LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060517\
Data File : BF095693.D
Acq On : 6 Jun 2017 1:54
Operator : SJ/MA
Sample : I3466-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-RO-6704-060217

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	1.601	8	11	29	rBV	343060	605101	28.46%	2.955%
2	4.613	520	523	544	rBV	63345	176312	8.29%	0.861%
3	5.295	635	639	667	rBV	1207433	2069892	97.35%	10.109%
4	6.954	917	921	933	rBV	1227089	1858729	87.42%	9.077%
5	7.054	933	938	952	rVB	1573422	2126301	100.00%	10.384%
6	7.395	992	996	1010	rBV	374688	494259	23.25%	2.414%
7	7.636	1032	1037	1054	rBV	1157033	1467062	69.00%	7.165%
8	8.313	1147	1152	1169	rBV	858455	1146961	53.94%	5.601%
9	9.424	1337	1341	1356	rBV	505693	680964	32.03%	3.326%
10	11.207	1638	1644	1657	rVB	1541494	1964240	92.38%	9.593%
11	11.901	1757	1762	1769	rBV	287269	351922	16.55%	1.719%
12	12.248	1816	1821	1826	rBV2	542097	679907	31.98%	3.320%
13	12.301	1826	1830	1837	rVB2	39810	55545	2.61%	0.271%
14	13.107	1963	1967	1970	rBV3	29391	35568	1.67%	0.174%
15	13.148	1970	1974	1985	rVB	33513	49693	2.34%	0.243%
16	13.542	2036	2041	2050	rBV	770397	992543	46.68%	4.847%
17	13.877	2094	2098	2106	rBV	37051	70058	3.29%	0.342%
18	14.612	2218	2223	2224	rBV	25919	31465	1.48%	0.154%
19	14.642	2224	2228	2231	rVV	465840	568987	26.76%	2.779%
20	14.677	2231	2234	2243	rVV	143772	199960	9.40%	0.977%
21	14.771	2247	2250	2257	rVB	42533	54109	2.54%	0.264%
22	15.289	2335	2338	2342	rBV2	16224	23806	1.12%	0.116%
23	15.442	2360	2364	2368	rBV2	67397	79386	3.73%	0.388%
24	15.489	2368	2372	2378	rVB2	44799	52673	2.48%	0.257%
25	15.559	2378	2384	2387	rBV	17839	22778	1.07%	0.111%
26	15.601	2387	2391	2395	rVV2	52688	74345	3.50%	0.363%
27	15.659	2395	2401	2412	rVB3	103332	157430	7.40%	0.769%
28	15.895	2437	2441	2447	rBV2	27682	41015	1.93%	0.200%
29	16.253	2497	2502	2506	rBV	47914	57015	2.68%	0.278%
30	16.295	2506	2509	2513	rVV5	22331	33416	1.57%	0.163%
31	16.377	2519	2523	2526	rBV3	24230	30199	1.42%	0.147%
32	16.412	2526	2529	2532	rVV	93980	100910	4.75%	0.493%
33	16.453	2532	2536	2542	rVB	251776	328729	15.46%	1.605%
34	16.759	2583	2588	2593	rBV	279020	330387	15.54%	1.613%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060517\
Data File : BF095693.D
Acq On : 6 Jun 2017 1:54
Operator : SJ/MA
Sample : I3466-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-RO-6704-060217

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	16.883	2606	2609	2613	rVB4	18624	24410	1.15%	0.119%
36	17.012	2624	2631	2637	rVB	1159940	1314251	61.81%	6.418%
37	17.089	2637	2644	2647	rBV3	23529	40276	1.89%	0.197%
38	17.206	2658	2664	2665	rBV5	21799	37894	1.78%	0.185%
39	17.224	2665	2667	2674	rVB2	40233	55009	2.59%	0.269%
40	17.318	2674	2683	2686	rBV2	38948	62709	2.95%	0.306%
41	17.359	2686	2690	2696	rBV2	42853	76661	3.61%	0.374%
42	17.477	2705	2710	2713	rBV2	34790	45535	2.14%	0.222%
43	17.512	2713	2716	2719	rVV	22034	22370	1.05%	0.109%
44	17.865	2773	2776	2782	rBV7	17667	33498	1.58%	0.164%
45	18.030	2798	2804	2807	rBV2	33784	56321	2.65%	0.275%
46	18.059	2807	2809	2812	rVB2	23969	23852	1.12%	0.116%
47	18.265	2839	2844	2853	rBV2	112727	225215	10.59%	1.100%
48	18.353	2853	2859	2862	rVV2	502809	665058	31.28%	3.248%
49	18.389	2862	2865	2871	rVB	87007	125567	5.91%	0.613%
50	18.477	2877	2880	2884	rVB4	25873	33142	1.56%	0.162%
51	19.624	3072	3075	3077	rBV	73722	92147	4.33%	0.450%
52	19.971	3131	3134	3138	rVB	72304	80187	3.77%	0.392%
53	20.018	3139	3142	3153	rVV2	320454	450896	21.21%	2.202%

Sum of corrected areas: 20476665

LSC Report - Integrated Chromatogram

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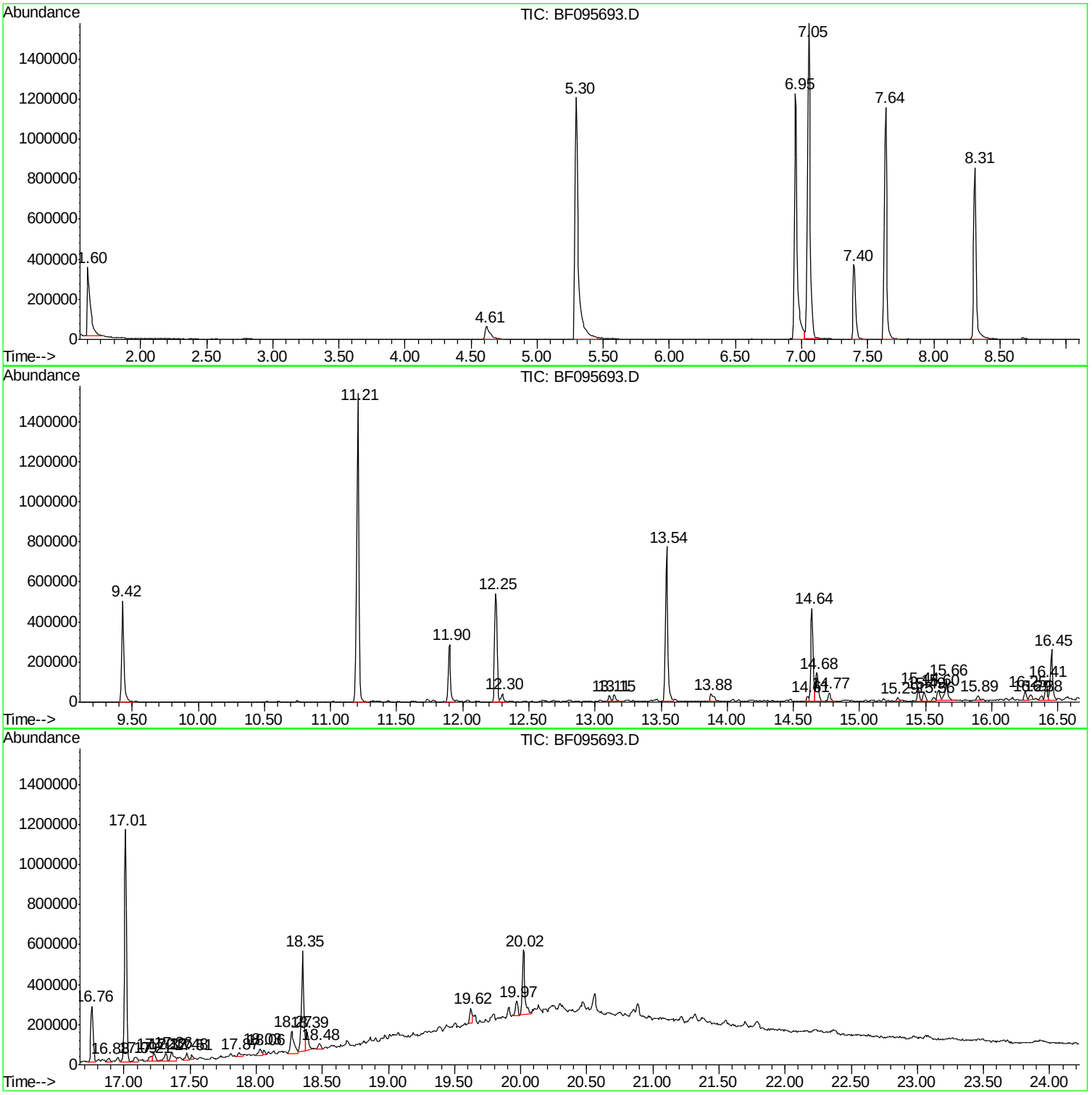
Data File : BF095693.D
Acq On : 6 Jun 2017 1:54
Operator : SJ/MA
Sample : I3466-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-RO-6704-060217

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\BF060517\
Data File : BF095693.D
Acq On : 6 Jun 2017 1:54
Operator : SJ/MA
Sample : I3466-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-RO-6704-060217

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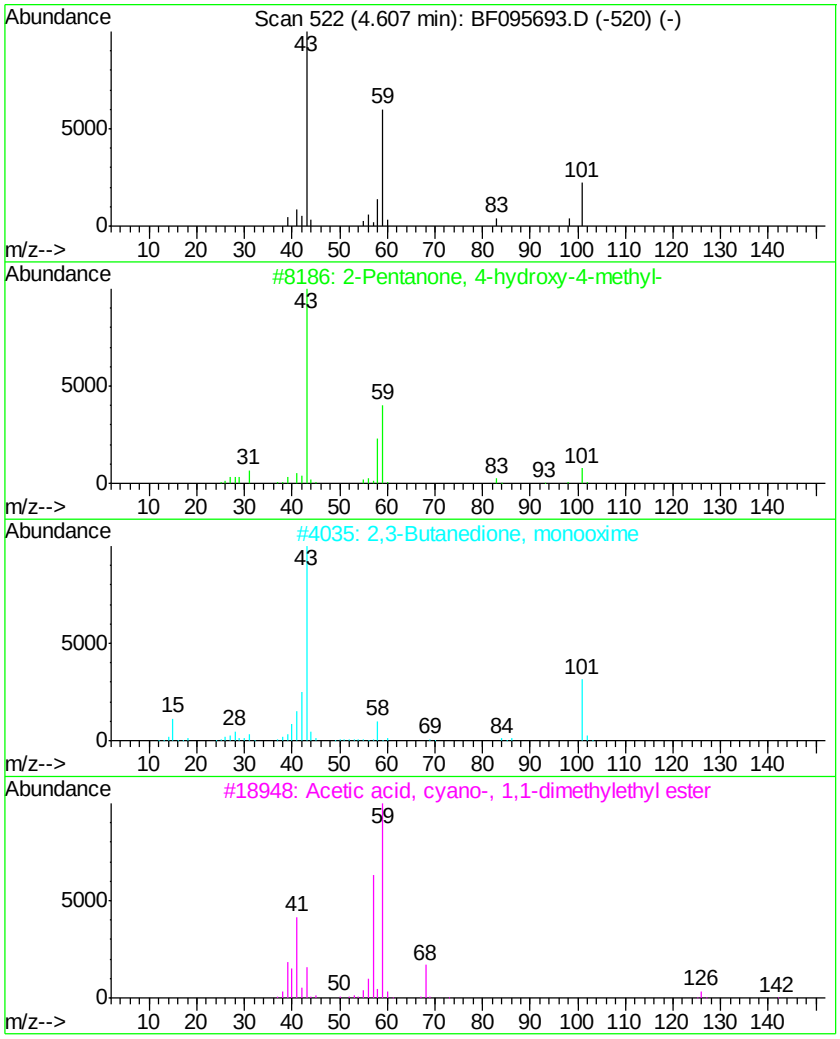
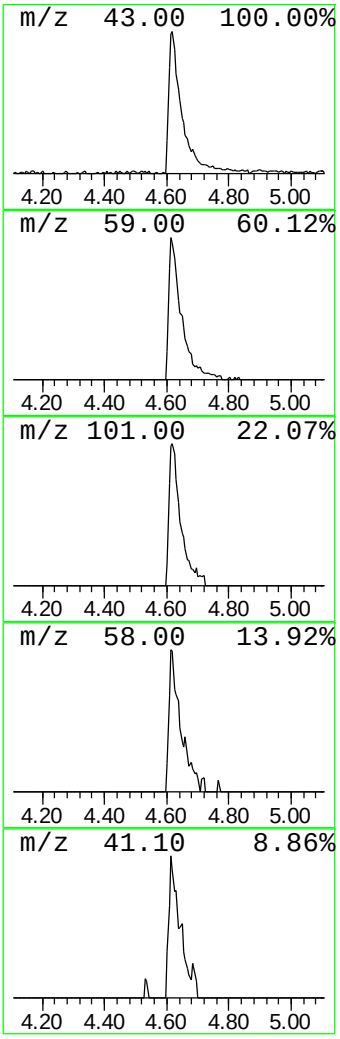
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.61	7.13 ng	176312	1,4-Dichlorobenzene-d4	7.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060517\
Data File : BF095693.D
Acq On : 6 Jun 2017 1:54
Operator : SJ/MA
Sample : I3466-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-RO-6704-060217

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

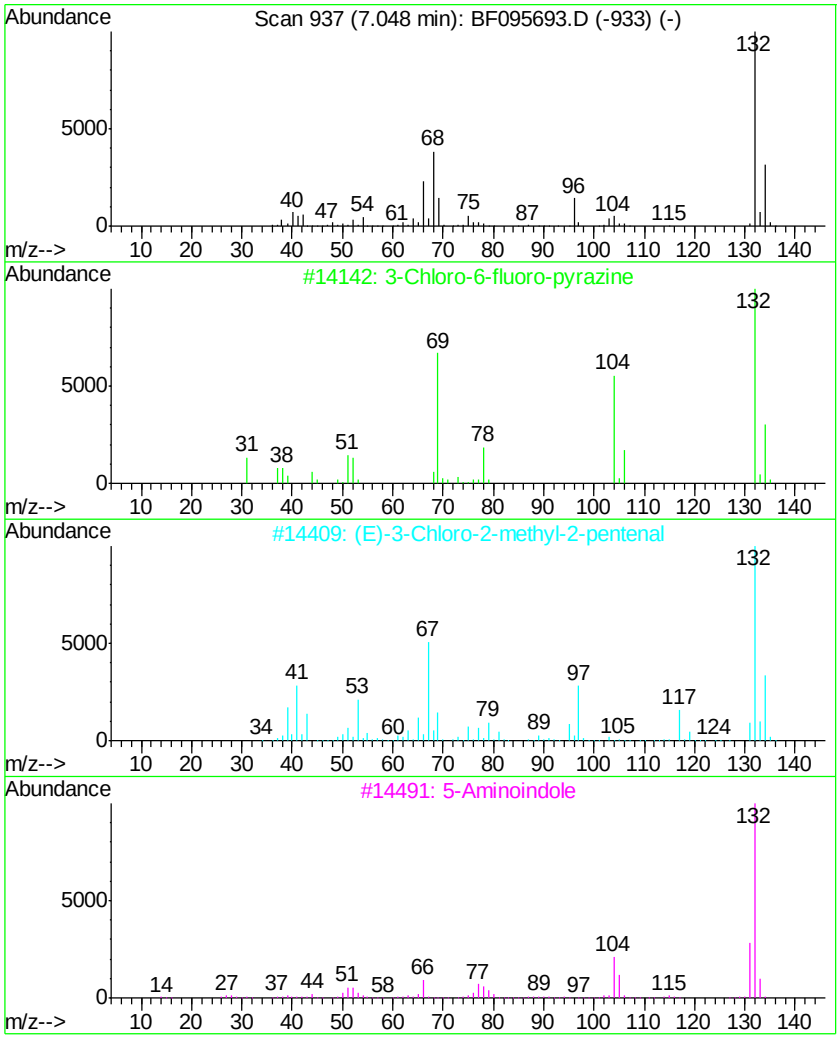
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

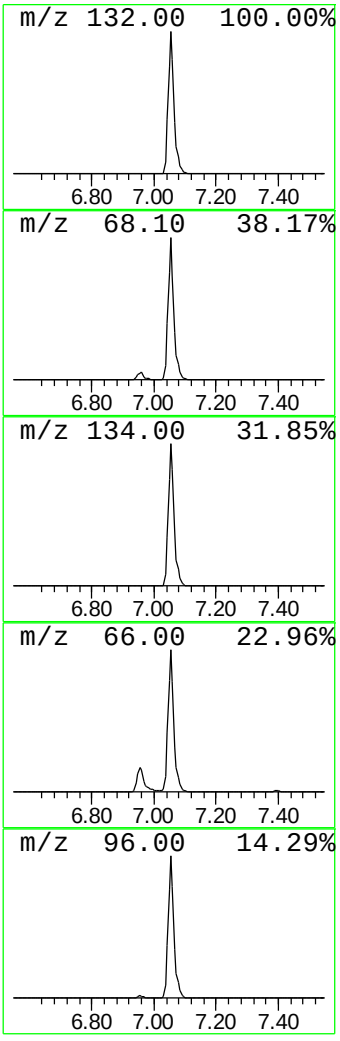
****

Peak Number 3 unknown7.05 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.05	86.04 ng	2126300	1,4-Dichlorobenzene-d4	7.40

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	25
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060517\
Data File : BF095693.D
Acq On : 6 Jun 2017 1:54
Operator : SJ/MA
Sample : I3466-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-RO-6704-060217

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

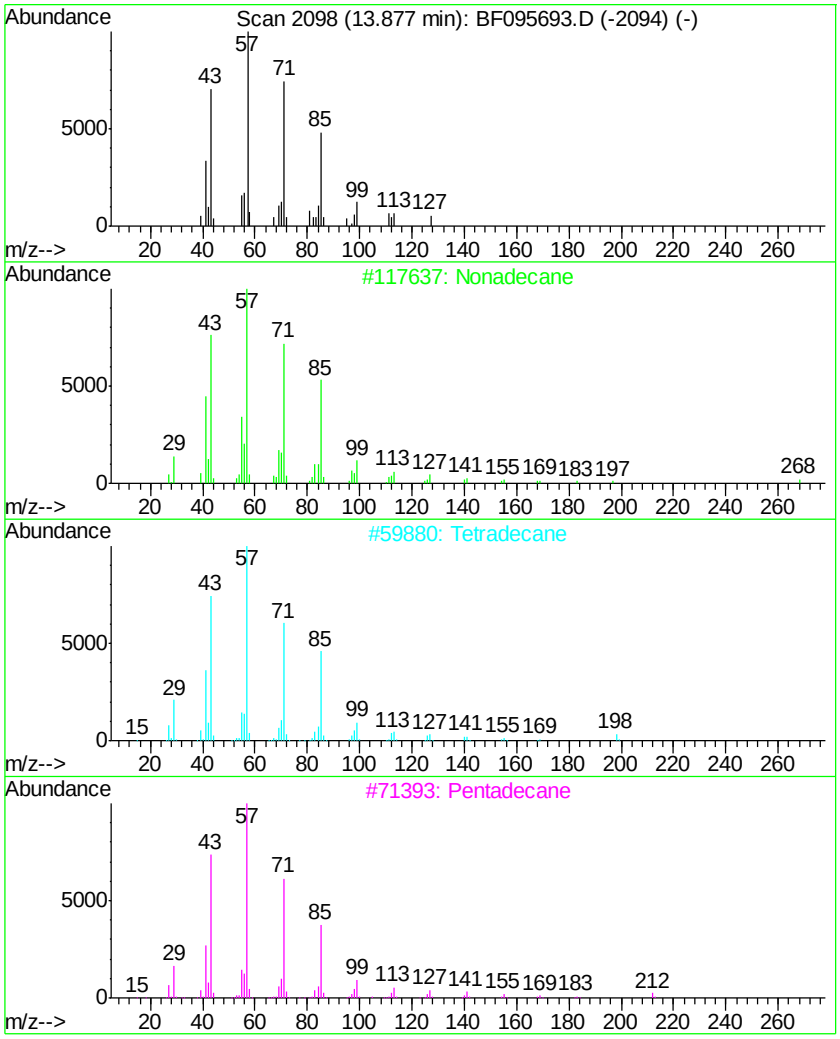
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

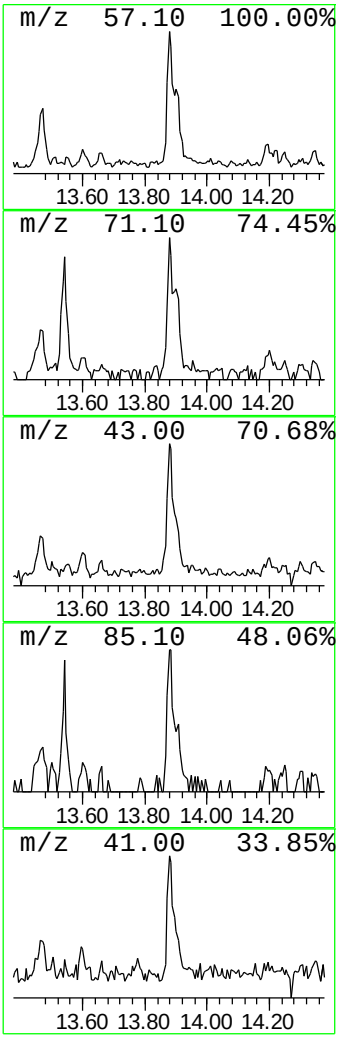
****

Peak Number 5 Nonadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	2.46 ng	70058	Phenanthrene-d10	14.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	91
2	Tetradecane	198	C14H30	000629-59-4	90
3	Pentadecane	212	C15H32	000629-62-9	90
4	Hexadecane	226	C16H34	000544-76-3	83
5	Tridecane	184	C13H28	000629-50-5	83





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060517\
Data File : BF095693.D
Acq On : 6 Jun 2017 1:54
Operator : SJ/MA
Sample : I3466-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-RO-6704-060217

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

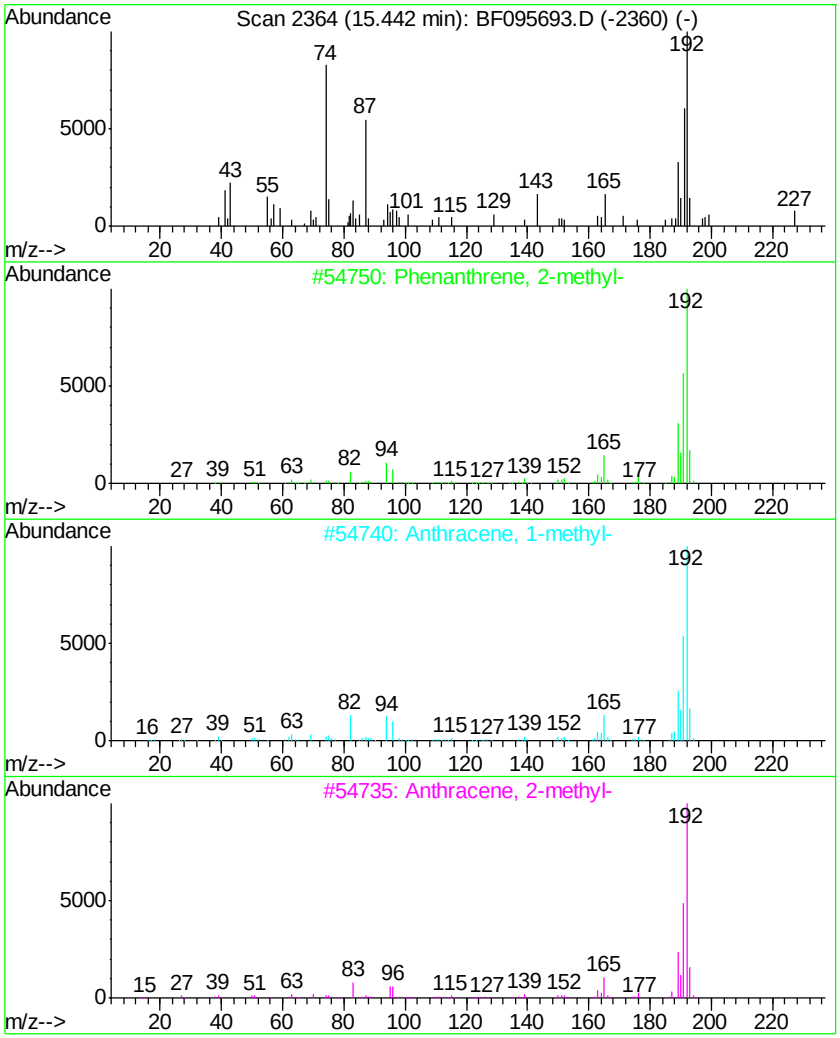
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

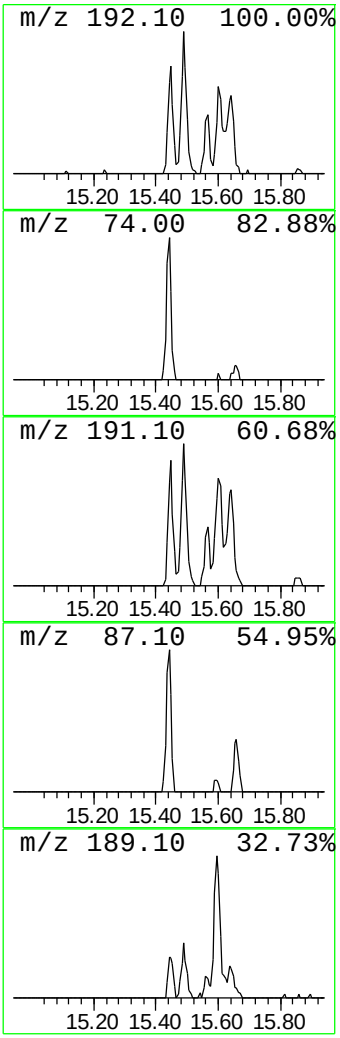
****

Peak Number 6 Phenanthrene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.44	2.79 ng	79386	Phenanthrene-d10	14.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	90
2	Anthracene, 1-methyl-	192	C15H12	000610-48-0	89
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	87
4	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	86
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	86





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Acq On : 6 Jun 2017 1:54
Operator : SJ/MA
Sample : I3466-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-RO-6704-060217

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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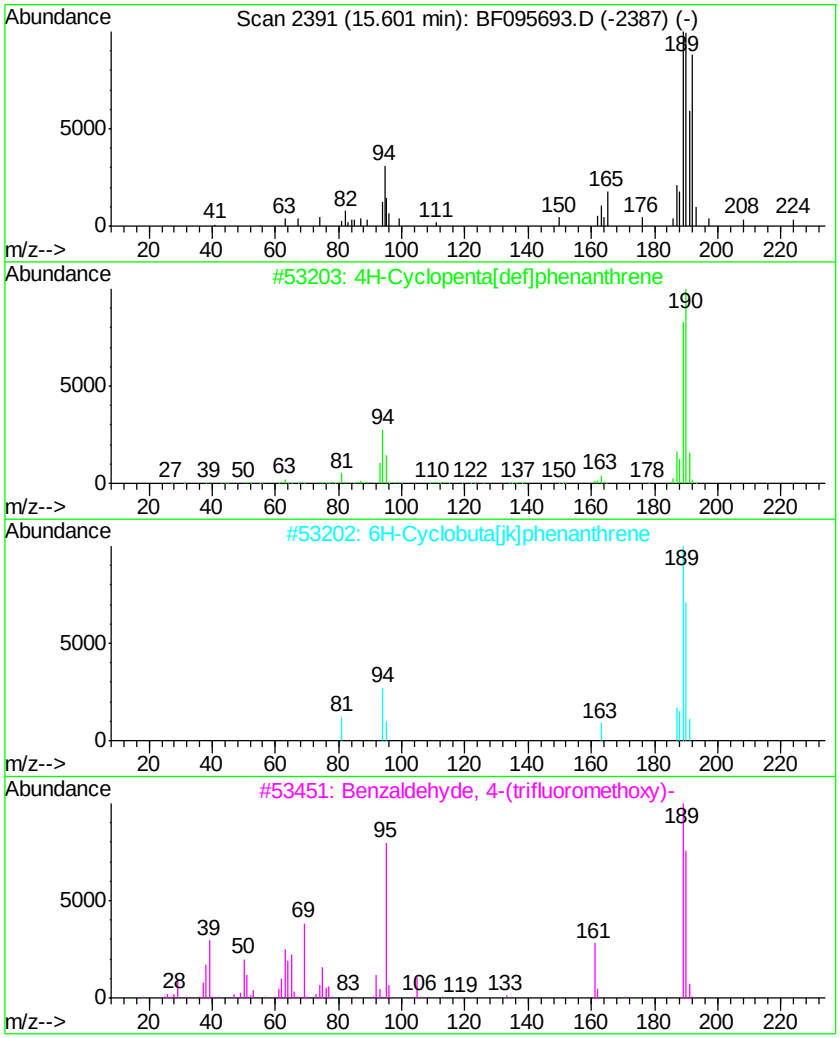
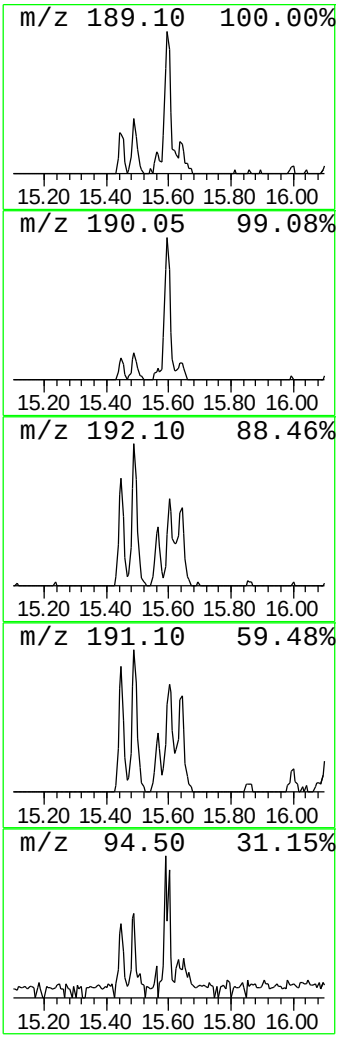
Peak Number 7 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.60	2.61 ng	74345	Phenanthrene-d10	14.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	49
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	49
3	Benzaldehyde, 4-(trifluoromethoxy)-	190	C8H5F3O2	000659-28-9	38
4	3-Bromo-2-furoic acid	190	C5H3BrO3	014903-90-3	35
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	30





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Operator : SJ/MA
Sample : I3466-05
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ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-RO-6704-060217

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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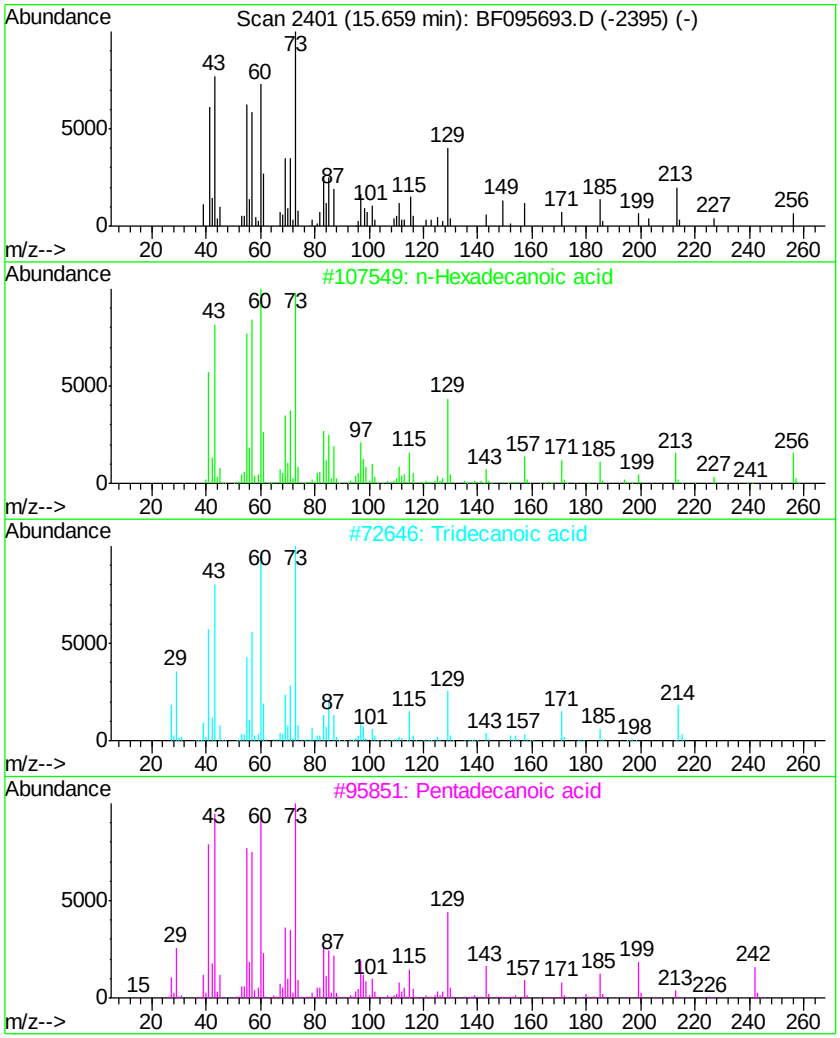
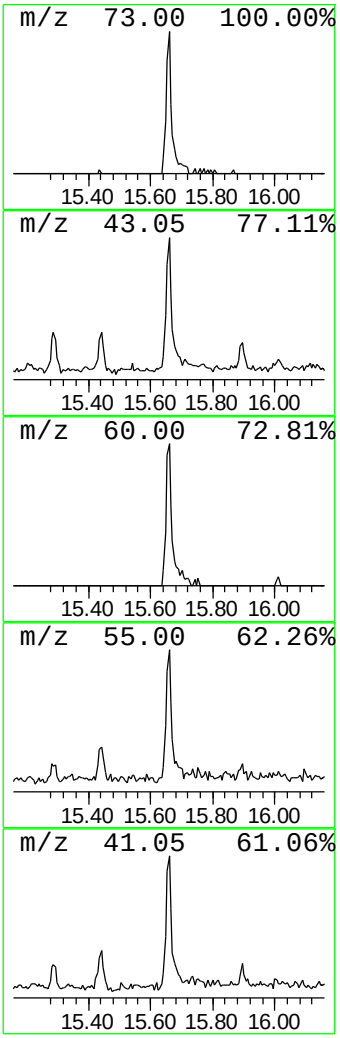
Peak Number 8 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.66	5.53 ng	157430	Phenanthrene-d10	14.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Tridecanoic acid	214	C13H26O2	000638-53-9	86
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5	Dodecanoic acid	200	C12H24O2	000143-07-7	50





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Acq On : 6 Jun 2017 1:54
Operator : SJ/MA
Sample : I3466-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-RO-6704-060217

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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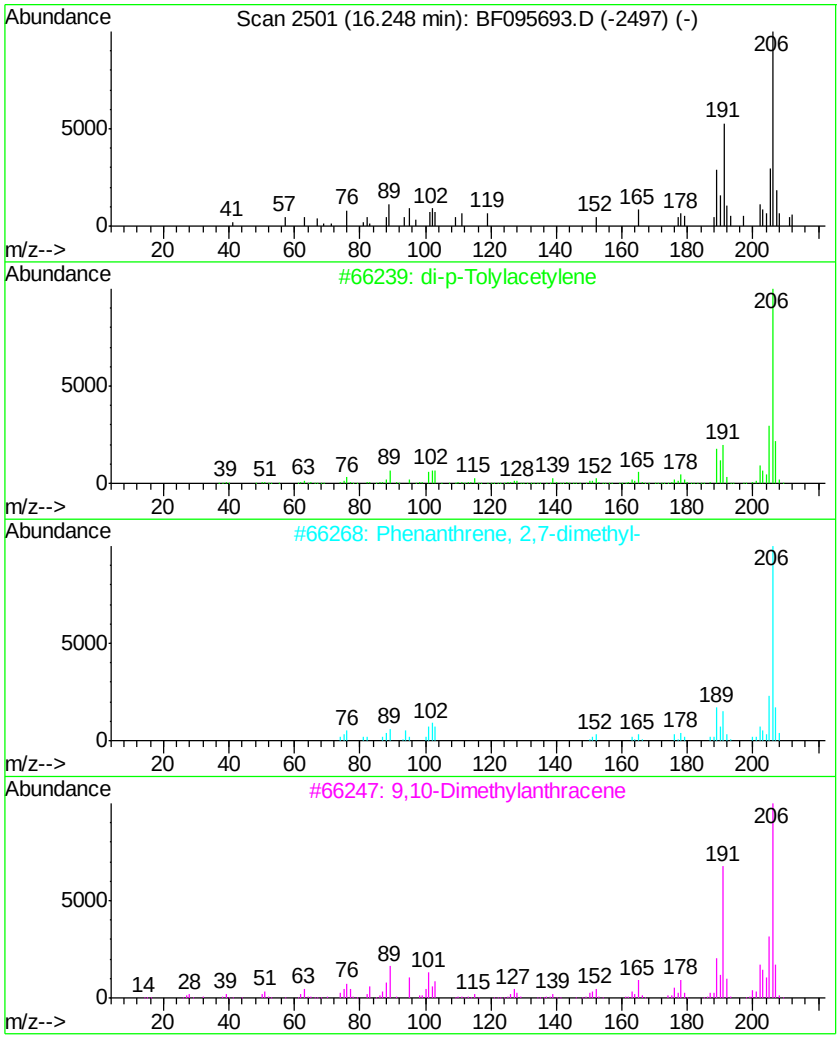
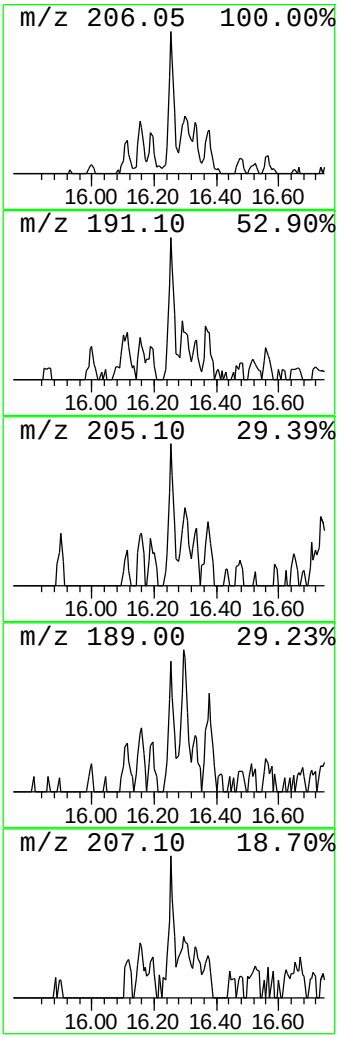
Peak Number 9 di-p-Tolylacetylene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.25	2.00 ng	57015	Phenanthrene-d10	14.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	di-p-Tolylacetylene	206	C16H14	002789-88-0	93
2	Phenanthrene, 2,7-dimethyl-	206	C16H14	001576-69-8	92
3	9,10-Dimethylanthracene	206	C16H14	000781-43-1	91
4	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	90
5	Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	89





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060517\
Data File : BF095693.D
Acq On : 6 Jun 2017 1:54
Operator : SJ/MA
Sample : I3466-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-RO-6704-060217

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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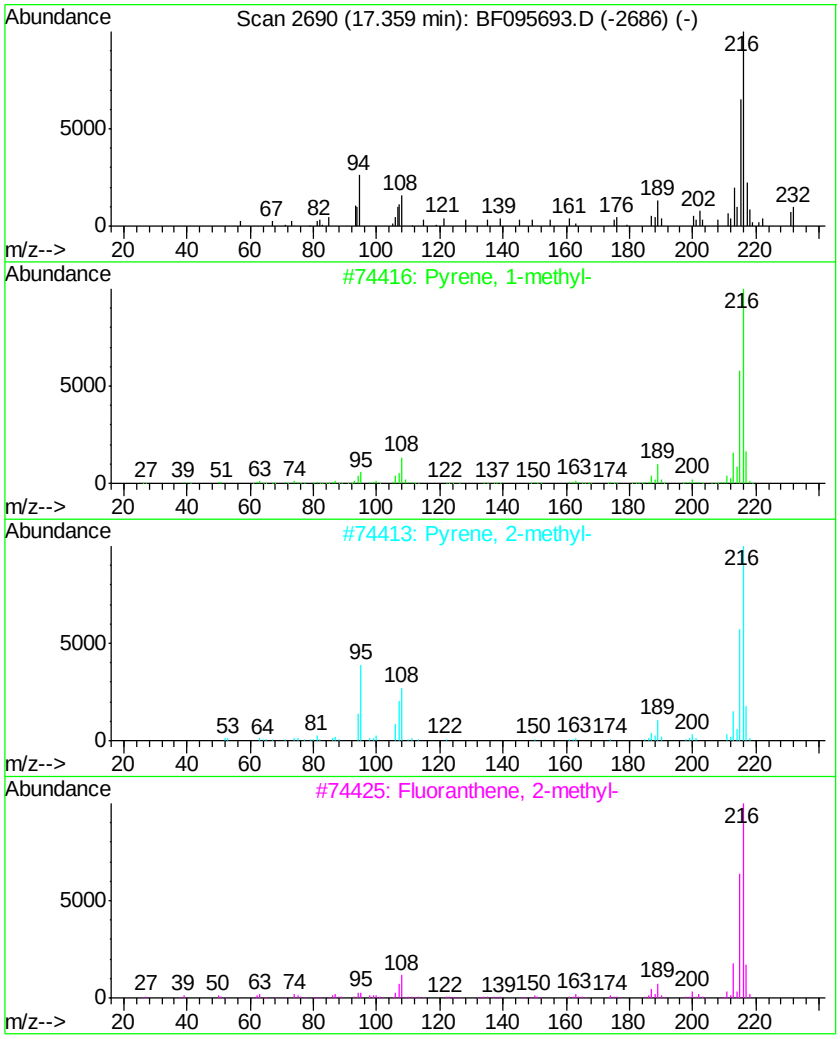
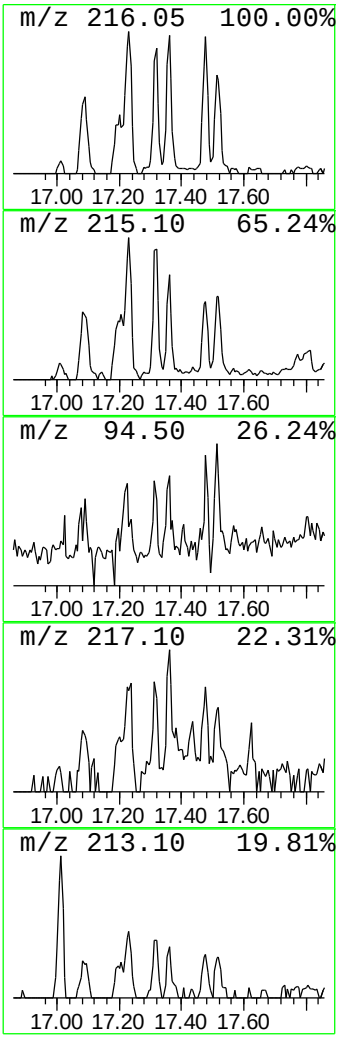
Peak Number 10 Pyrene, 1-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.36	2.31 ng	76661	Chrysene-d12	18.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	96
2	Pyrene, 2-methyl-	216	C17H12	003442-78-2	93
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	64
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	62
5	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	58





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060517\
Data File : BF095693.D
Acq On : 6 Jun 2017 1:54
Operator : SJ/MA
Sample : I3466-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-RO-6704-060217

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

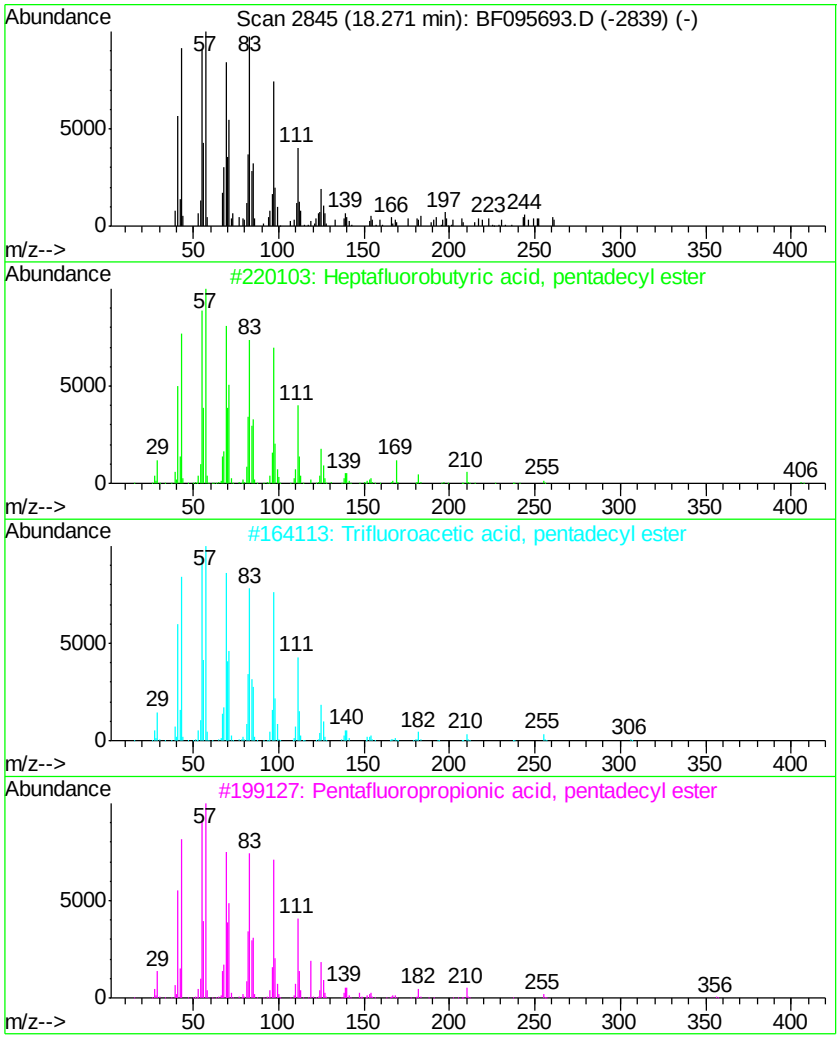
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

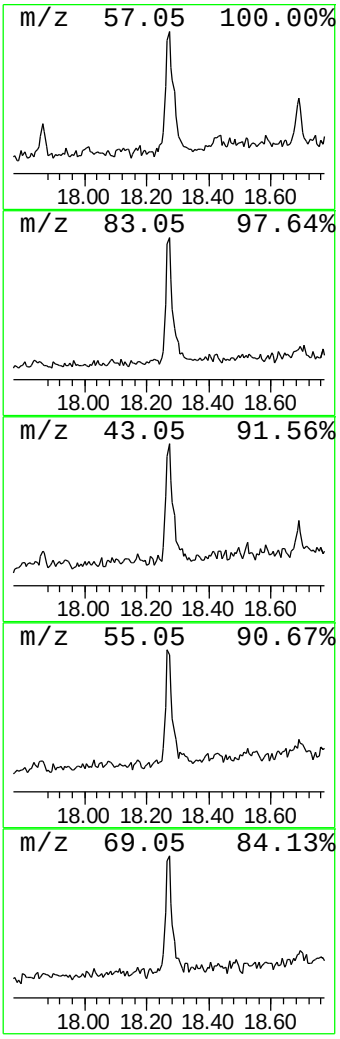
****

Peak Number 11 Heptafluorobutyric acid, pe... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.27	6.77 ng	225215	Chrysene-d12	18.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	95
2	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	95
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	95
4	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060517\
Data File : BF095693.D
Acq On : 6 Jun 2017 1:54
Operator : SJ/MA
Sample : I3466-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-RO-6704-060217

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...	4.61	7.1	ng	176312	1	7.40	494259	20.0
unknown7.05	7.05	86.0	ng	2126300	1	7.40	494259	20.0
Nonadecane	13.88	2.5	ng	70058	4	14.64	568987	20.0
Phenanthrene, 2-m...	15.44	2.8	ng	79386	4	14.64	568987	20.0
4H-Cyclopenta[def...	15.60	2.6	ng	74345	4	14.64	568987	20.0
n-Hexadecanoic acid	15.66	5.5	ng	157430	4	14.64	568987	20.0
di-p-Tolylacetylene	16.25	2.0	ng	57015	4	14.64	568987	20.0
Pyrene, 1-methyl-	17.36	2.3	ng	76661	5	18.35	665058	20.0
Heptafluorobutyri...	18.27	6.8	ng	225215	5	18.35	665058	20.0