LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060717\
Data File : BF095756.D
Acq On : 7 Jun 2017 20:35
Operator : SJ/MA
Sample : I3479-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4(0-2)20170604

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	503	507	521	rBV	54332	138476	8.54%	0.923%
2	5.269	622	626	653	rBV	744980	1324905	81.67%	8.828%
3	6.945	906	911	923	rBV	895636	1341610	82.70%	8.939%
4	7.039	923	927	942	rVB	1115754	1537474	94.77%	10.244%
5	7.381	981	985	1002	rBB	330852	430230	26.52%	2.867%
6	7.622	1021	1026	1044	rBV	887742	1095496	67.53%	7.299%
7	8.298	1136	1141	1166	rBV	621666	821913	50.66%	5.476%
8	9.416	1326	1331	1343	rBV	451757	560674	34.56%	3.736%
9	11.198	1628	1634	1650	rBV	1376855	1622291	100.00%	10.809%
10	11.886	1747	1751	1759	rBV	195444	217858	13.43%	1.452%
11	12.239	1806	1811	1816	rBV2	467374	550158	33.91%	3.666%
12	12.286	1816	1819	1825	rVB2	22854	28270	1.74%	0.188%
13	13.098	1950	1957	1961	rBV	29447	33032	2.04%	0.220%
14	13.533	2026	2031	2039	rBV	532033	697922	43.02%	4.650%
15	13.868	2084	2088	2098	rBV	29670	46112	2.84%	0.307%
16	14.598	2207	2212	2214	rBV2	17990	23144	1.43%	0.154%
17	14.633	2214	2218	2221	rVV	358561	443007	27.31%	2.952%
18	14.668	2221	2224	2231	rVB	72088	95876	5.91%	0.639%
19	14.762	2236	2240	2246	rVB	18542	25472	1.57%	0.170%
20	15.439	2352	2355	2359	rVV	14855	16846	1.04%	0.112%
21	15.480	2359	2362	2367	rVB	19492	21205	1.31%	0.141%
22	15.592	2377	2381	2384	rBV2	20176	25807	1.59%	0.172%
23	15.645	2384	2390	2398	rVB3	52826	71808	4.43%	0.478%
24	16.251	2488	2493	2496	rBV2	14746	20000	1.23%	0.133%
25	16.445	2522	2526	2532	rBV	204072	239128	14.74%	1.593%
26	16.751	2573	2578	2584	rBV	233412	269345	16.60%	1.795%
27	16.945	2607	2611	2616	rBV3	18917	21186	1.31%	0.141%
28	17.003	2616	2621	2625	rBV	1007456	1083696	66.80%	7.221%
29	17.192	2648	2653	2655	rBV4	11093	19180	1.18%	0.128%
30	17.221	2655	2658	2664	rVB	31536	37793	2.33%	0.252%
31	17.309	2668	2673	2677	rBV	26237	34137	2.10%	0.227%
32	17.356	2677	2681	2683	rBV3	22804	31730	1.96%	0.211%
33	17.415	2688	2691	2695	rVV4	13626	17708	1.09%	0.118%
34	17.468	2696	2700	2704	rVB2	16431	18173	1.12%	0.121%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060717\
Data File : BF095756.D
Acq On : 7 Jun 2017 20:35
Operator : SJ/MA
Sample : I3479-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4(0-2)20170604

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	17.856	2764	2766	2769	rBV3	17365	16841	1.04%	0.112%
36	18.056	2797	2800	2802	rVB2	20834	19646	1.21%	0.131%
37	18.121	2809	2811	2816	rVB5	13862	19001	1.17%	0.127%
38	18.186	2816	2822	2825	rBV	15609	23334	1.44%	0.155%
39	18.262	2830	2835	2843	rBV3	75973	145777	8.99%	0.971%
40	18.345	2843	2849	2853	rBV2	426759	589395	36.33%	3.927%
41	18.380	2853	2855	2861	rVB2	103062	113039	6.97%	0.753%
42	18.474	2867	2871	2876	rVB2	23816	28644	1.77%	0.191%
43	18.627	2894	2897	2901	rBV4	14385	17727	1.09%	0.118%
44	18.680	2902	2906	2909	rVB4	26023	32067	1.98%	0.214%
45	18.856	2933	2936	2938	rVB	22593	21924	1.35%	0.146%
46	18.968	2952	2955	2958	rBV5	19541	21732	1.34%	0.145%
47	19.068	2968	2972	2980	rVB4	44675	82400	5.08%	0.549%
48	19.456	3036	3038	3042	rVB3	21728	23363	1.44%	0.156%
49	19.615	3061	3065	3068	rBV	132558	172520	10.63%	1.149%
50	19.786	3092	3094	3096	rBV3	27845	31204	1.92%	0.208%
51	19.903	3110	3114	3117	rBV	83835	103428	6.38%	0.689%
52	19.962	3121	3124	3128	rBV	115626	124869	7.70%	0.832%
53	20.015	3129	3133	3137	rBV	281009	320666	19.77%	2.137%
54	21.197	3331	3334	3340	rVB2	52151	72214	4.45%	0.481%
55	21.533	3389	3391	3398	rVB2	41544	67110	4.14%	0.447%

Sum of corrected areas: 15008563

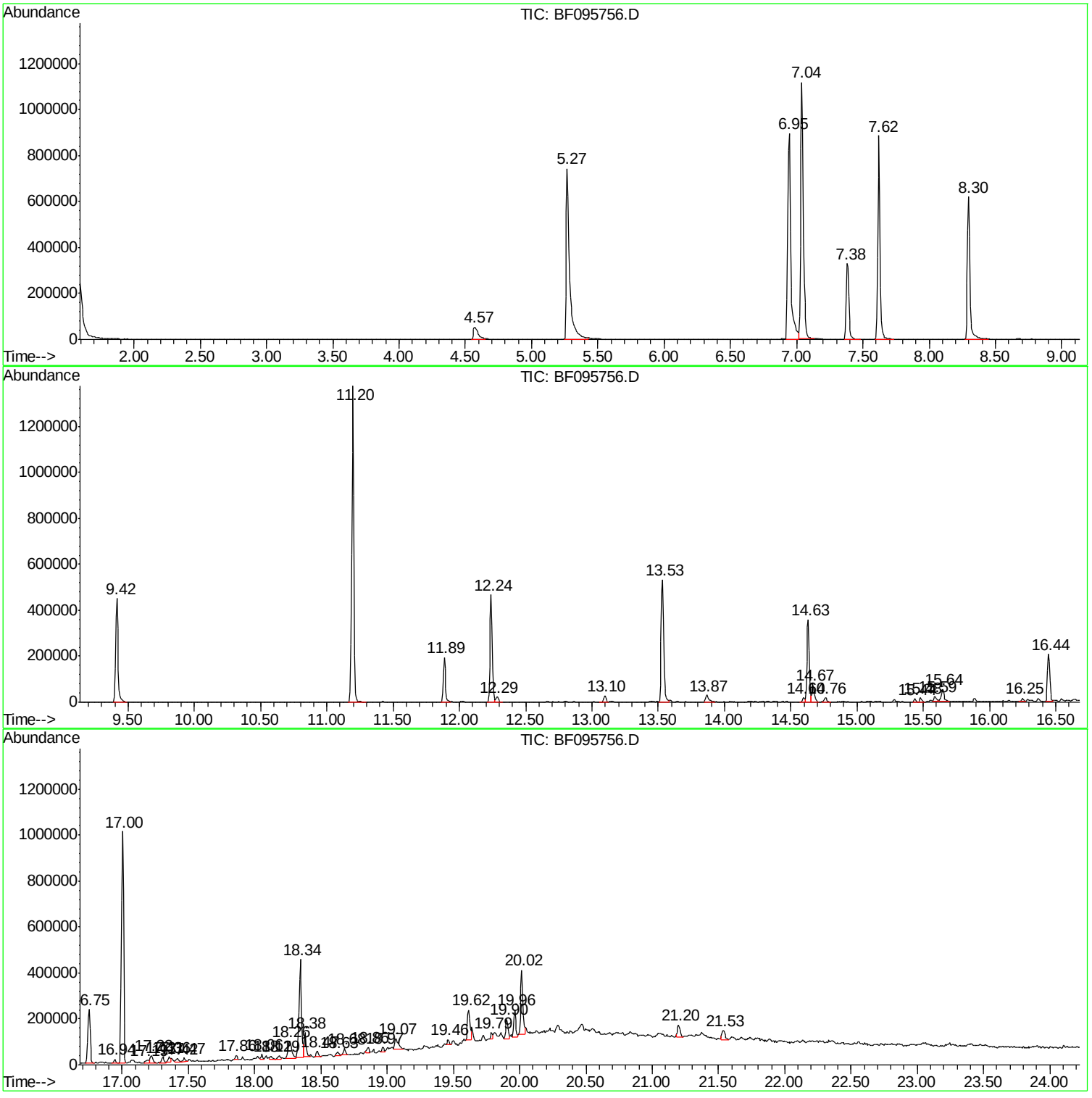
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060717\
Data File : BF095756.D
Acq On : 7 Jun 2017 20:35
Operator : SJ/MA
Sample : I3479-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4(0-2)20170604

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\BF060717\
Data File : BF095756.D
Acq On : 7 Jun 2017 20:35
Operator : SJ/MA
Sample : I3479-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4(0-2)20170604

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

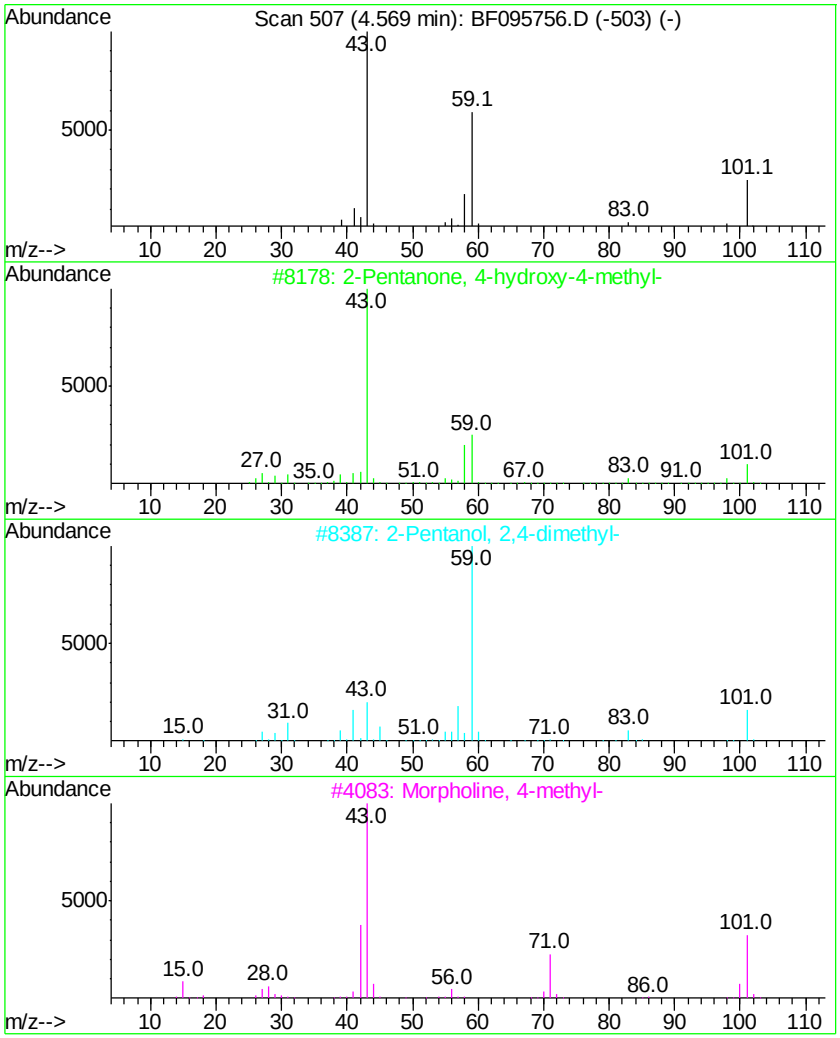
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

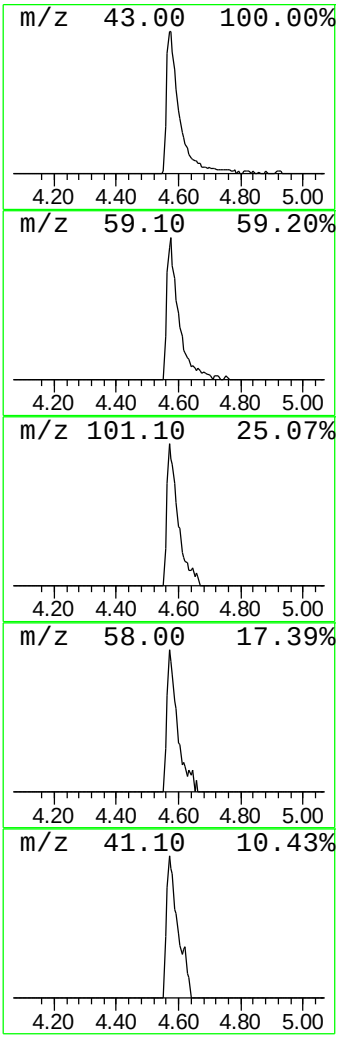
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.57	6.44 ng	138476	1,4-Dichlorobenzene-d4	7.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	25
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	Acetone	58	C3H6O	000067-64-1	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060717\
Data File : BF095756.D
Acq On : 7 Jun 2017 20:35
Operator : SJ/MA
Sample : I3479-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4(0-2)20170604

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

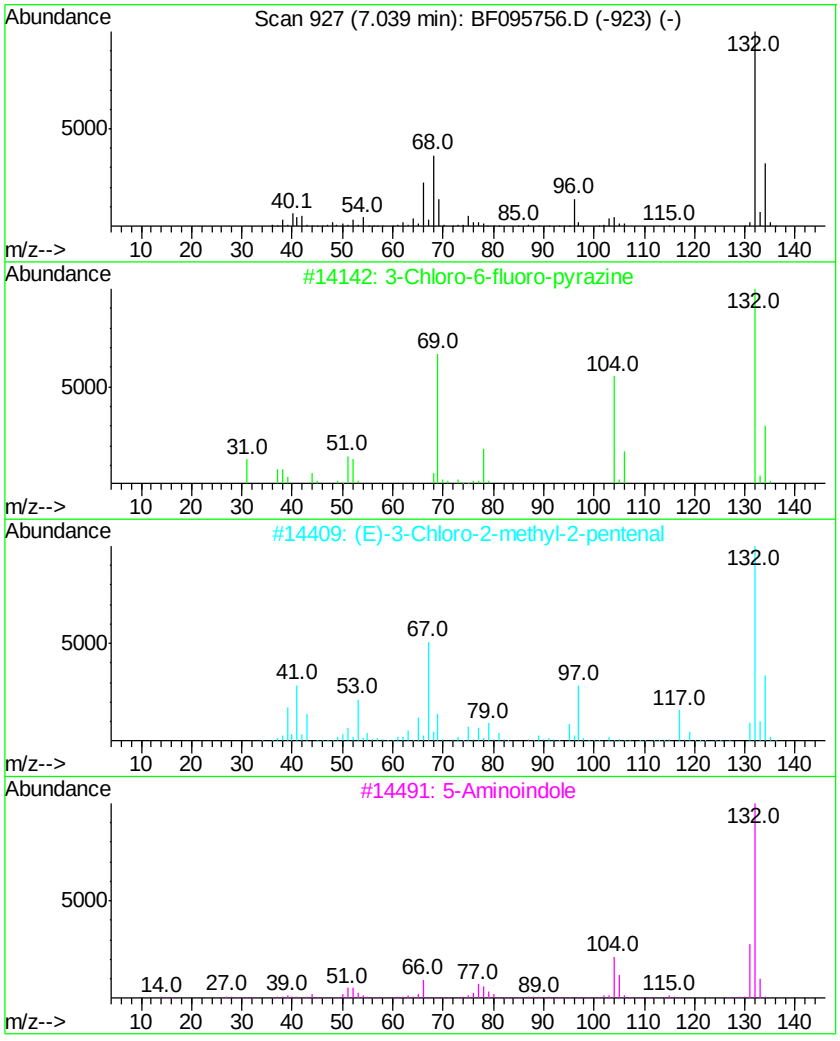
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

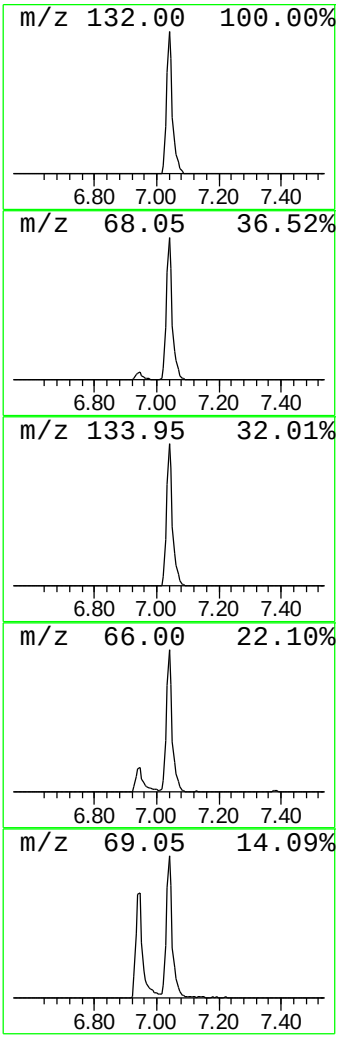
****

Peak Number 2 unknown7.04 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.04	71.47 ng	1537470	1,4-Dichlorobenzene-d4	7.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	Xenon	132	Xe	007440-63-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060717\
Data File : BF095756.D
Acq On : 7 Jun 2017 20:35
Operator : SJ/MA
Sample : I3479-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4(0-2)20170604

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

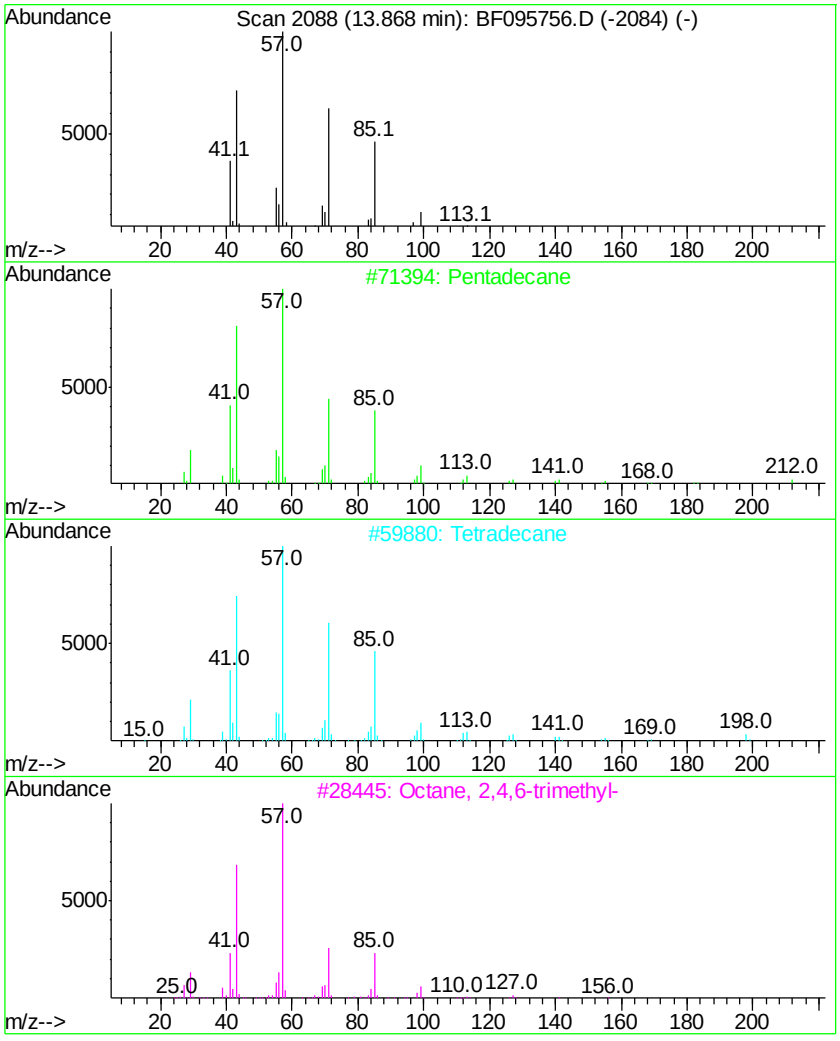
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

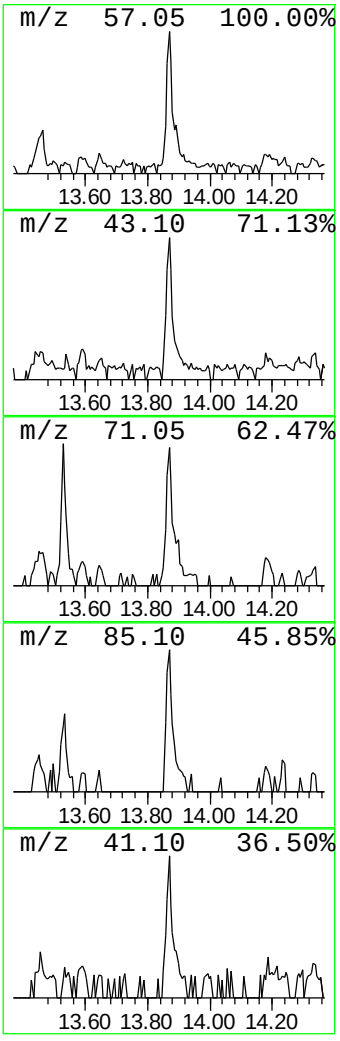
****

Peak Number 4 Pentadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	2.08 ng	46112	Phenanthrene-d10	14.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	78
2	Tetradecane	198	C14H30	000629-59-4	78
3	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	78
4	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	72
5	Tridecane	184	C13H28	000629-50-5	59





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060717\
Data File : BF095756.D
Acq On : 7 Jun 2017 20:35
Operator : SJ/MA
Sample : I3479-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4(0-2)20170604

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

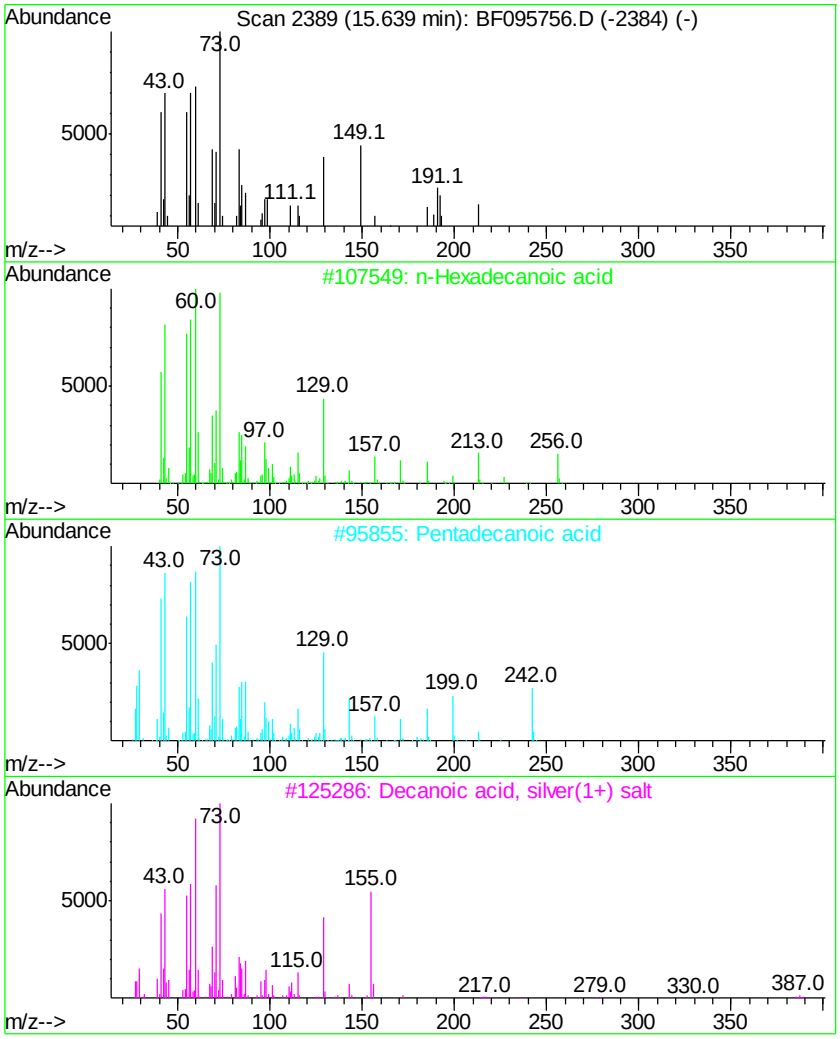
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

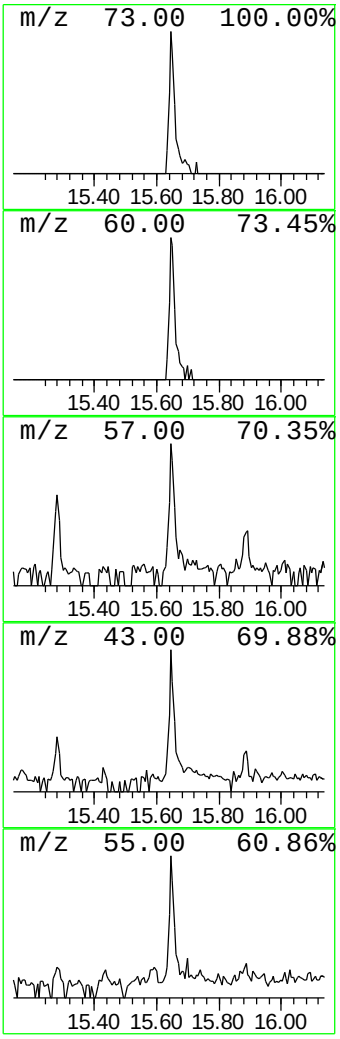
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.64	3.24 ng	71808	Phenanthrene-d10	14.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5	Tridecanoic acid	214	C13H26O2	000638-53-9	58





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Acq On : 7 Jun 2017 20:35
Operator : SJ/MA
Sample : I3479-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4(0-2)20170604

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

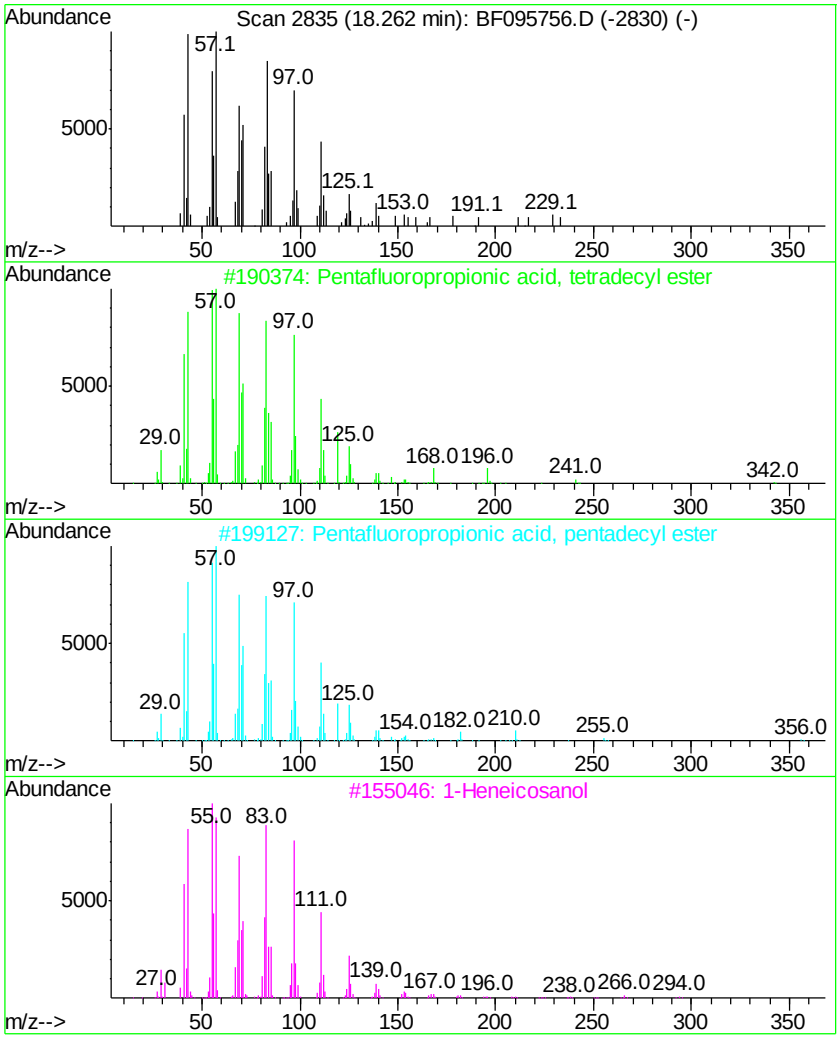
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

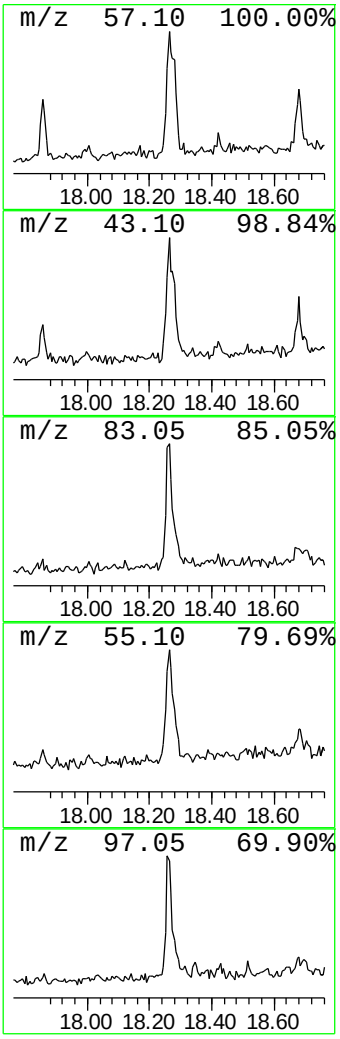
****

Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.26	4.95 ng	145777	Chrysene-d12	18.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	95
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	95
3	1-Heneicosanol	312	C21H44O	015594-90-8	93
4	1-Docosene	308	C22H44	001599-67-3	90
5	1-Heptacosanol	396	C27H56O	002004-39-9	90





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060717\
Data File : BF095756.D
Acq On : 7 Jun 2017 20:35
Operator : SJ/MA
Sample : I3479-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4(0-2)20170604

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

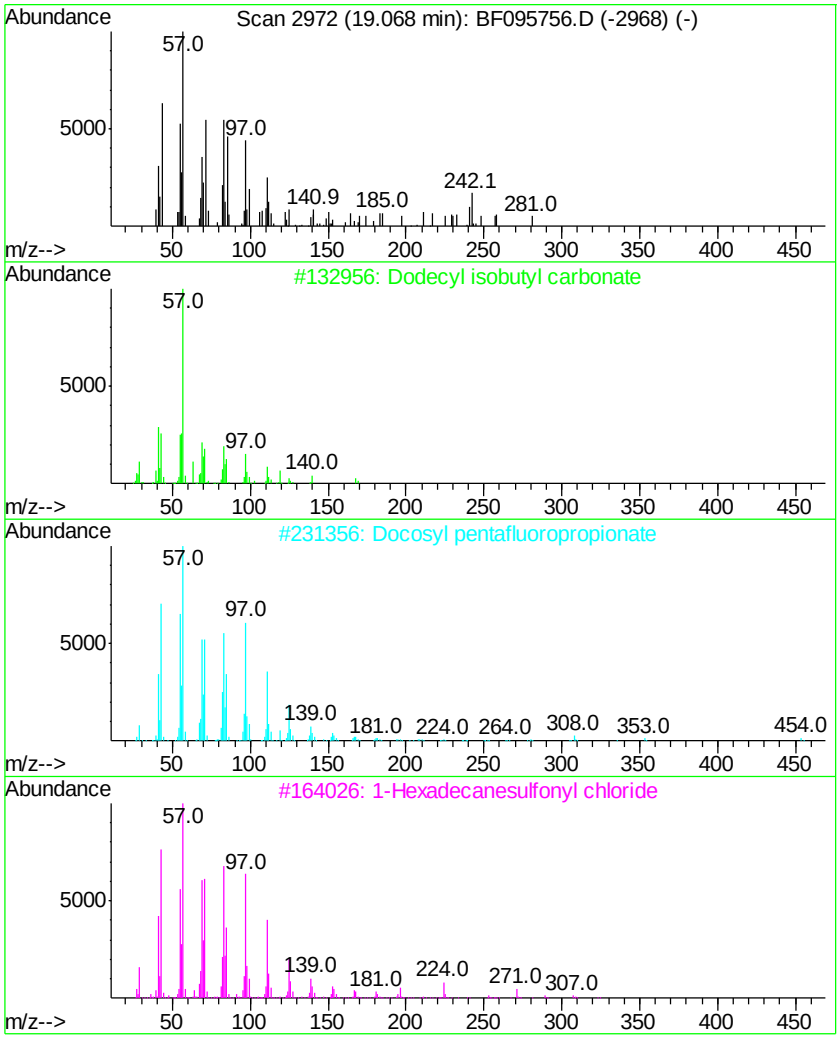
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

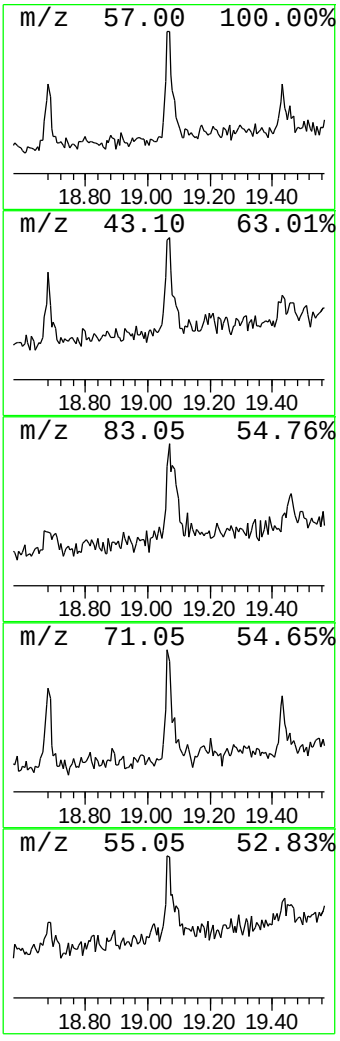
****

Peak Number 7 Dodecyl isobutyl carbonate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.07	2.80 ng	82400	Chrysene-d12	18.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecyl isobutyl carbonate	286	C17H34O3	959067-22-2	80
2	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	58
3	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	58
4	17-Pentatriacontene	491	C35H70	006971-40-0	58
5	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	58





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Data File : BF095756.D
Acq On : 7 Jun 2017 20:35
Operator : SJ/MA
Sample : I3479-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4(0-2)20170604

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

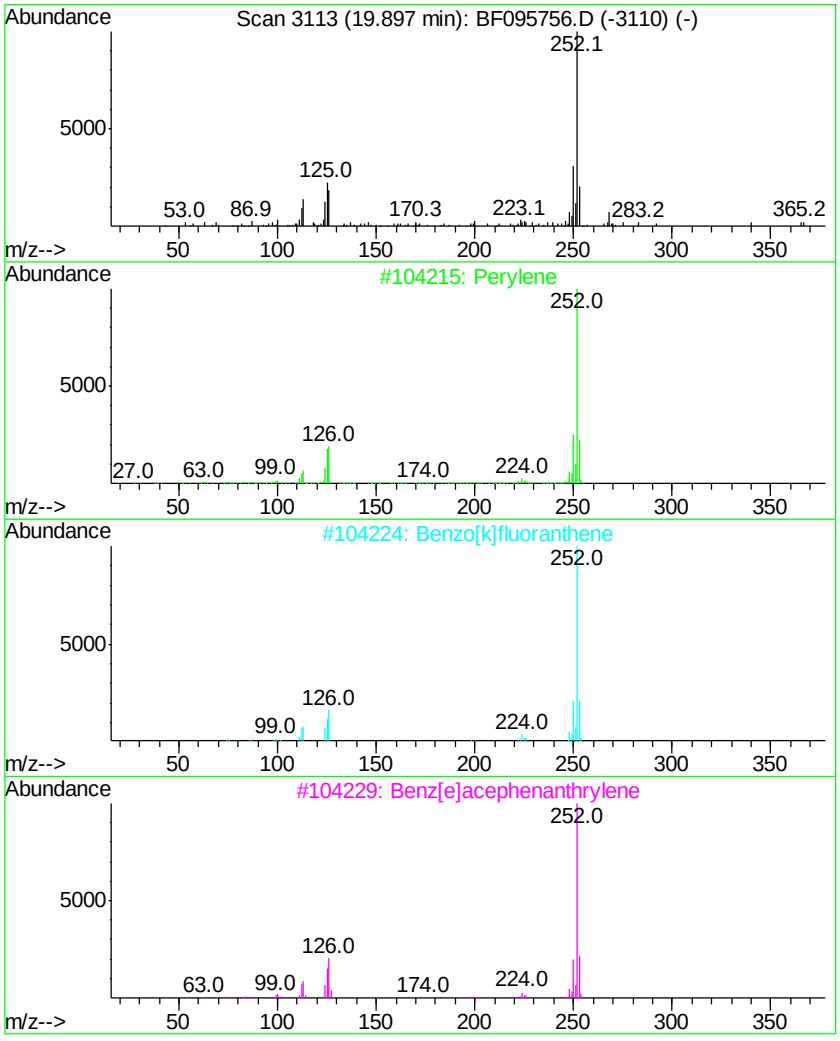
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

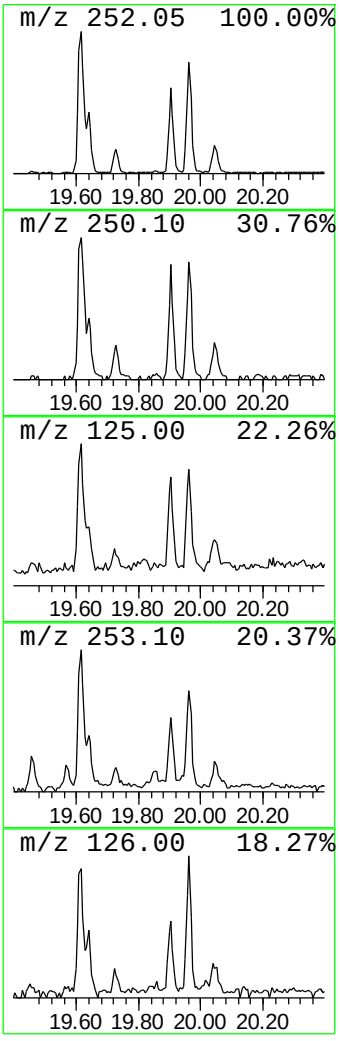
****

Peak Number 8 Perylene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.90	6.45 ng	103428	Perylene-d12	20.02

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





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060717\
Data File : BF095756.D
Acq On : 7 Jun 2017 20:35
Operator : SJ/MA
Sample : I3479-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-4(0-2)20170604

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	6.4	ng	138476	1	7.38	430230	20.0
unknown7.04	7.04	71.5	ng	1537470	1	7.38	430230	20.0
Pentadecane	13.87	2.1	ng	46112	4	14.63	443007	20.0
n-Hexadecanoic acid	15.64	3.2	ng	71808	4	14.63	443007	20.0
Pentafluoropropio...	18.26	5.0	ng	145777	5	18.34	589395	20.0
Dodecyl isobutyl ...	19.07	2.8	ng	82400	5	18.34	589395	20.0
Perylene	19.90	6.5	ng	103428	6	20.02	320666	20.0