LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095533.D
Acq On : 30 May 2017 13:59
Operator : SJ/MA
Sample : I3281-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R1-TP7-D34

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-BF050217.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	5.101	534	538	553	rBV	83694	221688	9.40%	0.982%
2	5.707	637	641	677	rBV	649559	1937786	82.15%	8.588%
3	7.284	905	909	925	rBV	728145	1751646	74.26%	7.763%
4	7.401	925	929	951	rVB	1238544	2358701	100.00%	10.453%
5	7.737	982	986	996	rBV	403156	516172	21.88%	2.288%
6	7.972	1021	1026	1040	rBV	1256586	1651331	70.01%	7.318%
7	8.642	1136	1140	1165	rBV	514109	1203653	51.03%	5.334%
8	9.766	1326	1331	1352	rBV	348030	749727	31.79%	3.323%
9	11.530	1626	1631	1654	rBV	1362497	2310081	97.94%	10.238%
10	12.236	1746	1751	1769	rBV	225629	426298	18.07%	1.889%
11	12.595	1807	1812	1828	rBV2	519842	873514	37.03%	3.871%
12	13.419	1949	1952	1958	rVB	30689	35775	1.52%	0.159%
13	13.777	2007	2013	2019	rBV4	13515	25238	1.07%	0.112%
14	13.895	2028	2033	2058	rBV	638640	1341549	56.88%	5.945%
15	14.195	2079	2084	2087	rBV	29753	41446	1.76%	0.184%
16	15.001	2216	2221	2225	rVV	491261	746137	31.63%	3.307%
17	15.036	2225	2227	2241	rVV	124478	218028	9.24%	0.966%
18	15.142	2241	2245	2252	rVB2	16351	29599	1.25%	0.131%
19	15.583	2317	2320	2329	rBV4	19691	31915	1.35%	0.141%
20	15.789	2351	2355	2358	rBV	33964	38957	1.65%	0.173%
21	15.830	2358	2362	2368	rVB	56193	68982	2.92%	0.306%
22	15.948	2377	2382	2386	rBV4	74702	142290	6.03%	0.631%
23	16.224	2425	2429	2439	rVB2	23430	47721	2.02%	0.211%
24	16.307	2439	2443	2448	rBV4	12463	24279	1.03%	0.108%
25	16.477	2469	2472	2476	rVV	27946	30850	1.31%	0.137%
26	16.577	2485	2489	2492	rVV	61096	74871	3.17%	0.332%
27	16.624	2492	2497	2500	rVV4	26017	52406	2.22%	0.232%
28	16.654	2500	2502	2505	rVV	23341	23704	1.00%	0.105%
29	16.689	2505	2508	2511	rVV3	24971	36551	1.55%	0.162%
30	16.718	2511	2513	2517	rVV2	26886	34138	1.45%	0.151%
31	16.783	2520	2524	2537	rVV	244382	333636	14.14%	1.479%
32	16.924	2543	2548	2554	rVB2	24761	40183	1.70%	0.178%
33	17.036	2561	2567	2571	rBV9	25725	47859	2.03%	0.212%
34	17.083	2571	2575	2582	rVB	257278	325830	13.81%	1.444%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095533.D
Acq On : 30 May 2017 13:59
Operator : SJ/MA
Sample : I3281-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R1-TP7-D34

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-BF050217.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	17.277	2603	2608	2609	rBV3	24884	31778	1.35%	0.141%
36	17.312	2609	2614	2624	rVV	1520082	1795077	76.10%	7.955%
37	17.401	2624	2629	2641	rVV6	39409	102162	4.33%	0.453%
38	17.512	2644	2648	2651	rVV2	36159	61643	2.61%	0.273%
39	17.548	2651	2654	2659	rVB3	30049	45315	1.92%	0.201%
40	17.683	2673	2677	2683	rBV2	77876	119980	5.09%	0.532%
41	17.801	2694	2697	2700	rVV	31184	34900	1.48%	0.155%
42	17.842	2701	2704	2709	rVV4	16397	25961	1.10%	0.115%
43	17.877	2709	2710	2719	rVB6	12672	28146	1.19%	0.125%
44	18.242	2767	2772	2778	rVB	46305	67909	2.88%	0.301%
45	18.354	2786	2791	2793	rBV3	14161	25693	1.09%	0.114%
46	18.383	2793	2796	2799	rVB2	33660	35731	1.51%	0.158%
47	18.524	2817	2820	2821	rBV	26074	27358	1.16%	0.121%
48	18.553	2821	2825	2829	rVV2	33194	56338	2.39%	0.250%
49	18.671	2839	2845	2849	rBV2	465412	721630	30.59%	3.198%
50	18.801	2862	2867	2870	rVB7	18227	33477	1.42%	0.148%
51	18.906	2882	2885	2892	rBV7	17666	38442	1.63%	0.170%
52	18.959	2892	2894	2900	rVB6	21904	26510	1.12%	0.117%
53	19.183	2925	2932	2936	rVV	50509	90532	3.84%	0.401%
54	19.218	2936	2938	2942	rVB2	29791	32667	1.38%	0.145%
55	19.277	2942	2948	2955	rVB10	17811	43392	1.84%	0.192%
56	19.336	2955	2958	2961	rBV2	28132	34327	1.46%	0.152%
57	19.600	2995	3003	3004	rBV8	11958	23790	1.01%	0.105%
58	19.671	3011	3015	3018	rVV5	26647	38978	1.65%	0.173%
59	19.706	3018	3021	3025	rVB5	27145	33329	1.41%	0.148%
60	19.783	3030	3034	3036	rBV5	17113	23930	1.01%	0.106%
61	19.948	3058	3062	3065	rBV	105058	144895	6.14%	0.642%
62	20.059	3078	3081	3085	rVB2	36662	38585	1.64%	0.171%
63	20.236	3107	3111	3117	rBV	78382	109363	4.64%	0.485%
64	20.300	3118	3122	3126	rVV	92451	117535	4.98%	0.521%
65	20.347	3126	3130	3138	rVV	331480	494382	20.96%	2.191%
66	20.406	3138	3140	3146	rVB4	39560	62428	2.65%	0.277%
67	20.783	3201	3204	3208	rBV2	25381	37646	1.60%	0.167%
68	21.700	3353	3360	3367	rVB4	44782	97966	4.15%	0.434%
69	22.094	3421	3427	3435	rBV3	29697	69879	2.96%	0.310%

Sum of corrected areas: 22564215

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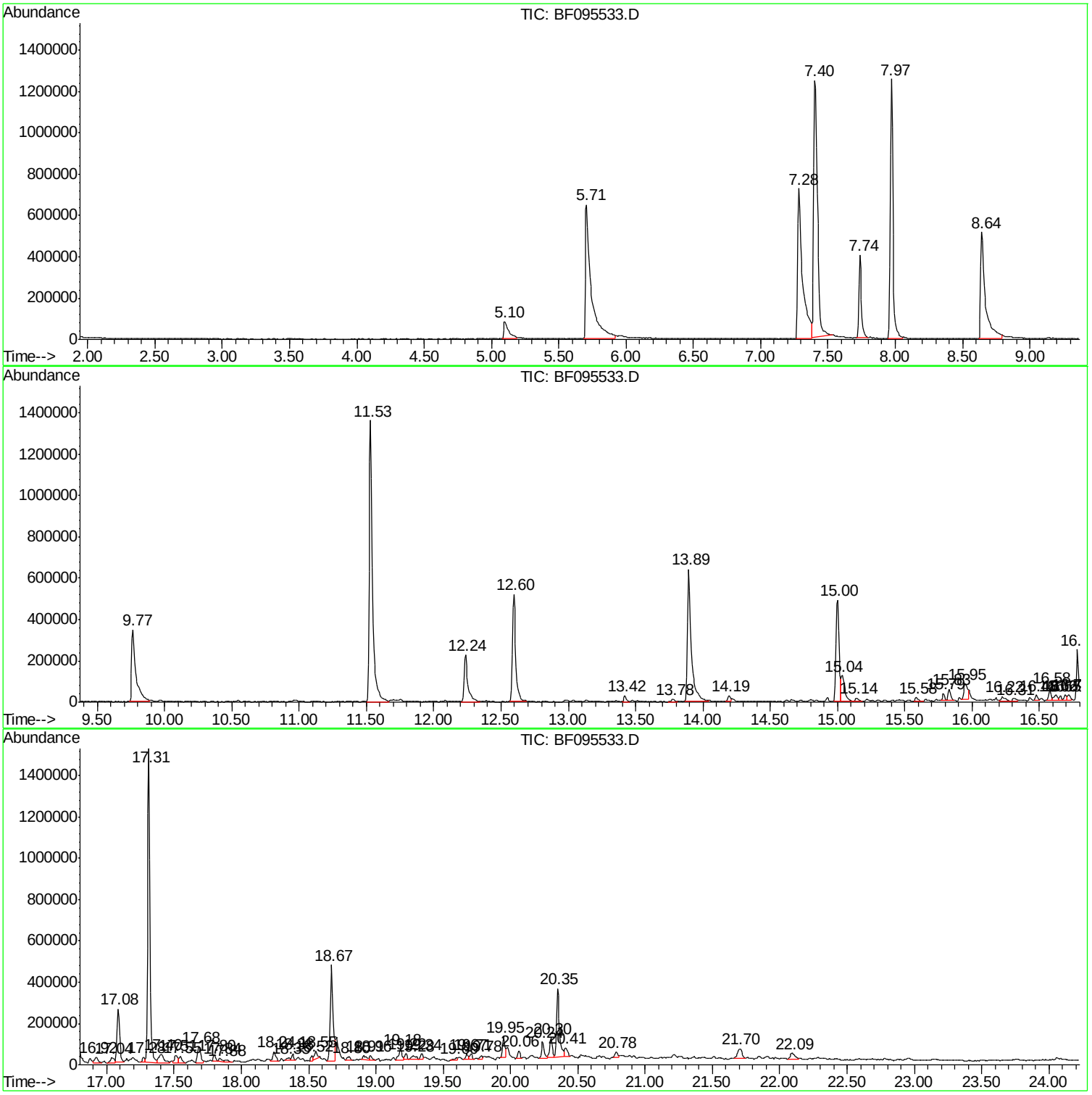
Acq On : 30 May 2017 13:59
Operator : SJ/MA
Sample : I3281-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
R1-TP7-D34

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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\BF053017\
Data File : BF095533.D
Acq On : 30 May 2017 13:59
Operator : SJ/MA
Sample : I3281-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R1-TP7-D34

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

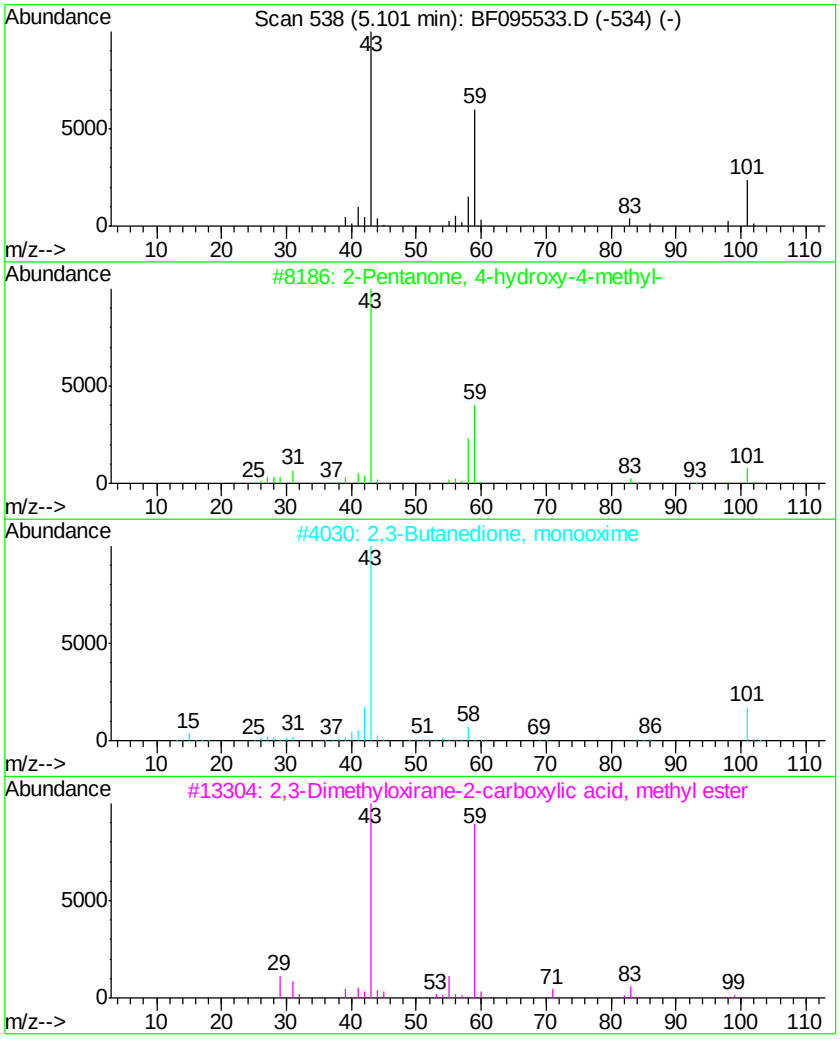
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

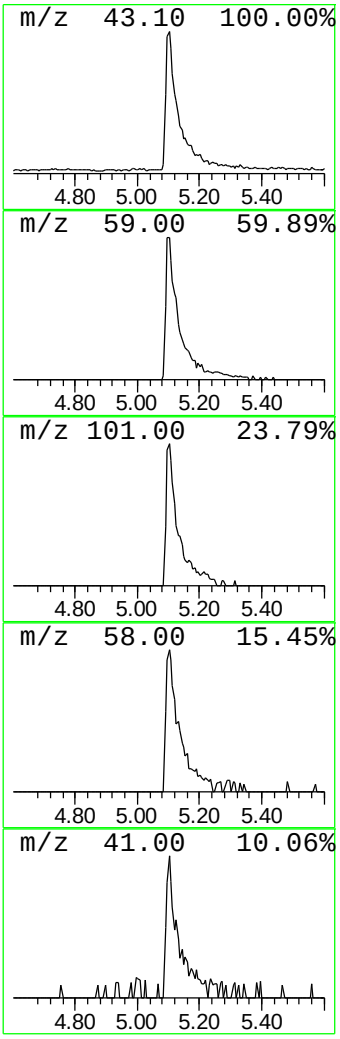
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	8.59 ng	221688	1,4-Dichlorobenzene-d4	7.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
3	2,3-Dimethyloxirane-2-carboxylic...	130	C6H10O3	1000306-64-4	28
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25
5	3-Hexanol	102	C6H14O	000623-37-0	25





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095533.D
Acq On : 30 May 2017 13:59
Operator : SJ/MA
Sample : I3281-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R1-TP7-D34

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

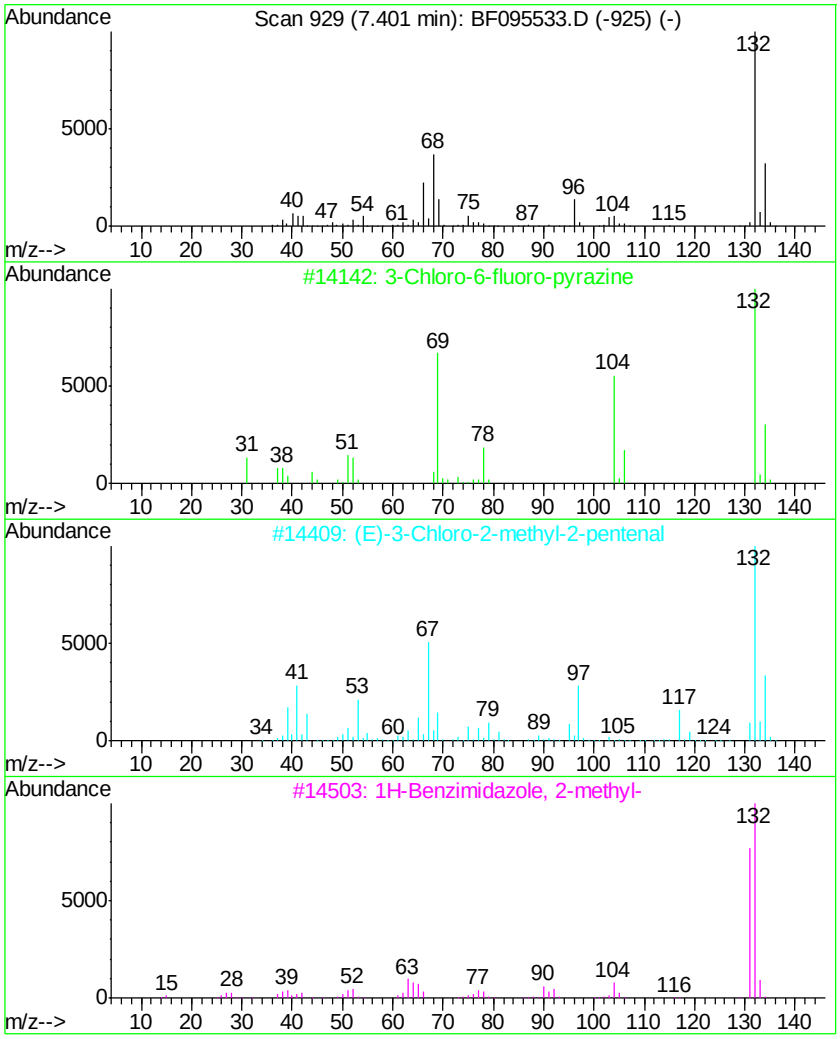
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

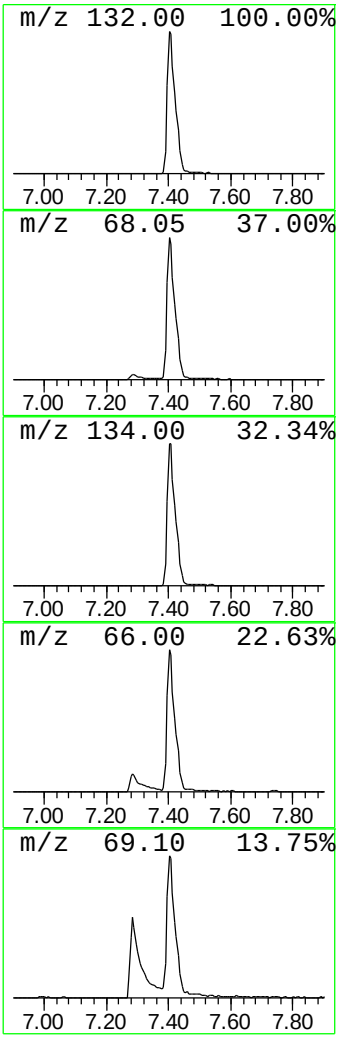
****

Peak Number 2 unknown7.40 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.40	91.39 ng	2358700	1,4-Dichlorobenzene-d4	7.74

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	17
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Operator : SJ/MA
Sample : I3281-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R1-TP7-D34

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

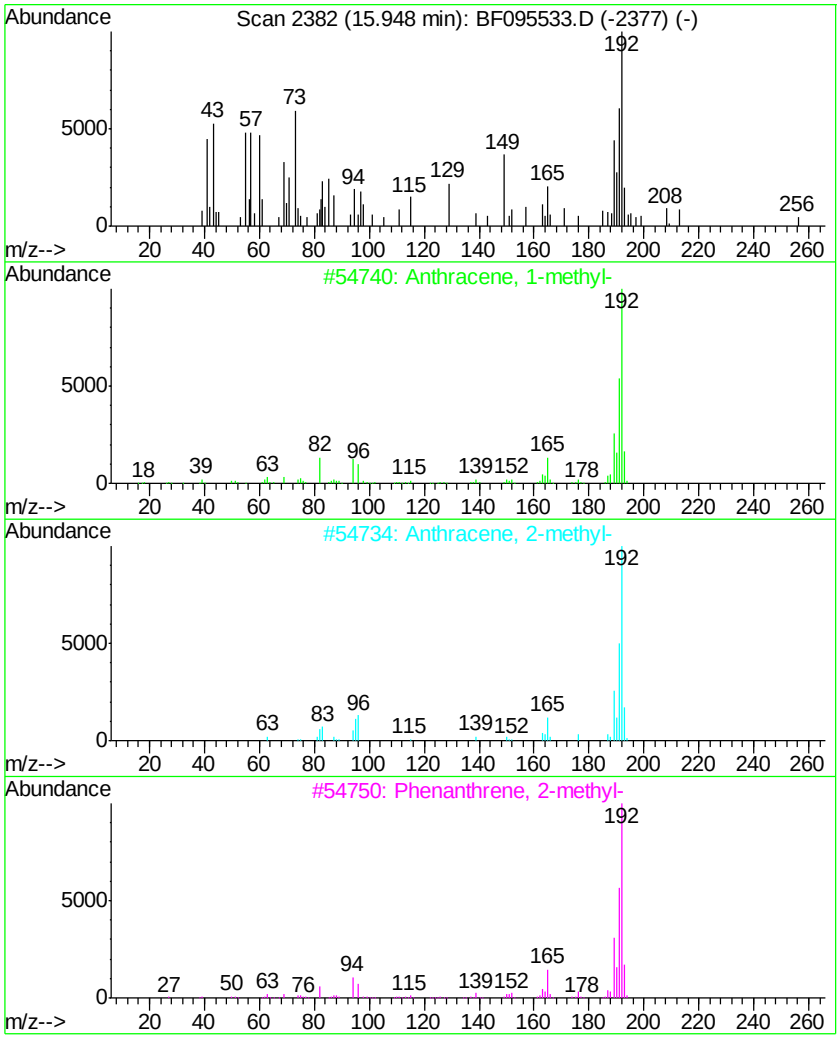
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

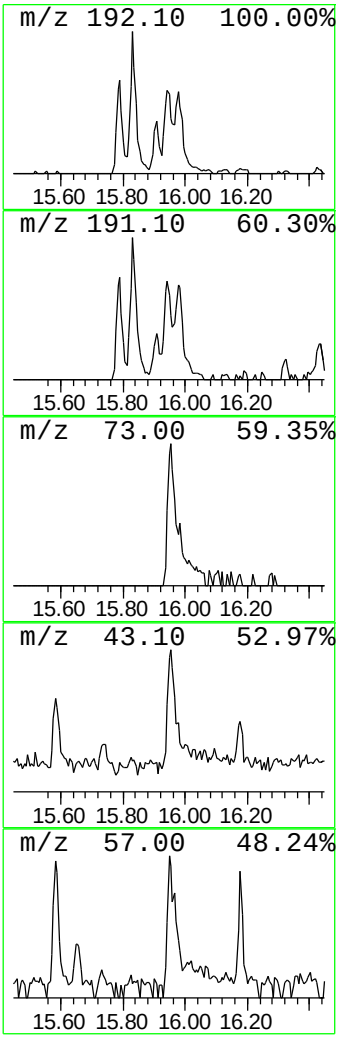
****

Peak Number 4 Anthracene, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.95	3.81 ng	142290	Phenanthrene-d10	15.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	64
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	53
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	50
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	50
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	50





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Acq On : 30 May 2017 13:59
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Sample : I3281-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R1-TP7-D34

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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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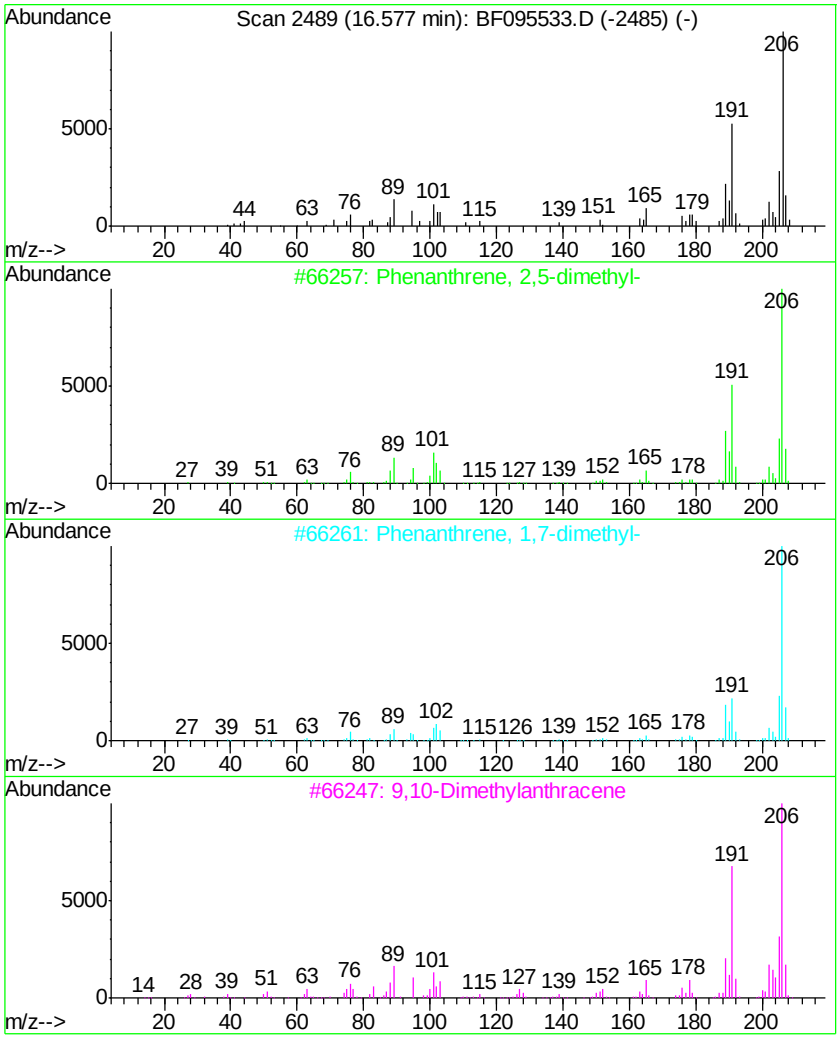
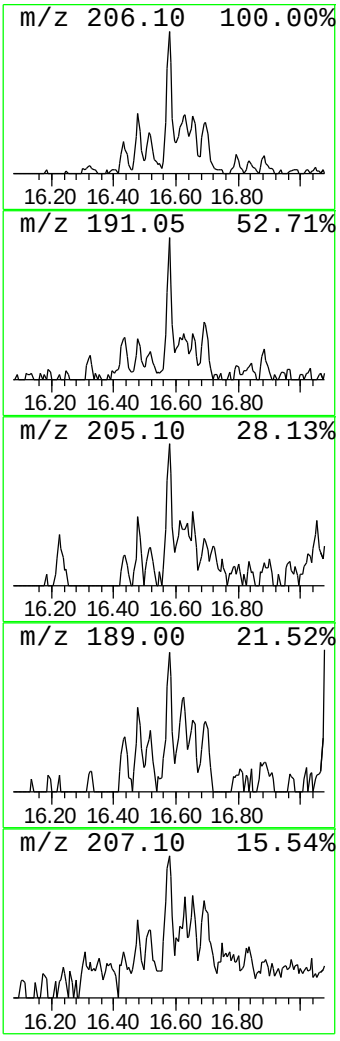
Peak Number 5 Phenanthrene, 2,5-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.58	2.01 ng	74871	Phenanthrene-d10	15.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	95
2	Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	94
3	9,10-Dimethylanthracene	206	C16H14	000781-43-1	93
4	di-p-Tolylacetylene	206	C16H14	002789-88-0	93
5	Anthracene, 1,4-dimethyl-	206	C16H14	000781-92-0	92





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
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Acq On : 30 May 2017 13:59
Operator : SJ/MA
Sample : I3281-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R1-TP7-D34

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

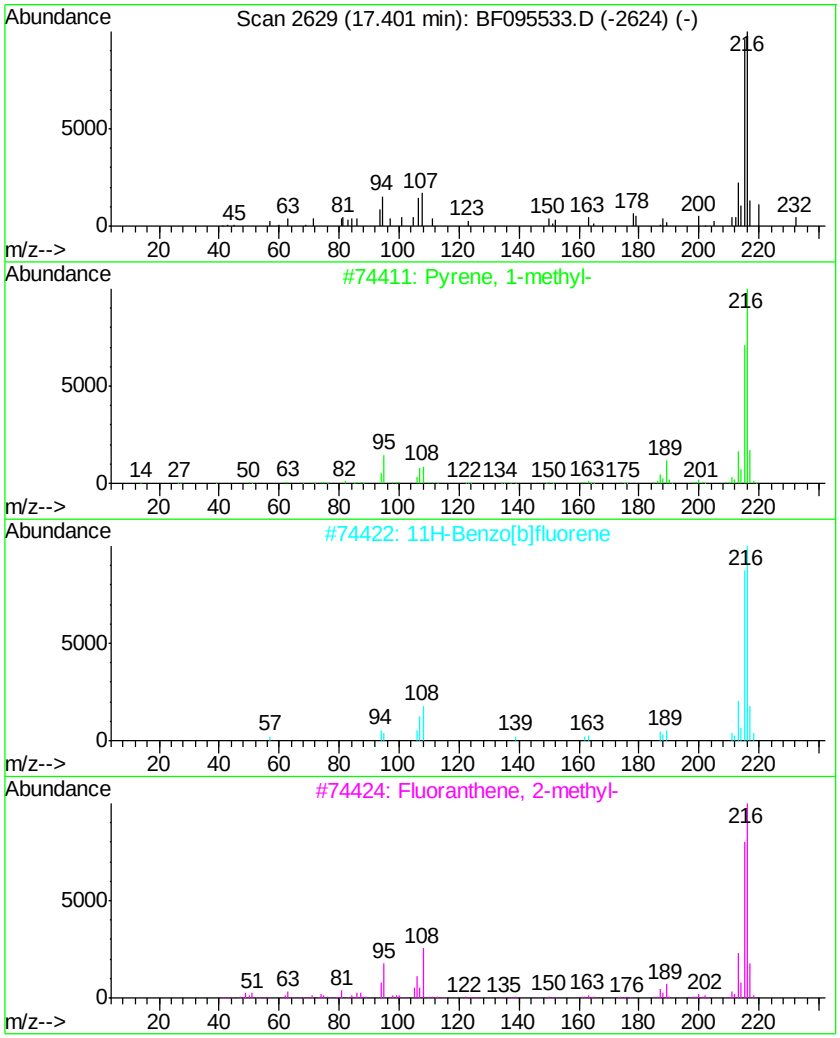
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

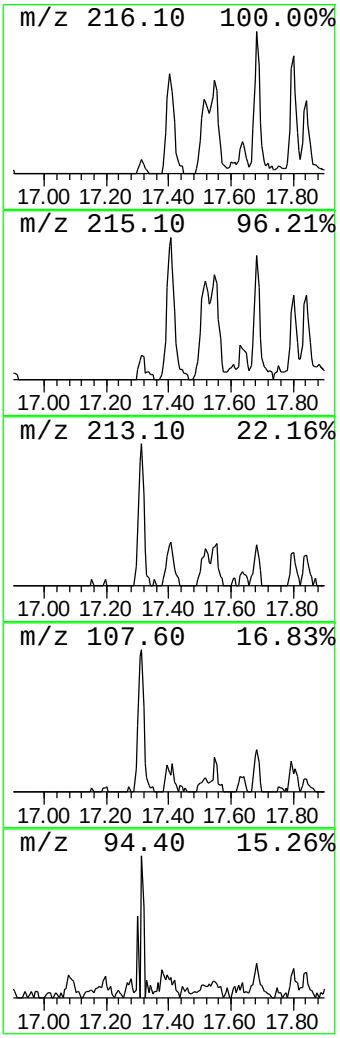
****

Peak Number 6 Pyrene, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.40	2.83 ng	102162	Chrysene-d12	18.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	87
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	74
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	68
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	64
5	trans-p-(Trifluoromethyl)cinnami...	216	C10H7F3O2	016642-92-5	59





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Data File : BF095533.D
Acq On : 30 May 2017 13:59
Operator : SJ/MA
Sample : I3281-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R1-TP7-D34

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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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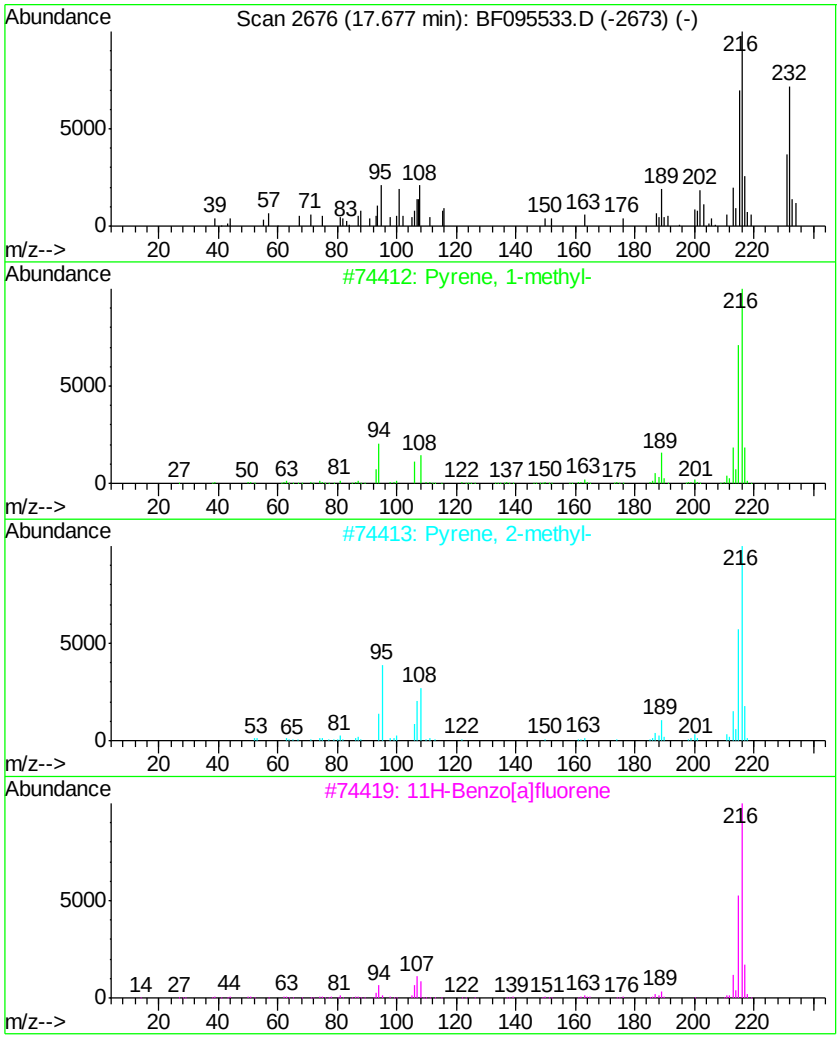
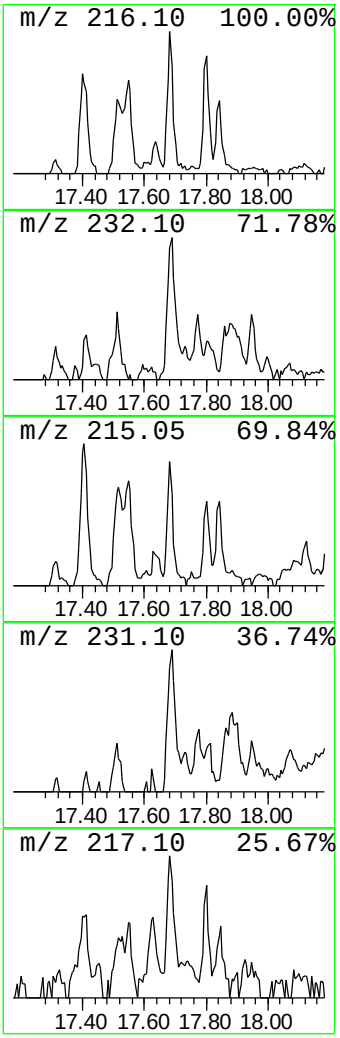
Peak Number 7 Pyrene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.68	3.33 ng	119980	Chrysene-d12	18.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	91
2	Pyrene, 2-methyl-	216	C17H12	003442-78-2	83
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	60
4	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	49
5	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	46





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095533.D
Acq On : 30 May 2017 13:59
Operator : SJ/MA
Sample : I3281-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R1-TP7-D34

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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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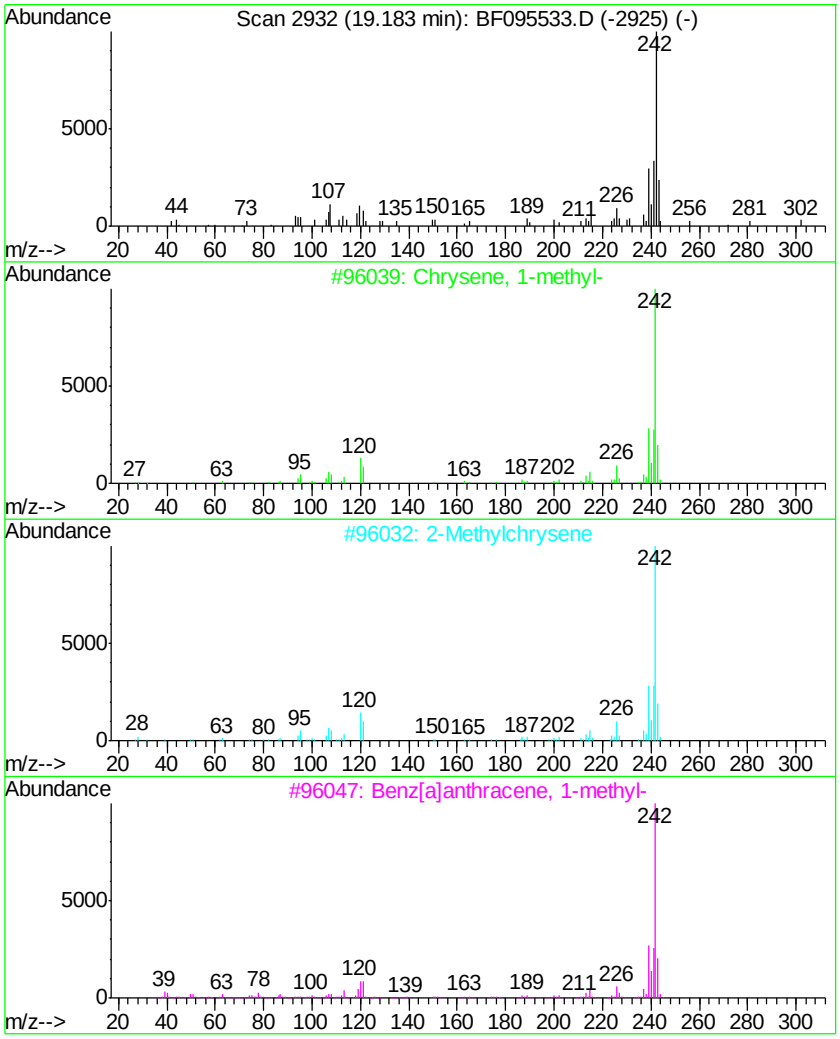
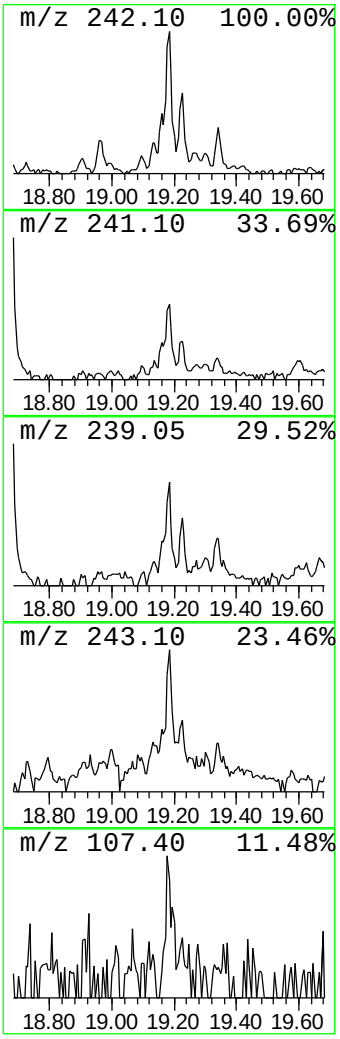
Peak Number 8 Chrysene, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.18	2.51 ng	90532	Chrysene-d12	18.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Chrysene, 1-methyl-	242	C19H14	003351-28-8	96
2	2-Methylchrysene	242	C19H14	003351-32-4	96
3	Benz[a]anthracene, 1-methyl-	242	C19H14	002498-77-3	93
4	Benz[a]anthracene, 8-methyl-	242	C19H14	002381-31-9	93
5	Chrysene, 3-methyl-	242	C19H14	003351-31-3	92





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Acq On : 30 May 2017 13:59
Operator : SJ/MA
Sample : I3281-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R1-TP7-D34

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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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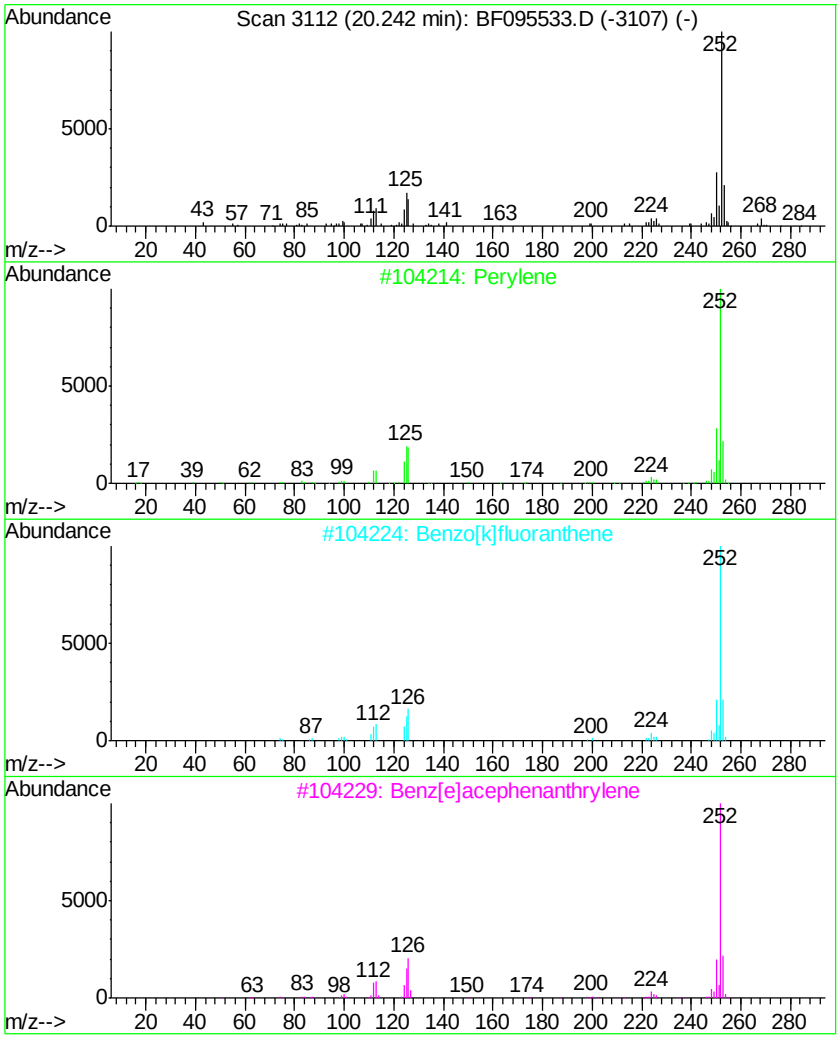
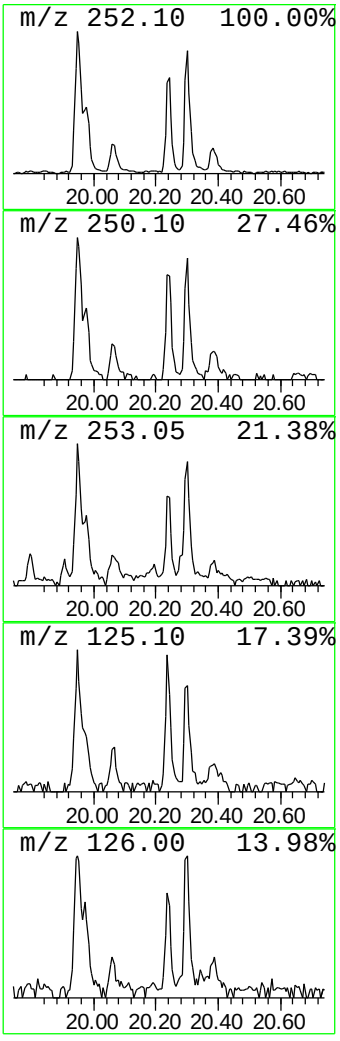
Peak Number 9 Perylene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.24	4.42 ng	109363	Perylene-d12	20.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	98
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95
4	Benzo[e]pyrene	252	C20H12	000192-97-2	95
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	93





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095533.D
Acq On : 30 May 2017 13:59
Operator : SJ/MA
Sample : I3281-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R1-TP7-D34

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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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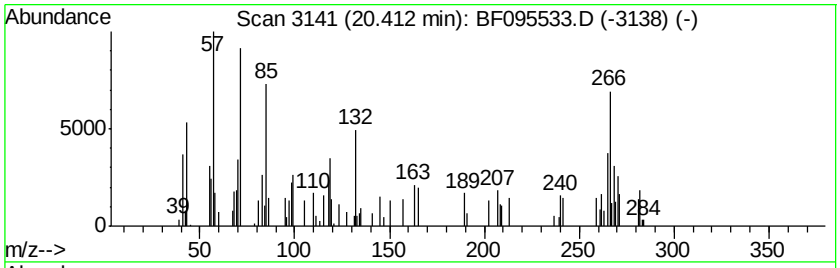
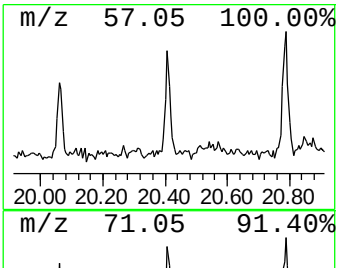
Peak Number 10 unknown20.41 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.41	2.53 ng	62428	Perylene-d12	20.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	42
2	Heptadecane	240	C17H36	000629-78-7	42
3	Hexacosane	366	C26H54	000630-01-3	30
4	Tetradecane	198	C14H30	000629-59-4	27
5	Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095533.D
Acq On : 30 May 2017 13:59
Operator : SJ/MA
Sample : I3281-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : R1-TP7-D34

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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...	5.10	8.6	ng	221688	1	7.74	516172	20.0
unknown7.40	7.40	91.4	ng	2358700	1	7.74	516172	20.0
Anthracene, 1-met...	15.95	3.8	ng	142290	4	15.00	746137	20.0
Phenanthrene, 2,5...	16.58	2.0	ng	74871	4	15.00	746137	20.0
Pyrene, 1-methyl-	17.40	2.8	ng	102162	5	18.67	721630	20.0
Pyrene, 2-methyl-	17.68	3.3	ng	119980	5	18.67	721630	20.0
Chrysene, 1-methyl-	19.18	2.5	ng	90532	5	18.67	721630	20.0
Perylene	20.24	4.4	ng	109363	6	20.35	494382	20.0
unknown20.41	20.41	2.5	ng	62428	6	20.35	494382	20.0