LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041516\
Data File : BF086233.D
Acq On : 15 Apr 2016 23:06
Operator : UM/SJ
Sample : H2402-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1-4-7-16

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-BF041516.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	2.156	4	6	24	rVB	122294	339555	4.16%	0.562%
2	5.082	259	262	266	rVB	179967	271063	3.32%	0.449%
3	5.482	294	297	300	rBV	3384969	3513594	43.04%	5.819%
4	6.510	384	387	389	rBV	2869723	2350489	28.79%	3.893%
5	6.659	397	400	402	rBV	5906959	6012563	73.65%	9.958%
6	6.887	418	420	423	rBV	1454420	1815167	22.23%	3.006%
7	7.047	431	434	437	rBV	5211434	5737859	70.28%	9.503%
8	7.459	466	470	472	rVB	4977839	5843111	71.57%	9.677%
9	7.688	485	490	494	rBV2	51388	114894	1.41%	0.190%
10	7.939	510	512	514	rVB	102712	158766	1.94%	0.263%
11	8.099	521	526	527	rBV3	114444	277298	3.40%	0.459%
12	8.133	527	529	530	rVV	132084	191526	2.35%	0.317%
13	8.179	530	533	535	rVV	2912046	2834108	34.71%	4.694%
14	8.213	535	536	538	rVB	198852	141409	1.73%	0.234%
15	8.305	541	544	546	rBV3	70561	192358	2.36%	0.319%
16	8.385	549	551	552	rVV	218161	233656	2.86%	0.387%
17	8.430	554	555	558	rVV2	83762	136750	1.68%	0.226%
18	8.499	559	561	563	rVB	280912	246223	3.02%	0.408%
19	8.545	563	565	569	rBV2	63650	114164	1.40%	0.189%
20	8.636	571	573	575	rVB2	104223	120966	1.48%	0.200%
21	8.693	575	578	580	rBV2	107944	181698	2.23%	0.301%
22	8.750	580	583	586	rVV2	129192	214108	2.62%	0.355%
23	8.796	586	587	589	rVB2	100929	99342	1.22%	0.165%
24	8.888	589	595	596	rBV3	123131	312955	3.83%	0.518%
25	8.945	596	600	602	rVB2	179293	346478	4.24%	0.574%
26	9.025	605	607	609	rVB	121077	134436	1.65%	0.223%
27	9.093	612	613	616	rBV2	76973	118978	1.46%	0.197%
28	9.196	621	622	624	rVB	96264	95836	1.17%	0.159%
29	9.265	624	628	630	rBV	5459566	8164135	100.00%	13.521%
30	9.333	633	634	639	rVB3	119757	200020	2.45%	0.331%
31	9.516	648	650	651	rBV2	60709	104138	1.28%	0.172%
32	9.539	651	652	655	rVB2	80831	123060	1.51%	0.204%
33	9.608	655	658	660	rBV2	59745	147199	1.80%	0.244%
34	9.653	660	662	664	rVB	121725	174680	2.14%	0.289%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041516\
Data File : BF086233.D
Acq On : 15 Apr 2016 23:06
Operator : UM/SJ
Sample : H2402-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1-4-7-16

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-BF041516.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	9.871	680	681	684	rVB	102526	95380	1.17%	0.158%
36	9.928	684	686	689	rBV	2040130	2521525	30.89%	4.176%
37	10.374	723	725	726	rVB	109549	94953	1.16%	0.157%
38	10.716	752	755	758	rBV2	3457902	4362189	53.43%	7.225%
39	10.842	764	766	771	rVB	159741	192467	2.36%	0.319%
40	11.288	803	805	807	rBV	147202	131577	1.61%	0.218%
41	11.414	813	816	818	rBV	2745975	2371939	29.05%	3.928%
42	11.471	818	821	828	rVB	49162	85661	1.05%	0.142%
43	11.951	861	863	871	rBV2	214853	381702	4.68%	0.632%
44	12.728	929	931	937	rBV2	238414	381235	4.67%	0.631%
45	13.002	952	955	958	rBV	5132667	5662421	69.36%	9.378%
46	13.894	1031	1033	1039	rBV3	52687	90667	1.11%	0.150%
47	14.042	1044	1046	1049	rBV	1476246	1602673	19.63%	2.654%
48	15.483	1169	1172	1175	rBV	1082455	1342498	16.44%	2.223%

Sum of corrected areas: 60379469

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041516\
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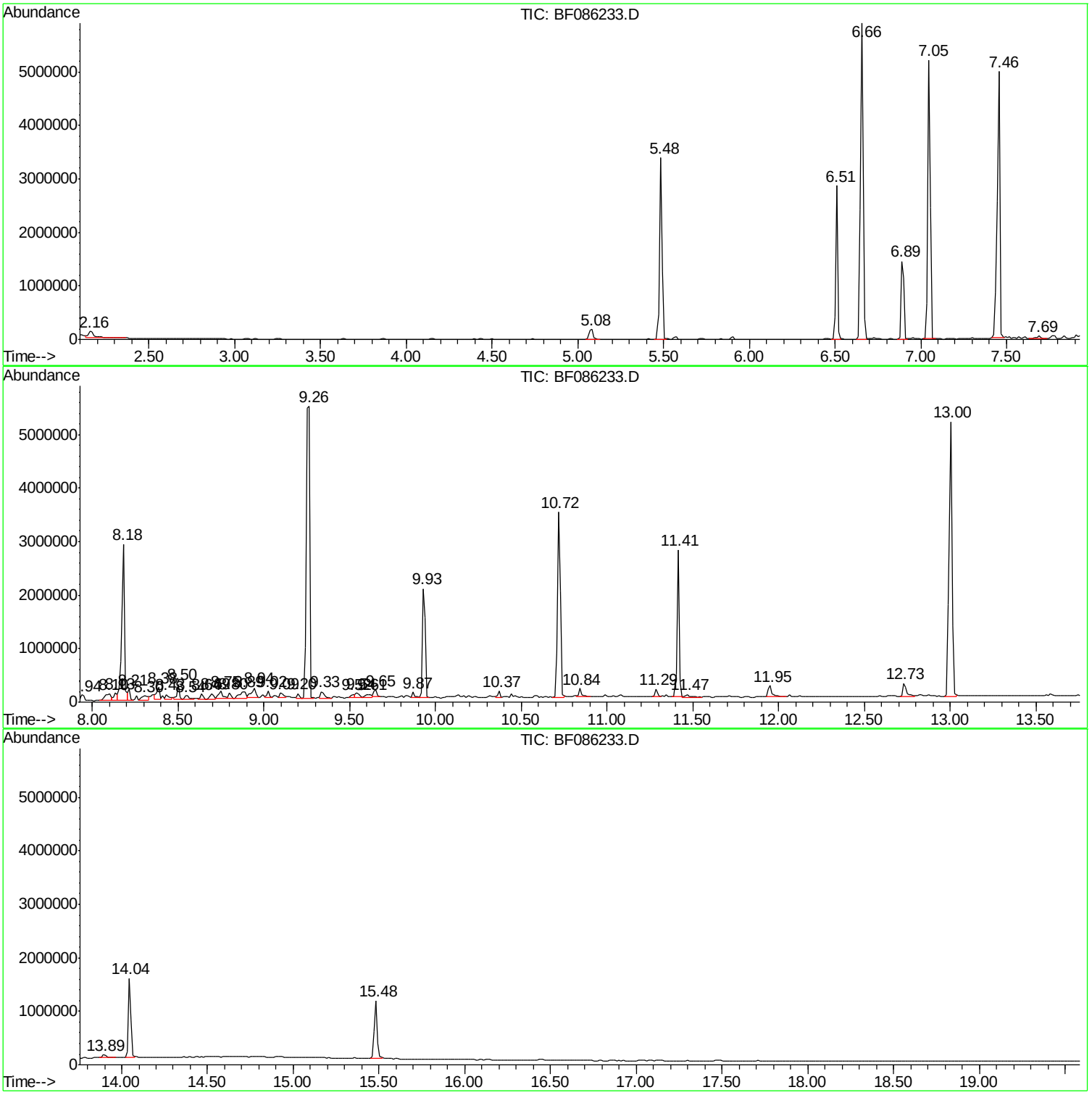
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1-4-7-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041516\
Data File : BF086233.D
Acq On : 15 Apr 2016 23:06
Operator : UM/SJ
Sample : H2402-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1-4-7-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

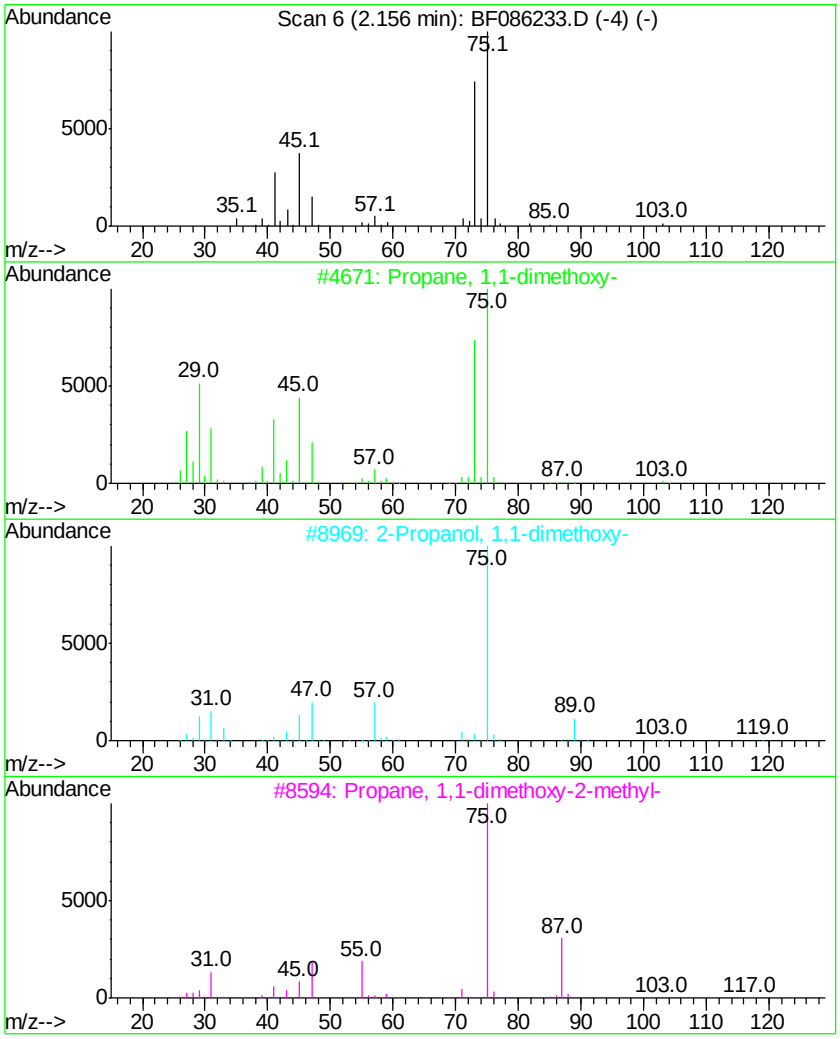
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

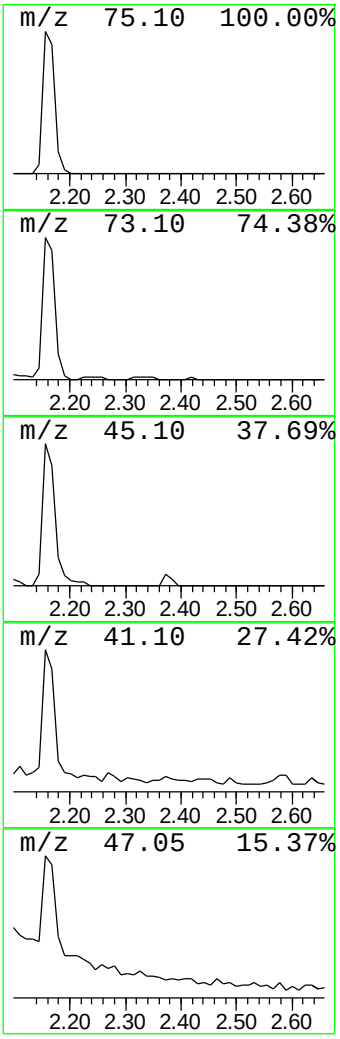
****

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	3.74 ng	339555	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2	2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	42
3	Propane, 1,1-dimethoxy-2-methyl-	118	C6H14O2	041632-89-7	33
4	Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9
5	Ethane, 1,1,2-trimethoxy-	120	C5H12O3	024332-20-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041516\
Data File : BF086233.D
Acq On : 15 Apr 2016 23:06
Operator : UM/SJ
Sample : H2402-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1-4-7-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041516.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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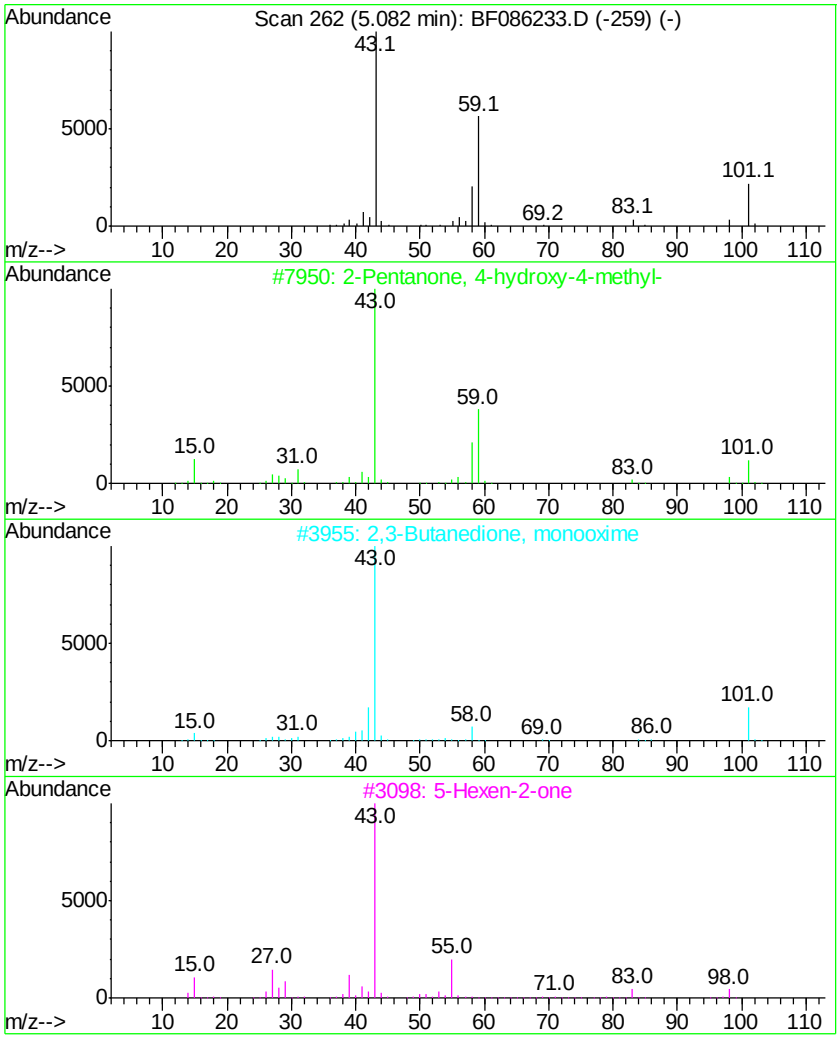
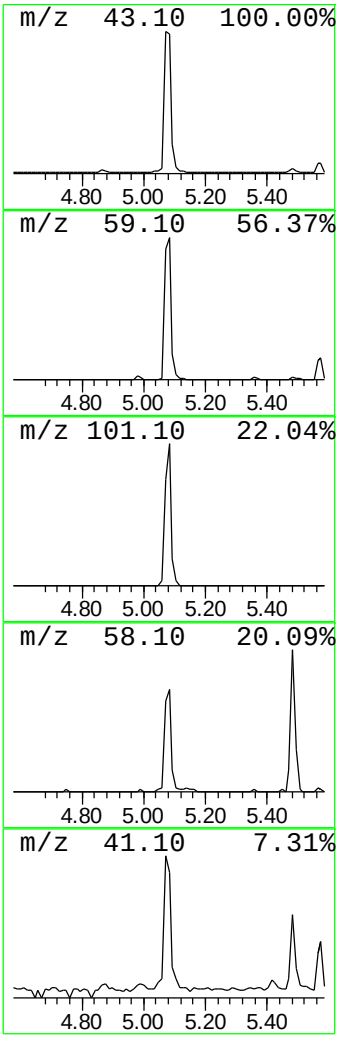
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	2.99 ng	271063	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Acetone	58	C3H6O	000067-64-1	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041516\
Data File : BF086233.D
Acq On : 15 Apr 2016 23:06
Operator : UM/SJ
Sample : H2402-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1-4-7-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

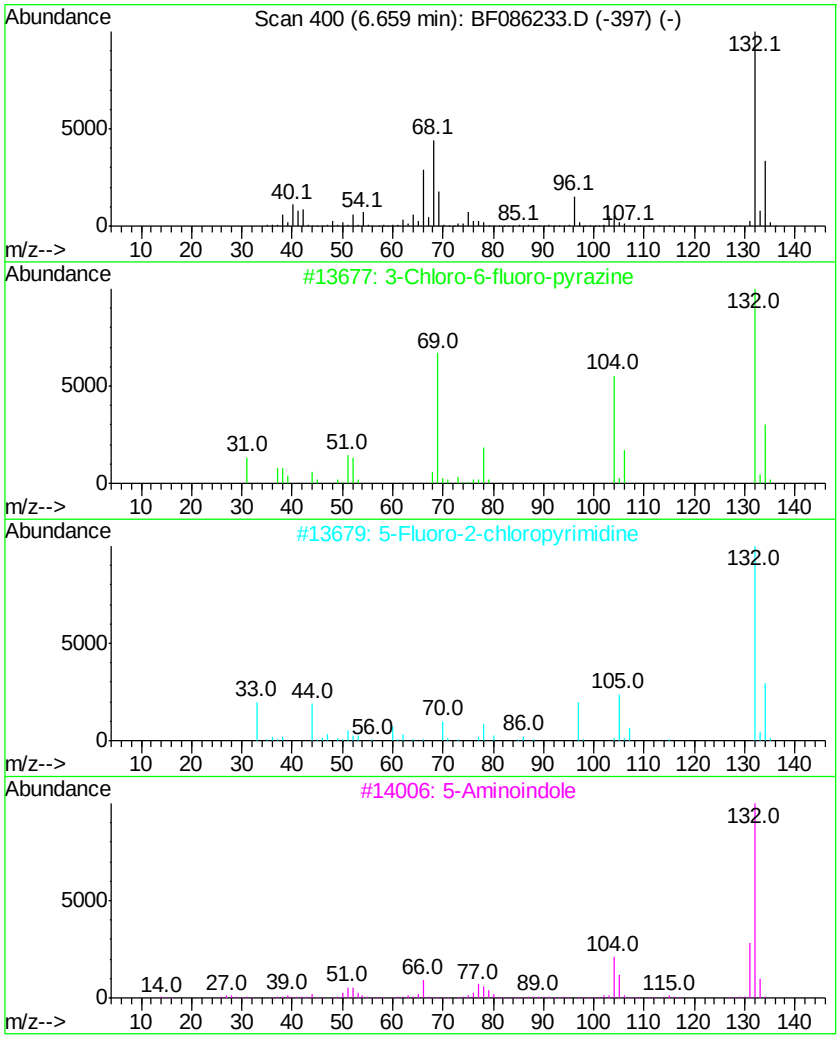
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

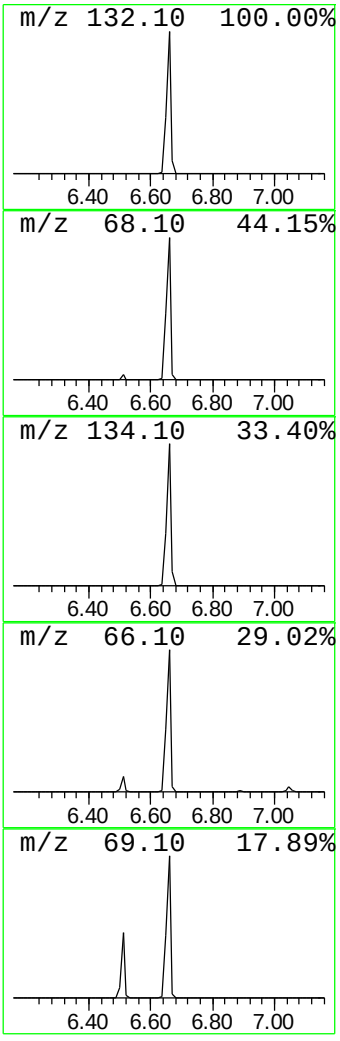
****

Peak Number 3 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	66.25 ng	6012560	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





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Data File : BF086233.D
Acq On : 15 Apr 2016 23:06
Operator : UM/SJ
Sample : H2402-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1-4-7-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041516.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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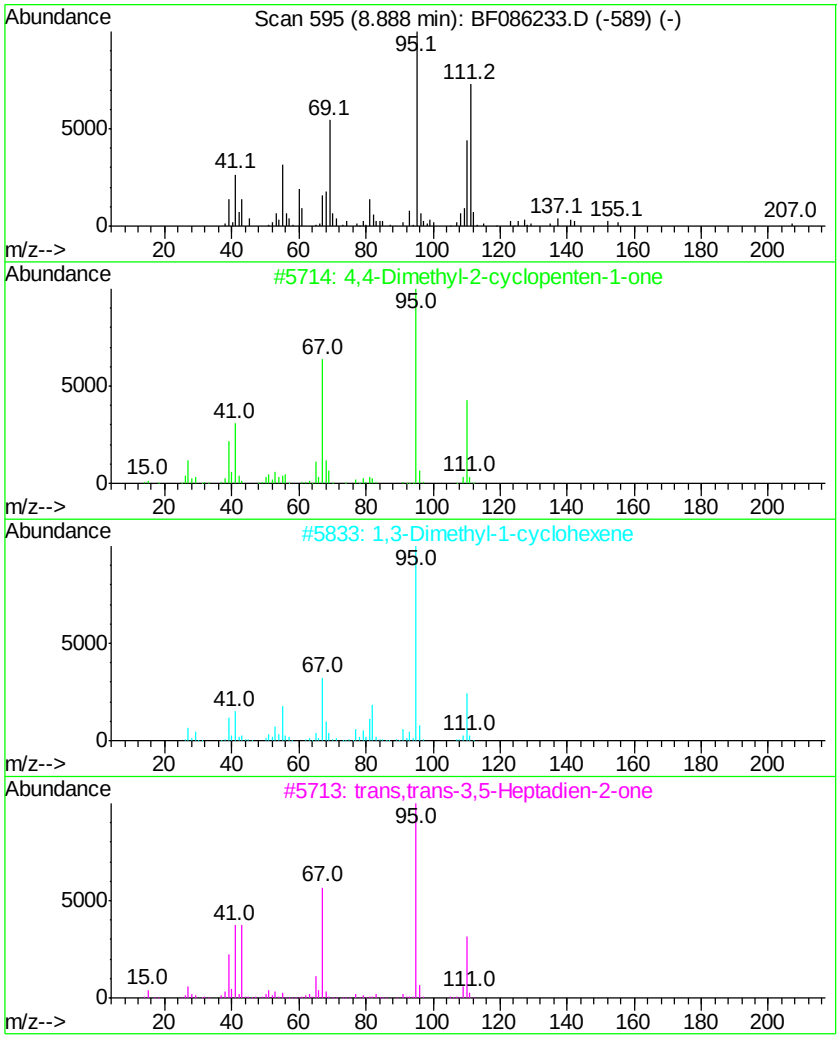
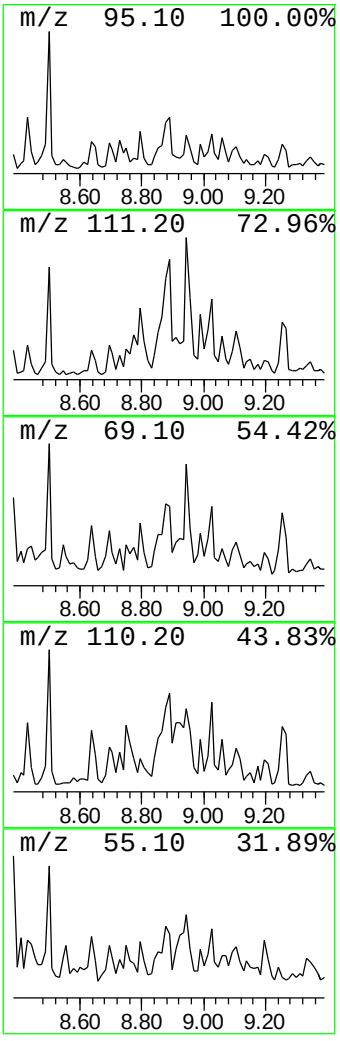
Peak Number 5 4,4-Dimethyl-2-cyclopenten-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.89	2.21 ng	312955	Naphthalene-d8	8.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4-Dimethyl-2-cyclopenten-1-one	110	C7H10O	022748-16-9	50
2	1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	50
3	trans,trans-3,5-Heptadien-2-one	110	C7H10O	018402-90-9	50
4	Ethanone, 1-(2-furanyl)-	110	C6H6O2	001192-62-7	47
5	Ethanone, 1-(1H-pyrazol-4-yl)-	110	C5H6N2O	025016-16-4	47





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041516\
Data File : BF086233.D
Acq On : 15 Apr 2016 23:06
Operator : UM/SJ
Sample : H2402-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1-4-7-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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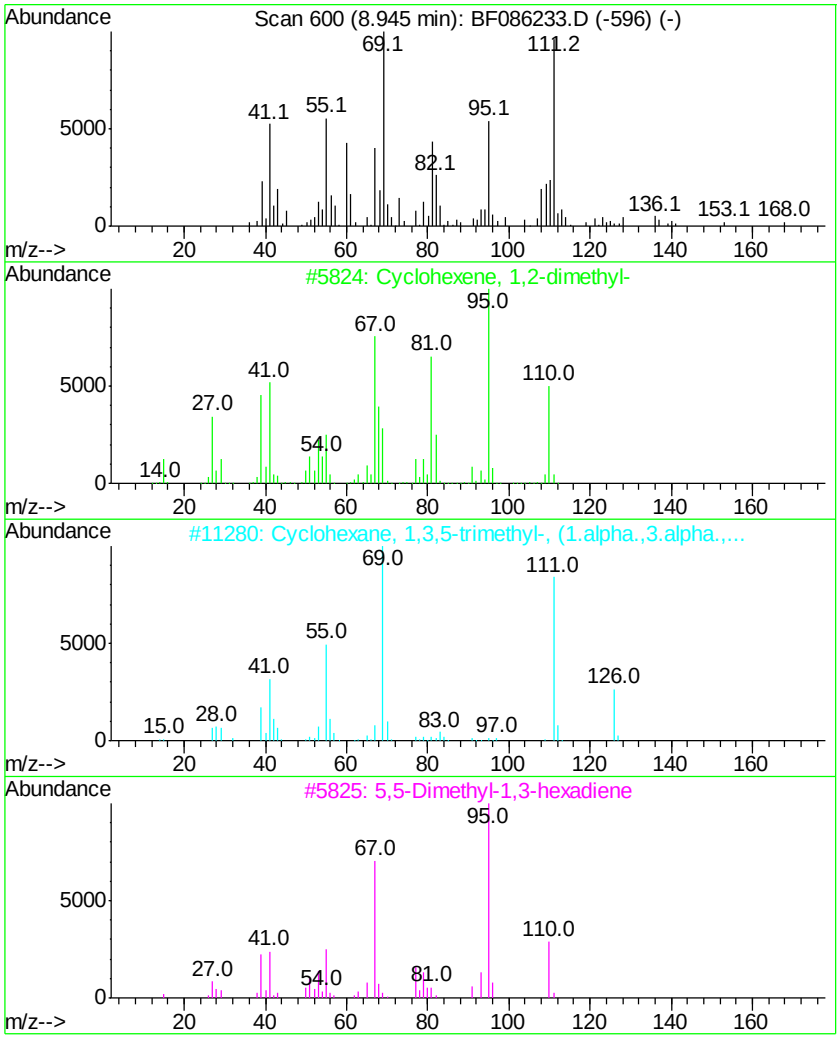
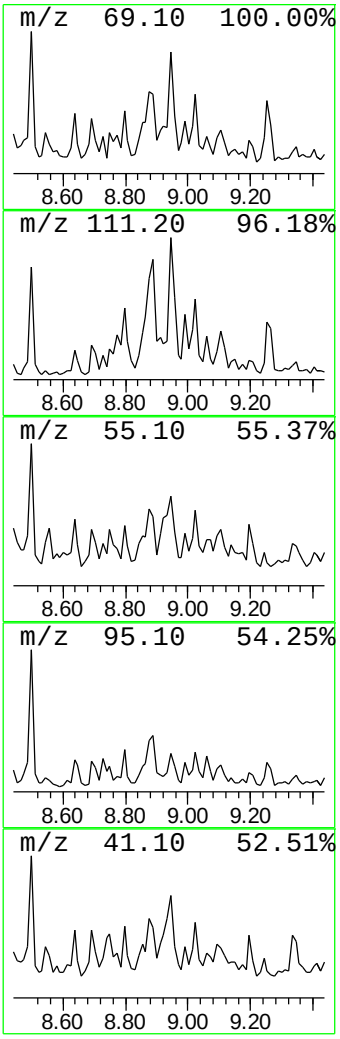
****

Peak Number 6 unknown8.94 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.94	2.45 ng	346478	Naphthalene-d8	8.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene, 1,2-dimethyl-	110	C8H14	001674-10-8	35
2	Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-27-3	35
3	5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	25
4	6-Methyl-1,5-heptadiene	110	C8H14	007270-50-0	25
5	Cyclohexane, 1-ethyl-2,4-dimethyl-	140	C10H20	061142-69-6	25





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Operator : UM/SJ
Sample : H2402-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1-4-7-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

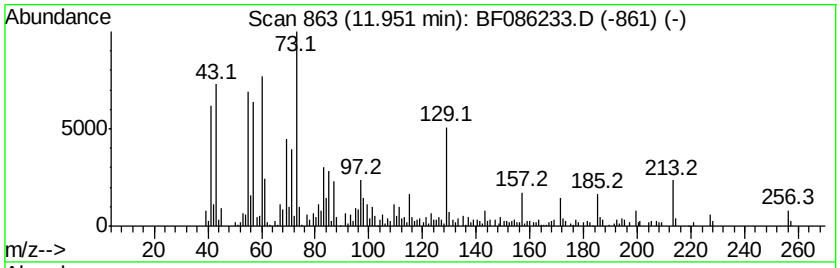
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

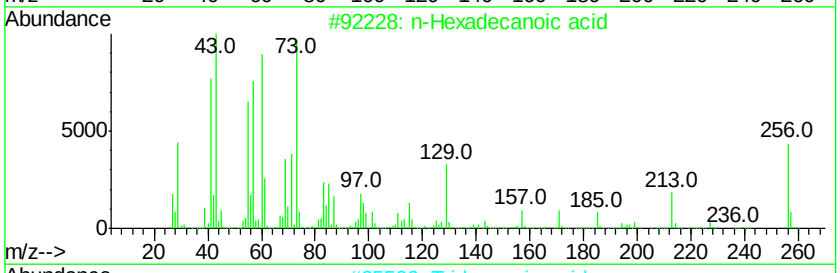
****

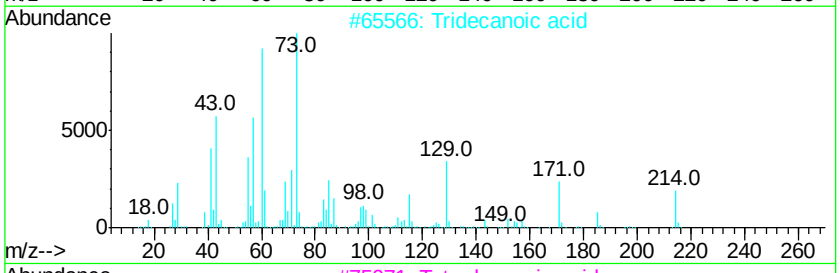
Peak Number 7 n-Hexadecanoic acid Concentration Rank 4

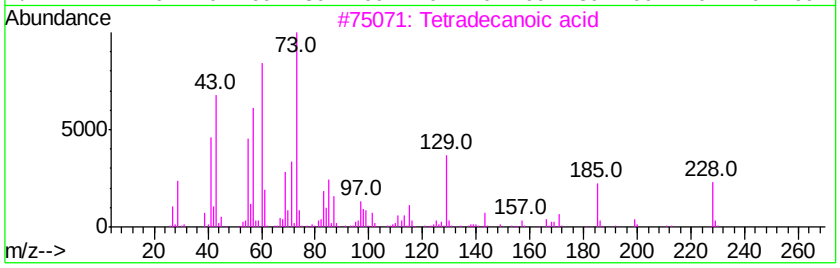
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	3.22 ng	381702	Phenanthrene-d10	11.41

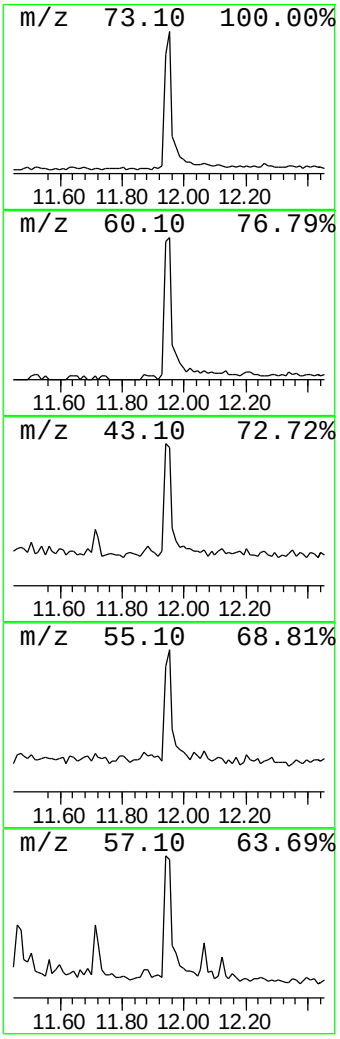
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76











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Acq On : 15 Apr 2016 23:06
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Sample : H2402-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1-4-7-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

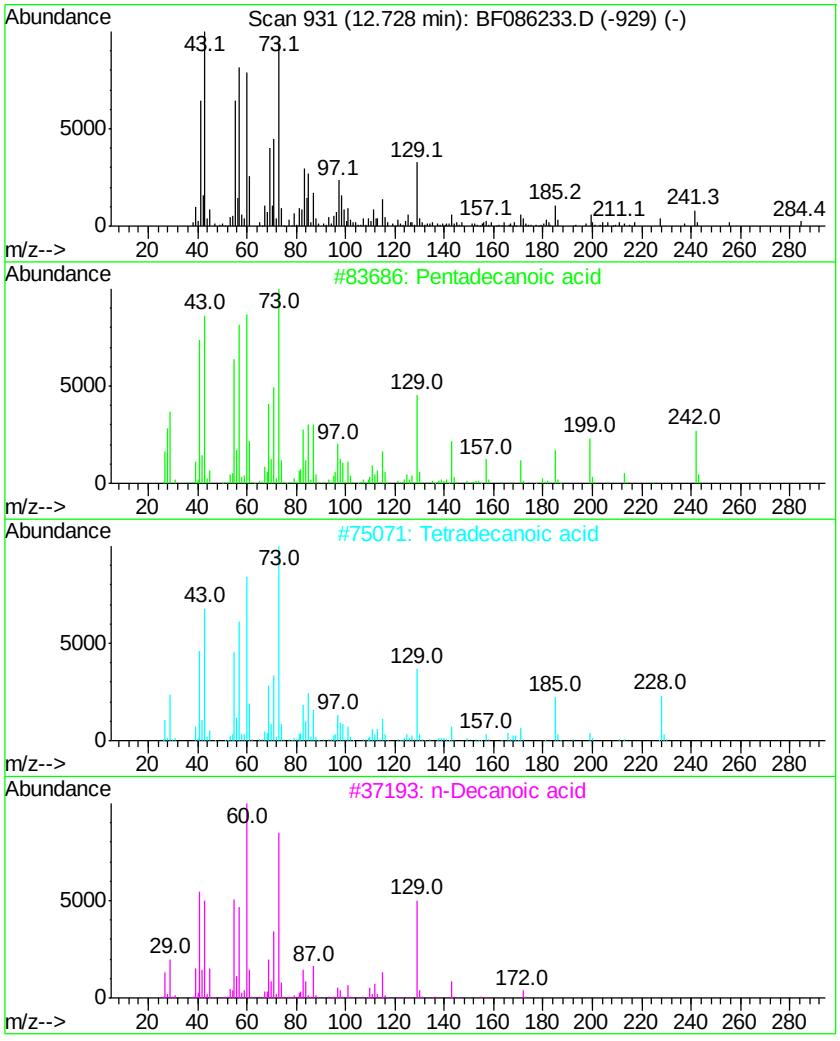
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

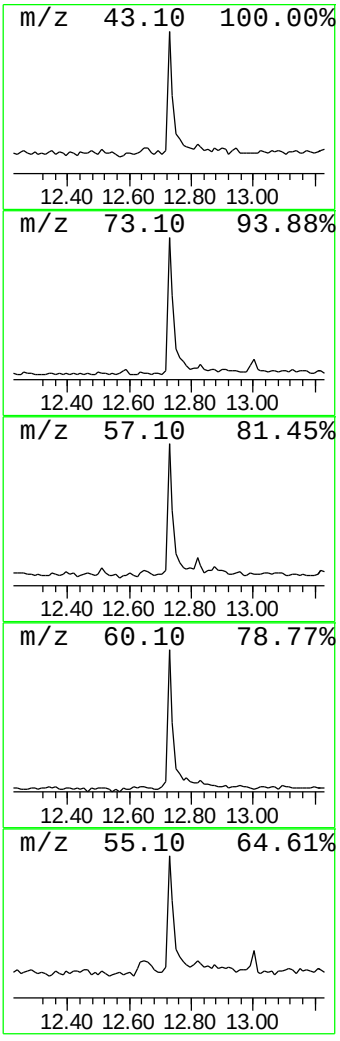
****

Peak Number 8 Pentadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	3.21 ng	381235	Phenanthrene-d10	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
3	n-Decanoic acid	172	C10H20O2	000334-48-5	49
4	Undecane	156	C11H24	001120-21-4	25
5	Hexadecane	226	C16H34	000544-76-3	11





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041516\
Data File : BF086233.D
Acq On : 15 Apr 2016 23:06
Operator : UM/SJ
Sample : H2402-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1-4-7-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041516.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
Propane, 1,1-dime...	2.16	3.7	ng	339555	1	6.90	1815170	20.0
2-Pentanone, 4-hy...	5.08	3.0	ng	271063	1	6.90	1815170	20.0
unknown6.66	6.66	66.3	ng	6012560	1	6.90	1815170	20.0
4,4-Dimethyl-2-cy...	8.89	2.2	ng	312955	2	8.18	2834110	20.0
unknown8.94	8.94	2.5	ng	346478	2	8.18	2834110	20.0
n-Hexadecanoic acid	11.95	3.2	ng	381702	4	11.41	2371940	20.0
Pentadecanoic acid	12.73	3.2	ng	381235	4	11.41	2371940	20.0