LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062616\
Data File : BG022602.D
Acq On : 26 Jun 2016 9:25
Operator : UM/SJ
Sample : H3701-08
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TEC-COMP-B2D

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-BG062516.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	3.057	32	37	54	rBV	8256266	13461672	100.00%	17.914%
2	5.237	403	408	417	rBV	174884	279358	2.08%	0.372%
3	5.707	480	488	497	rVB	2717858	4354231	32.35%	5.794%
4	7.311	752	761	771	rBV	2782333	5014384	37.25%	6.673%
5	7.693	816	826	834	rBV	2704585	4740265	35.21%	6.308%
6	8.163	899	906	915	rVB2	460820	803703	5.97%	1.070%
7	8.486	951	961	972	rVB	1980509	3506952	26.05%	4.667%
8	9.332	1097	1105	1114	rVB	1739273	3164453	23.51%	4.211%
9	10.989	1376	1387	1394	rBV	594991	1119492	8.32%	1.490%
10	13.421	1793	1801	1812	rVB	4372280	6917854	51.39%	9.206%
11	14.238	1934	1940	1949	rVB	847025	1232753	9.16%	1.640%
12	14.796	2028	2035	2046	rVB2	1039979	1678392	12.47%	2.234%
13	16.289	2280	2289	2300	rBV	4570379	7297889	54.21%	9.712%
14	16.488	2317	2323	2327	rBV3	95858	155854	1.16%	0.207%
15	17.552	2498	2504	2511	rBV	1458369	2313750	17.19%	3.079%
16	18.427	2647	2653	2663	rBV	557982	835318	6.21%	1.112%
17	19.691	2864	2868	2874	rBV	435589	603746	4.48%	0.803%
18	20.155	2941	2947	2953	rBV	8136360	11682865	86.79%	15.547%
19	21.465	3166	3170	3179	rBV7	196652	353679	2.63%	0.471%
20	21.847	3229	3235	3244	rVB	1686912	2827321	21.00%	3.762%
21	25.208	3798	3807	3819	rVB2	918200	2802165	20.82%	3.729%

Sum of corrected areas: 75146096

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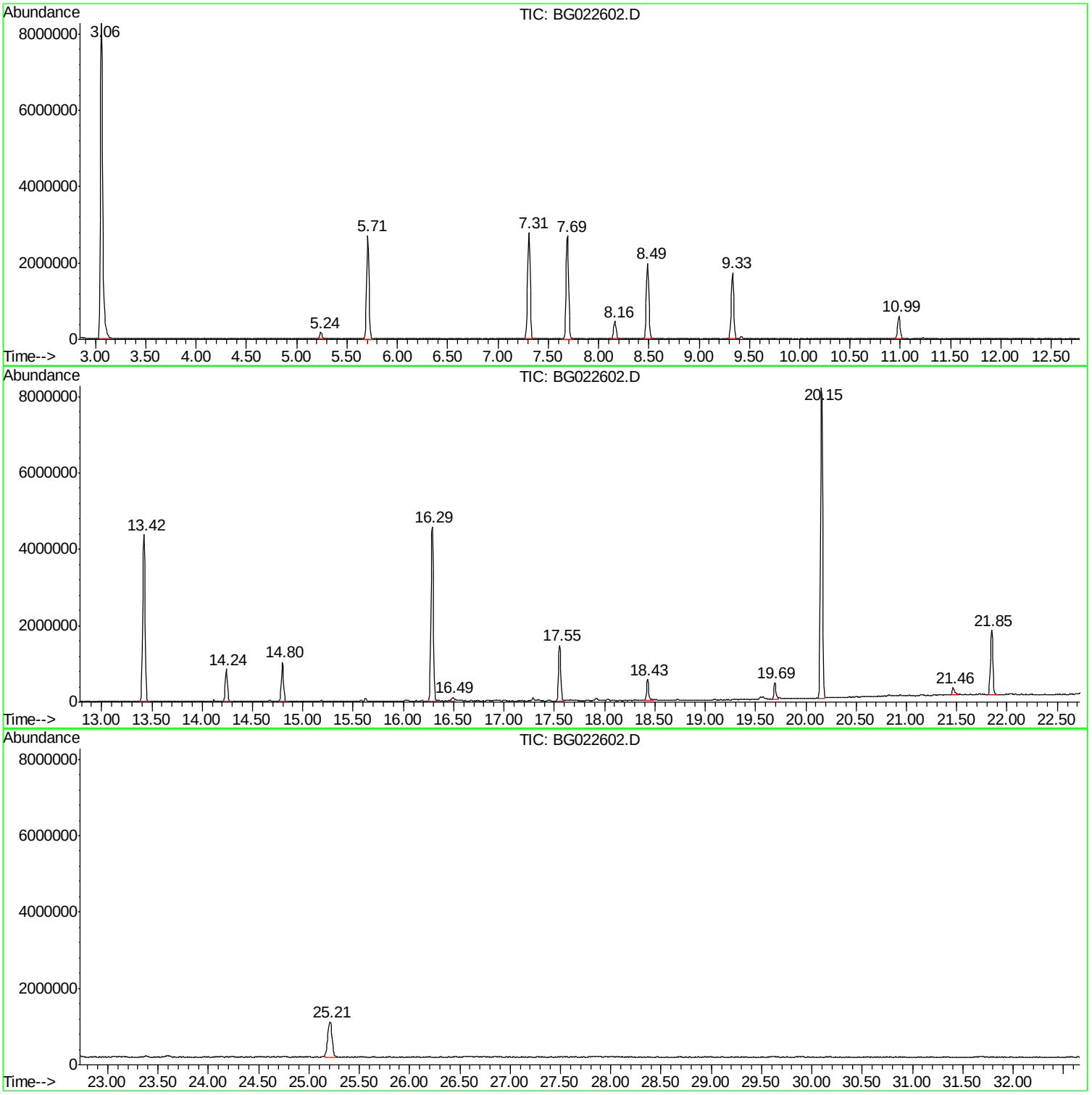
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TEC-COMP-B2D

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062516.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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Data File : BG022602.D
Acq On : 26 Jun 2016 9:25
Operator : UM/SJ
Sample : H3701-08
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TEC-COMP-B2D

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

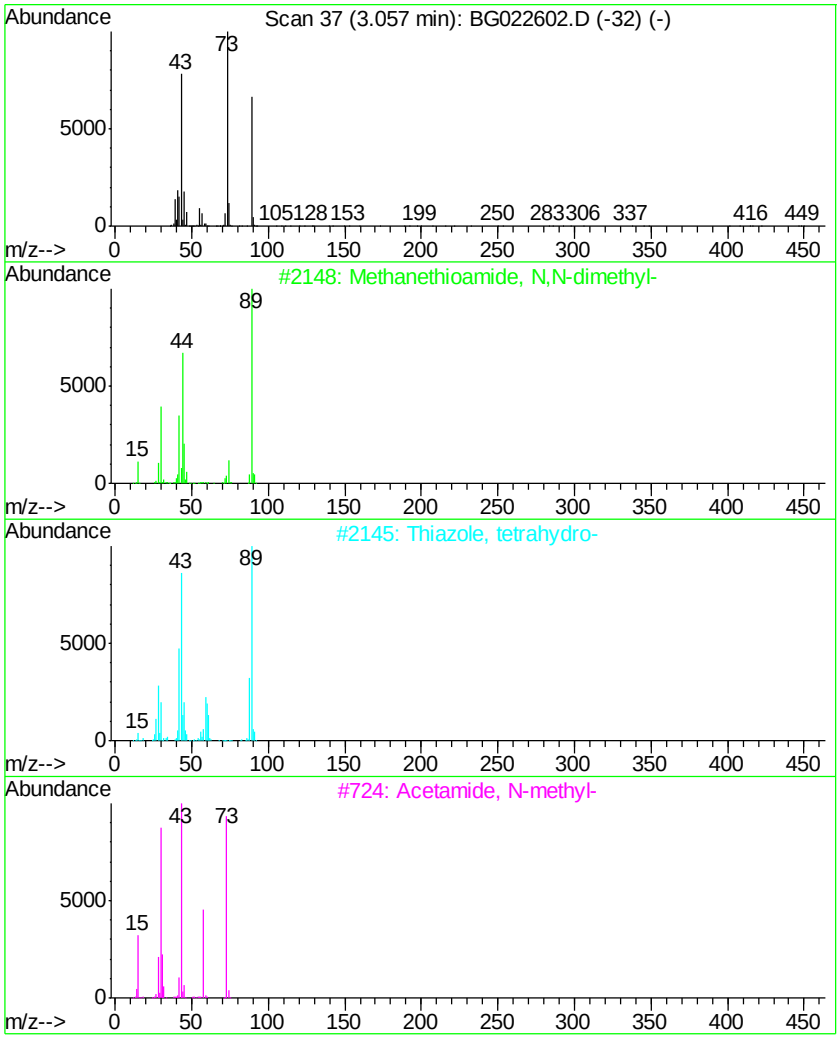
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

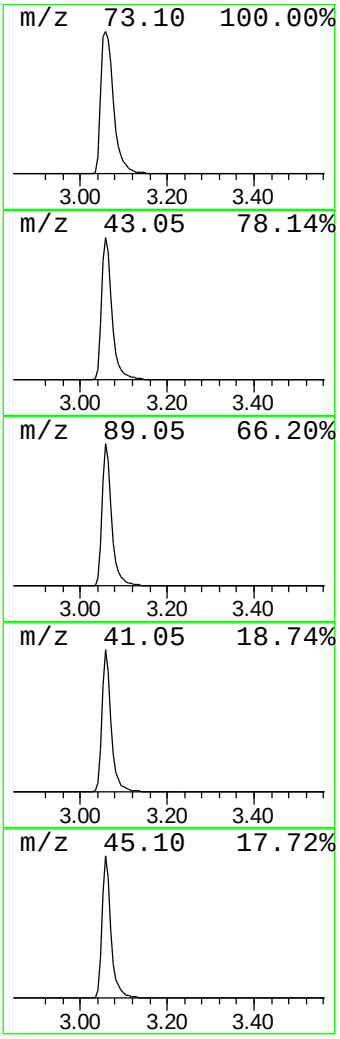
****

Peak Number 1 unknown3.06 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.06	334.99 ng	13461700	1,4-Dichlorobenzene-d4	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanethioamide, N,N-dimethyl-	89	C3H7NS	000758-16-7	43
2	Thiazole, tetrahydro-	89	C3H7NS	000504-78-9	28
3	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	25
4	1-Hepten-4-ol	114	C7H14O	003521-91-3	23
5	2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	17





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062616\
Data File : BG022602.D
Acq On : 26 Jun 2016 9:25
Operator : UM/SJ
Sample : H3701-08
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TEC-COMP-B2D

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062516.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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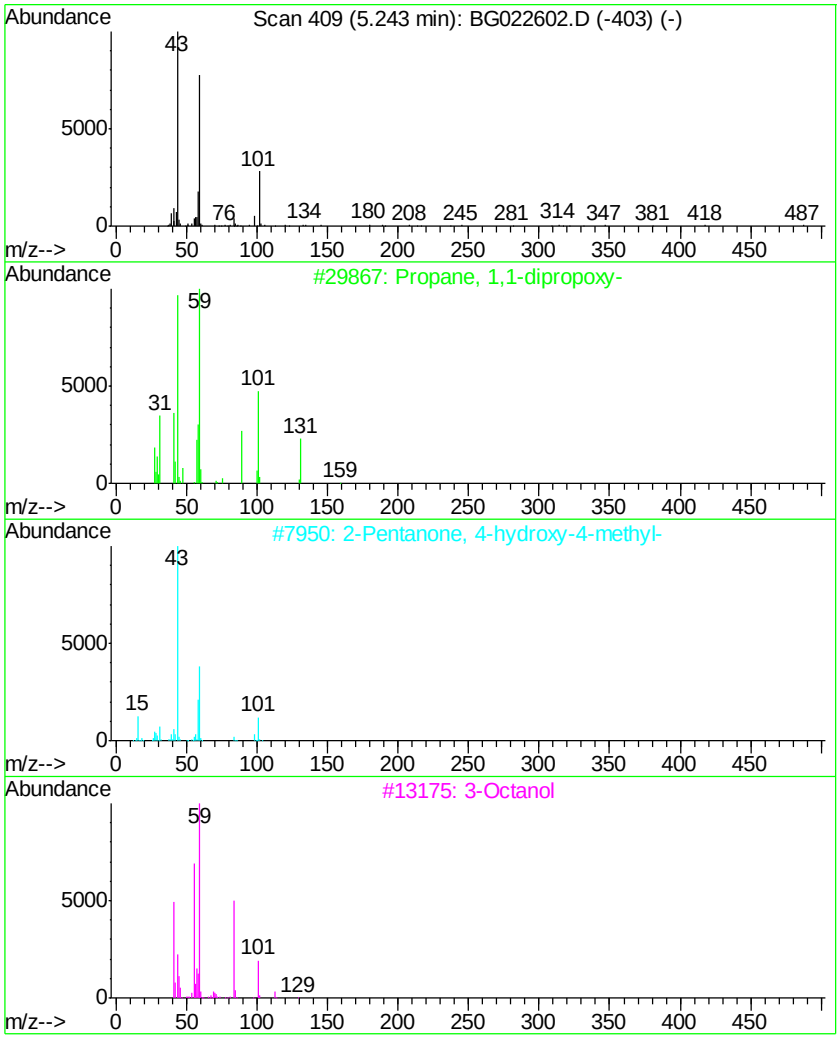
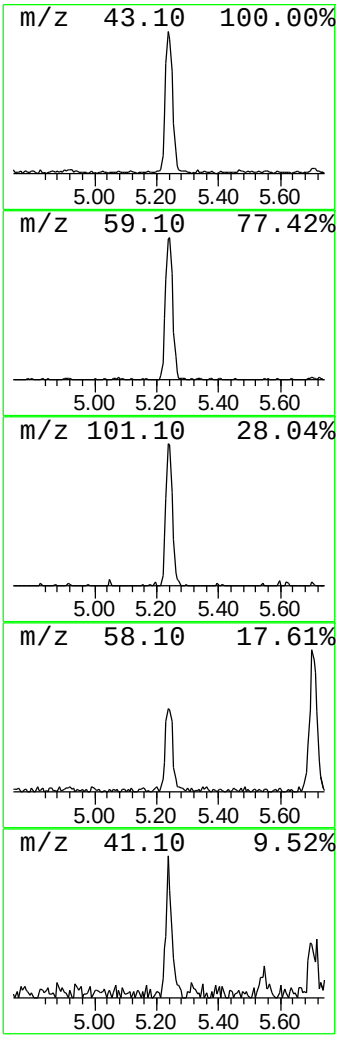
Peak Number 2 Propane, 1,1-dipropoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.24	6.95 ng	279358	1,4-Dichlorobenzene-d4	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	50
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
3	3-Octanol	130	C8H18O	020296-29-1	28
4	4-Ethyl-3-octanol	158	C10H22O	019781-26-1	23
5	3-Heptadecanol	256	C17H36O	084534-30-5	23





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062616\
Data File : BG022602.D
Acq On : 26 Jun 2016 9:25
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Sample : H3701-08
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TEC-COMP-B2D

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062516.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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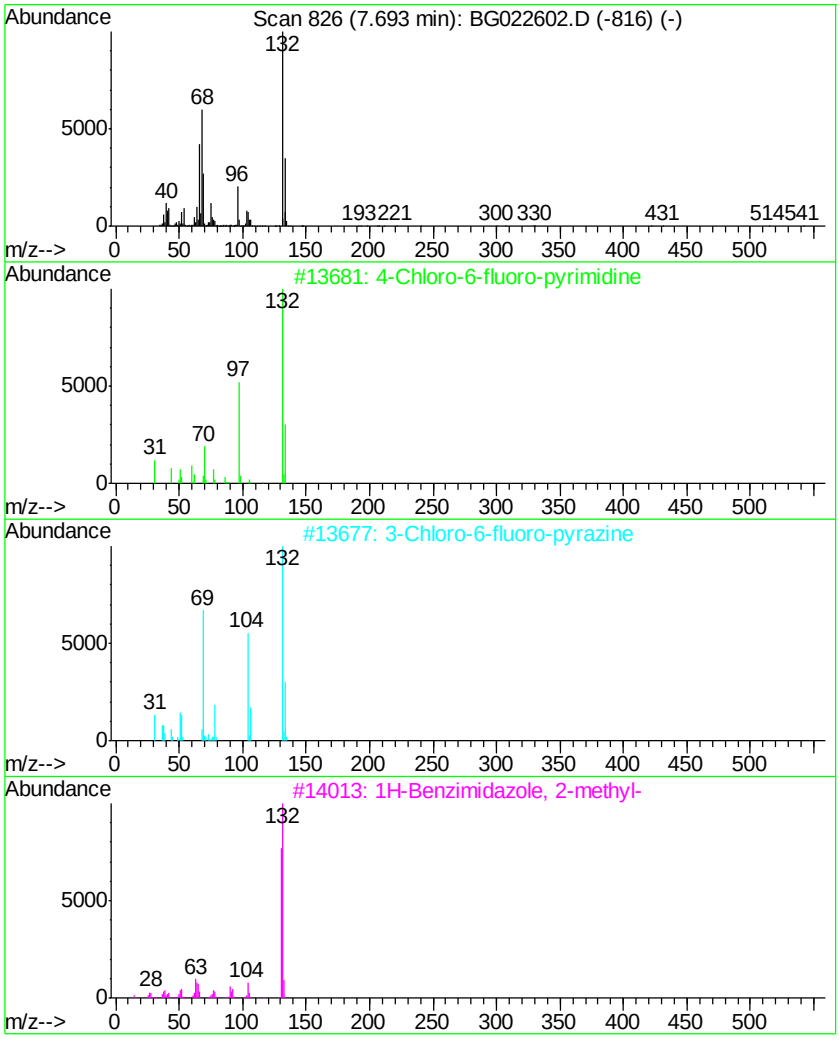
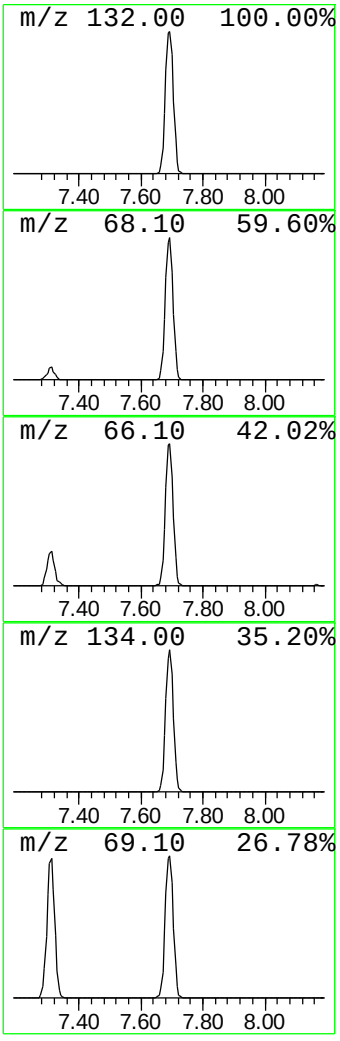
Peak Number 3 unknown7.69 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.69	117.96 ng	4740270	1,4-Dichlorobenzene-d4	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	10
5	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	10





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Data File : BG022602.D
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Operator : UM/SJ
Sample : H3701-08
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TEC-COMP-B2D

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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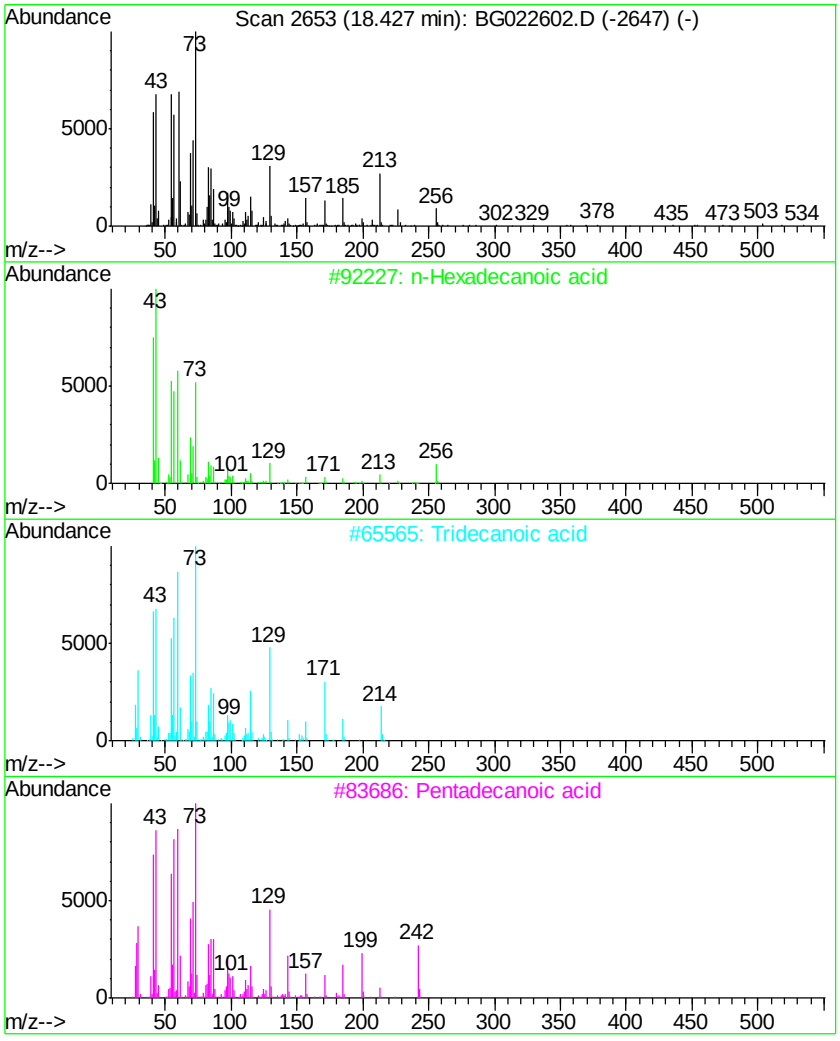
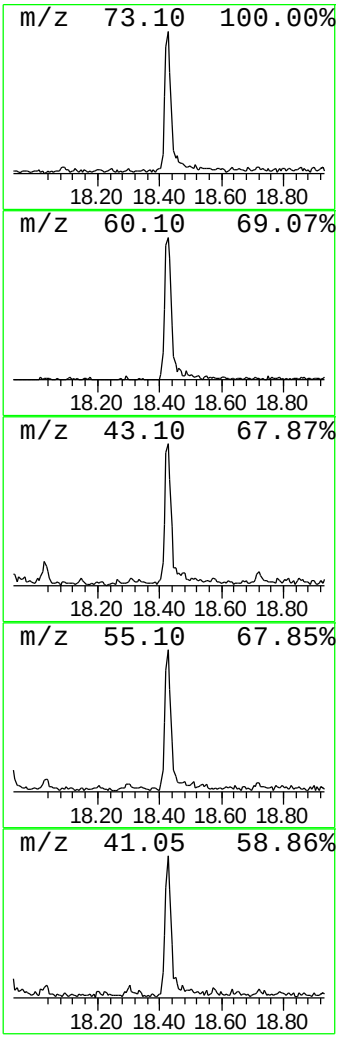
Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.43	7.22 ng	835318	Phenanthrene-d10	17.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Tridecanoic acid	214	C13H26O2	000638-53-9	62
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	58
4	Undecane, 5-methyl-	170	C12H26	001632-70-8	35
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	18





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Data File : BG022602.D
Acq On : 26 Jun 2016 9:25
Operator : UM/SJ
Sample : H3701-08
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TEC-COMP-B2D

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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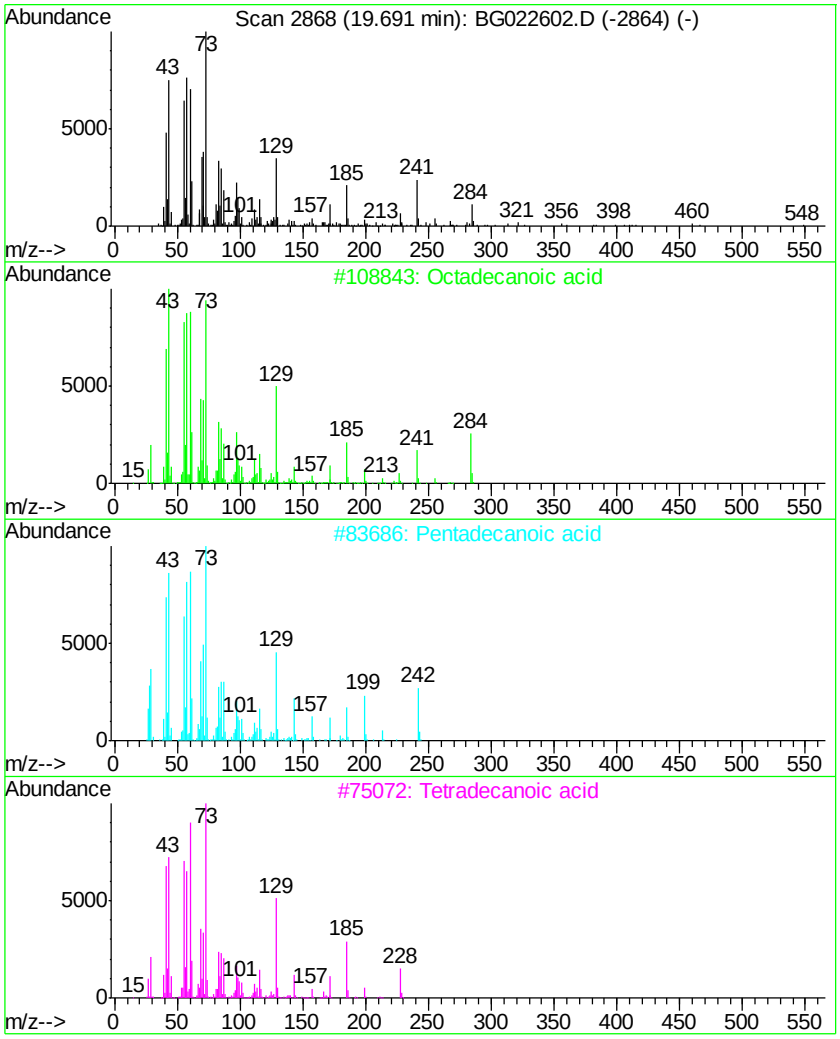
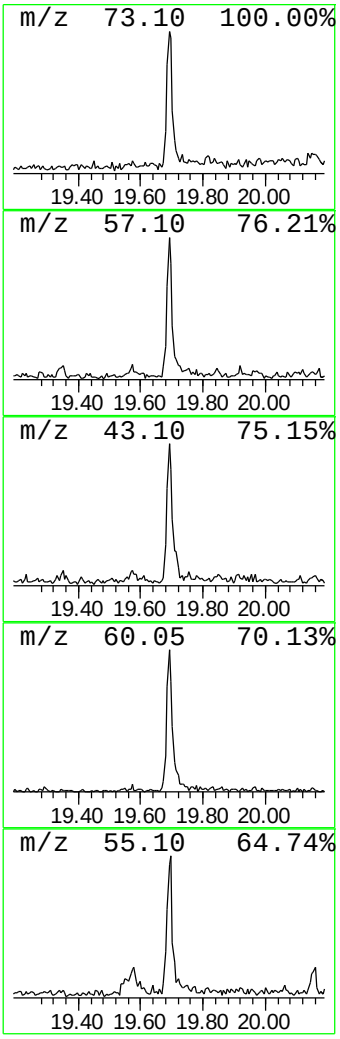
Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.69	5.22 ng	603746	Phenanthrene-d10	17.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	60
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58
5	Nonadecane	268	C19H40	000629-92-5	56





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Operator : UM/SJ
Sample : H3701-08
Misc :
ALS Vial : 57 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TEC-COMP-B2D

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

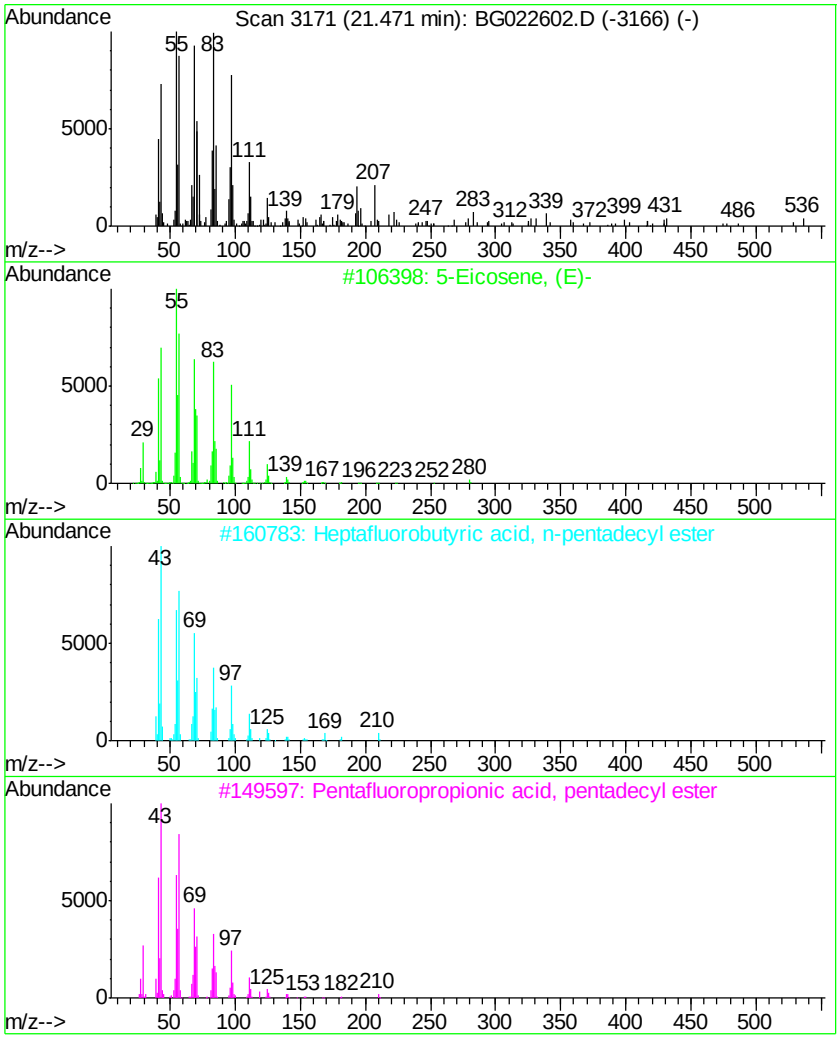
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

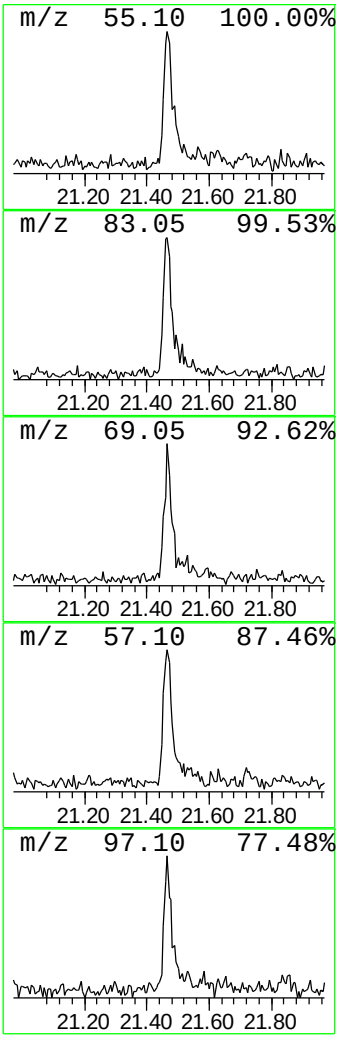
****

Peak Number 7 5-Eicosene, (E)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.47	2.50 ng	353679	Chrysene-d12	21.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	93
2	Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	91
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	1000280-07-5	91
4	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
5	1-Hexadecene	224	C16H32	000629-73-2	91





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_G
ClientSampleId : TEC-COMP-B2D

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062516.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
unknown3.06	3.06	335.0	ng	13461700	1	8.16	803703	20.0
Propane, 1,1-dipr...	5.24	7.0	ng	279358	1	8.16	803703	20.0
unknown7.69	7.69	118.0	ng	4740270	1	8.16	803703	20.0
n-Hexadecanoic acid	18.43	7.2	ng	835318	4	17.55	2313750	20.0
Octadecanoic acid	19.69	5.2	ng	603746	4	17.55	2313750	20.0
5-Eicosene, (E)-	21.47	2.5	ng	353679	5	21.85	2827320	20.0