LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052717\
Data File : BF095516.D
Acq On : 28 May 2017 1:34
Operator : SJ/MA
Sample : I3244-12
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM13-COMP-6-18

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	5.095	533	537	562	rBV	86158	230825	10.17%	1.308%
2	5.701	636	640	673	rBV	729037	1976944	87.09%	11.206%
3	7.283	905	909	925	rBV	728008	1748057	77.01%	9.909%
4	7.401	925	929	950	rVB	1325810	2269890	100.00%	12.867%
5	7.736	982	986	999	rVB	428425	537109	23.66%	3.045%
6	7.972	1021	1026	1047	rBV	1228036	1597547	70.38%	9.056%
7	8.642	1136	1140	1167	rBV	485144	1128757	49.73%	6.398%
8	9.766	1327	1331	1355	rBV	258617	613278	27.02%	3.476%
9	11.530	1626	1631	1654	rBV	1096299	2013820	88.72%	11.415%
10	12.242	1747	1752	1769	rBV	105779	207775	9.15%	1.178%
11	12.595	1807	1812	1828	rBV2	426829	751291	33.10%	4.259%
12	13.418	1948	1952	1959	rBV	28819	37926	1.67%	0.215%
13	13.895	2029	2033	2058	rBV	465759	985120	43.40%	5.584%
14	14.195	2080	2084	2093	rBV2	27480	40312	1.78%	0.229%
15	15.001	2217	2221	2244	rVB	306320	625676	27.56%	3.547%
16	15.483	2298	2303	2316	rBV2	37929	89020	3.92%	0.505%
17	15.848	2360	2365	2370	rBV4	35236	61658	2.72%	0.350%
18	15.954	2379	2383	2396	rVB5	49199	99149	4.37%	0.562%
19	16.789	2521	2525	2534	rBV	80475	116194	5.12%	0.659%
20	17.095	2572	2577	2586	rVB	91023	135803	5.98%	0.770%
21	17.312	2609	2614	2625	rBV	844230	1000244	44.07%	5.670%
22	18.553	2817	2825	2838	rBV5	25804	82595	3.64%	0.468%
23	18.677	2840	2846	2850	rBV2	332605	520090	22.91%	2.948%
24	19.783	3031	3034	3038	rBV	22713	24507	1.08%	0.139%
25	19.953	3060	3063	3066	rBV	57454	79776	3.51%	0.452%
26	20.065	3079	3082	3087	rBV2	20818	25134	1.11%	0.142%
27	20.241	3109	3112	3118	rBV	36546	44709	1.97%	0.253%
28	20.300	3119	3122	3126	rBV	45262	52054	2.29%	0.295%
29	20.353	3127	3131	3139	rBV	254393	410236	18.07%	2.325%
30	20.788	3201	3205	3210	rBV6	15622	24068	1.06%	0.136%
31	21.718	3358	3363	3370	rBV5	29285	56672	2.50%	0.321%
32	22.112	3426	3430	3439	rVB8	25147	54878	2.42%	0.311%

LSC Area Percent Report

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Misc :
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Instrument :
BNA_F
ClientSampleId :
NM13-COMP-6-18

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

Sum of corrected areas: 17641114

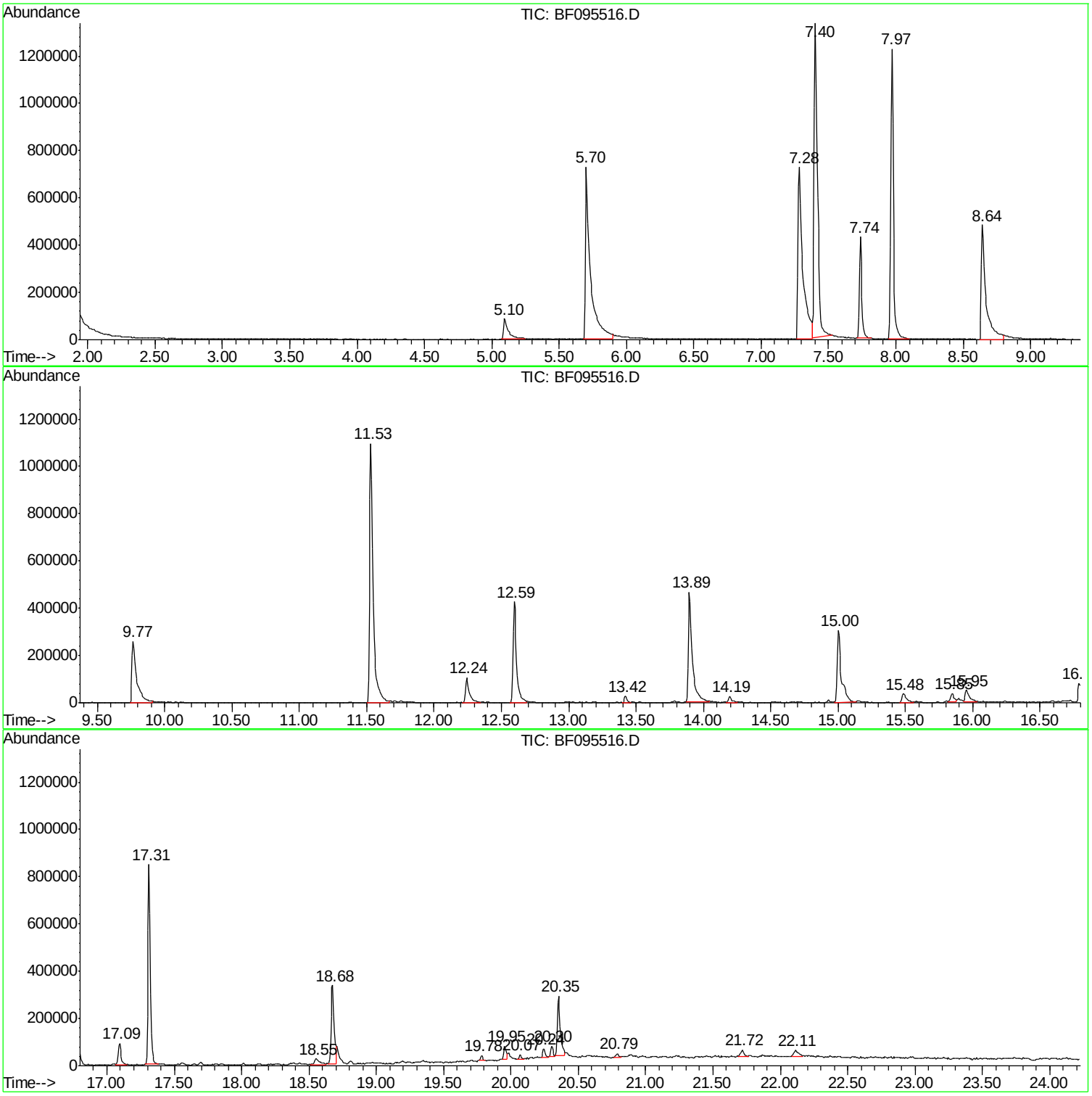
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052717\
Data File : BF095516.D
Acq On : 28 May 2017 1:34
Operator : SJ/MA
Sample : I3244-12
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM13-COMP-6-18

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\BF052717\
Data File : BF095516.D
Acq On : 28 May 2017 1:34
Operator : SJ/MA
Sample : I3244-12
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM13-COMP-6-18

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

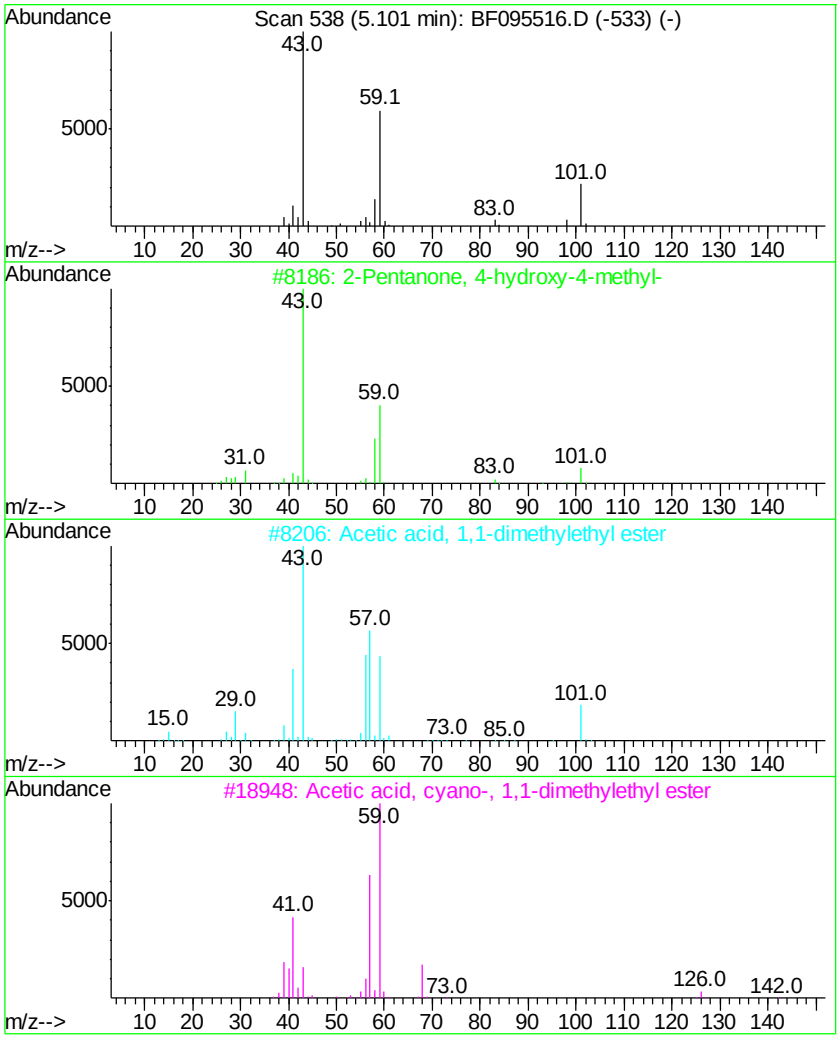
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

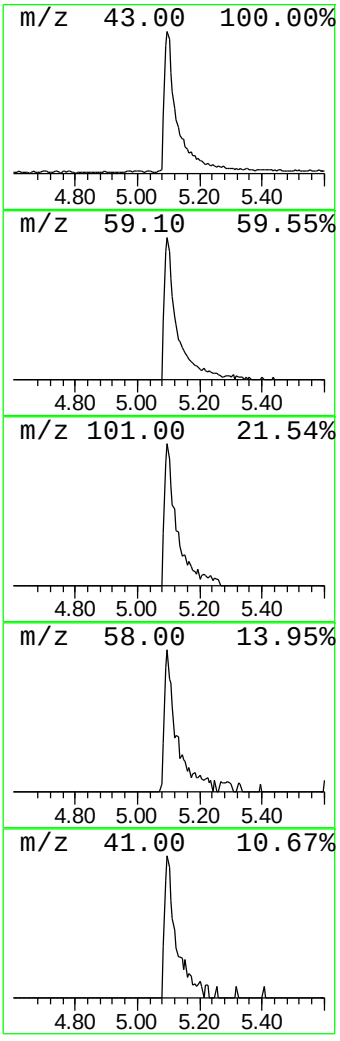
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	8.60 ng	230825	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	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Acetone	58	C3H6O	000067-64-1	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052717\
Data File : BF095516.D
Acq On : 28 May 2017 1:34
Operator : SJ/MA
Sample : I3244-12
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM13-COMP-6-18

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

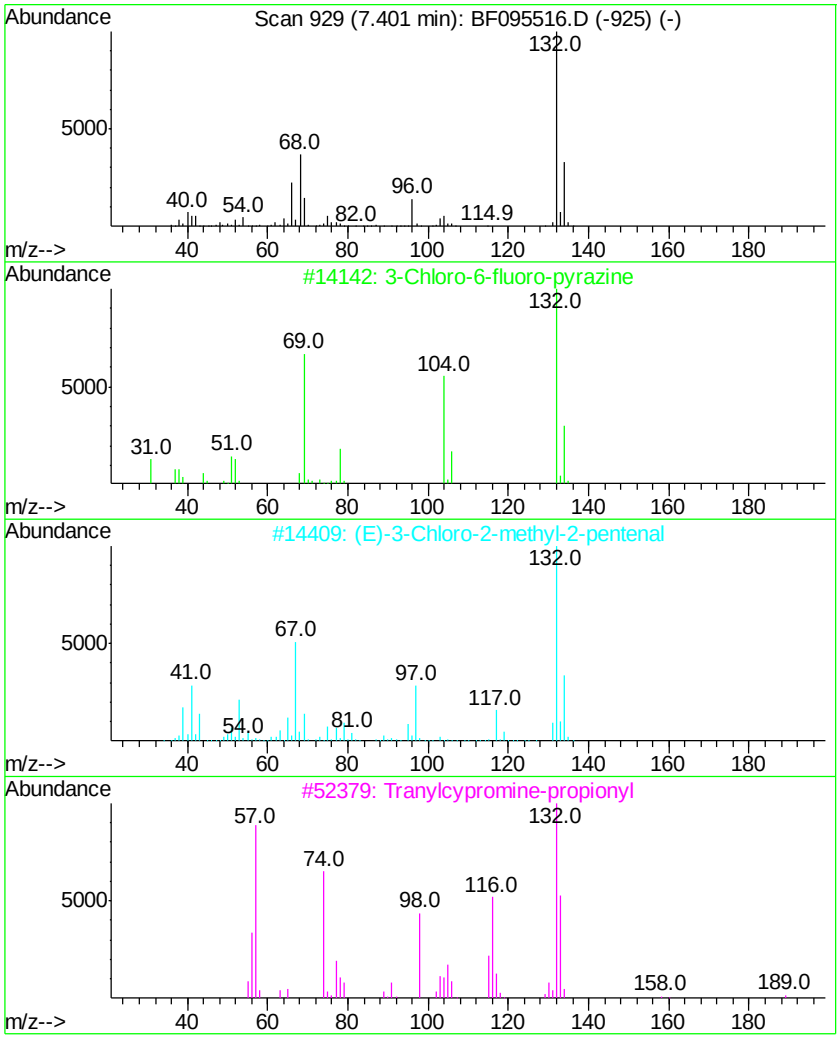
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

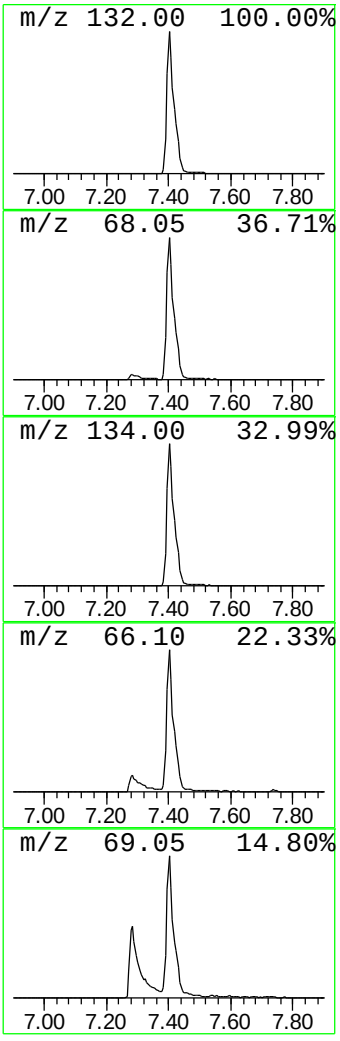
****

Peak Number 2 unknown7.40 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.40	84.52 ng	2269890	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	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Xenon	132	Xe	007440-63-3	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052717\
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Acq On : 28 May 2017 1:34
Operator : SJ/MA
Sample : I3244-12
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM13-COMP-6-18

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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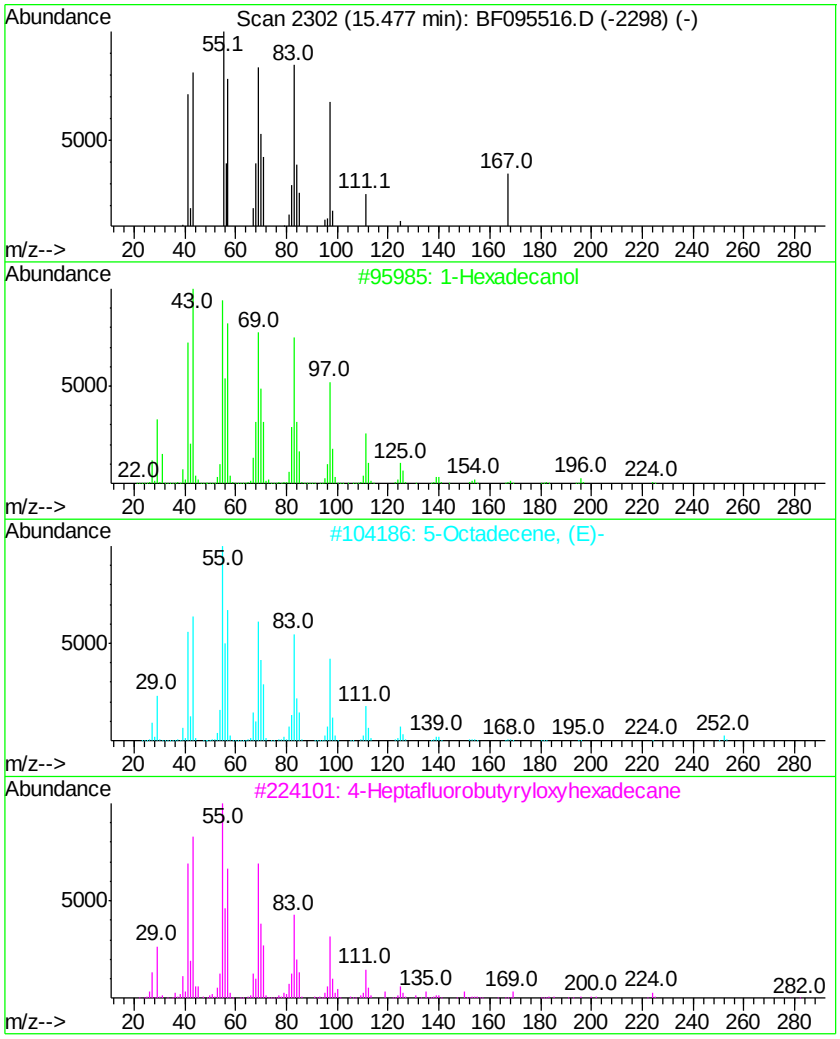
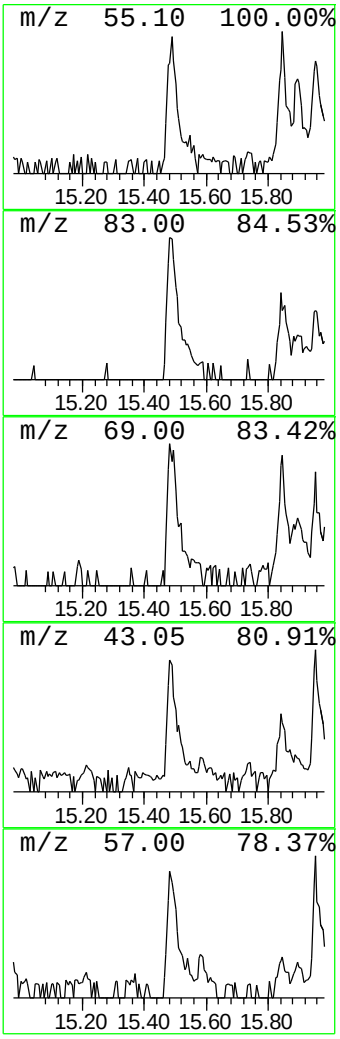
Peak Number 4 1-Hexadecanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.48	2.85 ng	89020	Phenanthrene-d10	15.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4	91
2	5-Octadecene, (E)-	252	C18H36	007206-21-5	90
3	4-Heptafluorobutyryloxyhexadecane	438	C20H33F7O2	1000282-97-2	90
4	1-Heptadecene	238	C17H34	006765-39-5	90
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	87





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052717\
Data File : BF095516.D
Acq On : 28 May 2017 1:34
Operator : SJ/MA
Sample : I3244-12
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM13-COMP-6-18

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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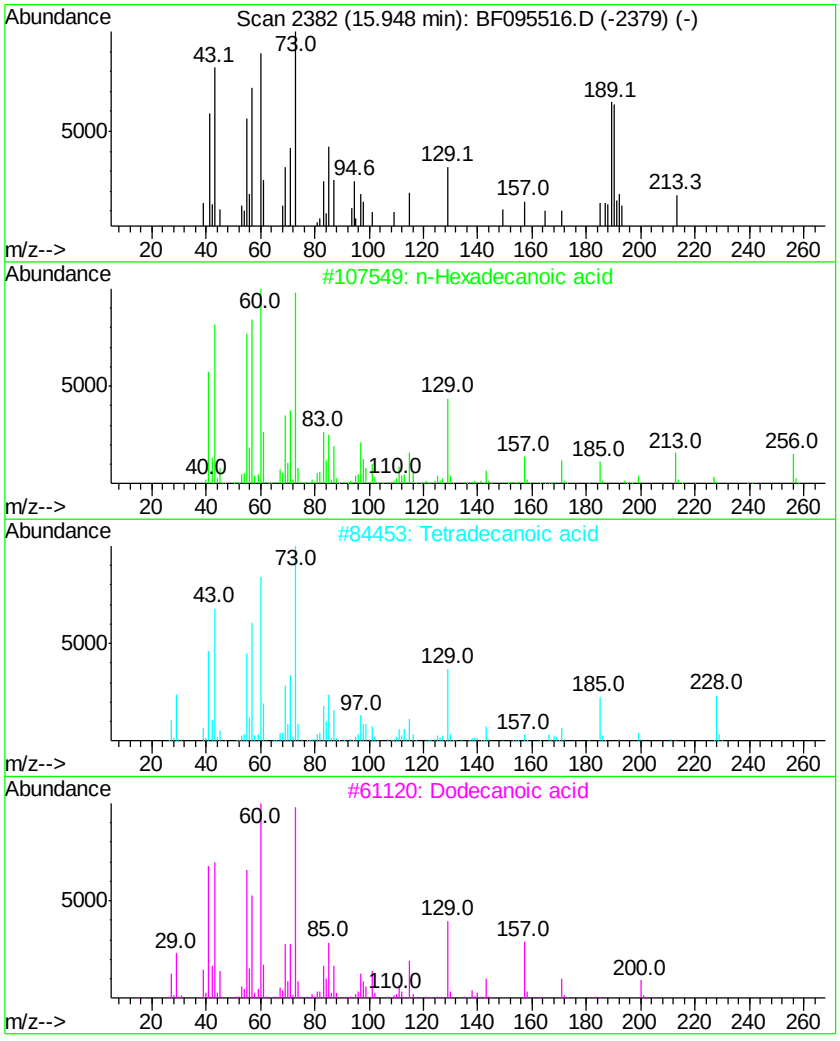
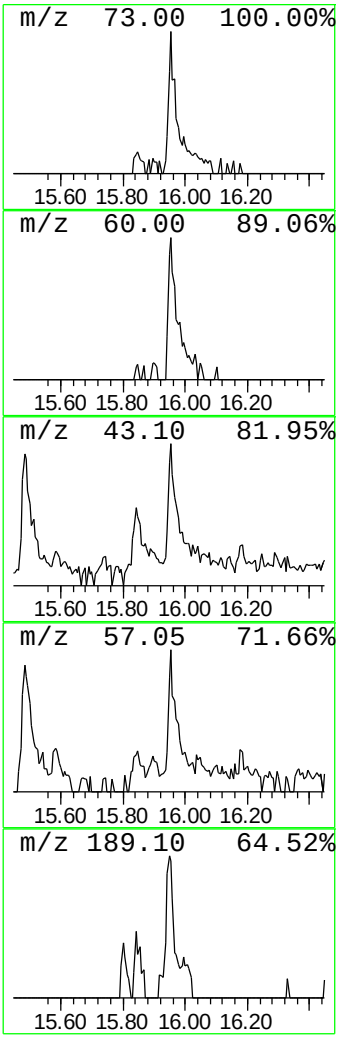
Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.95	3.17 ng	99149	Phenanthrene-d10	15.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	49
3	Dodecanoic acid	200	C12H24O2	000143-07-7	43
4	Tridecanoic acid	214	C13H26O2	000638-53-9	43
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	38





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Sample : I3244-12
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM13-COMP-6-18

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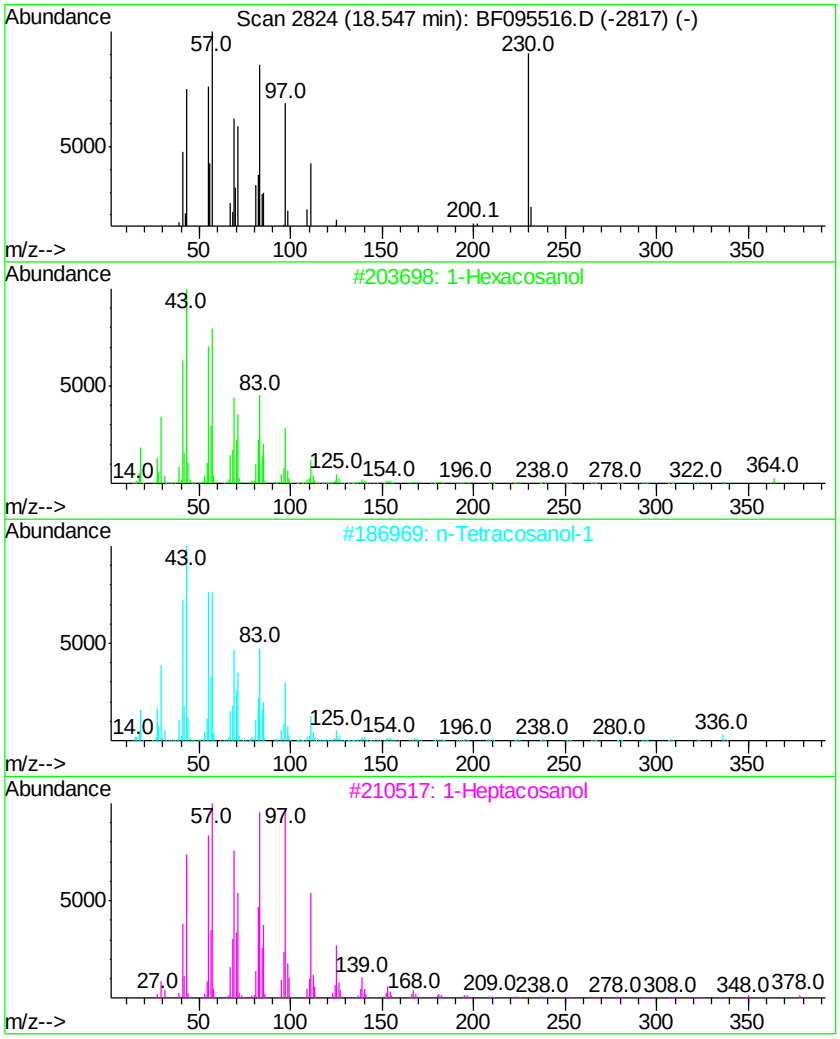
TIC Integration Parameters: LSCINT.P

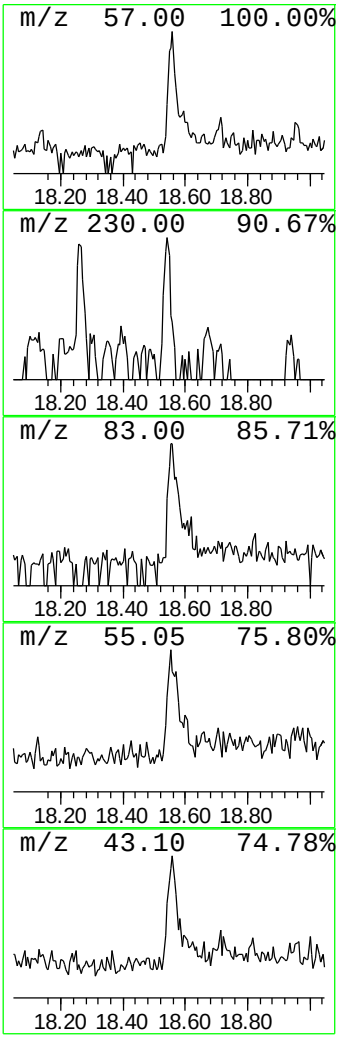
****

Peak Number 6 1-Hexacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.55	3.18 ng	82595	Chrysene-d12	18.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosanol	382	C26H54O	000506-52-5	81
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	76
3	1-Heptacosanol	396	C27H56O	002004-39-9	64
4	Dichloroacetic acid, tridecyl ester	310	C15H28Cl2O2	1000280-48-3	58
5	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	58





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_F
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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	230825	1	7.74	537109	20.0
unknown7.40	7.40	84.5	ng	2269890	1	7.74	537109	20.0
1-Hexadecanol	15.48	2.9	ng	89020	4	15.00	625676	20.0
n-Hexadecanoic acid	15.95	3.2	ng	99149	4	15.00	625676	20.0
1-Hexacosanol	18.55	3.2	ng	82595	5	18.68	520090	20.0