LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG022716\
Data File : BG021123.D
Acq On : 27 Feb 2016 20:21
Operator : UM/SJ
Sample : H1565-06
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CEB-4(12-14)20160223

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_G\METHODS\8270-BG022616.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	3.084	37	42	62	rBV	1073572	1552081	100.00%	29.531%
2	3.237	62	68	76	rVB3	10901	21844	1.41%	0.416%
3	5.258	406	412	418	rBV	35713	51913	3.34%	0.988%
4	5.722	484	491	498	rBB	155692	247352	15.94%	4.706%
5	7.309	754	761	769	rVB	171976	292208	18.83%	5.560%
6	7.696	820	827	834	rBB	165943	274237	17.67%	5.218%
7	8.166	901	907	913	rBB	25385	40109	2.58%	0.763%
8	8.490	955	962	969	rBB	109117	180364	11.62%	3.432%
9	9.330	1097	1105	1112	rBB	104743	181007	11.66%	3.444%
10	10.975	1378	1385	1392	rBB	36118	63282	4.08%	1.204%
11	13.401	1791	1798	1805	rBB	251854	370280	23.86%	7.045%
12	14.218	1931	1937	1942	rBB	45479	61357	3.95%	1.167%
13	14.770	2025	2031	2037	rBB2	60704	93963	6.05%	1.788%
14	16.251	2275	2283	2289	rBB2	256074	360570	23.23%	6.860%
15	17.508	2491	2497	2502	rBV2	89011	132295	8.52%	2.517%
16	18.372	2640	2644	2650	rBV3	18733	24659	1.59%	0.469%
17	20.100	2932	2938	2943	rVB	560737	724257	46.66%	13.780%
18	20.769	3047	3052	3058	rBV	55499	99195	6.39%	1.887%
19	20.822	3058	3061	3067	rVB	25569	35902	2.31%	0.683%
20	21.392	3153	3158	3169	rBV	85918	121929	7.86%	2.320%
21	21.768	3216	3222	3228	rBV	105268	170056	10.96%	3.236%
22	25.053	3770	3781	3790	rBV2	50016	140336	9.04%	2.670%
23	26.357	3997	4003	4010	rBV8	6356	16648	1.07%	0.317%

Sum of corrected areas: 5255844

LSC Report - Integrated Chromatogram

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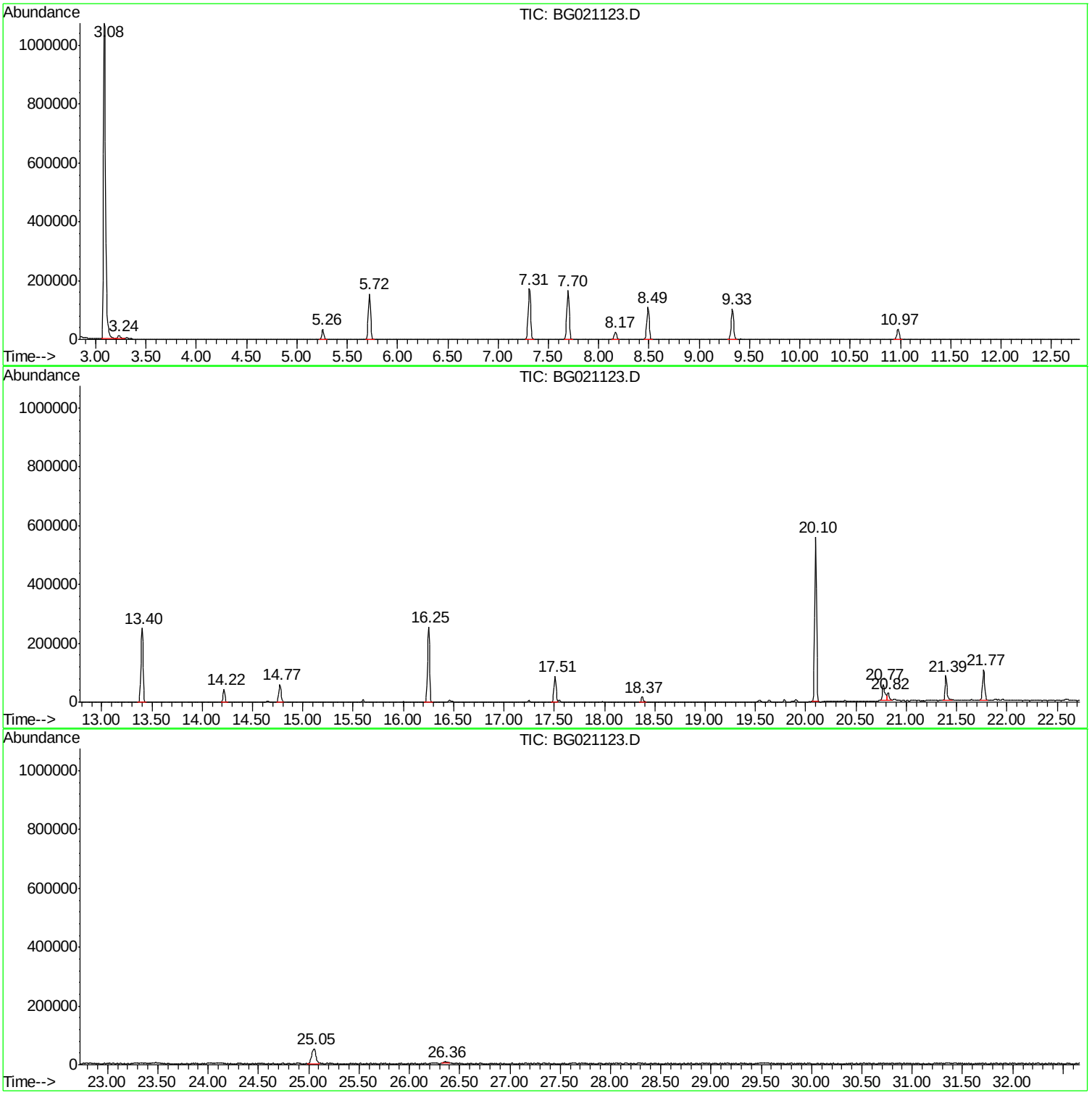
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CEB-4(12-14)20160223

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022616.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 G\DATA\BG022716\
Data File : BG021123.D
Acq On : 27 Feb 2016 20:21
Operator : UM/SJ
Sample : H1565-06
Misc :
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Instrument : BNA_G
ClientSampleId : CEB-4(12-14)20160223

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

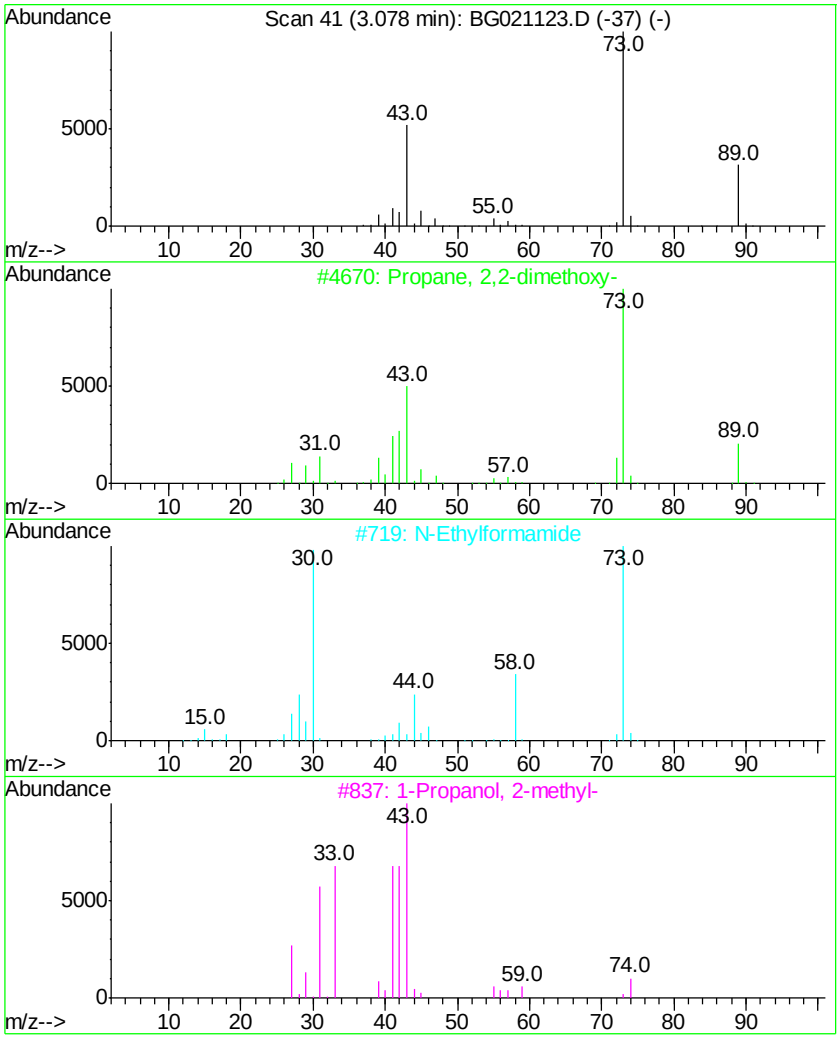
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

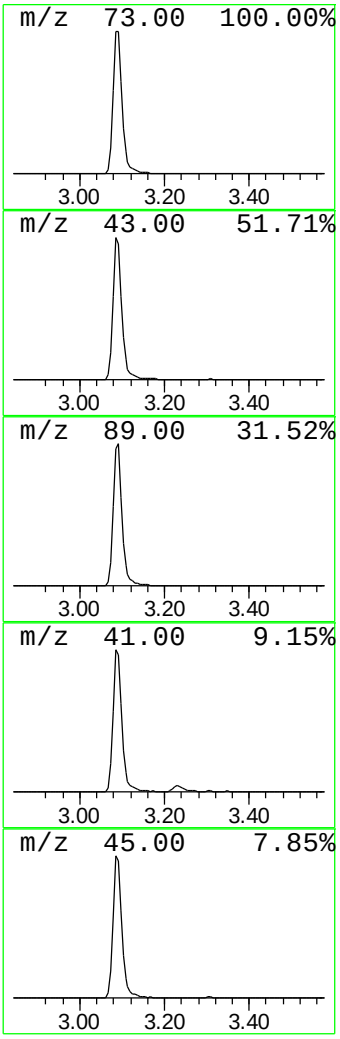
****

Peak Number 1 unknown3.08 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.08	773.93 ng	1552080	1,4-Dichlorobenzene-d4	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2	N-Ethylformamide	73	C3H7NO	000627-45-2	9
3	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
4	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
5	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9





Library Search Compound Report

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Operator : UM/SJ
Sample : H1565-06
Misc :
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Instrument : BNA_G
ClientSampleId : CEB-4(12-14)20160223

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022616.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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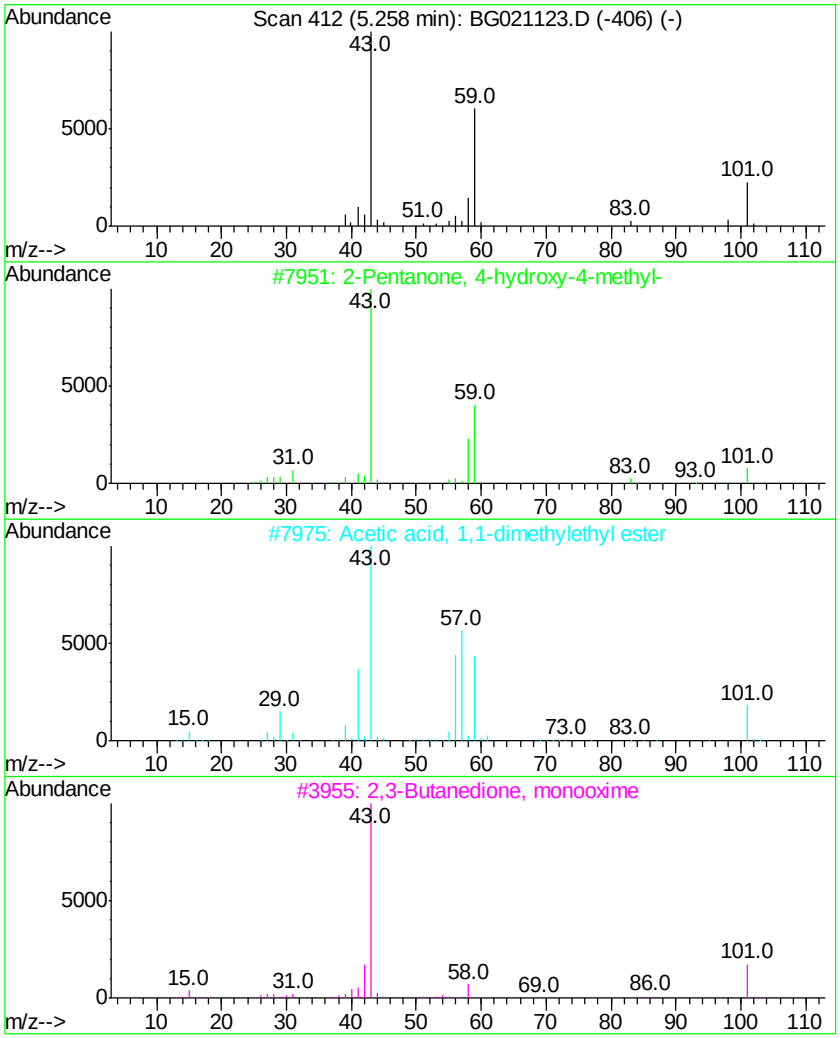
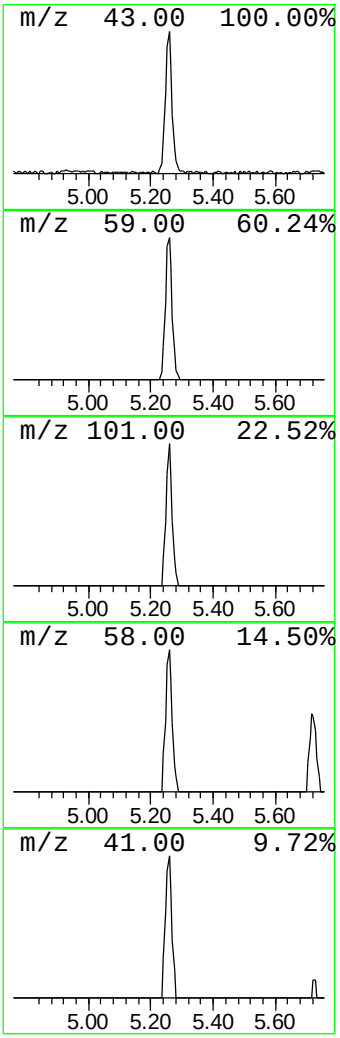
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.26	25.89 ng	51913	1,4-Dichlorobenzene-d4	8.17

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	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG022716\
Data File : BG021123.D
Acq On : 27 Feb 2016 20:21
Operator : UM/SJ
Sample : H1565-06
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CEB-4(12-14)20160223

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022616.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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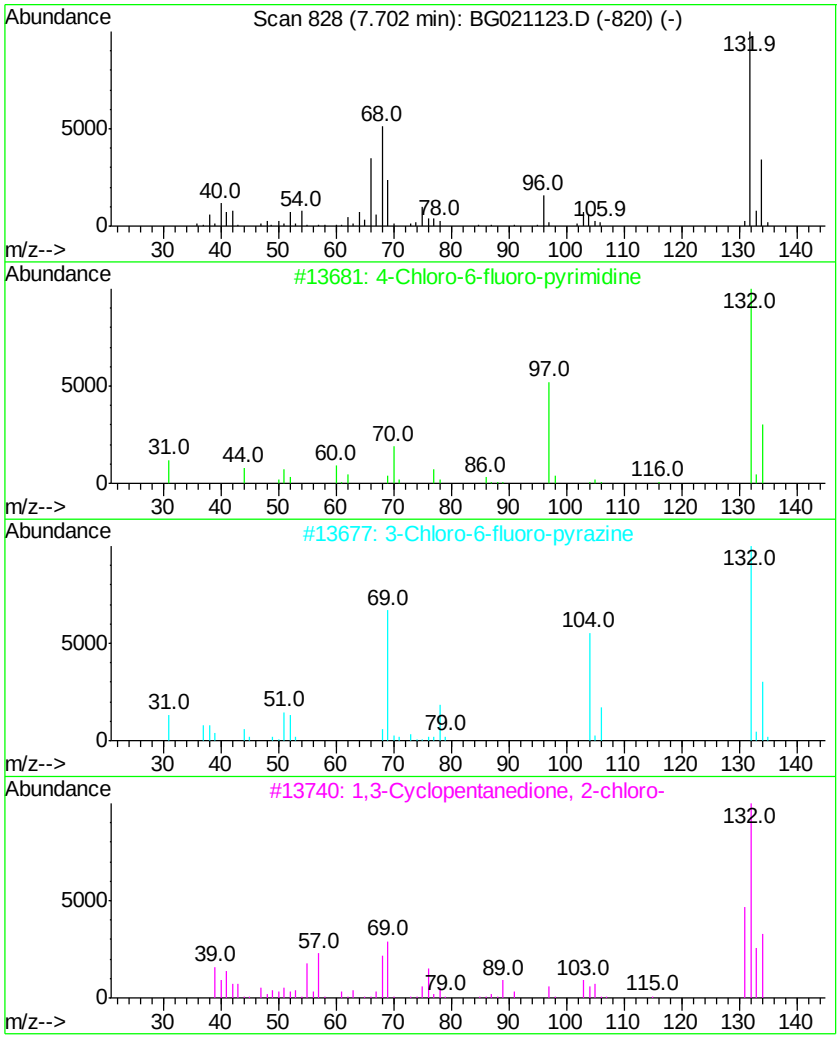
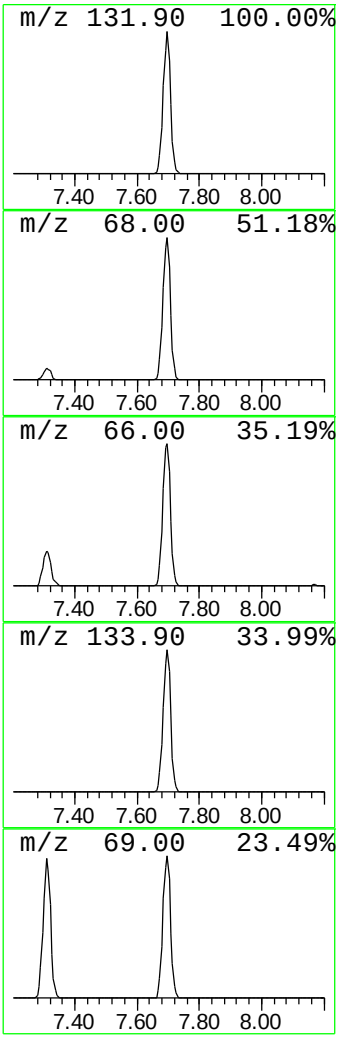
Peak Number 4 unknown7.70 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.70	136.75 ng	274237	1,4-Dichlorobenzene-d4	8.17

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	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	25
4	5-Aminoindole	132	C8H8N2	005192-03-0	22
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22





Data Path : Z:\HPCHEM1\BNA G\DATA\BG022716\
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Operator : UM/SJ
Sample : H1565-06
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CEB-4(12-14)20160223

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022616.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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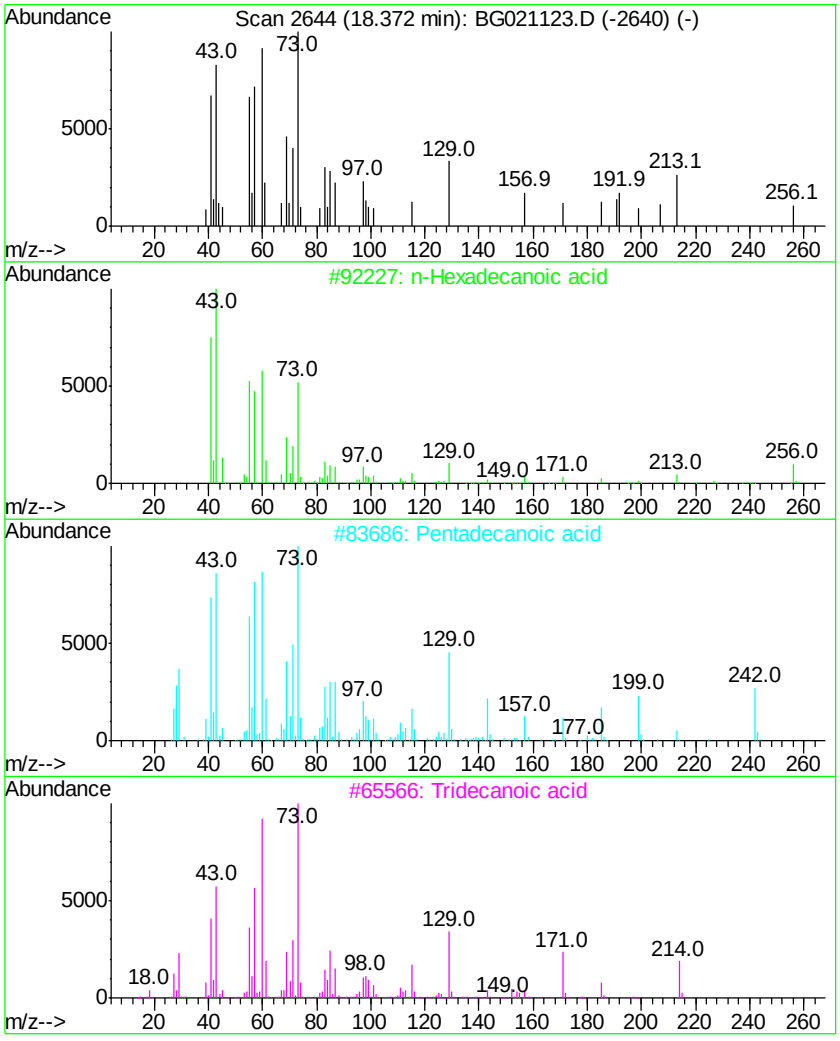
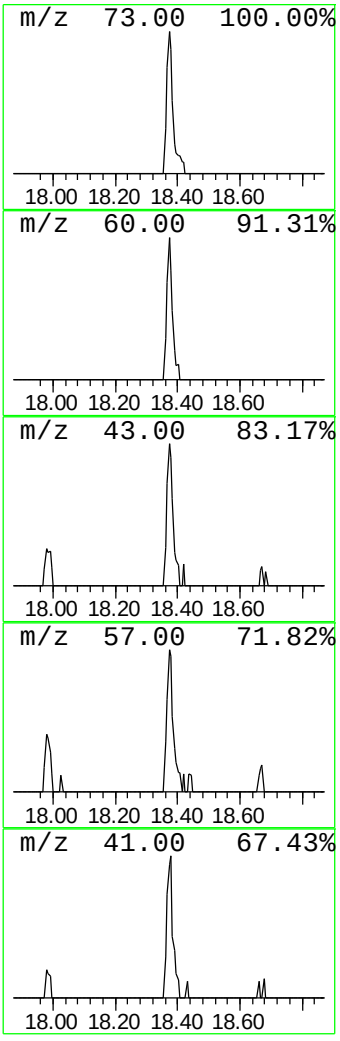
Peak Number 6 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.37	3.73 ng	24659	Phenanthrene-d10	17.51

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	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	59





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Operator : UM/SJ
Sample : H1565-06
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CEB-4(12-14)20160223

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022616.M
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TIC Library : C:\DATABASE\NIST02.L
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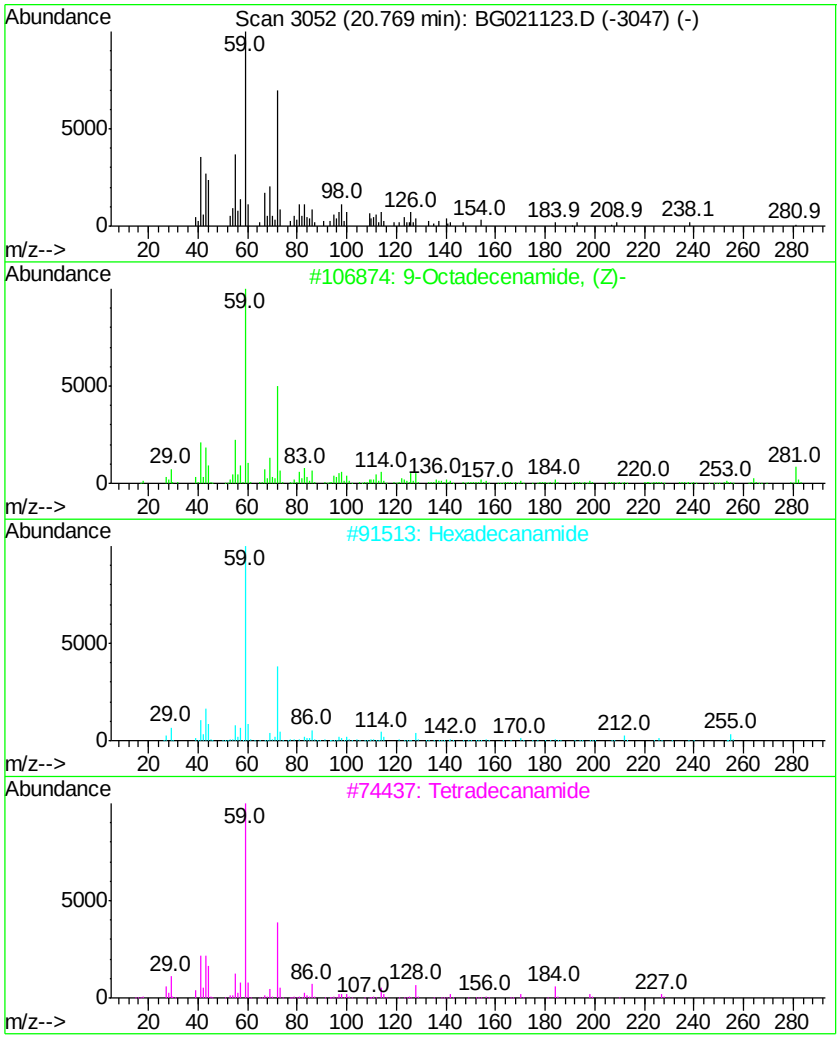
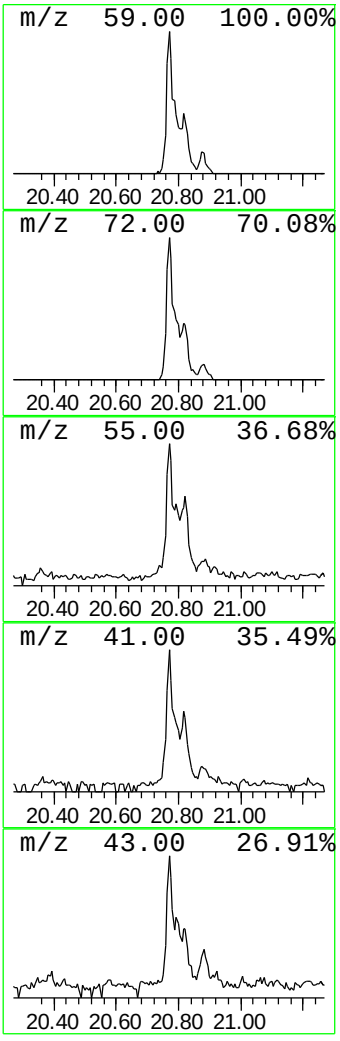
****

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.77	11.67 ng	99195	Chrysene-d12	21.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	72
2	Hexadecanamide	255	C16H33NO	000629-54-9	64
3	Tetradecanamide	227	C14H29NO	000638-58-4	56
4	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	50
5	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	50





Library Search Compound Report

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Instrument : BNA_G
ClientSampleId : CEB-4(12-14)20160223

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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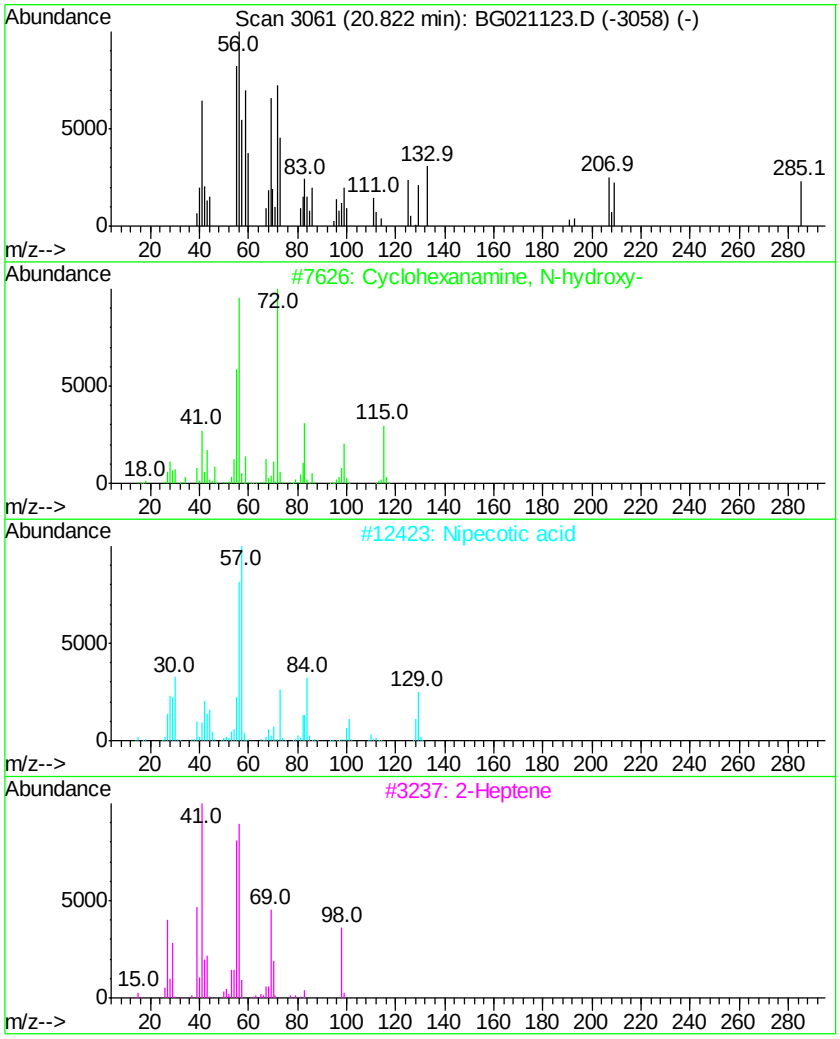
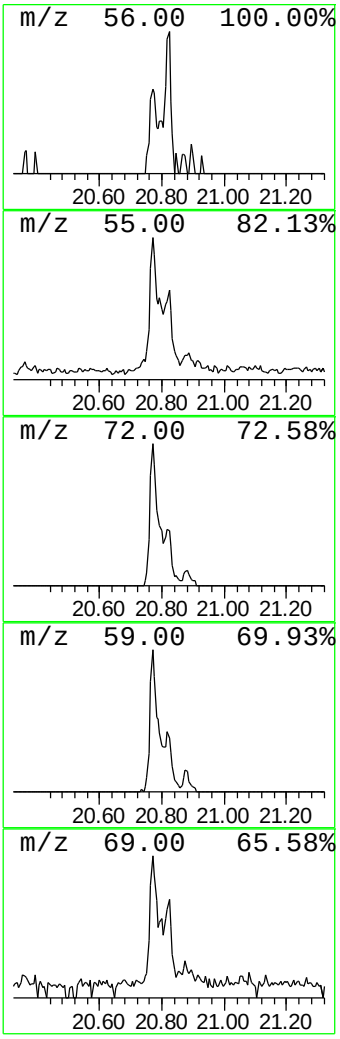
****

Peak Number 8 unknown20.82 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.82	4.22 ng	35902	Chrysene-d12	21.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanamine, N-hydroxy-	115	C6H13NO	002211-64-5	38
2	Nipecotic acid	129	C6H11NO2	000498-95-3	14
3	2-Heptene	98	C7H14	000592-77-8	11
4	1-Heptene, 6-methyl-	112	C8H16	005026-76-6	11
5	1-Undecene, 10-methyl-	168	C12H24	022370-55-4	10





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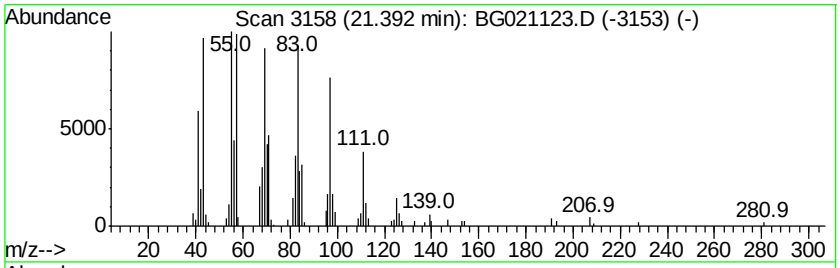
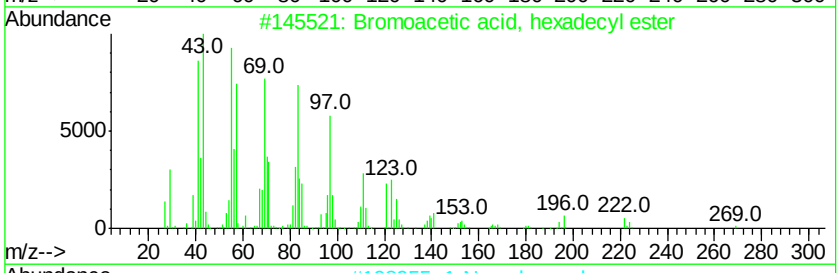
****

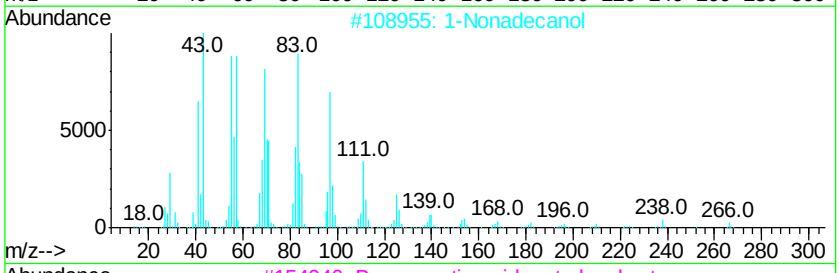
Peak Number 9 Bromoacetic acid, hexadecyl... Concentration Rank 5

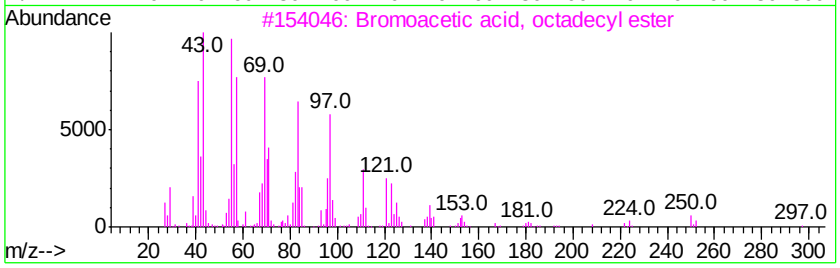
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.39	14.34 ng	121929	Chrysene-d12	21.77

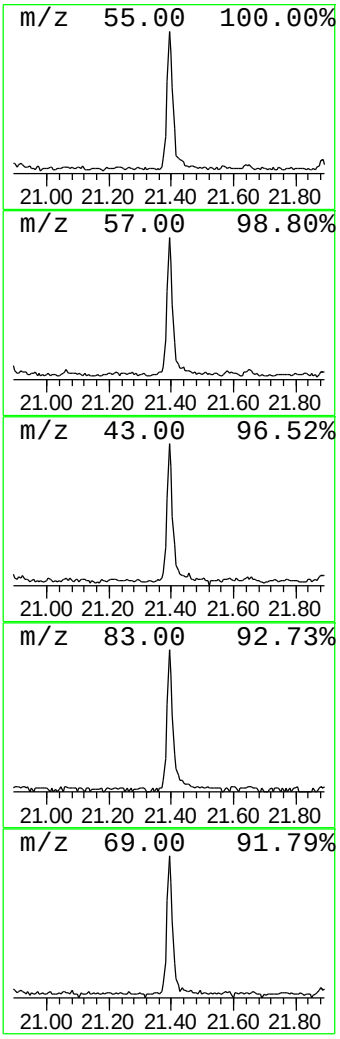
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	94
2	1-Nonadecanol	284	C19H40O	001454-84-8	91
3	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
4	1-Nonadecene	266	C19H38	018435-45-5	91
5	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	91











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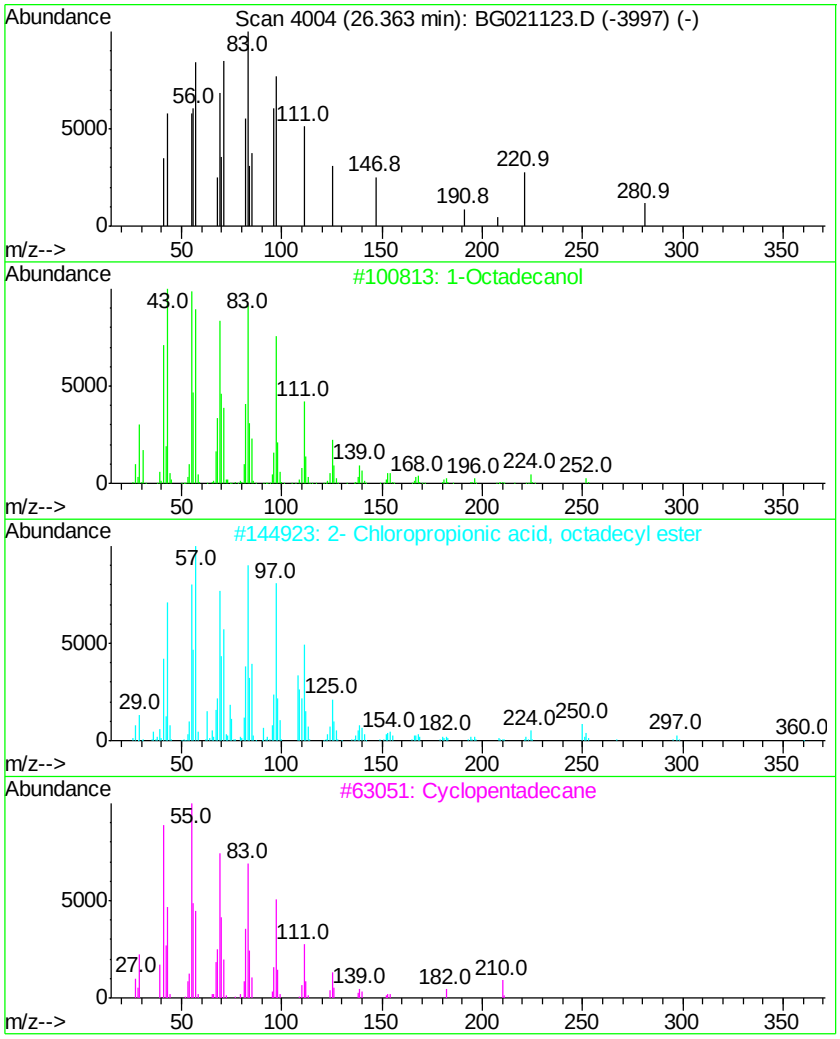
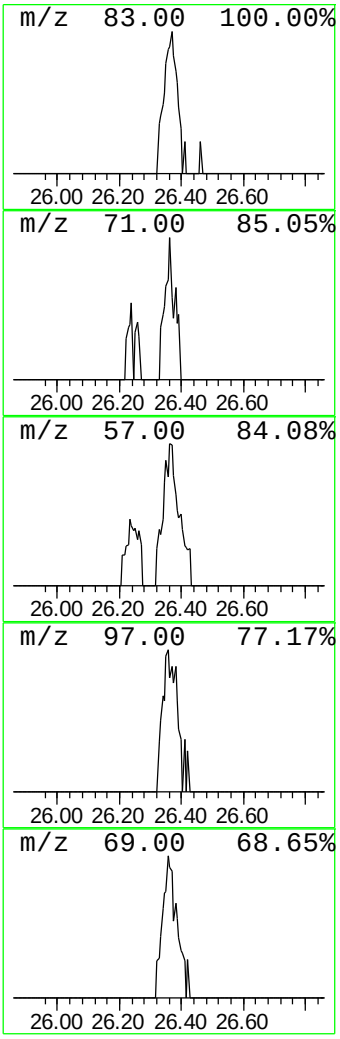
****

Peak Number 10 1-Octadecanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.36	2.37 ng	16648	Perylene-d12	25.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecanol	270	C18H38O	000112-92-5	72
2	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	72
3	Cyclopentadecane	210	C15H30	000295-48-7	72
4	17-Pentatriacontene	491	C35H70	006971-40-0	68
5	Bacteriochlorophyll-c-stearyl	841	C52H72MgN4O4	1000164-49-7	64





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_G
ClientSampleId : CEB-4(12-14)20160223

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022616.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
unknown3.08	3.08	773.9	ng	1552080	1	8.17	40109	20.0
2-Pentanone, 4-hy...	5.26	25.9	ng	51913	1	8.17	40109	20.0
unknown7.70	7.70	136.8	ng	274237	1	8.17	40109	20.0
n-Hexadecanoic acid	18.37	3.7	ng	24659	4	17.51	132295	20.0
9-Octadecenamide,...	20.77	11.7	ng	99195	5	21.77	170056	20.0
unknown20.82	20.82	4.2	ng	35902	5	21.77	170056	20.0
Bromoacetic acid,...	21.39	14.3	ng	121929	5	21.77	170056	20.0
1-Octadecanol	26.36	2.4	ng	16648	6	25.05	140336	20.0