LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016446.D
Acq On : 16 Apr 2015 6:36
Operator : TP/IZ
Sample : G1829-23
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TE-PMW-11S

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-BG040615.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	2.761	6	12	21	rBV	331555	598421	14.94%	2.380%
2	2.837	21	25	38	rVB	422100	570165	14.23%	2.267%
3	4.782	351	356	363	rBV	59888	84909	2.12%	0.338%
4	5.258	431	437	448	rBV	716436	986388	24.62%	3.923%
5	6.181	589	594	605	rBV	24538	46745	1.17%	0.186%
6	6.856	702	709	725	rVB	456901	713814	17.81%	2.839%
7	7.203	760	768	778	rBV	1291242	1986146	49.57%	7.898%
8	7.667	838	847	853	rBV	297364	461396	11.52%	1.835%
9	7.984	893	901	908	rBV	1113451	1718942	42.90%	6.836%
10	8.825	1036	1044	1054	rBV	893608	1434484	35.80%	5.704%
11	10.452	1313	1321	1329	rBV	439027	716755	17.89%	2.850%
12	12.932	1734	1743	1752	rBV	2312117	3493929	87.20%	13.894%
13	13.766	1880	1885	1890	rBV	31529	40633	1.01%	0.162%
14	14.306	1971	1977	1987	rVB2	634781	966835	24.13%	3.845%
15	15.669	2202	2209	2215	rBV	108399	138268	3.45%	0.550%
16	15.799	2224	2231	2240	rBV	1785464	2378491	59.36%	9.458%
17	17.050	2437	2444	2454	rBV2	838746	1208028	30.15%	4.804%
18	17.949	2592	2597	2605	rBV	187343	276255	6.89%	1.099%
19	19.089	2787	2791	2793	rBV3	45132	61710	1.54%	0.245%
20	19.230	2811	2815	2830	rVB	117872	194469	4.85%	0.773%
21	19.682	2886	2892	2900	rBV	3239803	4006817	100.00%	15.934%
22	20.946	3103	3107	3118	rBV	293046	399671	9.97%	1.589%
23	21.145	3138	3141	3147	rBV	102072	114720	2.86%	0.456%
24	21.228	3150	3155	3161	rBV	994789	1221887	30.50%	4.859%
25	22.068	3294	3298	3304	rBV	97080	127726	3.19%	0.508%
26	23.460	3529	3535	3547	rVB2	623411	1199148	29.93%	4.769%

Sum of corrected areas: 25146752

LSC Report - Integrated Chromatogram

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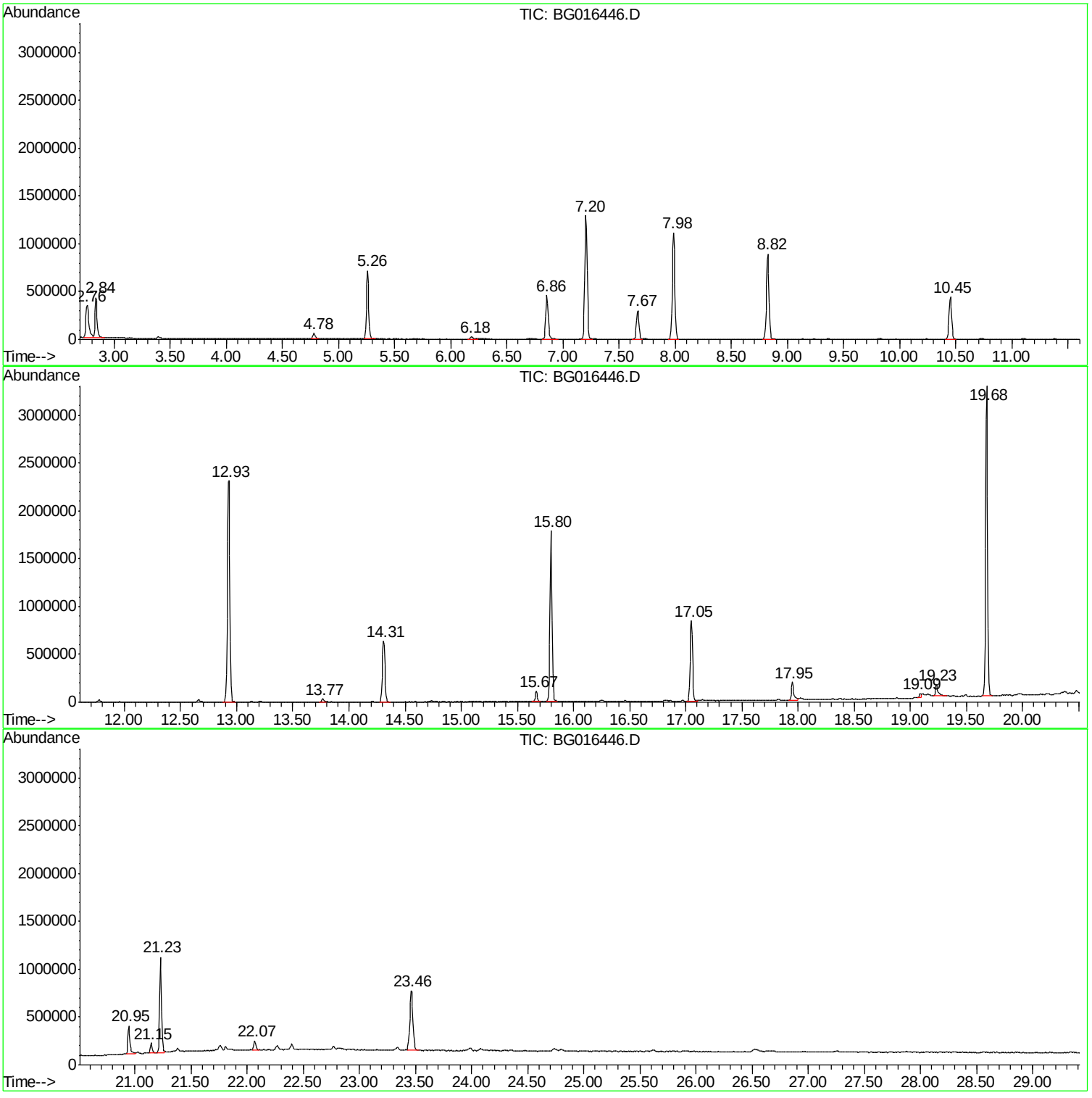
Acq On : 16 Apr 2015 6:36
Operator : TP/IZ
Sample : G1829-23
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TE-PMW-11S

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.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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Operator : TP/IZ
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Instrument : BNA_G
ClientSampleId : TE-PMW-11S

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

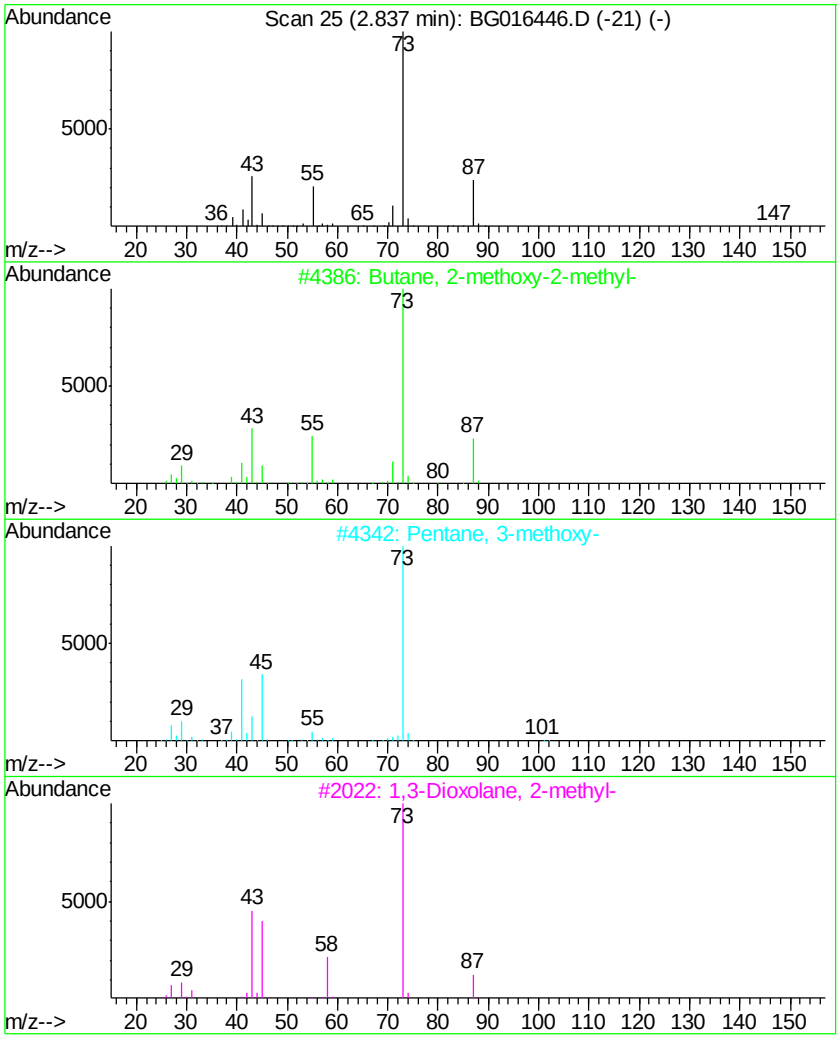
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

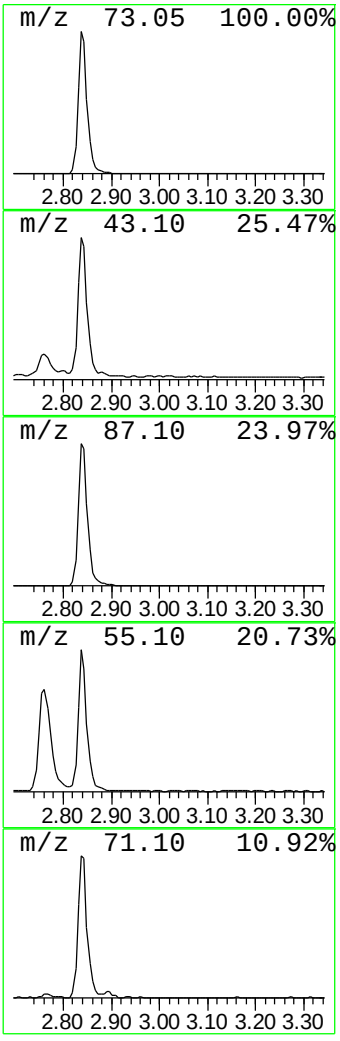
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.84	24.71 ng	570165	1,4-Dichlorobenzene-d4	7.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9





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Data File : BG016446.D
Acq On : 16 Apr 2015 6:36
Operator : TP/IZ
Sample : G1829-23
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TE-PMW-11S

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

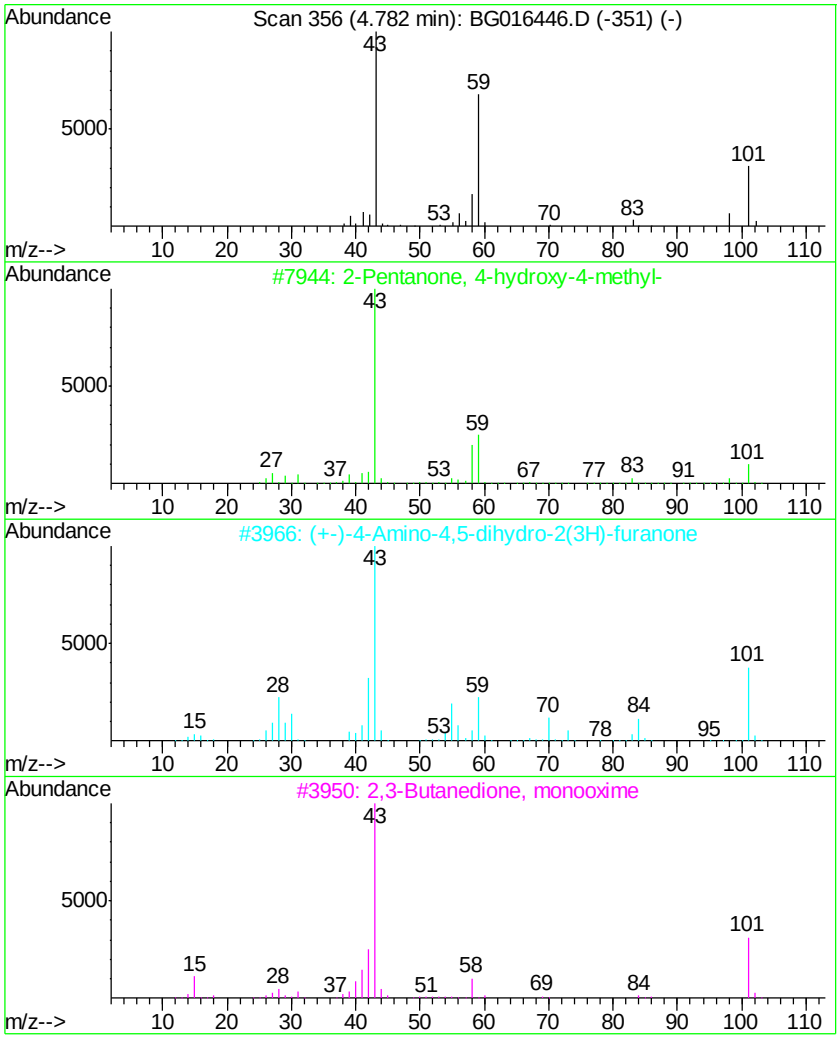
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

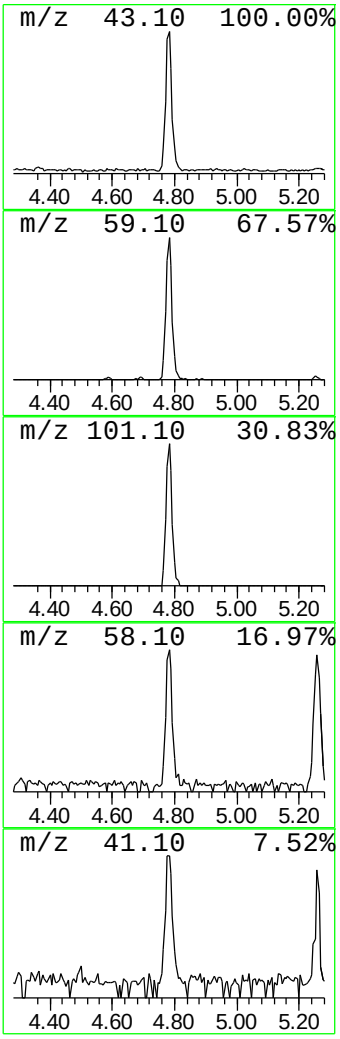
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.78	3.68 ng	84909	1,4-Dichlorobenzene-d4	7.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	47
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	32
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	16





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Operator : TP/IZ
Sample : G1829-23
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TE-PMW-11S

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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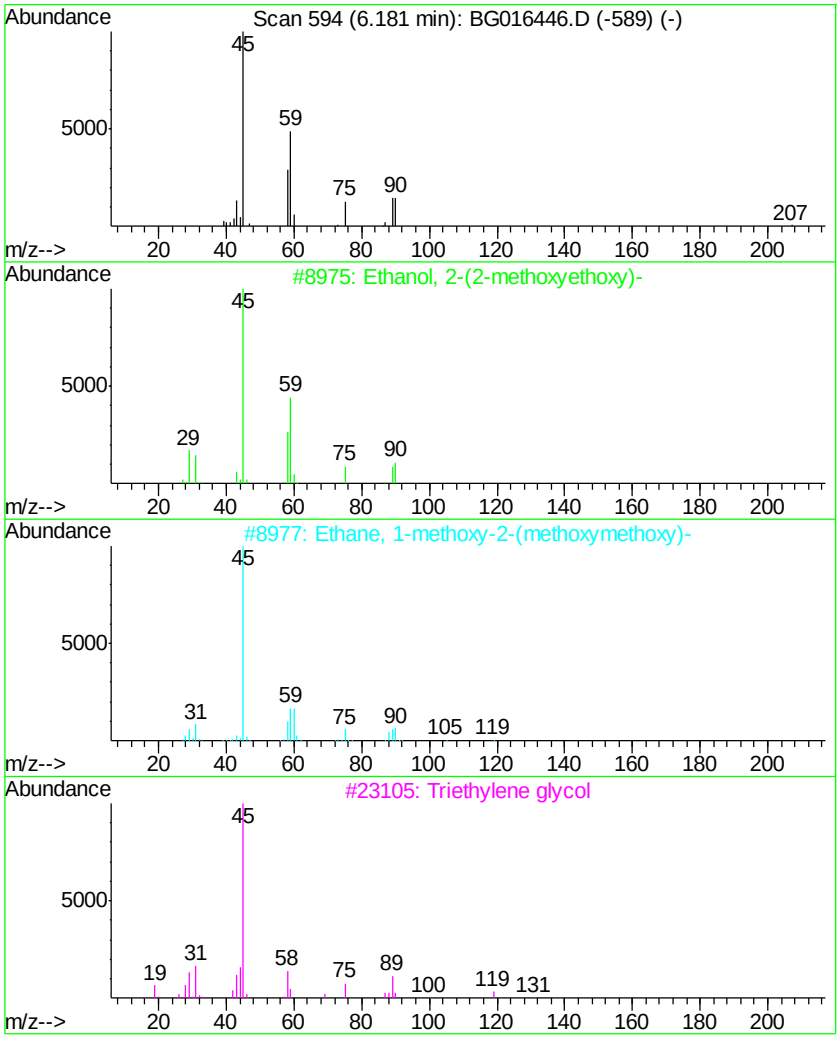
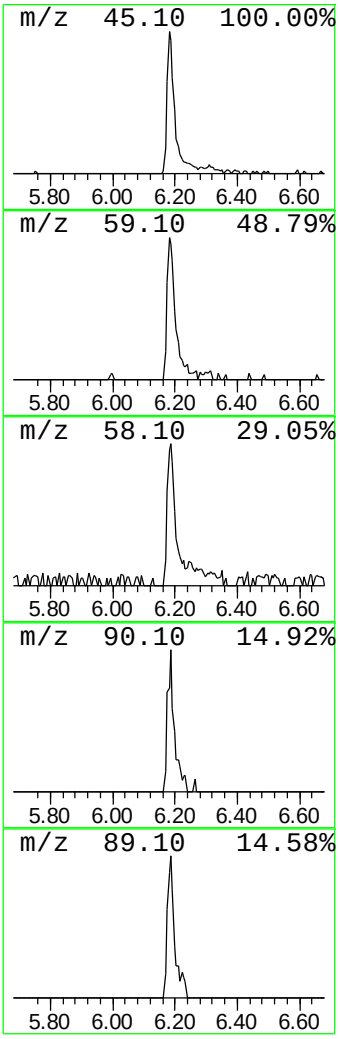
Peak Number 4 Ethanol, 2-(2-methoxyethoxy)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.18	2.03 ng	46745	1,4-Dichlorobenzene-d4	7.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	83
2	Ethane, 1-methoxy-2-(methoxymeth...	120	C5H12O3	074498-88-7	23
3	Triethylene glycol	150	C6H14O4	000112-27-6	9
4	1,4-Dioxan-2-ol	104	C4H8O3	022347-47-3	9
5	Propane, 2,2'-[ethylidenebis(oxy...	146	C8H18O2	004285-59-0	9





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Sample : G1829-23
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TE-PMW-11S

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

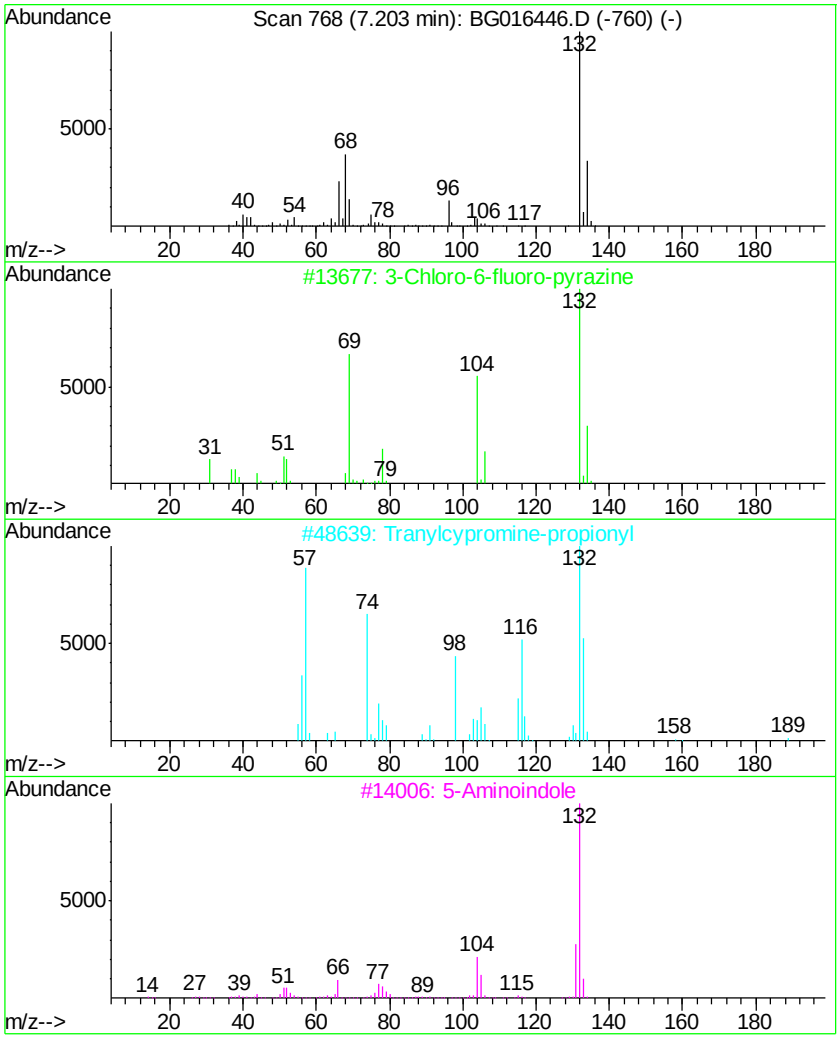
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

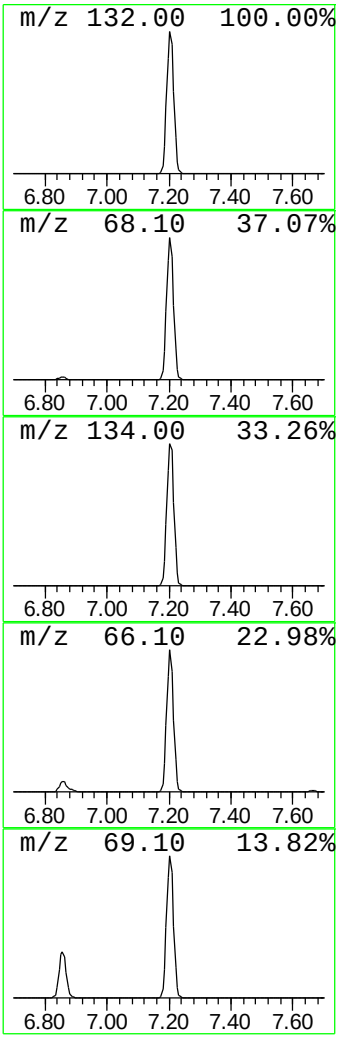
****

Peak Number 5 unknown7.20 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.20	86.09 ng	1986150	1,4-Dichlorobenzene-d4	7.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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Sample : G1829-23
Misc :
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Instrument : BNA_G
ClientSampleId : TE-PMW-11S

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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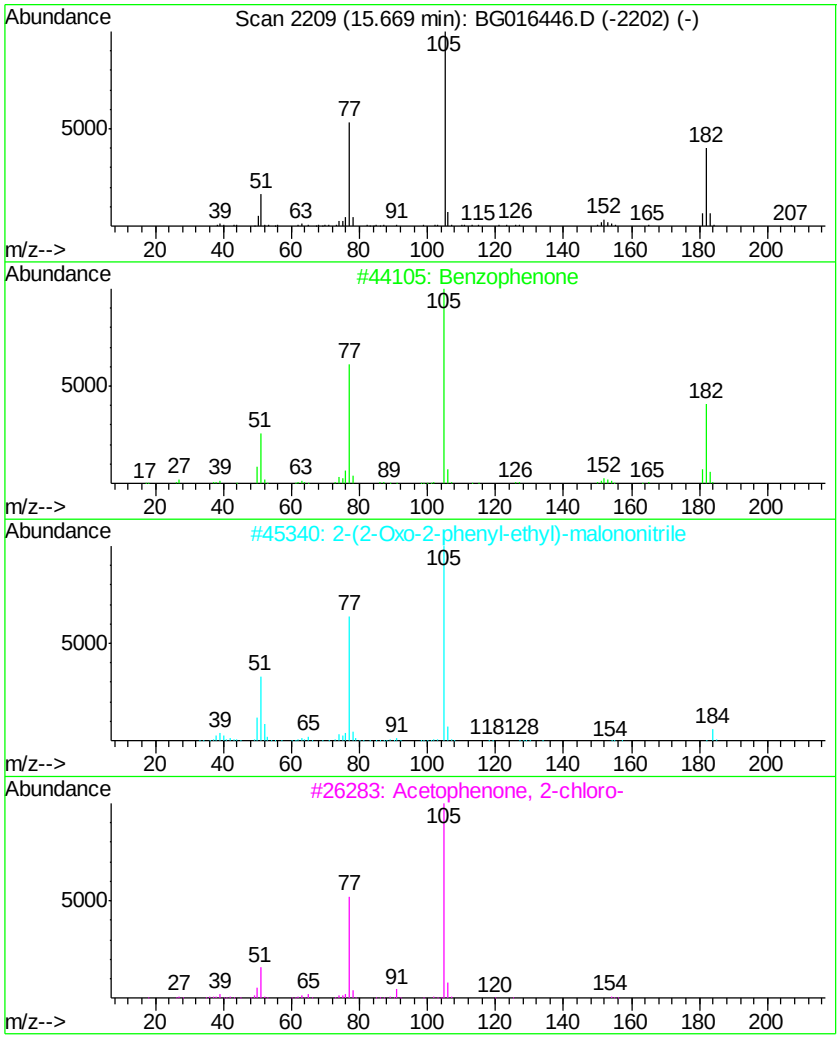
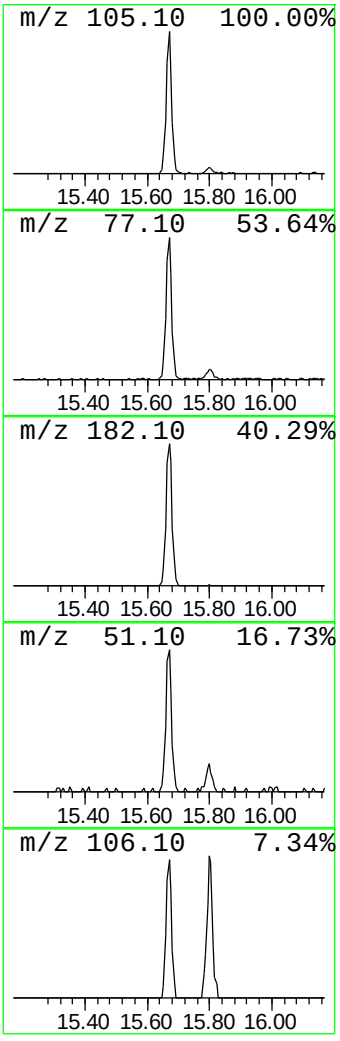
Peak Number 7 Benzophenone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.67	2.86 ng	138268	Acenaphthene-d10	14.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	95
2	2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47
3	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	46
4	3-(Benzoylthio)-2-methylpropanoi...	224	C11H12O3S	067714-34-5	43
5	Ethanone, 2,2,2-trifluoro-1-phenyl-	174	C8H5F3O	000434-45-7	43





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

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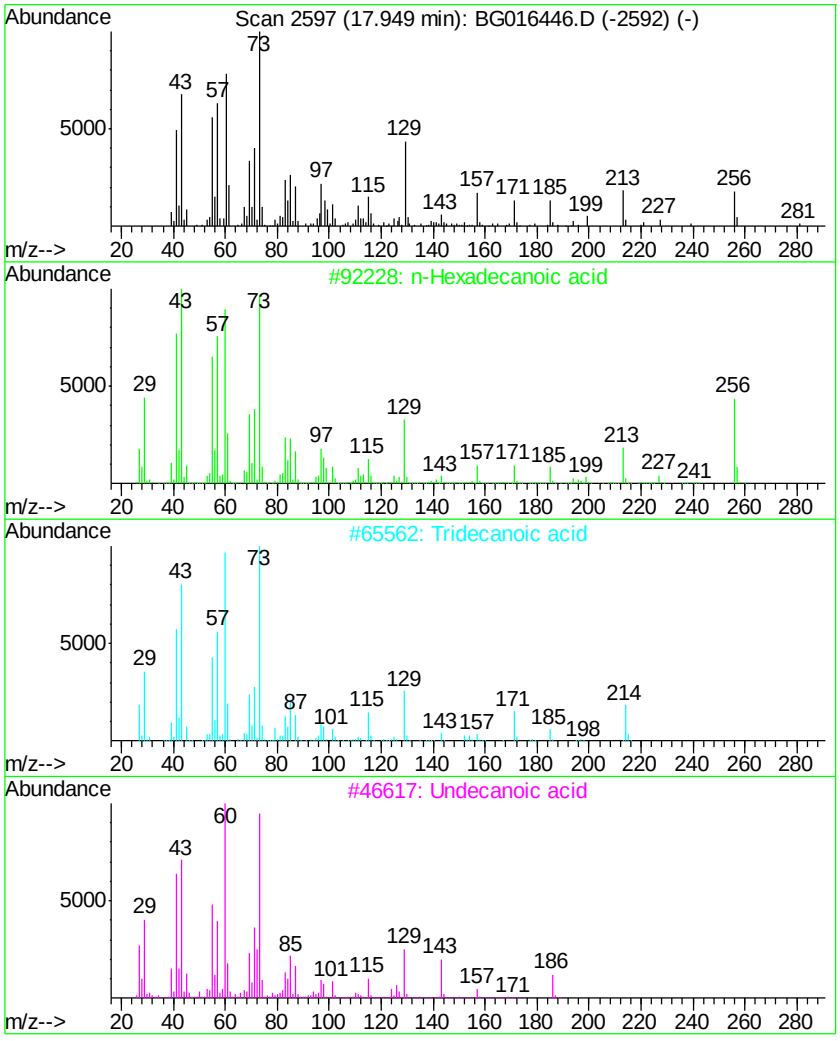
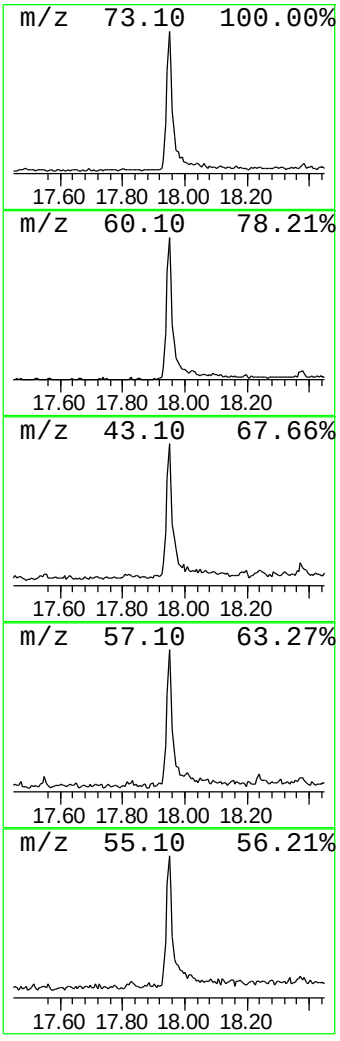
Peak Number 8 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.95	4.57 ng	276255	Phenanthrene-d10	17.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Undecanoic acid	186	C11H22O2	000112-37-8	87
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68





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Instrument : BNA_G
ClientSampleId : TE-PMW-11S

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

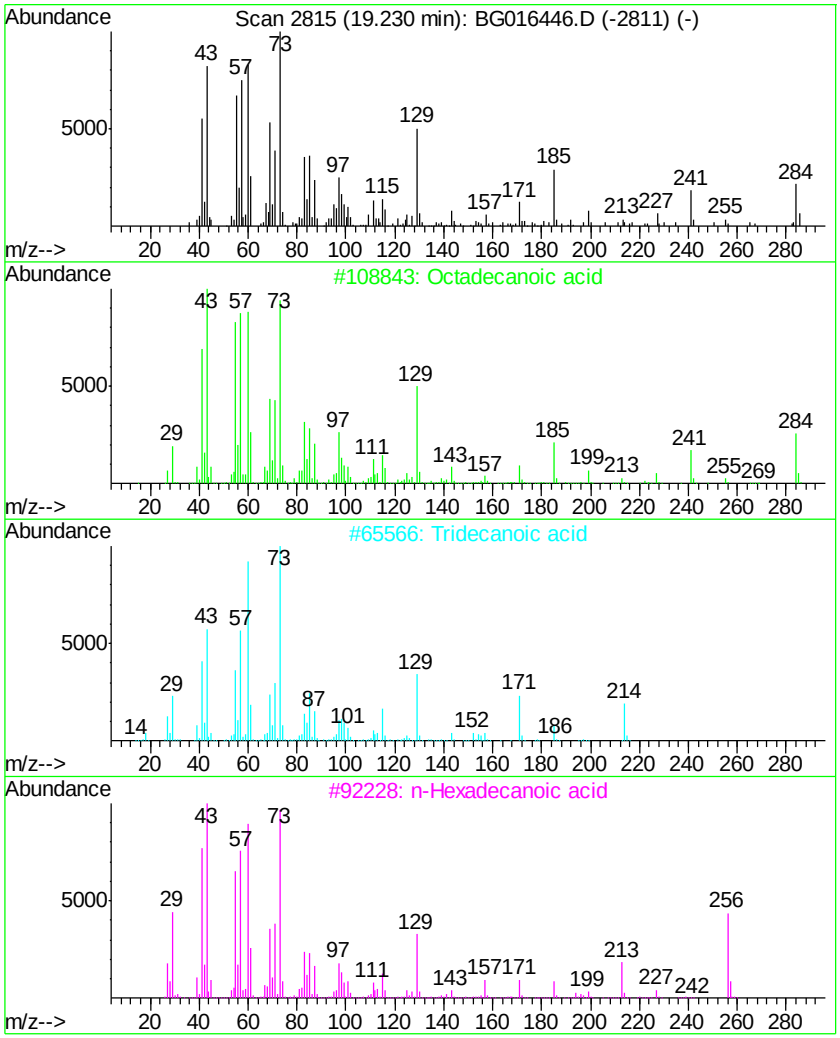
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

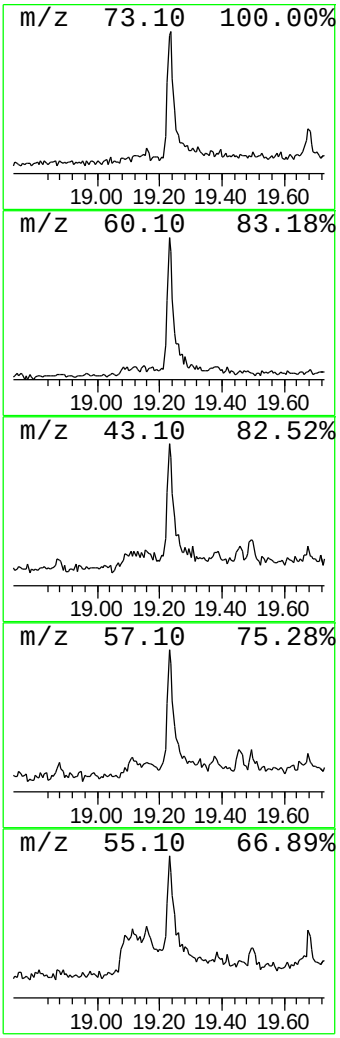
****

Peak Number 9 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.23	3.18 ng	194469	Chrysene-d12	21.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72





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Misc :
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Instrument : BNA_G
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
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TIC Library : C:\DATABASE\NIST02.L
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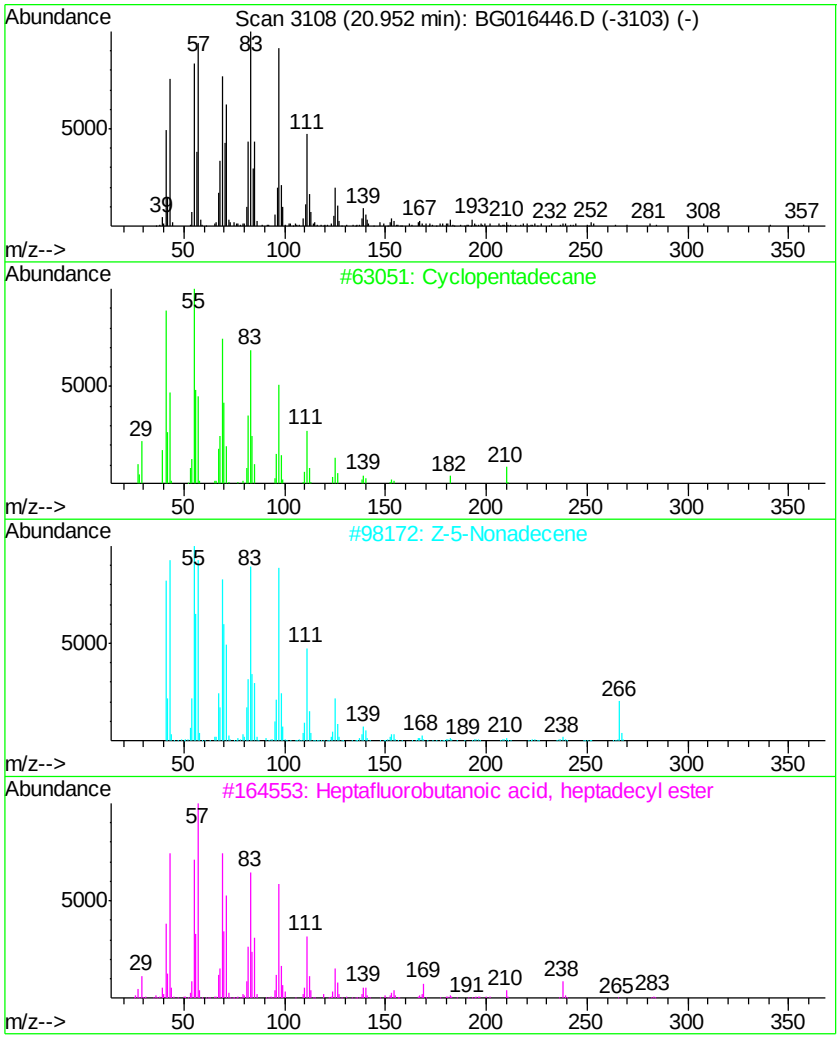
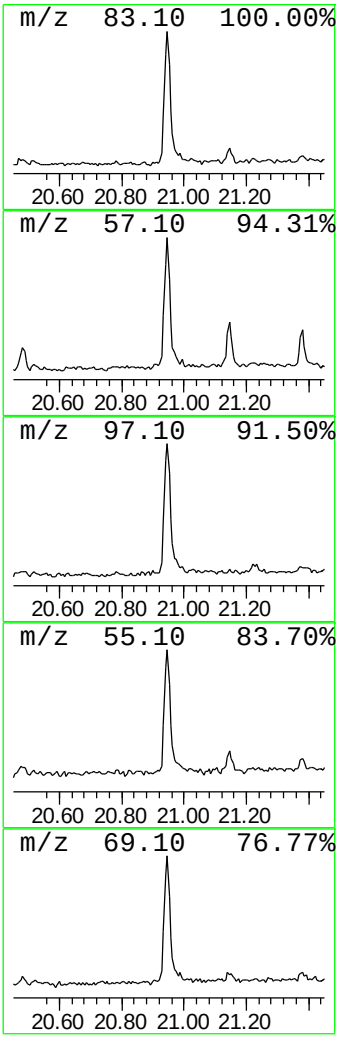
Peak Number 10 Cyclopentadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.95	6.54 ng	399671	Chrysene-d12	21.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	97
2	Z-5-Nonadecene	266	C19H38	1000131-11-8	97
3	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	93
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
5	1-Nonadecene	266	C19H38	018435-45-5	92





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Instrument : BNA_G
ClientSampleId : TE-PMW-11S

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.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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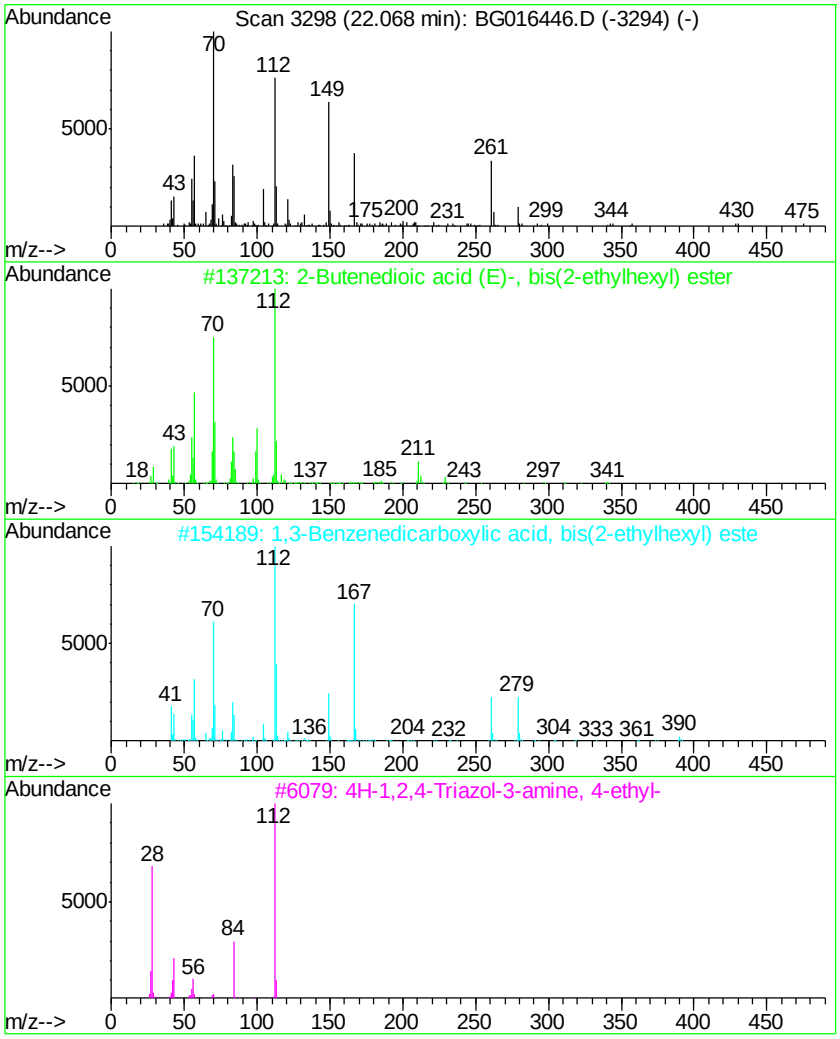
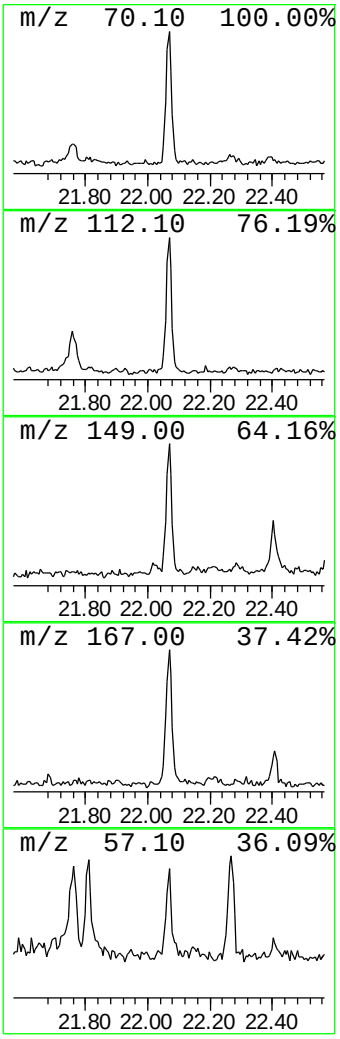
Peak Number 11 unknown22.07 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.07	2.09 ng	127726	Chrysene-d12	21.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenedioic acid (E)-, bis(2-e...	340	C20H36O4	000141-02-6	25
2	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	25
3	4H-1,2,4-Triazol-3-amine, 4-ethyl-	112	C4H8N4	042786-06-1	22
4	1,3-Cyclohexanedione, 4-propyl-	154	C9H14O2	018456-81-0	16
5	Phenol, 3-fluoro-	112	C6H5FO	000372-20-3	14





Tentatively Identified Compound (LSC) summary

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Data File : BG016446.D
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Operator : TP/IZ
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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
Butane, 2-methoxy...	2.84	24.7	ng	570165	1	7.67	461396	20.0
2-Pentanone, 4-hy...	4.78	3.7	ng	84909	1	7.67	461396	20.0
Ethanol, 2-(2-met...	6.18	2.0	ng	46745	1	7.67	461396	20.0
unknown7.20	7.20	86.1	ng	1986150	1	7.67	461396	20.0
Benzophenone	15.67	2.9	ng	138268	3	14.31	966835	20.0
n-Hexadecanoic acid	17.95	4.6	ng	276255	4	17.05	1208030	20.0
Octadecanoic acid	19.23	3.2	ng	194469	5	21.23	1221890	20.0
Cyclopentadecane	20.95	6.5	ng	399671	5	21.23	1221890	20.0
unknown22.07	22.07	2.1	ng	127726	5	21.23	1221890	20.0