LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086759.D
Acq On : 7 May 2016 8:03
Operator : UM/SJ
Sample : H2863-01
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-MICHELINI-001

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-BF050416.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	4.899	244	246	253	rBV	202739	382437	6.65%	0.813%
2	5.310	280	282	296	rBV	4439614	4782221	83.14%	10.167%
3	6.362	371	374	382	rBV	4299089	4938967	85.87%	10.501%
4	6.476	382	384	387	rBV	4817882	4758580	82.73%	10.117%
5	6.704	402	404	406	rBV	1082310	1111553	19.33%	2.363%
6	6.864	415	418	420	rBV	2876018	3956919	68.79%	8.413%
7	7.276	451	454	456	rBV	3238713	3498764	60.83%	7.439%
8	7.390	462	464	469	rVB2	44078	74552	1.30%	0.159%
9	7.985	514	516	519	rBV	1135955	1368089	23.79%	2.909%
10	9.070	607	611	613	rBV	5174743	5751818	100.00%	12.229%
11	9.150	616	618	621	rVB	57953	73069	1.27%	0.155%
12	9.470	643	646	648	rBV	792781	805592	14.01%	1.713%
13	9.676	662	664	666	rBV	170671	170569	2.97%	0.363%
14	9.733	667	669	672	rVV	1179260	1526205	26.53%	3.245%
15	9.916	681	685	688	rBV2	30288	81737	1.42%	0.174%
16	10.179	704	708	710	rBV	246435	263780	4.59%	0.561%
17	10.396	724	727	730	rBV	77108	131137	2.28%	0.279%
18	10.533	736	739	741	rBV2	2556684	3597718	62.55%	7.649%
19	10.648	747	749	756	rVB	271999	345079	6.00%	0.734%
20	11.093	786	788	790	rBV	161574	160039	2.78%	0.340%
21	11.219	797	799	801	rBV	1502372	1471869	25.59%	3.129%
22	11.756	844	846	857	rBV	202455	280633	4.88%	0.597%
23	12.545	912	915	920	rBV	41864	73347	1.28%	0.156%
24	12.636	920	923	925	rVV	68810	86474	1.50%	0.184%
25	12.808	935	938	940	rBV	3972308	4977235	86.53%	10.582%
26	13.288	978	980	983	rBV	239139	274660	4.78%	0.584%
27	13.334	983	984	986	rVB	73725	60369	1.05%	0.128%
28	13.711	1015	1017	1026	rBV	28221	74945	1.30%	0.159%
29	13.848	1026	1029	1031	rBV	922704	1094556	19.03%	2.327%
30	15.220	1147	1149	1156	rBV	534754	861510	14.98%	1.832%

Sum of corrected areas: 47034423

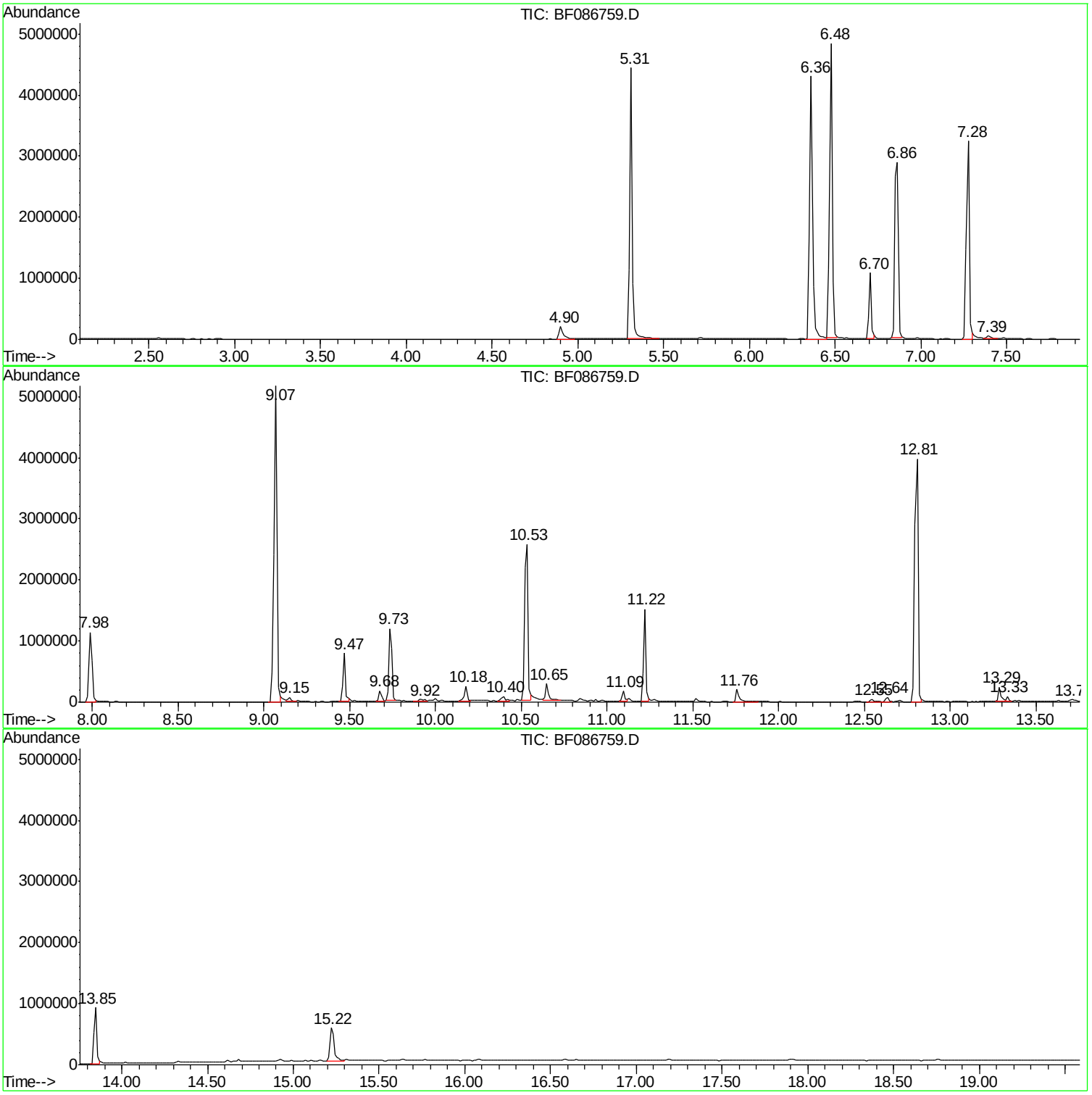
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086759.D
Acq On : 7 May 2016 8:03
Operator : UM/SJ
Sample : H2863-01
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
IM-MICHELINI-001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086759.D
Acq On : 7 May 2016 8:03
Operator : UM/SJ
Sample : H2863-01
Misc :
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Instrument : BNA_F
ClientSampleId : IM-MICHELINI-001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

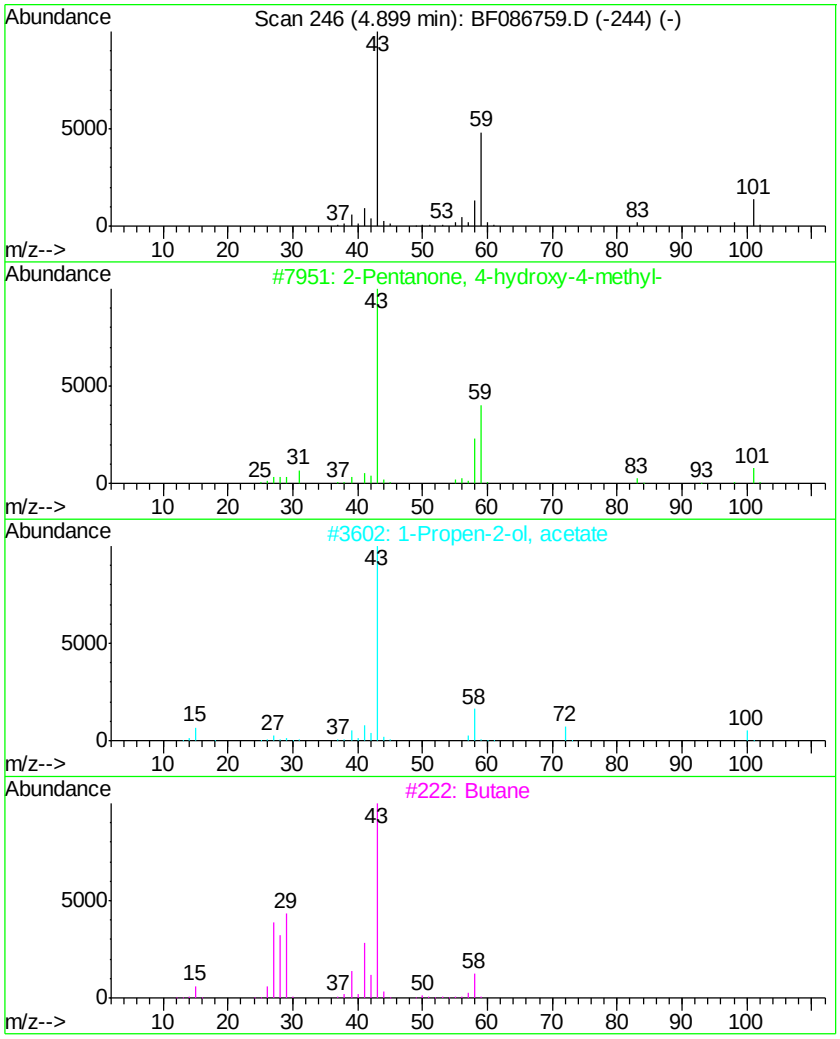
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

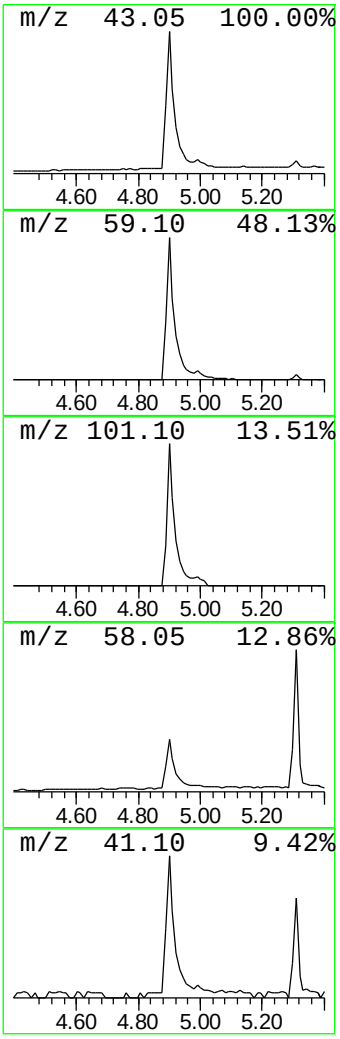
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	13.76 ng	382437	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3	Butane	58	C4H10	000106-97-8	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Diacetamide	101	C4H7NO2	000625-77-4	9





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Data File : BF086759.D
Acq On : 7 May 2016 8:03
Operator : UM/SJ
Sample : H2863-01
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-MICHELINI-001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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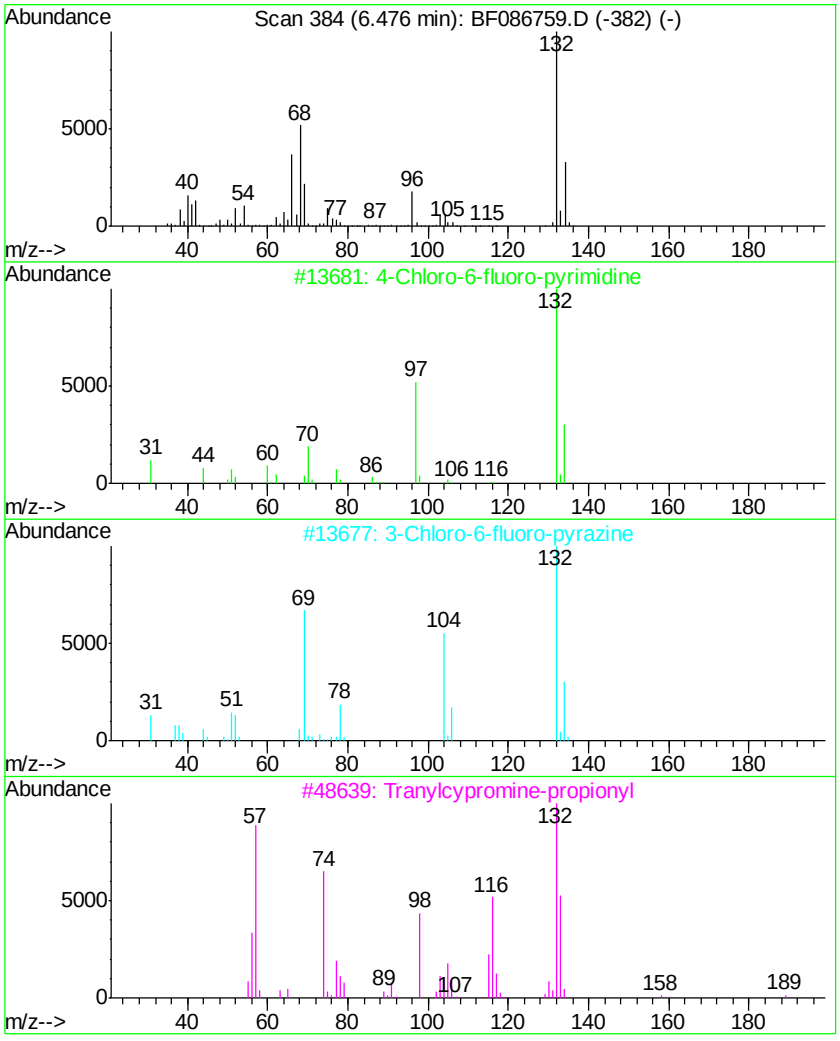
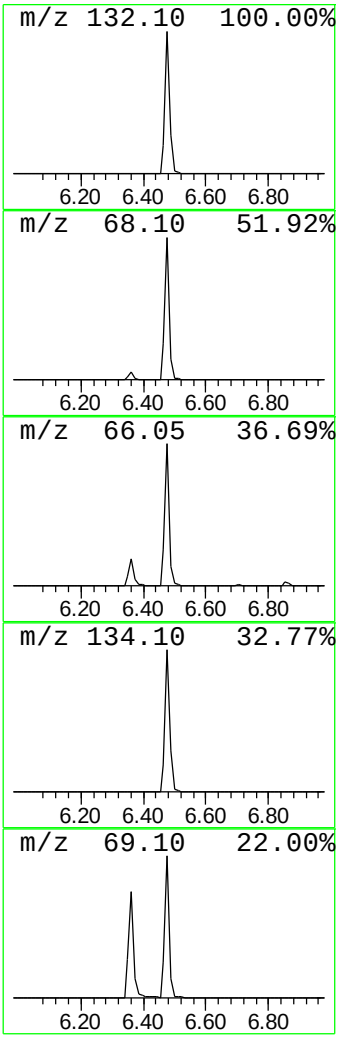
Peak Number 2 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	171.24 ng	4758580	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
4	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	22
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086759.D
Acq On : 7 May 2016 8:03
Operator : UM/SJ
Sample : H2863-01
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-MICHELINI-001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

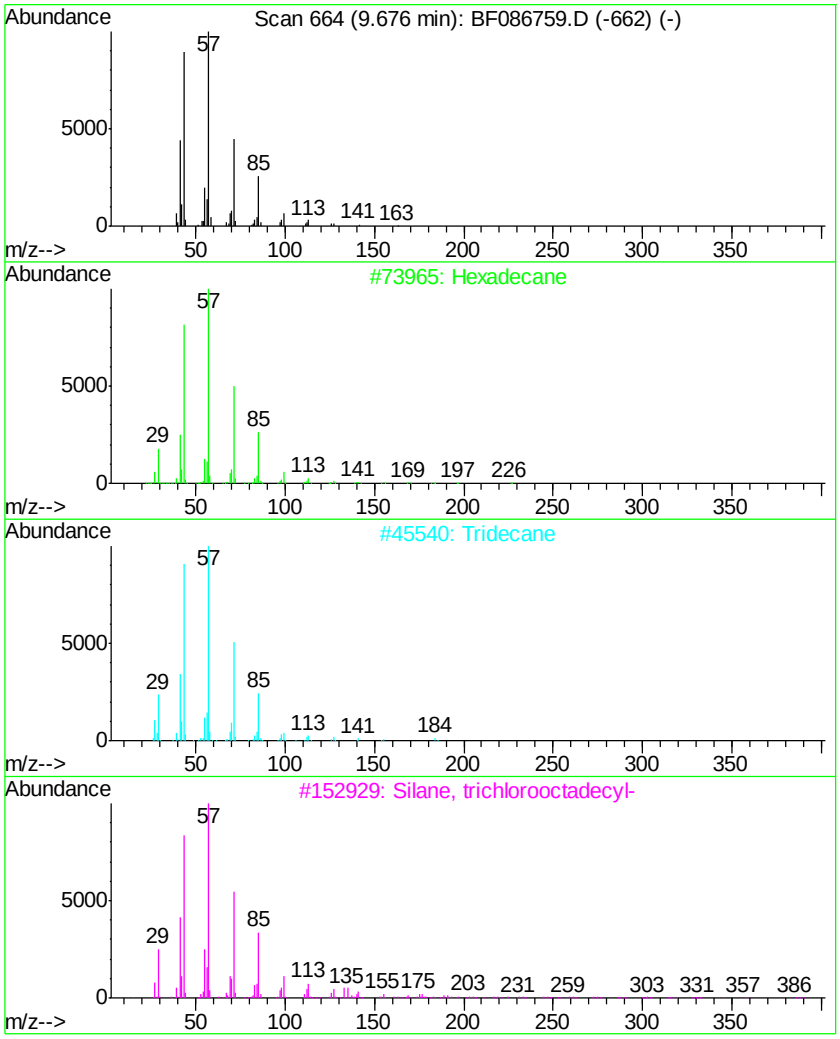
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

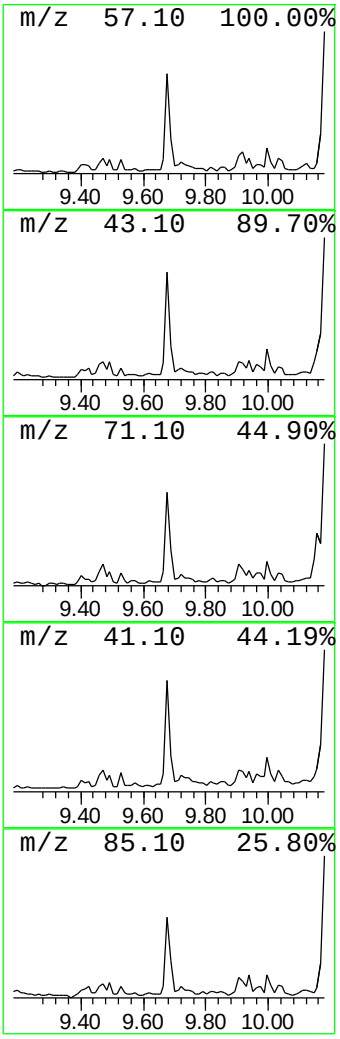
****

Peak Number 4 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.68	4.47 ng	170569	Acenaphthene-d10	9.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Tridecane	184	C13H28	000629-50-5	90
3	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	90
4	Pentadecane	212	C15H32	000629-62-9	86
5	Eicosane	282	C20H42	000112-95-8	83





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086759.D
Acq On : 7 May 2016 8:03
Operator : UM/SJ
Sample : H2863-01
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-MICHELINI-001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

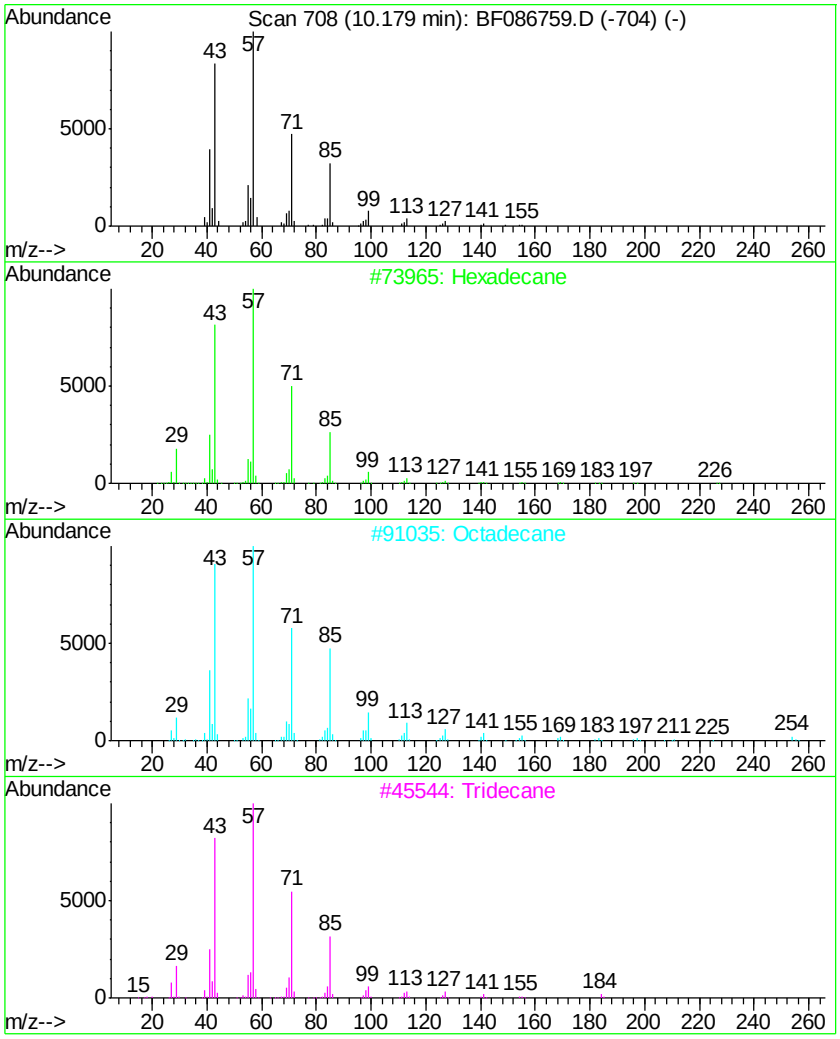
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

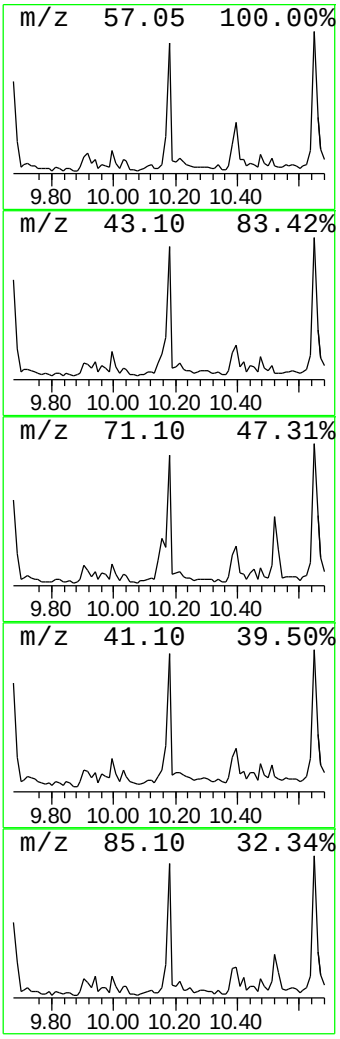
****

Peak Number 5 Octadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.18	6.91 ng	263780	Acenaphthene-d10	9.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Octadecane	254	C18H38	000593-45-3	86
3	Tridecane	184	C13H28	000629-50-5	86
4	Pentadecane	212	C15H32	000629-62-9	86
5	Decane, 3-bromo-	220	C10H21Br	030571-71-2	80





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086759.D
Acq On : 7 May 2016 8:03
Operator : UM/SJ
Sample : H2863-01
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-MICHELINI-001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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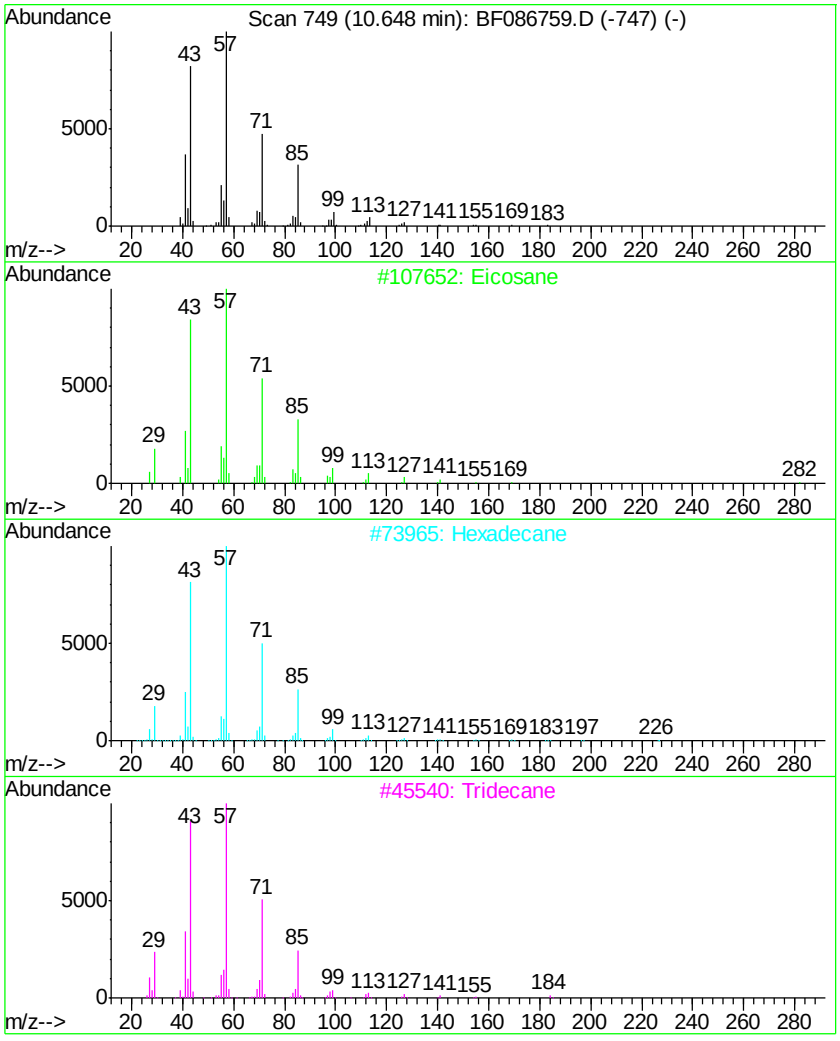
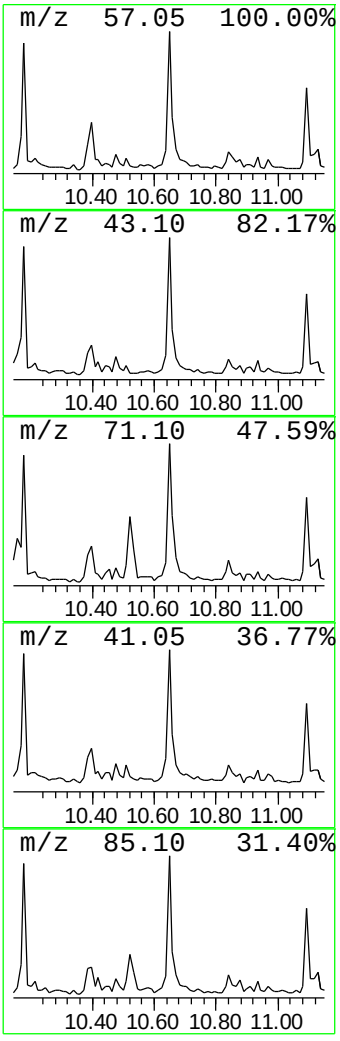
Peak Number 6 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	9.38 ng	345079	Phenanthrene-d10	11.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Hexadecane	226	C16H34	000544-76-3	91
3	Tridecane	184	C13H28	000629-50-5	90
4	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	90
5	Tridecane, 7-propyl-	226	C16H34	055045-09-5	86





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Operator : UM/SJ
Sample : H2863-01
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-MICHELINI-001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

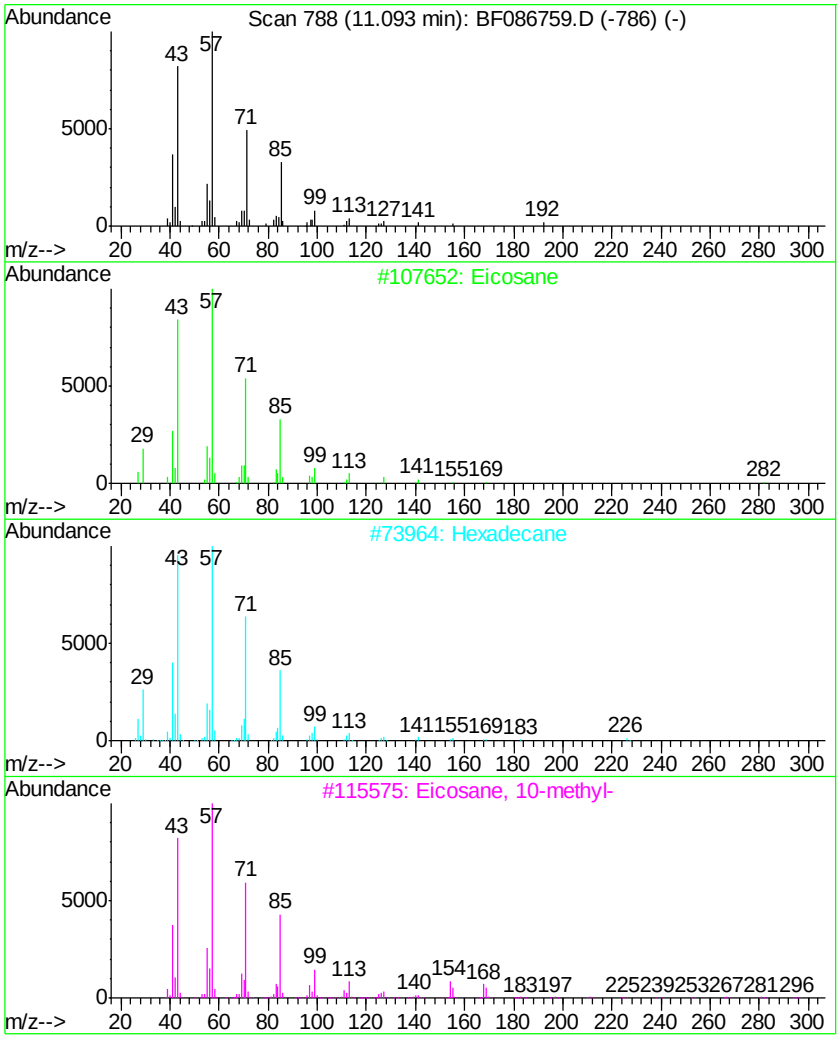
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

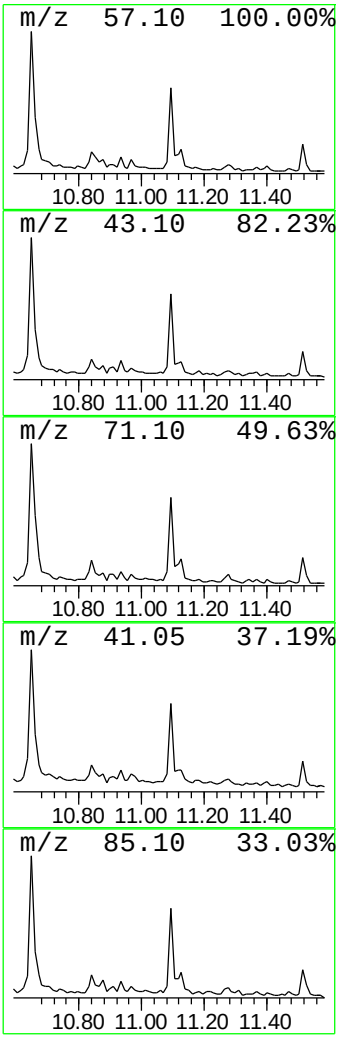
****

Peak Number 7 Eicosane, 10-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.09	4.35 ng	160039	Phenanthrene-d10	11.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Hexadecane	226	C16H34	000544-76-3	91
3	Eicosane, 10-methyl-	296	C21H44	054833-23-7	90
4	Tridecane	184	C13H28	000629-50-5	90
5	Dodecane	170	C12H26	000112-40-3	90





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Operator : UM/SJ
Sample : H2863-01
Misc :
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Instrument : BNA_F
ClientSampleId : IM-MICHELINI-001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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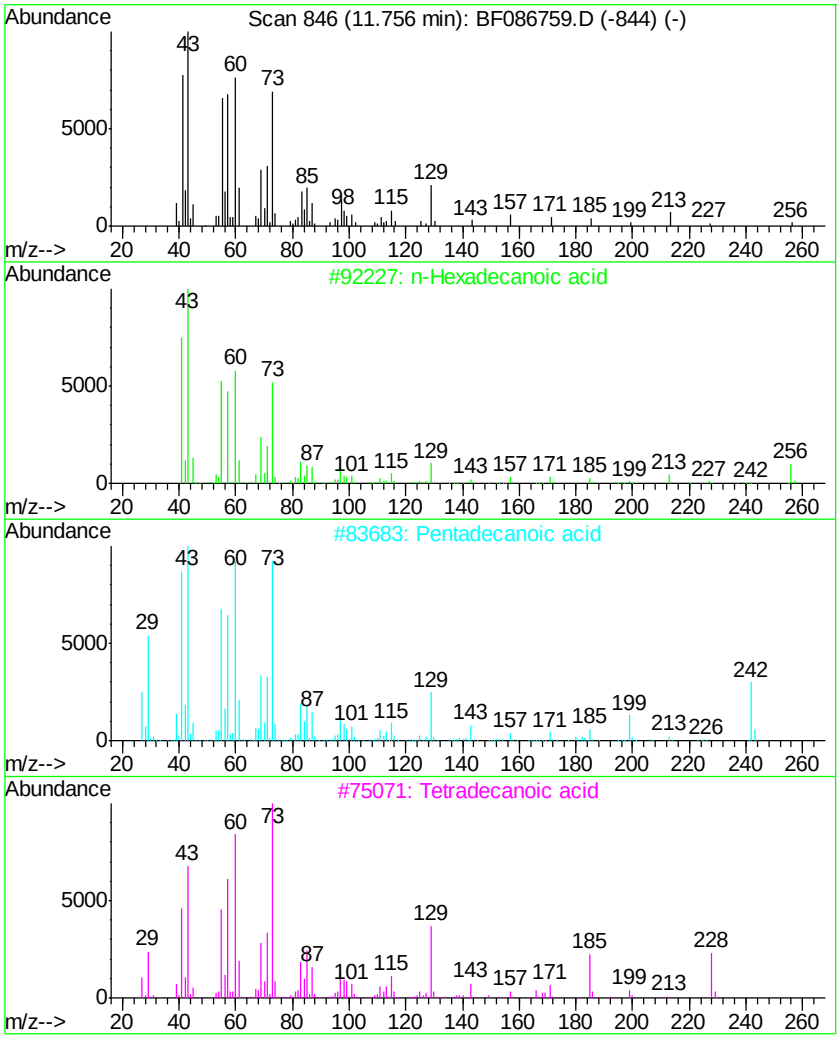
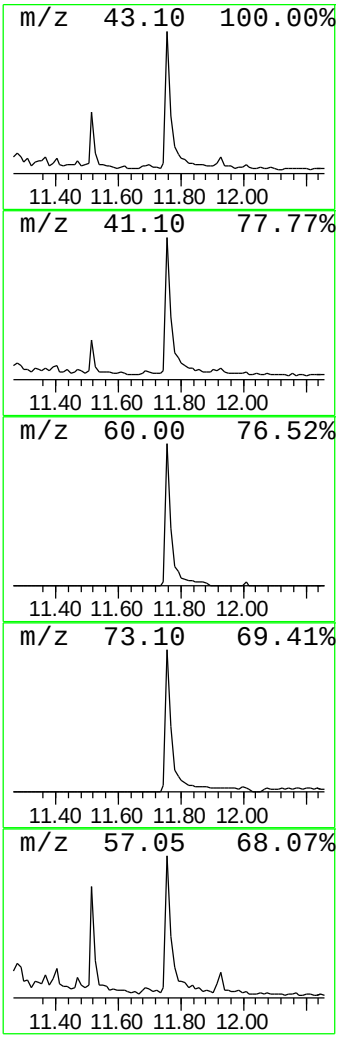
Peak Number 8 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.76	7.63 ng	280633	Phenanthrene-d10	11.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Undecanoic acid	186	C11H22O2	000112-37-8	80
5	Dodecanoic acid	200	C12H24O2	000143-07-7	59





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Sample : H2863-01
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-MICHELINI-001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

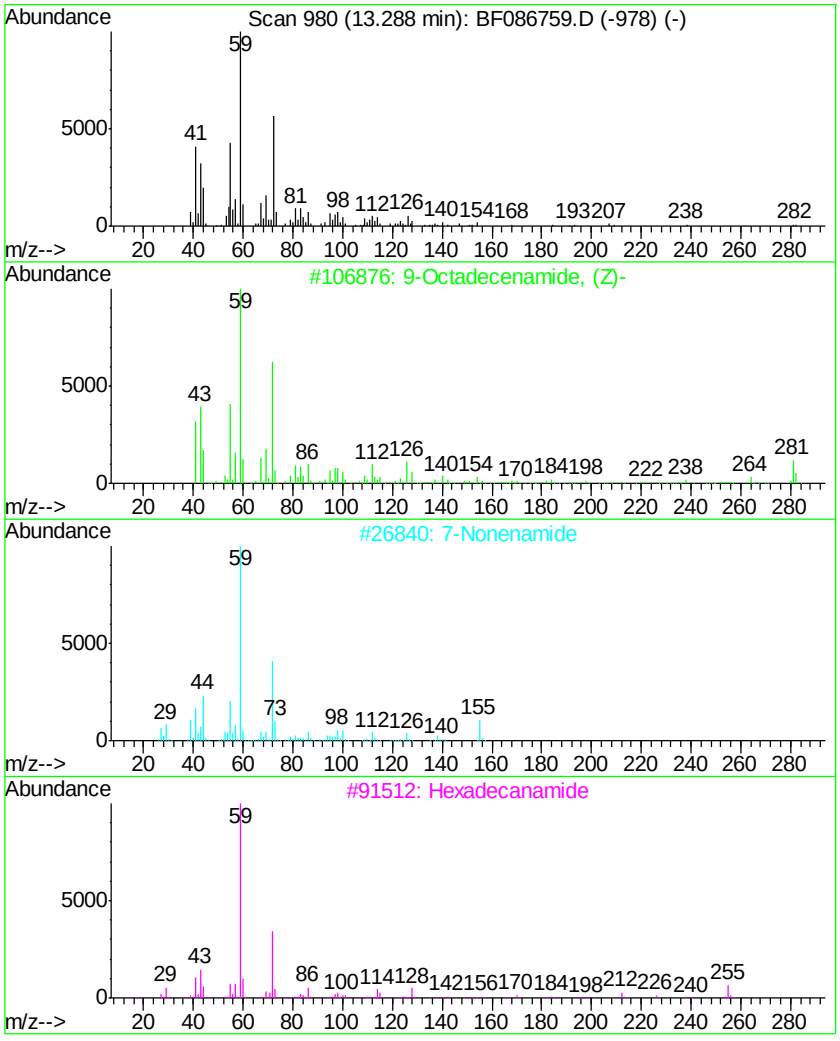
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

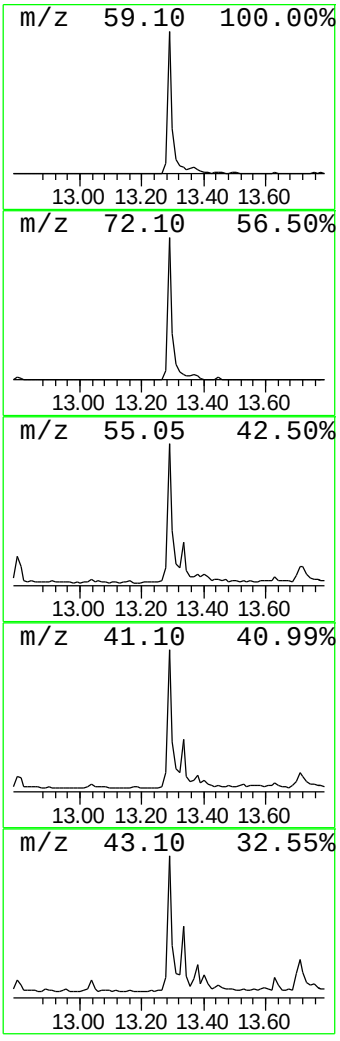
****

Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.29	10.04 ng	274660	Chrysene-d12	13.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	76
2	7-Nonenamide	155	C9H17NO	090949-53-4	64
3	Hexadecanamide	255	C16H33NO	000629-54-9	59
4	Hexanamide	115	C6H13NO	000628-02-4	58
5	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	56





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086759.D
Acq On : 7 May 2016 8:03
Operator : UM/SJ
Sample : H2863-01
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IM-MICHELINI-001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.90	13.8	ng	382437	1	6.70	1111550	40.0
unknown6.48	6.48	171.2	ng	4758580	1	6.70	1111550	40.0
Hexadecane	9.68	4.5	ng	170569	3	9.73	1526210	40.0
Octadecane	10.18	6.9	ng	263780	3	9.73	1526210	40.0
Eicosane	10.65	9.4	ng	345079	4	11.22	1471870	40.0
Eicosane, 10-methyl-	11.09	4.3	ng	160039	4	11.22	1471870	40.0
n-Hexadecanoic acid	11.76	7.6	ng	280633	4	11.22	1471870	40.0
9-Octadecenamide,...	13.29	10.0	ng	274660	5	13.85	1094560	40.0