LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF043015\
Data File : BF078861.D
Acq On : 30 Apr 2015 21:47
Operator : TP/IZ
Sample : G2067-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SINGSING-SS2-0-6

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-BF043015.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	1.541	28	31	34	rVB	6685891	7710678	100.00%	18.598%
2	1.678	39	43	46	rVB	220431	466783	6.05%	1.126%
3	1.781	50	52	57	rBV	356022	664432	8.62%	1.603%
4	1.861	57	59	62	rVB	278001	343166	4.45%	0.828%
5	1.907	62	63	105	rVB	3314563	6201635	80.43%	14.959%
6	5.176	347	349	357	rVB	591217	746520	9.68%	1.801%
7	5.667	389	392	395	rBV	2377556	2335431	30.29%	5.633%
8	6.913	499	501	504	rBV	1954300	2414753	31.32%	5.824%
9	7.085	513	516	518	rBV	1937613	2581910	33.48%	6.228%
10	7.370	538	541	543	rVB	554086	487930	6.33%	1.177%
11	7.553	555	557	560	rVB	1705032	1957931	25.39%	4.723%
12	8.056	599	601	604	rBV	1497643	1471282	19.08%	3.549%
13	8.948	677	679	681	rBV	726058	655485	8.50%	1.581%
14	10.296	794	797	799	rBV	3206909	3234622	41.95%	7.802%
15	10.799	839	841	843	rBV	158238	175404	2.27%	0.423%
16	11.119	867	869	872	rVB	603082	705994	9.16%	1.703%
17	12.102	952	955	958	rBV	2084672	2015403	26.14%	4.861%
18	12.297	970	972	977	rBV	55943	97244	1.26%	0.235%
19	12.971	1028	1031	1033	rBV	807365	799008	10.36%	1.927%
20	14.754	1184	1187	1191	rBV2	46824	89208	1.16%	0.215%
21	14.971	1203	1206	1208	rBV	3526978	3769958	48.89%	9.093%
22	15.600	1255	1261	1264	rBV	147882	309906	4.02%	0.748%
23	15.645	1264	1265	1268	rVB	85488	89510	1.16%	0.216%
24	16.125	1305	1307	1315	rBV	287607	430429	5.58%	1.038%
25	16.263	1316	1319	1321	rBV	800819	863959	11.20%	2.084%
26	18.011	1469	1472	1475	rBV	673007	840025	10.89%	2.026%

Sum of corrected areas: 41458606

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF043015\
Data File : BF078861.D
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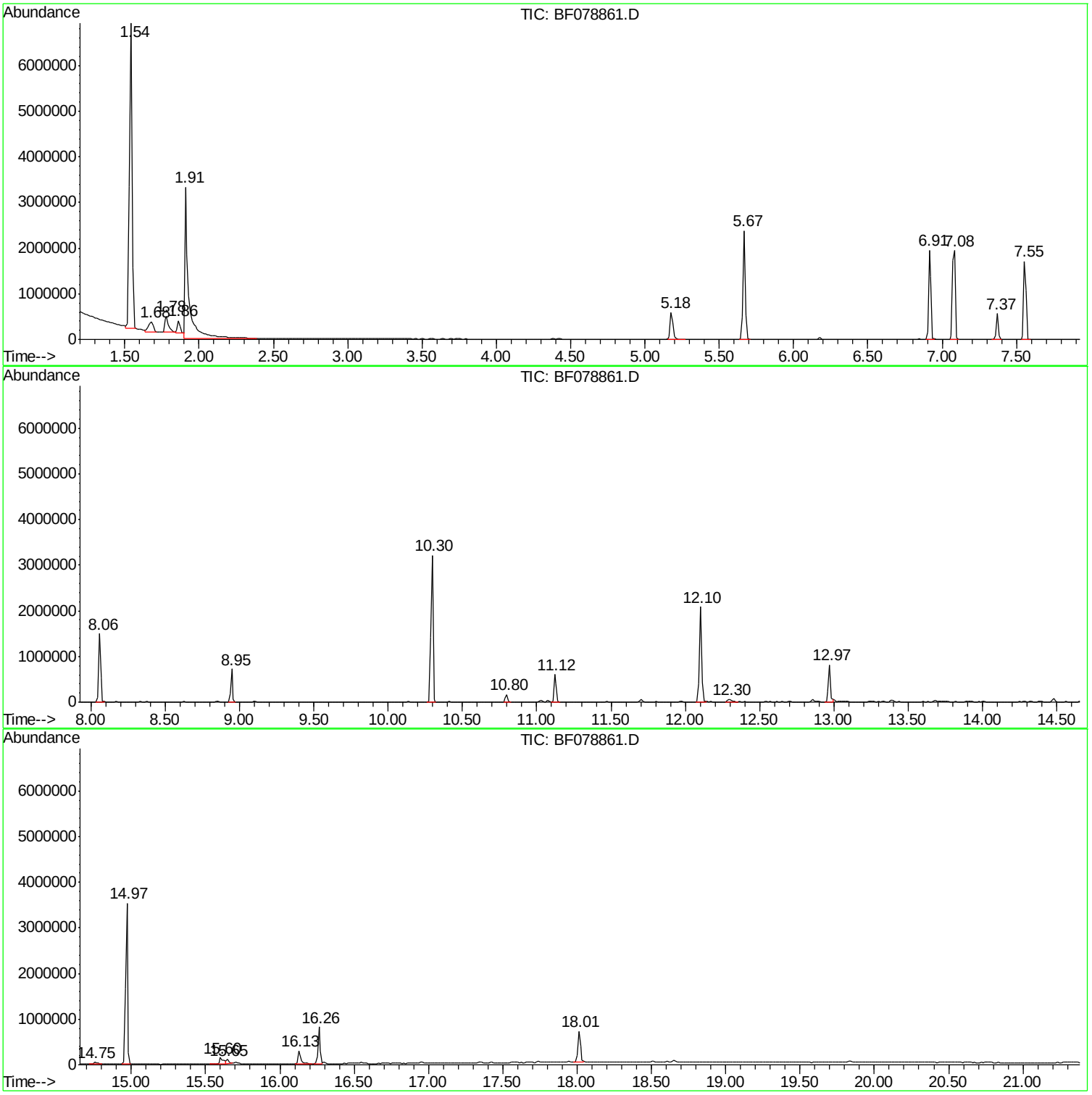
Operator : TP/IZ
Sample : G2067-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SINGSING-SS2-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.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\BF043015\
Data File : BF078861.D
Acq On : 30 Apr 2015 21:47
Operator : TP/IZ
Sample : G2067-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SINGSING-SS2-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

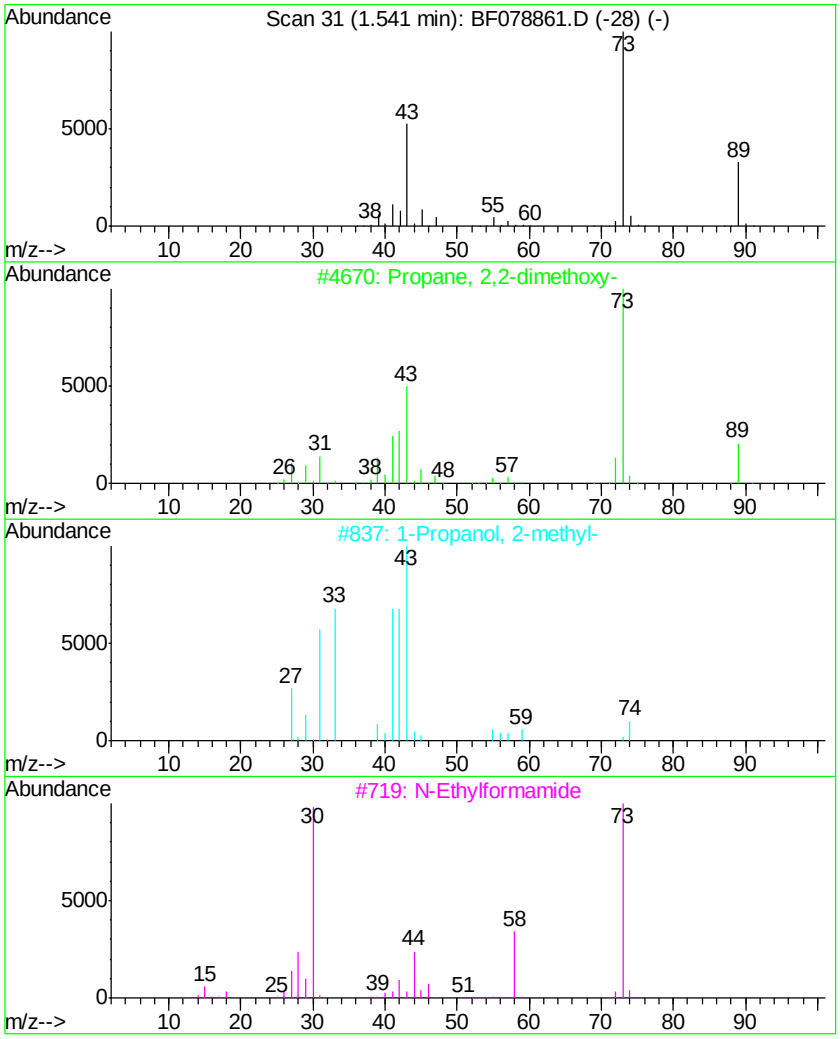
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

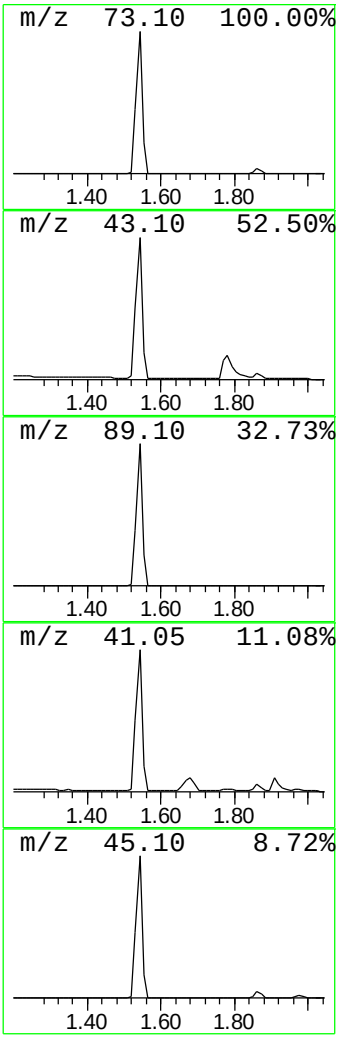
****

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.54	316.06 ng	7710680	1,4-Dichlorobenzene-d4	7.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
5	Oxirane-2-carboxylic acid, ethyl...	116	C5H8O3	1000192-50-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF043015\
Data File : BF078861.D
Acq On : 30 Apr 2015 21:47
Operator : TP/IZ
Sample : G2067-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SINGSING-SS2-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.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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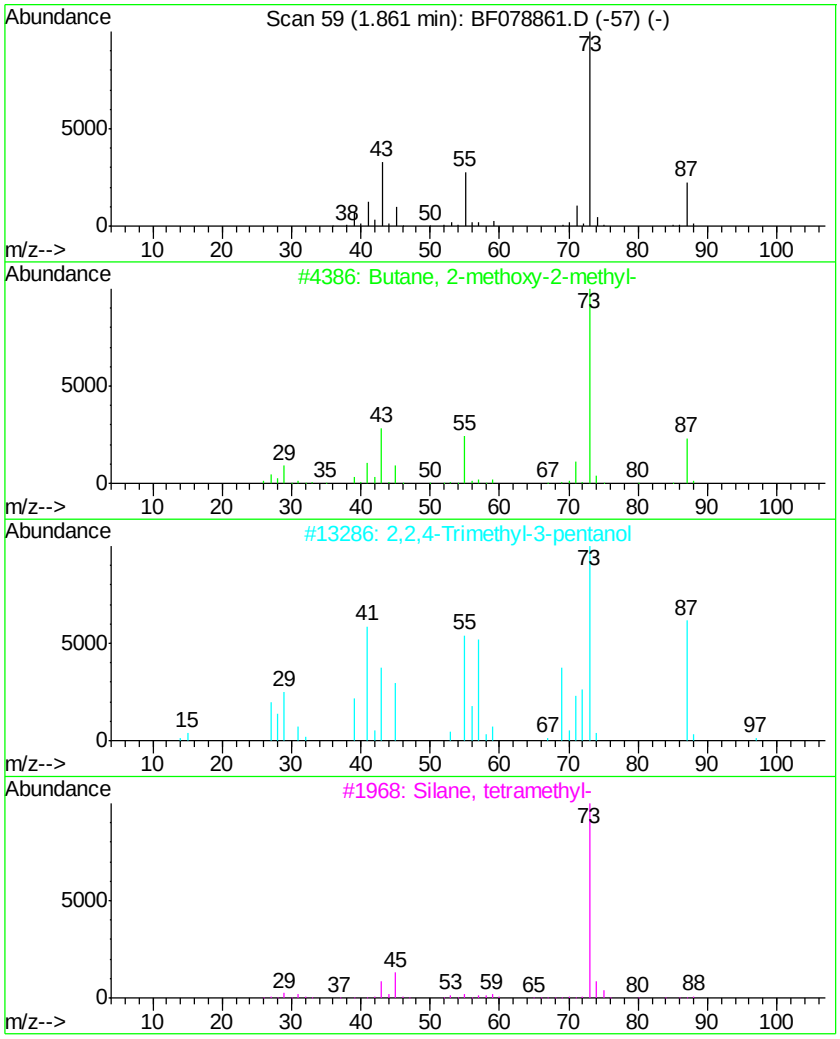
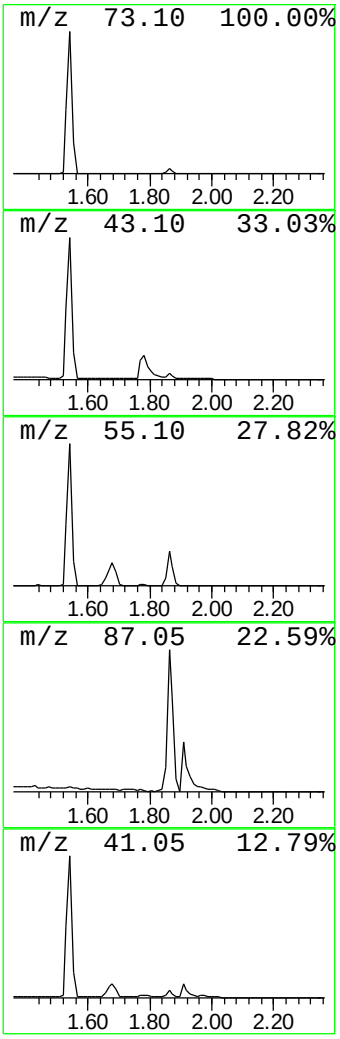
Peak Number 4 Butane, 2-methoxy-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.86	14.07 ng	343166	1,4-Dichlorobenzene-d4	7.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF043015\
Data File : BF078861.D
Acq On : 30 Apr 2015 21:47
Operator : TP/IZ
Sample : G2067-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SINGSING-SS2-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

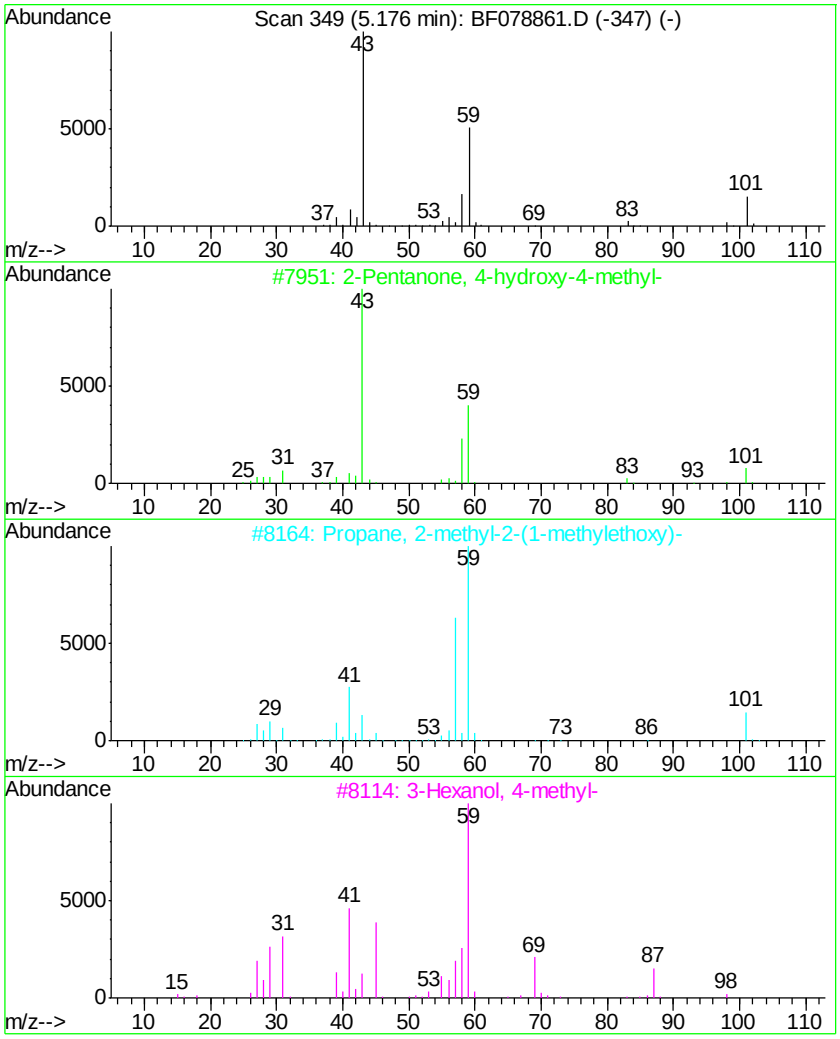
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

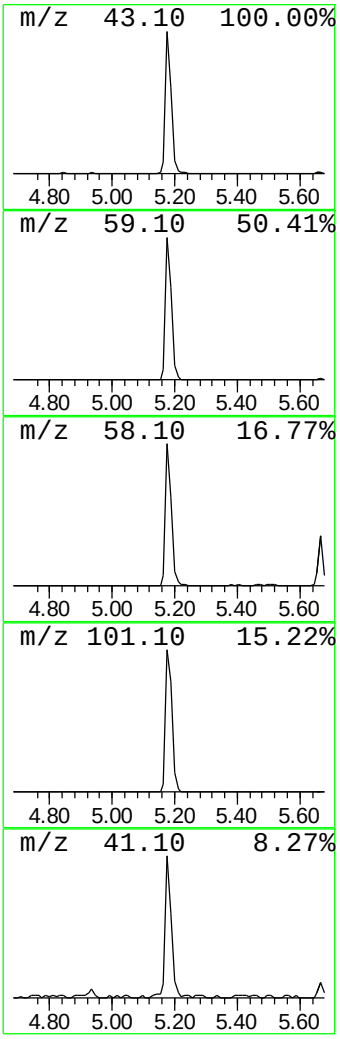
****

Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	30.60 ng	746520	1,4-Dichlorobenzene-d4	7.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF043015\
Data File : BF078861.D
Acq On : 30 Apr 2015 21:47
Operator : TP/IZ
Sample : G2067-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SINGSING-SS2-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

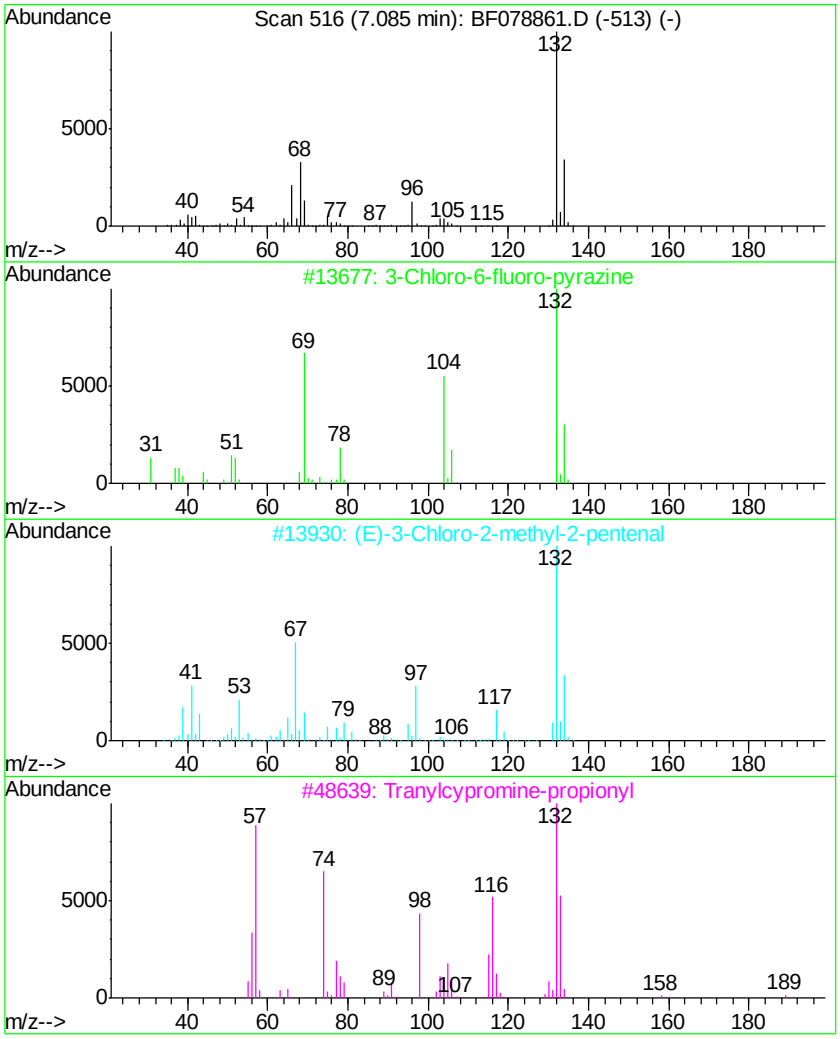
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

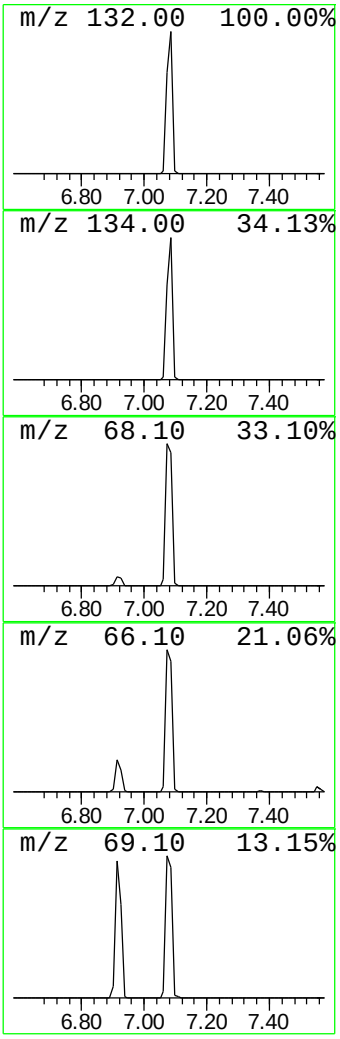
****

Peak Number 7 unknown7.08 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.08	105.83 ng	2581910	1,4-Dichlorobenzene-d4	7.37

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	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Amphetaminil	250	C17H18N2	017590-01-1	12
5	5-Aminoindole	132	C8H8N2	005192-03-0	12





Data Path : Z:\HPCHEM1\BNA F\DATA\BF043015\
Data File : BF078861.D
Acq On : 30 Apr 2015 21:47
Operator : TP/IZ
Sample : G2067-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SINGSING-SS2-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.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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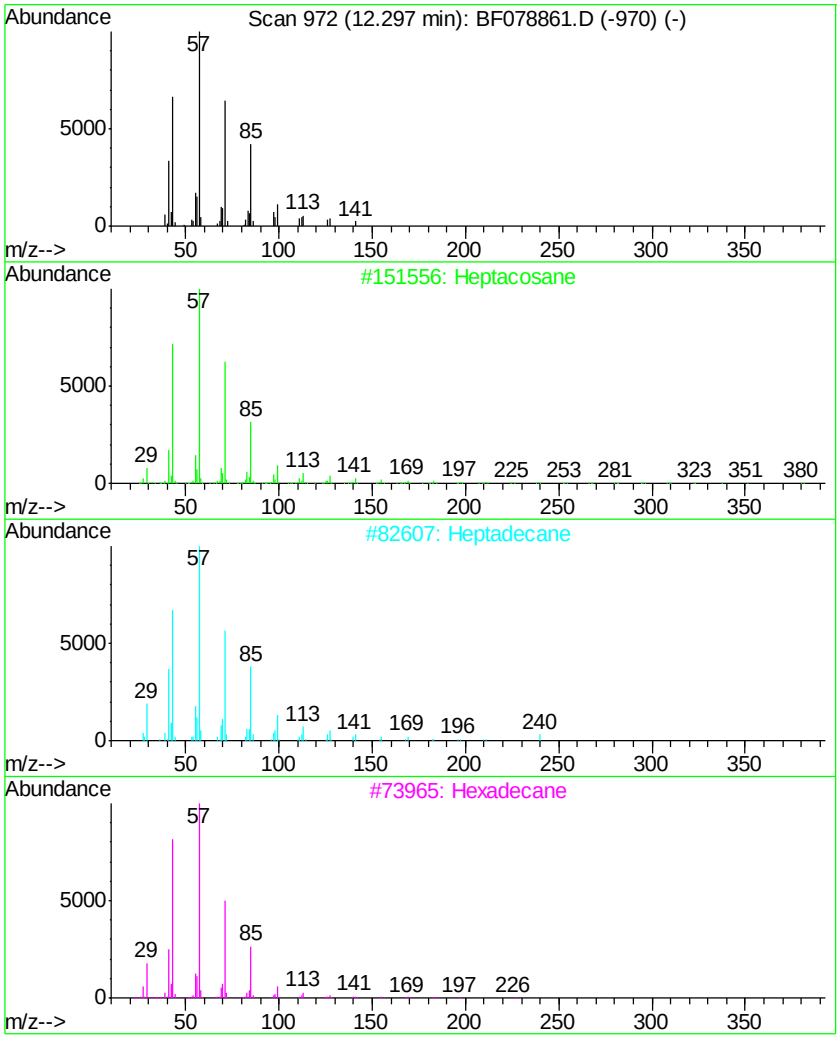
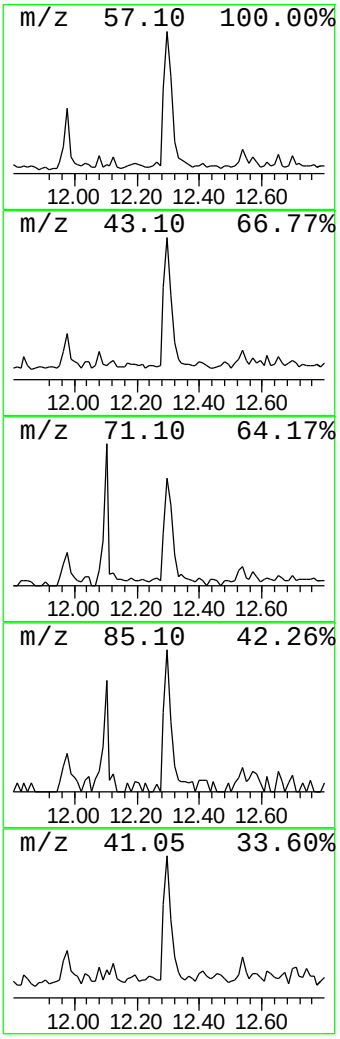
Peak Number 9 Heptacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	2.43 ng	97244	Phenanthrene-d10	12.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	90
2	Heptadecane	240	C17H36	000629-78-7	90
3	Hexadecane	226	C16H34	000544-76-3	90
4	Tetradecane	198	C14H30	000629-59-4	86
5	Eicosane	282	C20H42	000112-95-8	86





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Sample : G2067-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SINGSING-SS2-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.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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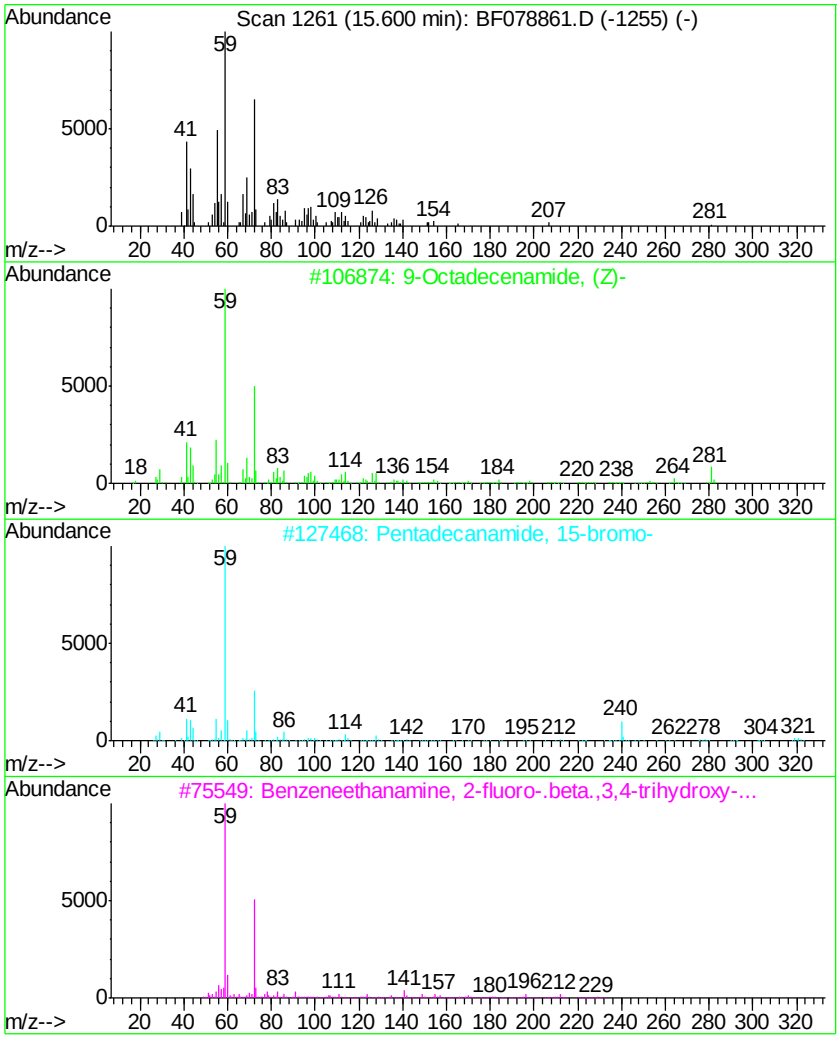
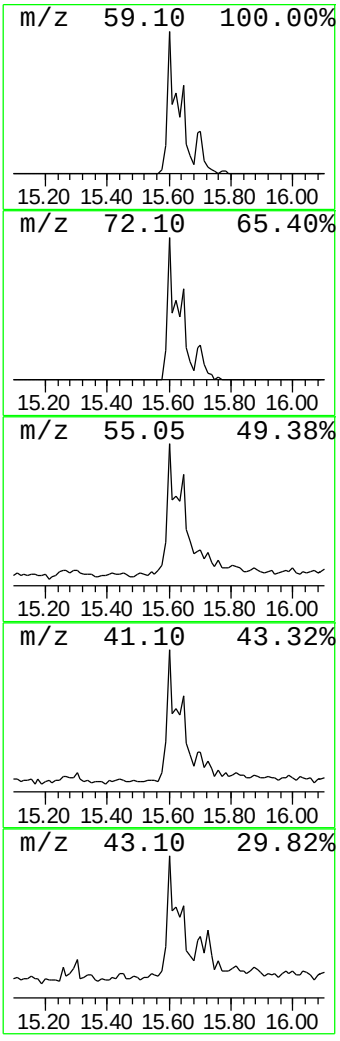
Peak Number 11 9-Octadecenamide, (Z)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.60	7.17 ng	309906	Chrysene-d12	16.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	72
2	Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	64
3	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	53
4	Dodecanamide	199	C12H25NO	001120-16-7	50
5	2-Propanone, 1-cyclohexyl-	140	C9H16O	000103-78-6	46





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Sample : G2067-02
Misc :
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Instrument : BNA_F
ClientSampleId : SINGSING-SS2-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.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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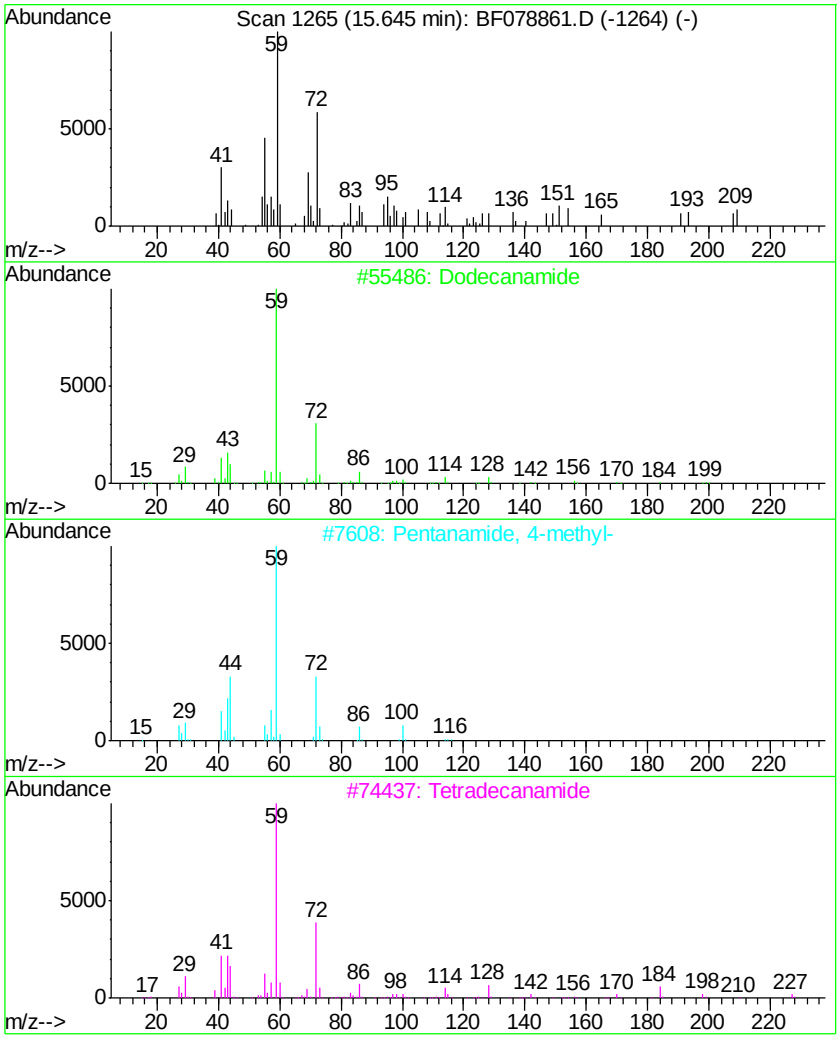
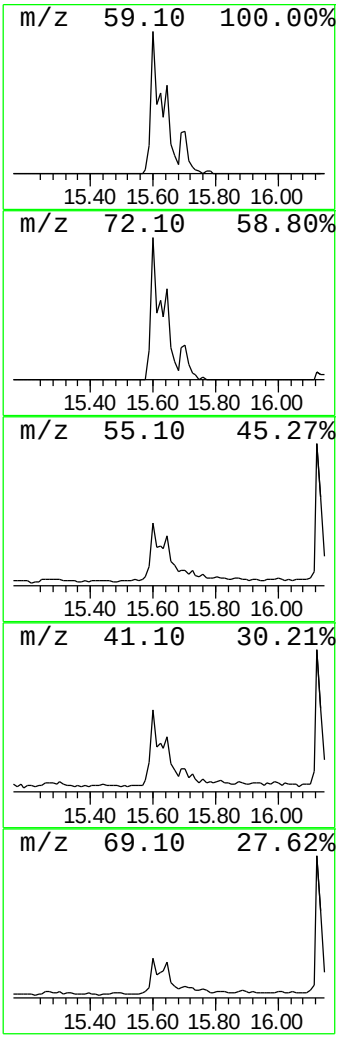
Peak Number 12 Dodecanamide Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.65	2.07 ng	89510	Chrysene-d12	16.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanamide	199	C12H25NO	001120-16-7	53
2	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	50
3	Tetradecanamide	227	C14H29NO	000638-58-4	42
4	Decanamide-	171	C10H21NO	002319-29-1	40
5	Octanamide	143	C8H17NO	000629-01-6	40





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Sample : G2067-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SINGSING-SS2-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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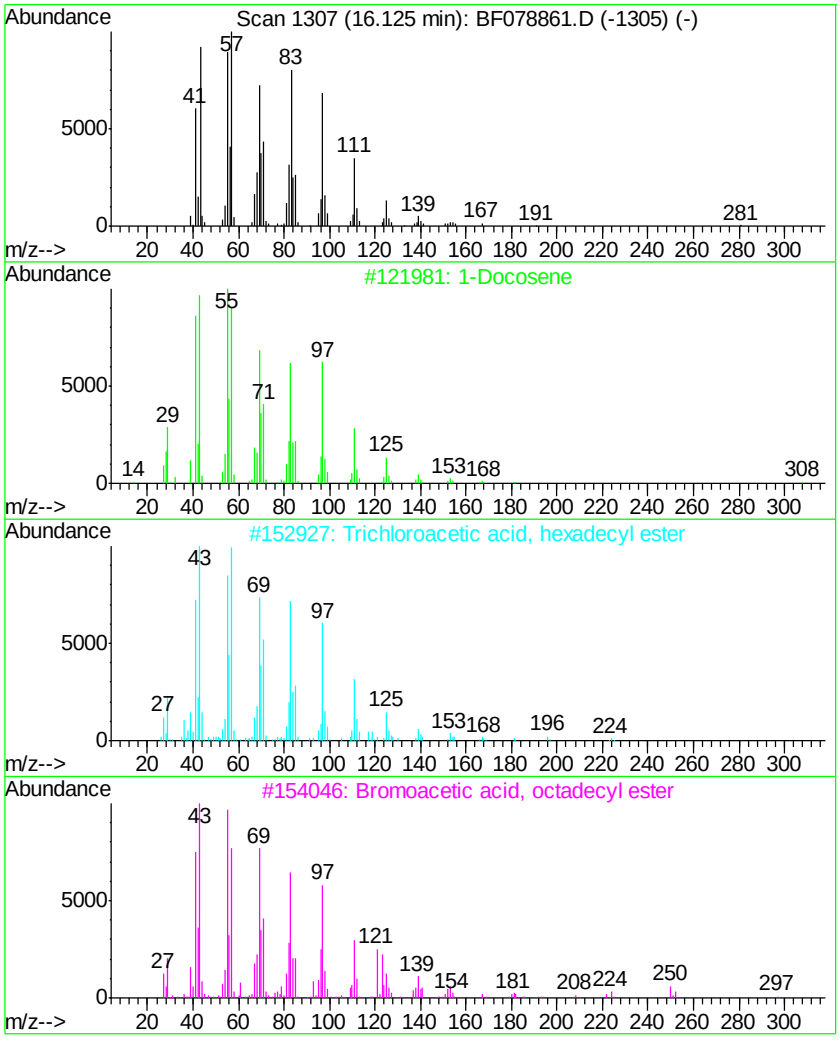
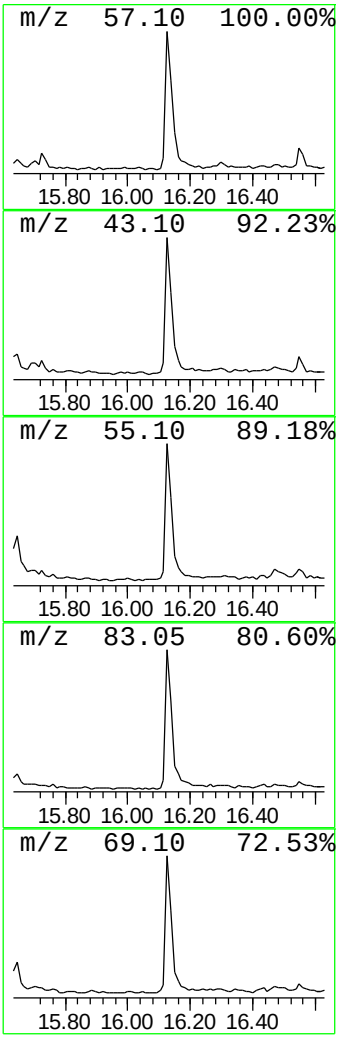
Peak Number 13 1-Docosene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	9.96 ng	430429	Chrysene-d12	16.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	94
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	94
4	1-Nonadecanol	284	C19H40O	001454-84-8	94
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF043015\
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Operator : TP/IZ
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.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, 2,2-dime...	1.54	316.1	ng	7710680	1	7.37	487930	20.0
Butane, 2-methoxy...	1.86	14.1	ng	343166	1	7.37	487930	20.0
2-Pentanone, 4-hy...	5.18	30.6	ng	746520	1	7.37	487930	20.0
unknown7.08	7.08	105.8	ng	2581910	1	7.37	487930	20.0
Heptacosane	12.30	2.4	ng	97244	4	12.97	799008	20.0
9-Octadecenamide,...	15.60	7.2	ng	309906	5	16.26	863959	20.0
Dodecanamide	15.65	2.1	ng	89510	5	16.26	863959	20.0
1-Docosene	16.13	10.0	ng	430429	5	16.26	863959	20.0