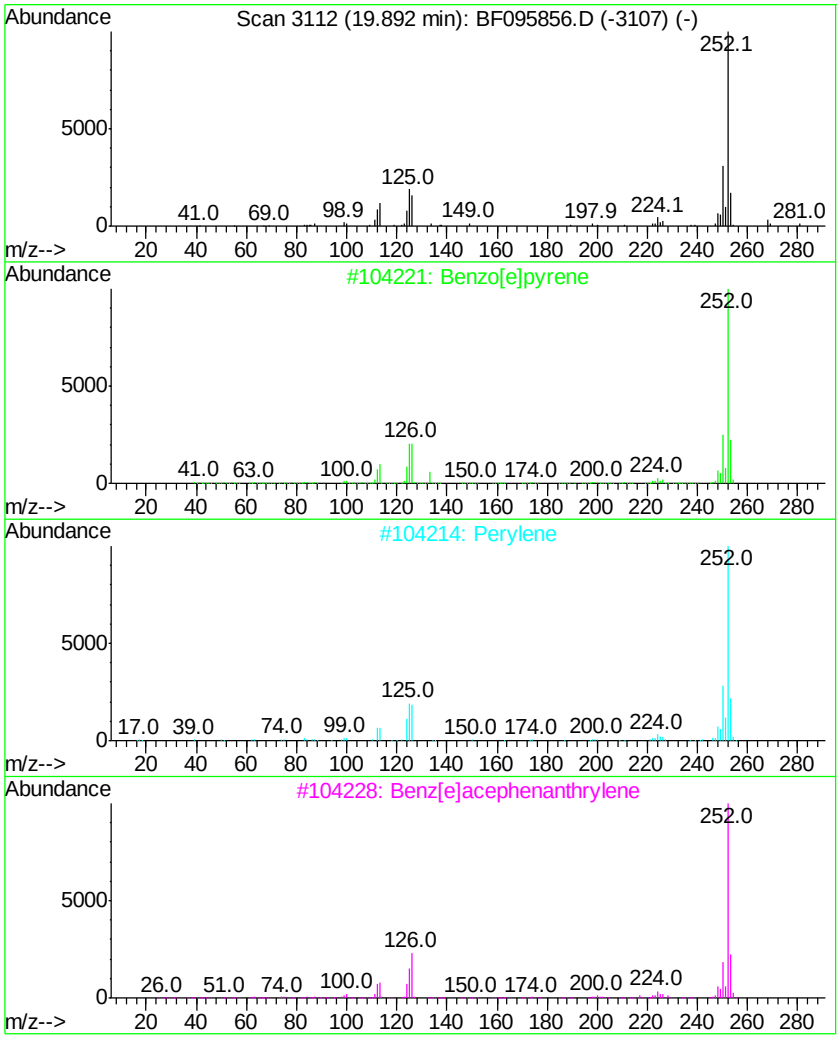
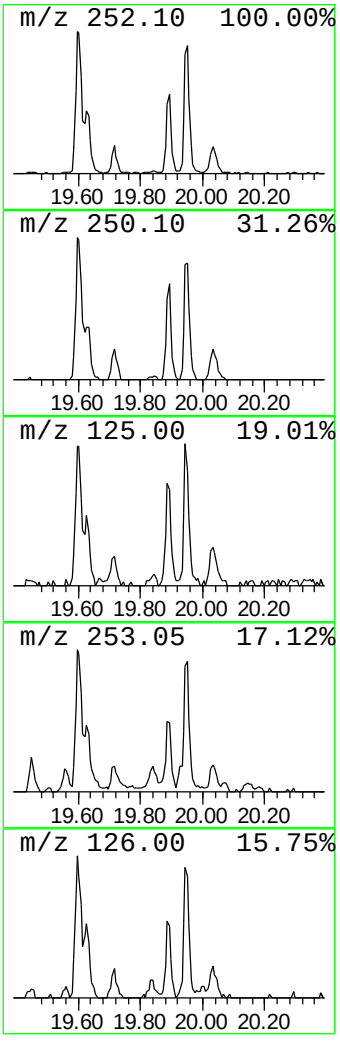
Peak Number 10 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.89	6.33 ng	119084	Perylene-d12	20.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	94
2	Perylene	252	C20H12	000198-55-0	93
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93
4	Benzo[a]pyrene	252	C20H12	000050-32-8	89
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	89





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061017\
Data File : BF095856.D
Acq On : 10 Jun 2017 19:39
Operator : SJ/MA
Sample : I3583-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-2669

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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...	4.57	6.2	ng	104851	1	7.37	341046	20.0
unknown7.02	7.02	80.9	ng	1379510	1	7.37	341046	20.0
Phenanthrene, 2-m...	15.47	2.4	ng	62920	4	14.62	533410	20.0
4H-Cyclopenta[def...	15.57	3.8	ng	100652	4	14.62	533410	20.0
Anthracene, 9-met...	15.62	2.1	ng	56171	4	14.62	533410	20.0
11H-Benzo[b]fluorene	17.21	2.5	ng	89617	5	18.33	723909	20.0
Pyrene, 2-methyl-	17.34	2.2	ng	81214	5	18.33	723909	20.0
Pentafluoropropio...	18.24	2.3	ng	83043	5	18.33	723909	20.0
Benzo[e]pyrene	19.89	6.3	ng	119084	6	20.00	376045	20.0