LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051217\
Data File : BF095111.D
Acq On : 12 May 2017 14:44
Operator : SJ/MA
Sample : I3100-08
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5A-051017

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	4.990	515	519	529	rBV	60913	127993	3.92%	0.624%
2	5.648	628	631	661	rVB	373696	902297	27.66%	4.398%
3	7.260	901	905	918	rBV	185340	498349	15.28%	2.429%
4	7.360	918	922	942	rVV	1238546	2005018	61.47%	9.772%
5	7.501	942	946	954	rVB	36964	47599	1.46%	0.232%
6	7.695	976	979	990	rBV	364100	482531	14.79%	2.352%
7	7.784	990	994	1000	rVB3	26346	49235	1.51%	0.240%
8	7.937	1015	1020	1041	rVB	1481997	1887967	57.88%	9.202%
9	8.301	1077	1082	1089	rVB2	29300	43057	1.32%	0.210%
10	8.601	1128	1133	1149	rBV	1100567	1560466	47.84%	7.605%
11	8.719	1149	1153	1157	rVB	56643	66902	2.05%	0.326%
12	9.719	1319	1323	1333	rBV	495788	702920	21.55%	3.426%
13	9.801	1333	1337	1340	rVB	59485	62248	1.91%	0.303%
14	9.925	1354	1358	1363	rVB	26203	33959	1.04%	0.166%
15	10.789	1501	1505	1513	rVB	31485	36295	1.11%	0.177%
16	11.495	1619	1625	1638	rBV	2713346	3261703	100.00%	15.897%
17	12.195	1740	1744	1755	rBV	69493	103779	3.18%	0.506%
18	12.548	1799	1804	1816	rBV2	565507	795019	24.37%	3.875%
19	13.842	2019	2024	2044	rBV	1181659	1815129	55.65%	8.847%
20	14.954	2208	2213	2232	rBV	510810	798756	24.49%	3.893%
21	15.918	2372	2377	2388	rBV2	134493	207444	6.36%	1.011%
22	17.007	2557	2562	2578	rBV2	222338	385097	11.81%	1.877%
23	17.124	2578	2582	2586	rVV	52287	57995	1.78%	0.283%
24	17.283	2602	2609	2612	rBV	2496799	3219826	98.72%	15.693%
25	18.077	2741	2744	2750	rVB	52190	59632	1.83%	0.291%
26	18.454	2805	2808	2812	rVB	62896	70159	2.15%	0.342%
27	18.624	2833	2837	2844	rBV	534871	729898	22.38%	3.557%
28	20.295	3117	3121	3131	rBV	327672	506513	15.53%	2.469%

Sum of corrected areas: 20517786

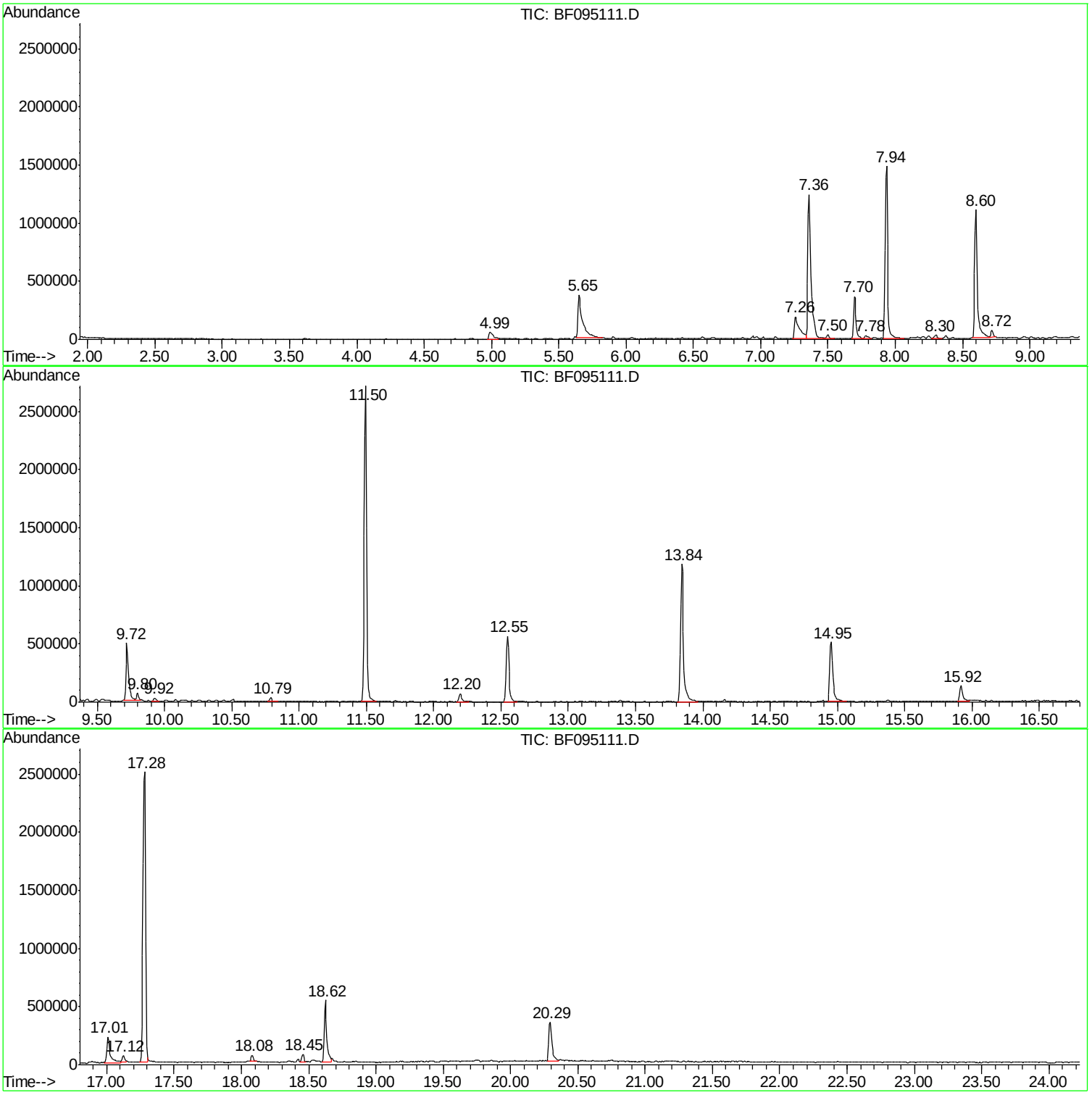
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051217\
Data File : BF095111.D
Acq On : 12 May 2017 14:44
Operator : SJ/MA
Sample : I3100-08
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5A-051017

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051217\
Data File : BF095111.D
Acq On : 12 May 2017 14:44
Operator : SJ/MA
Sample : I3100-08
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ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5A-051017

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

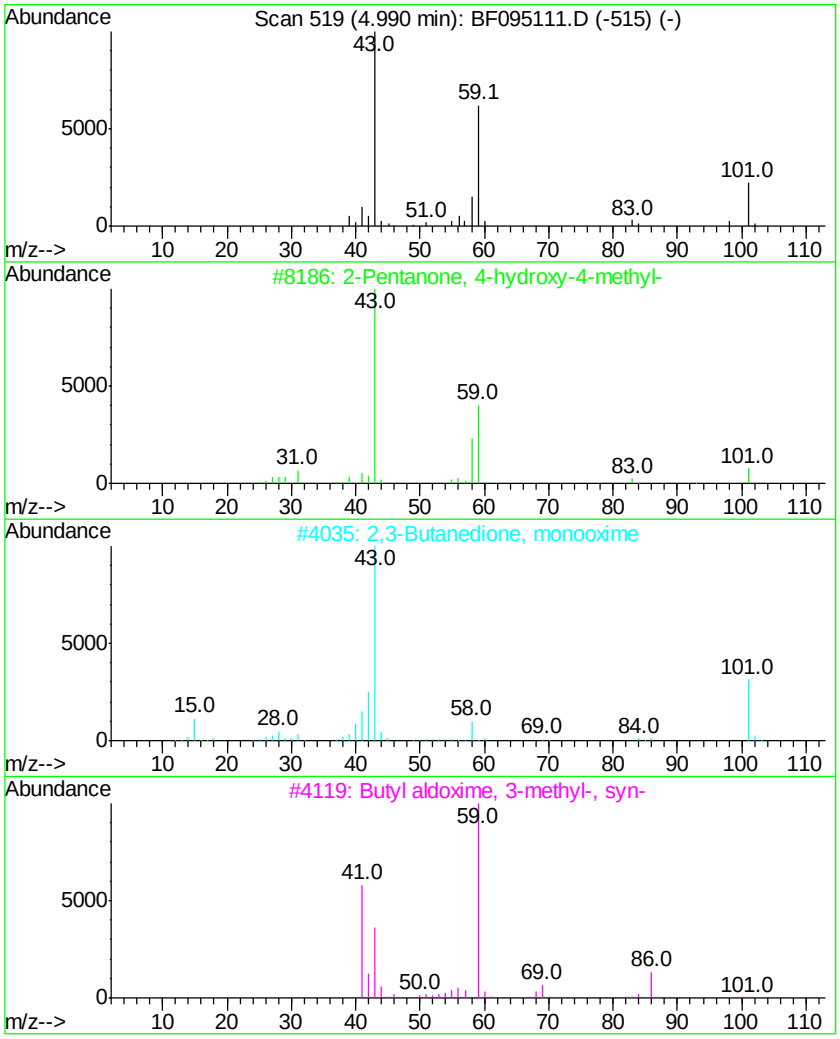
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

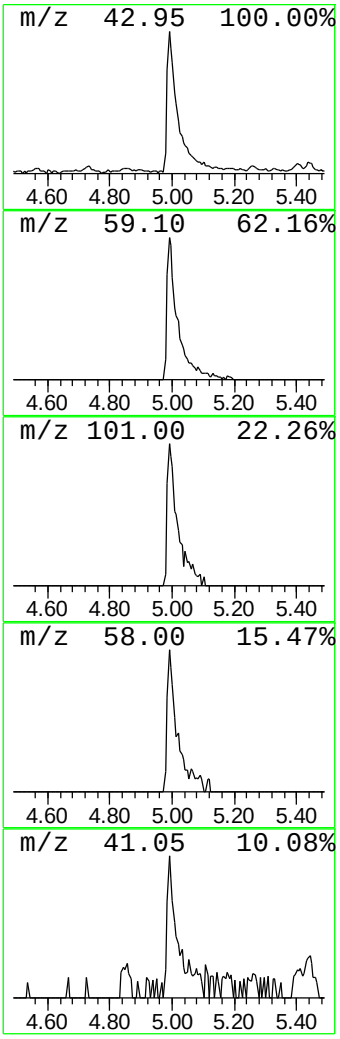
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	5.31 ng	127993	1,4-Dichlorobenzene-d4	7.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	32
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF051217\
Data File : BF095111.D
Acq On : 12 May 2017 14:44
Operator : SJ/MA
Sample : I3100-08
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5A-051017

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

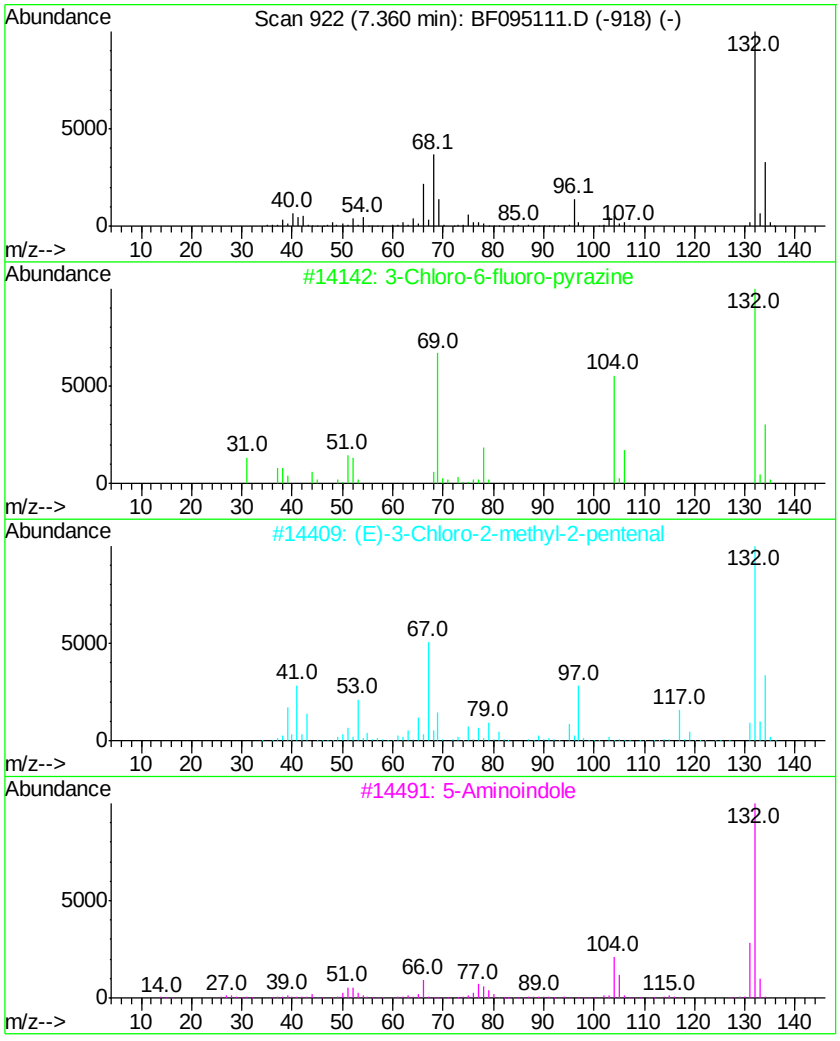
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

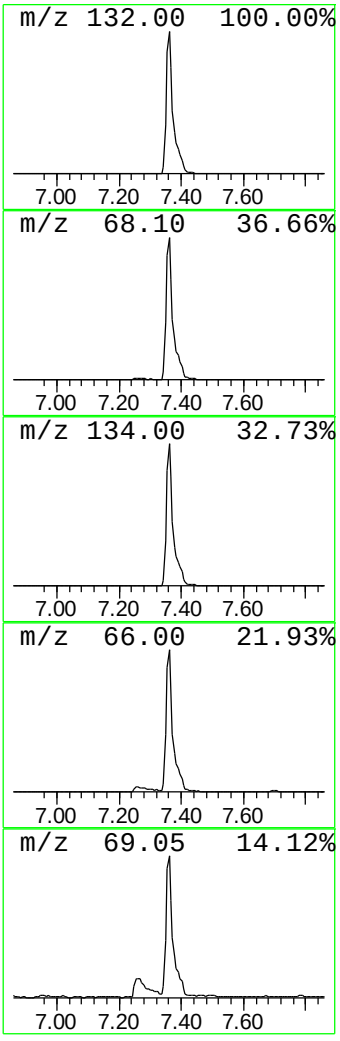
****

Peak Number 2 unknown7.36 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.36	83.10 ng	2005020	1,4-Dichlorobenzene-d4	7.70

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	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Xenon	132	Xe	007440-63-3	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051217\
Data File : BF095111.D
Acq On : 12 May 2017 14:44
Operator : SJ/MA
Sample : I3100-08
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5A-051017

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

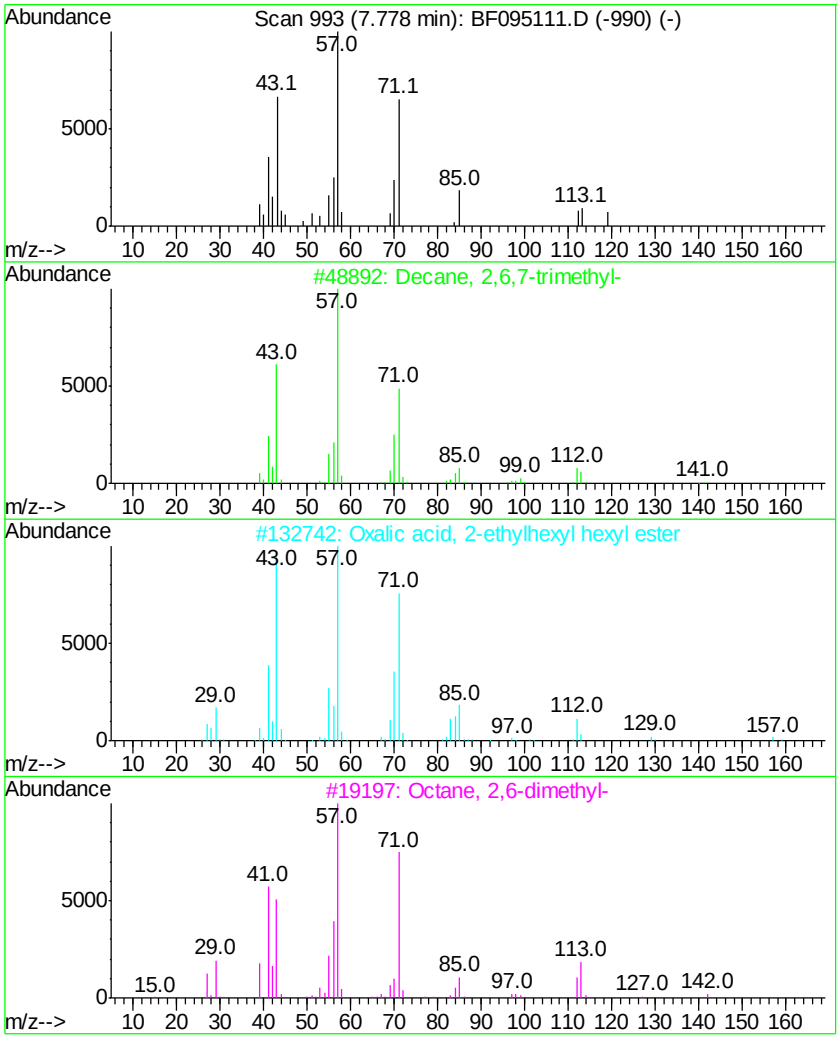
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

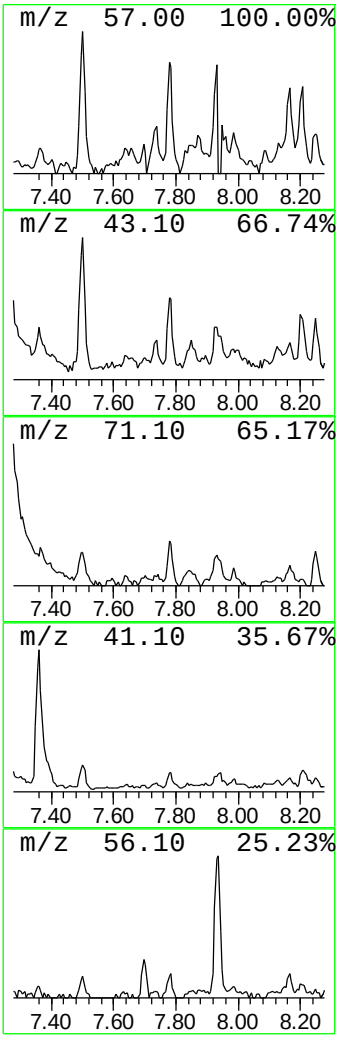
****

Peak Number 3 Decane, 2,6,7-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.78	2.04 ng	49235	1,4-Dichlorobenzene-d4	7.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 2,6,7-trimethyl-	184	C13H28	062108-25-2	86
2	Oxalic acid, 2-ethylhexyl hexyl ...	286	C16H30O4	1000309-38-9	64
3	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	59
4	Nonane, 3-methyl-	142	C10H22	005911-04-6	59
5	Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	59





Data Path : Z:\HPCHEM1\BNA F\DATA\BF051217\
Data File : BF095111.D
Acq On : 12 May 2017 14:44
Operator : SJ/MA
Sample : I3100-08
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5A-051017

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

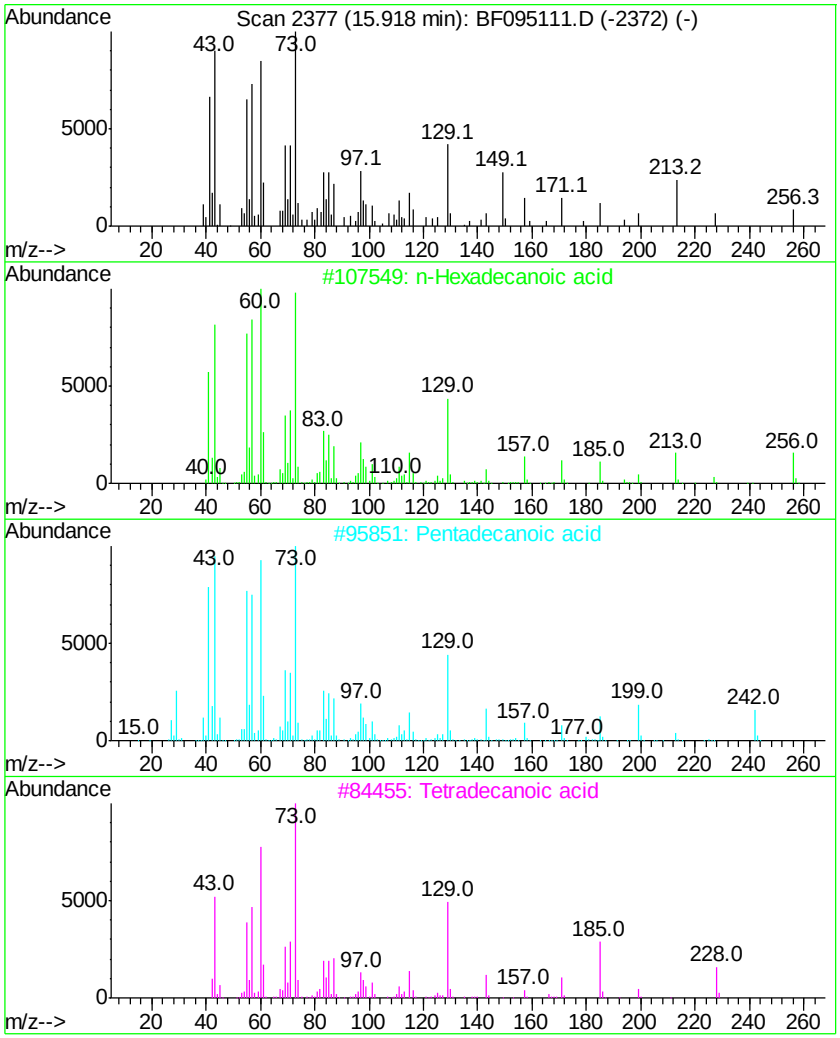
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

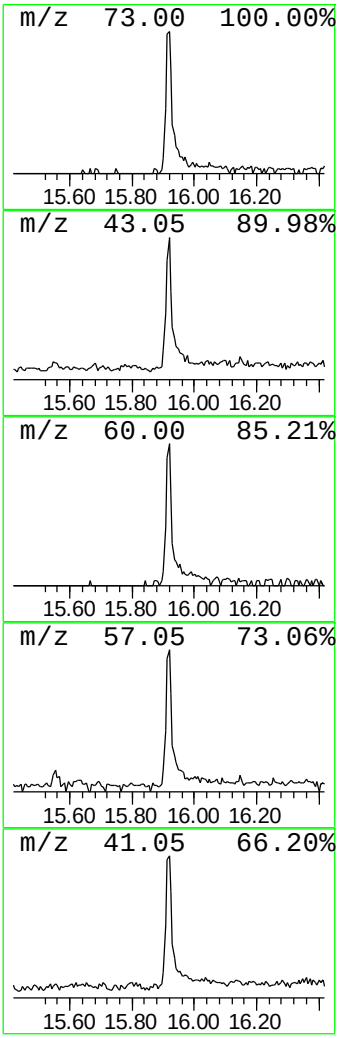
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.92	5.19 ng	207444	Phenanthrene-d10	14.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4	Tridecanoic acid	214	C13H26O2	000638-53-9	52
5	Oxalic acid, allyl dodecyl ester	298	C17H30O4	1000309-24-0	14





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051217\
Data File : BF095111.D
Acq On : 12 May 2017 14:44
Operator : SJ/MA
Sample : I3100-08
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5A-051017

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

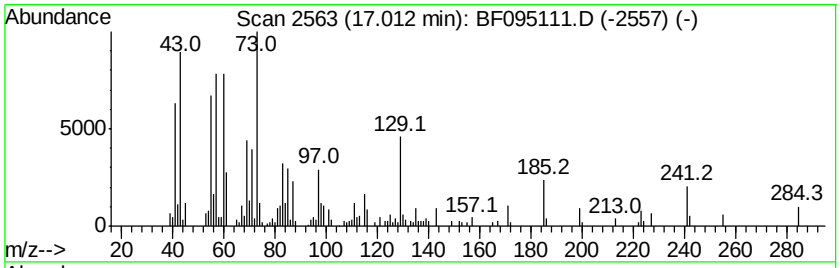
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

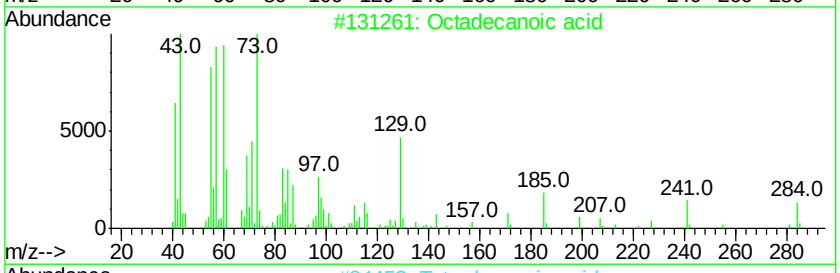
****

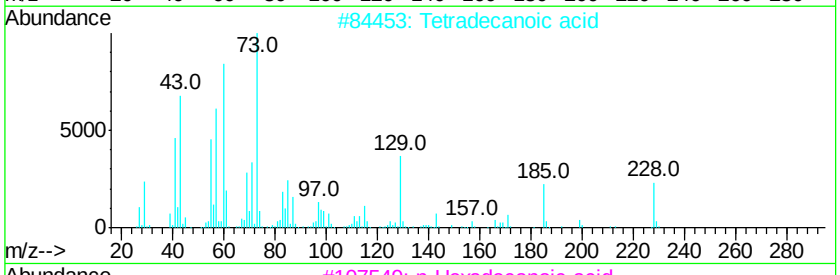
Peak Number 6 Octadecanoic acid Concentration Rank 3

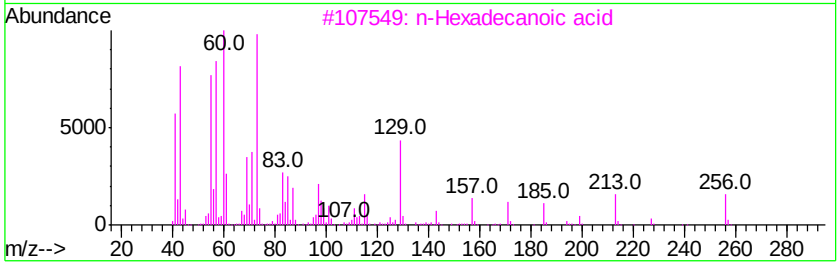
R.T.	EstConc	Area	Relative to ISTD	R.T.
17.01	10.55 ng	385097	Chrysene-d12	18.62

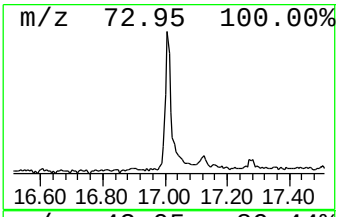
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76

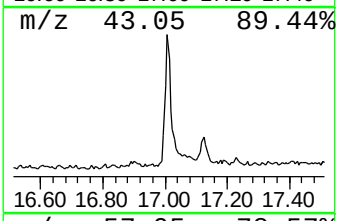


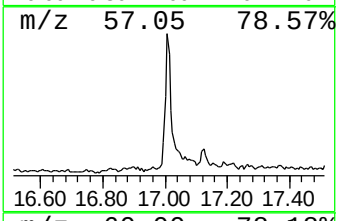


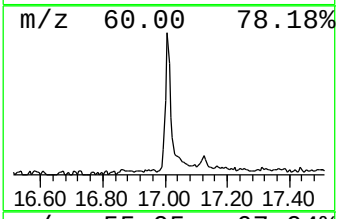


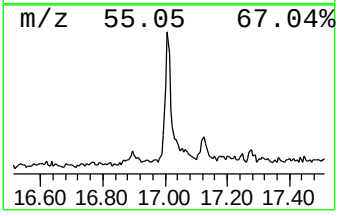












Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051217\
Data File : BF095111.D
Acq On : 12 May 2017 14:44
Operator : SJ/MA
Sample : I3100-08
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5A-051017

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...	4.99	5.3	ng	127993	1	7.70	482531	20.0
unknown7.36	7.36	83.1	ng	2005020	1	7.70	482531	20.0
Decane, 2,6,7-tri...	7.78	2.0	ng	49235	1	7.70	482531	20.0
n-Hexadecanoic acid	15.92	5.2	ng	207444	4	14.95	798756	20.0
Octadecanoic acid	17.01	10.6	ng	385097	5	18.62	729898	20.0