LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062616\
Data File : BG022601.D
Acq On : 26 Jun 2016 8:45
Operator : UM/SJ
Sample : H3663-18
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-11

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	3.055	32	37	56	rBV	5909104	8986967	70.93%	11.381%
2	5.241	402	409	419	rBV	736270	1159658	9.15%	1.469%
3	5.705	481	488	497	rBV	3106004	4986208	39.36%	6.315%
4	7.309	752	761	771	rBV	3304866	5813327	45.88%	7.362%
5	7.691	818	826	834	rBV	3167159	5409877	42.70%	6.851%
6	8.161	898	906	914	rBV	553443	963025	7.60%	1.220%
7	8.490	955	962	973	rVB	2065962	3634000	28.68%	4.602%
8	9.336	1096	1106	1114	rVB	1956687	3603962	28.45%	4.564%
9	10.987	1379	1387	1389	rBV	735207	1206259	9.52%	1.528%
10	11.005	1389	1390	1398	rVB5	691921	306376	2.42%	0.388%
11	13.420	1793	1801	1810	rBV	4367149	6889218	54.38%	8.725%
12	14.236	1935	1940	1947	rBV	728937	1057150	8.34%	1.339%
13	14.794	2027	2035	2043	rBV2	1244563	2020496	15.95%	2.559%
14	15.382	2125	2135	2146	rBV4	63886	187467	1.48%	0.237%
15	16.287	2277	2289	2297	rBV	5460377	8389679	66.22%	10.625%
16	17.550	2498	2504	2511	rBV	1770703	2712436	21.41%	3.435%
17	18.425	2648	2653	2663	rBV	416068	648902	5.12%	0.822%
18	19.689	2864	2868	2874	rBV2	208772	328515	2.59%	0.416%
19	19.841	2890	2894	2898	rVB2	145481	171371	1.35%	0.217%
20	20.159	2941	2948	2954	rBV	9083296	12669454	100.00%	16.045%
21	21.463	3166	3170	3181	rBV2	561563	922282	7.28%	1.168%
22	21.845	3228	3235	3242	rBV2	1933701	3291217	25.98%	4.168%
23	22.697	3376	3380	3389	rVB9	152001	351838	2.78%	0.446%
24	22.938	3417	3421	3426	rVB8	100832	164449	1.30%	0.208%
25	25.212	3798	3808	3821	rVB2	997136	3088571	24.38%	3.911%

Sum of corrected areas: 78962704

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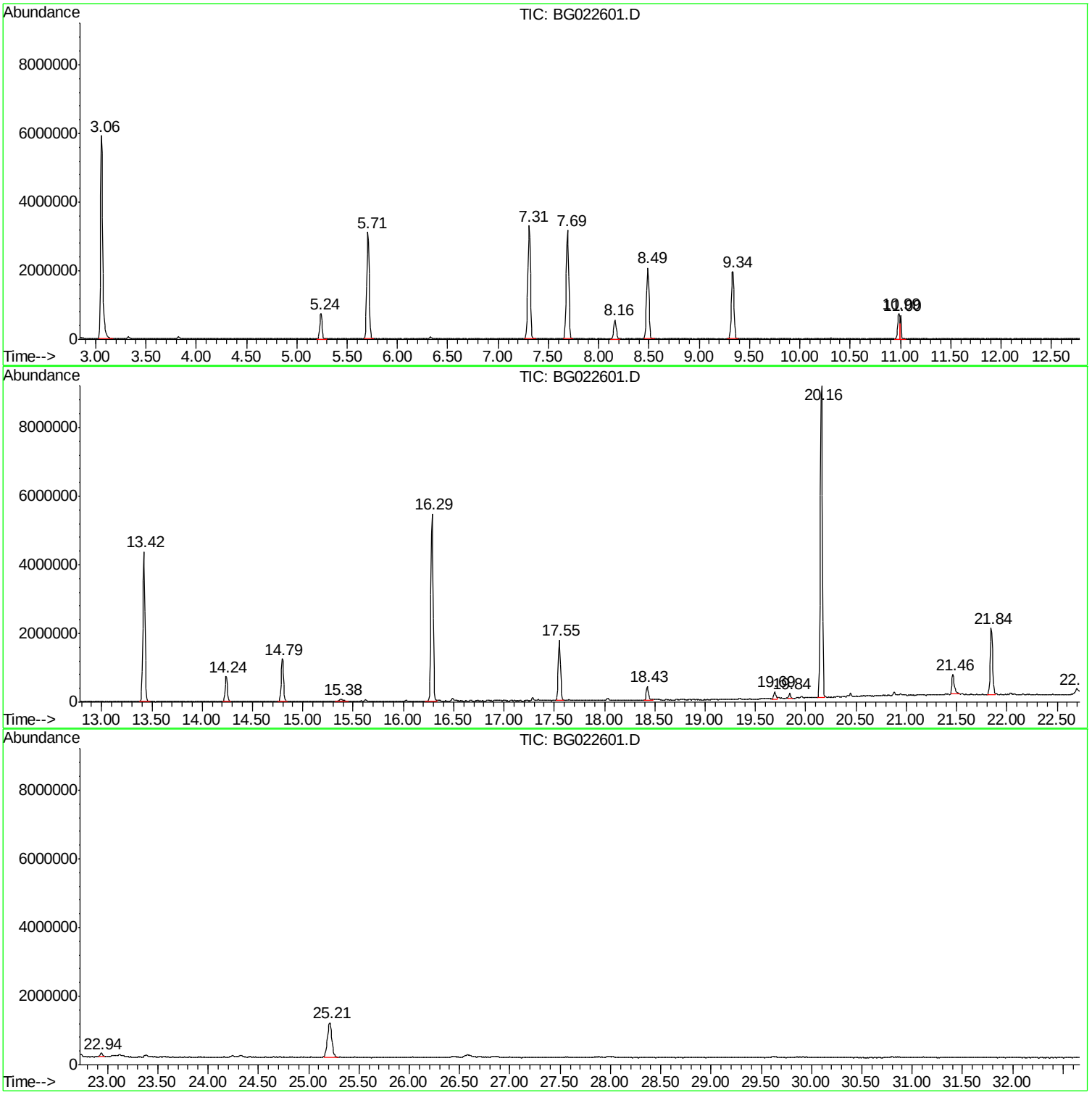
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-11

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062616\
Data File : BG022601.D
Acq On : 26 Jun 2016 8:45
Operator : UM/SJ
Sample : H3663-18
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-11

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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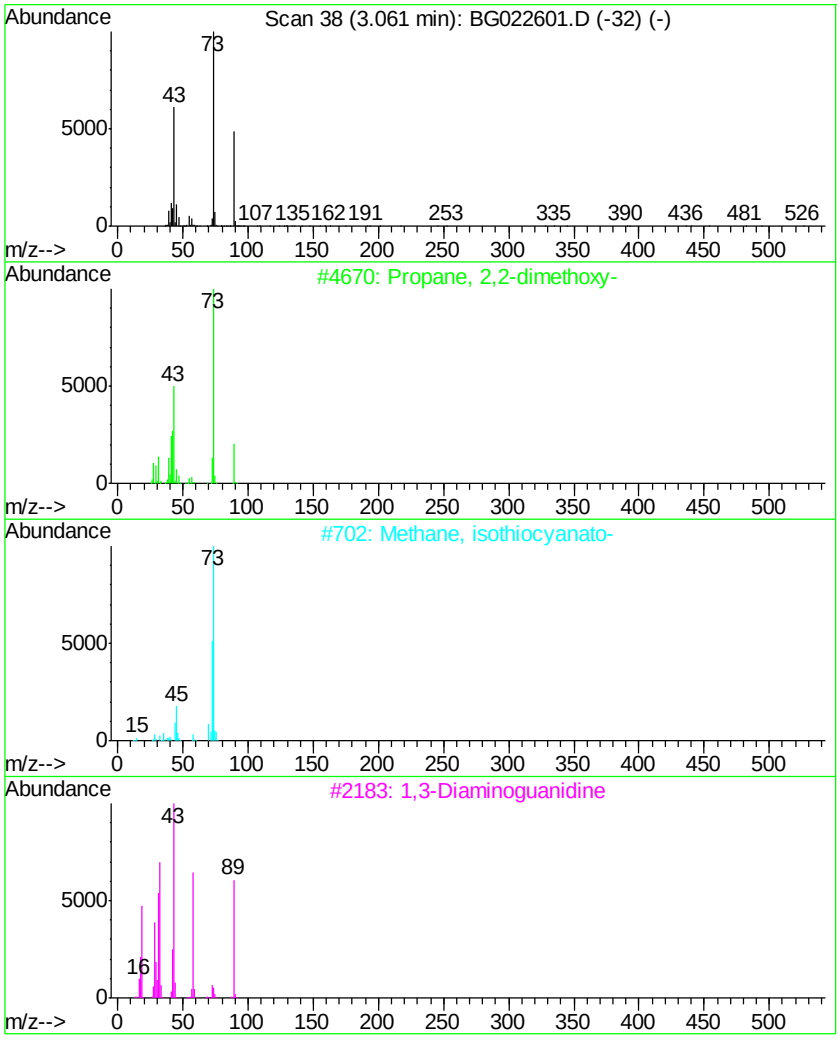
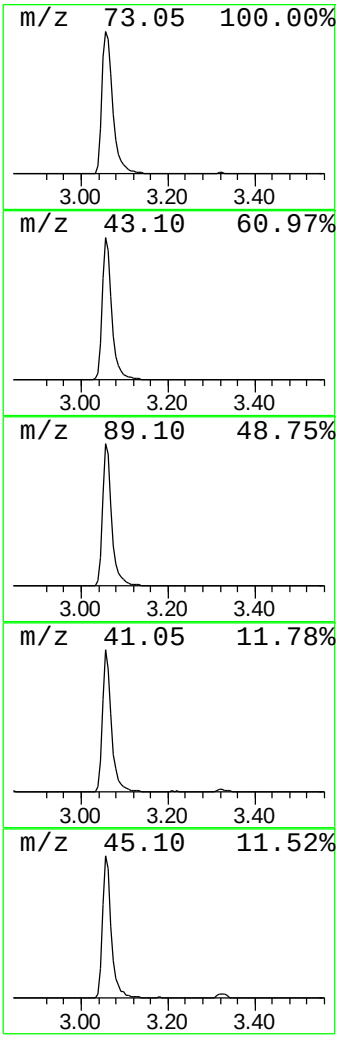
Peak Number 1 unknown3.06 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.06	186.64 ng	8986970	1,4-Dichlorobenzene-d4	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	10
3	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
4	1,3-Dioxolane, 2-(3-bromo-5,5,5-...	352	C10H16BrCl3O2	1000115-31-4	9
5	1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9





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Data File : BG022601.D
Acq On : 26 Jun 2016 8:45
Operator : UM/SJ
Sample : H3663-18
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-11

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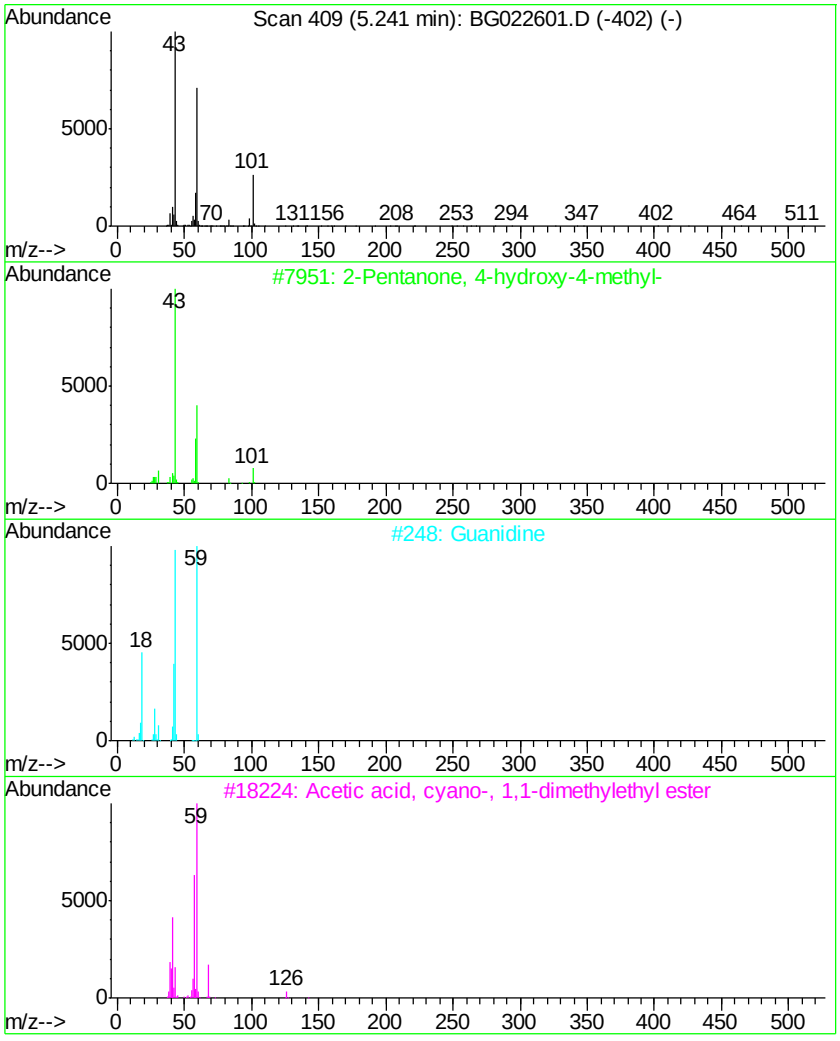
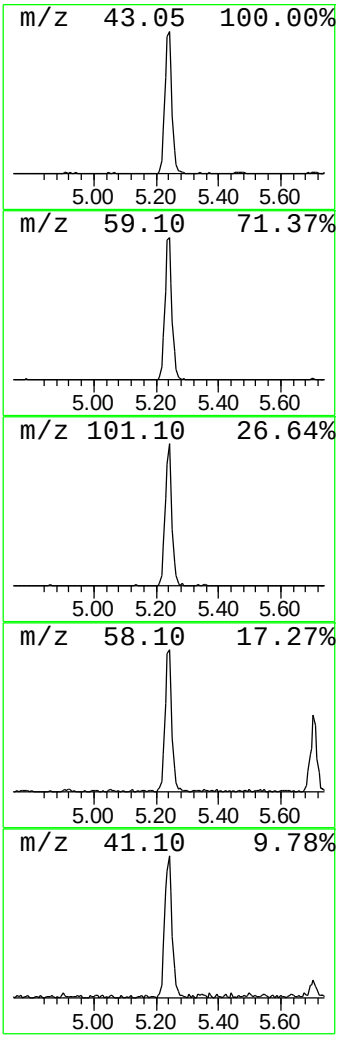
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.24	24.08 ng	1159660	1,4-Dichlorobenzene-d4	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Guanidine	59	CH5N3	000113-00-8	43
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Acetone	58	C3H6O	000067-64-1	10
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062616\
Data File : BG022601.D
Acq On : 26 Jun 2016 8:45
Operator : UM/SJ
Sample : H3663-18
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-11

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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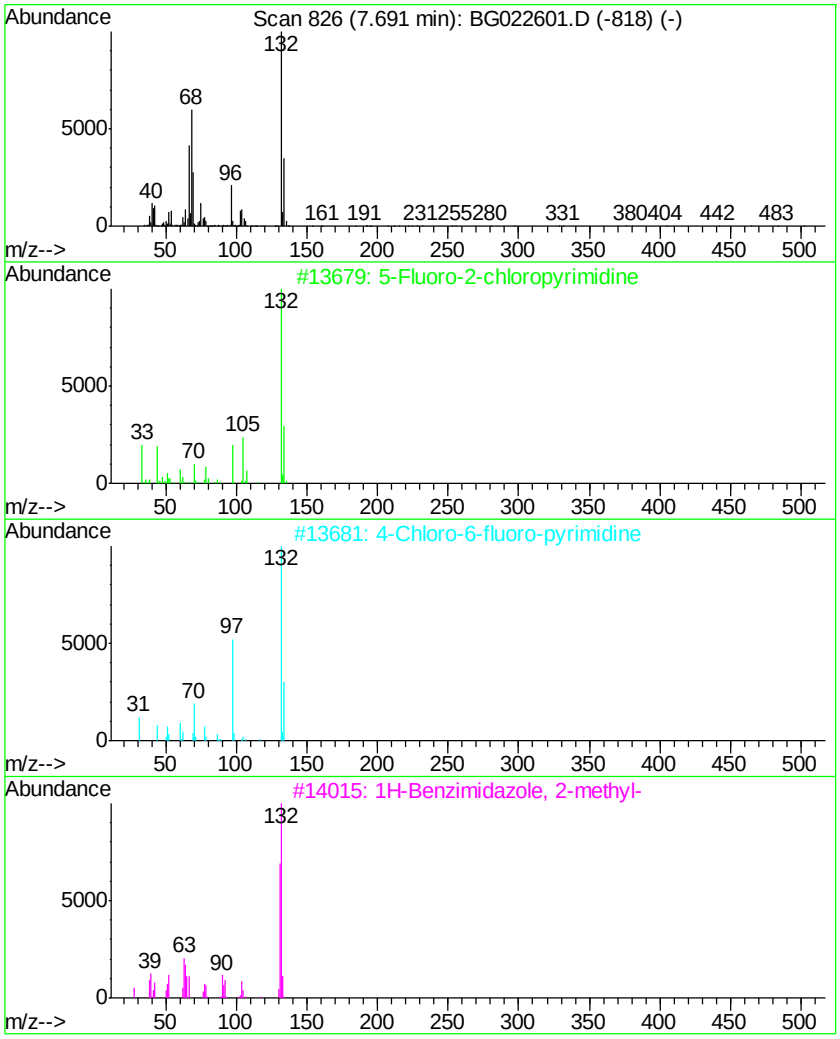
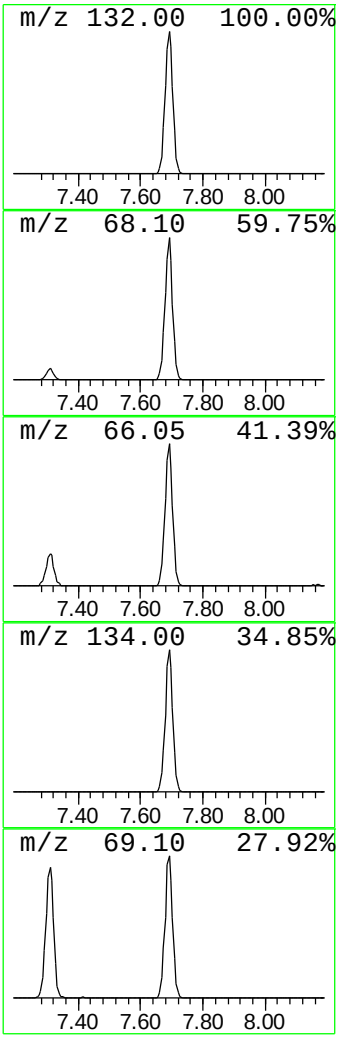
Peak Number 3 unknown7.69 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.69	112.35 ng	5409880	1,4-Dichlorobenzene-d4	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
4	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062616\
Data File : BG022601.D
Acq On : 26 Jun 2016 8:45
Operator : UM/SJ
Sample : H3663-18
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-11

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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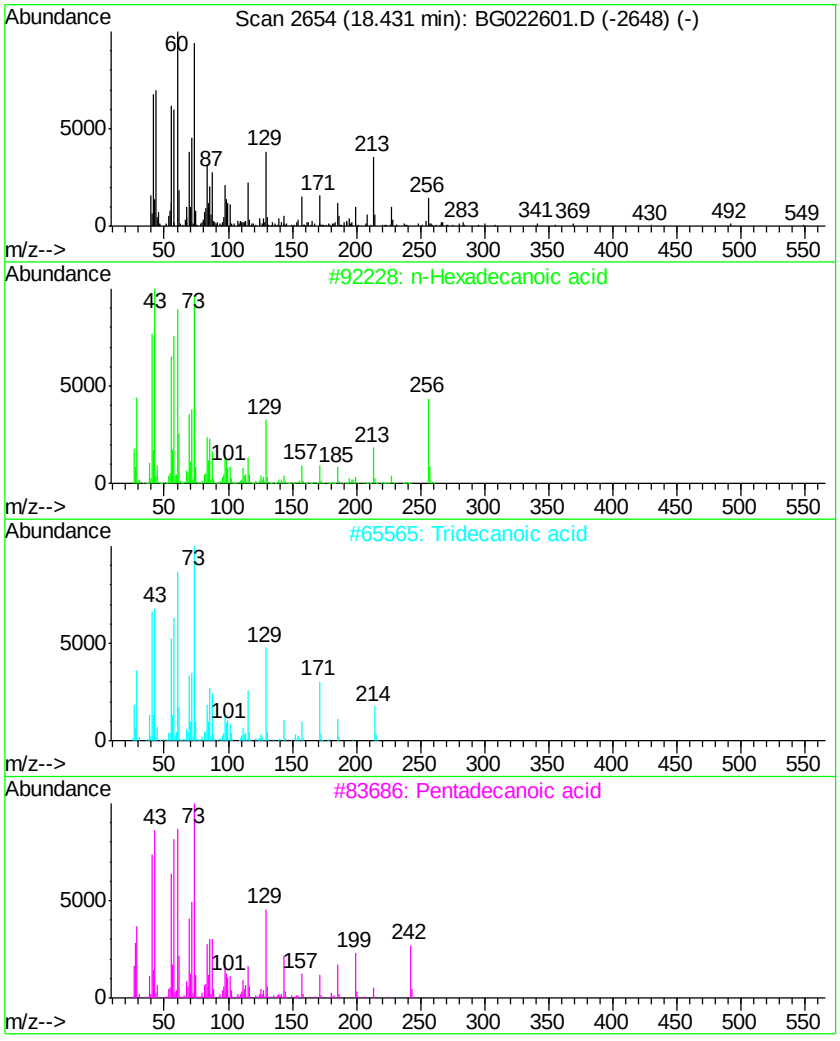
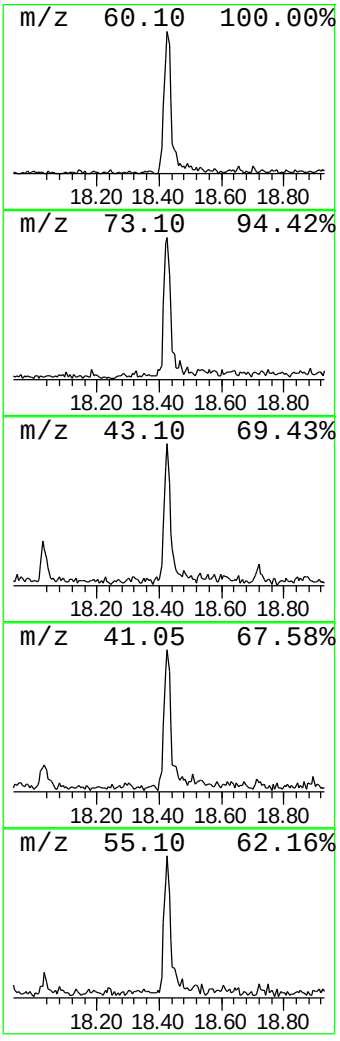
Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.43	4.78 ng	648902	Phenanthrene-d10	17.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062616\
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Operator : UM/SJ
Sample : H3663-18
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-11

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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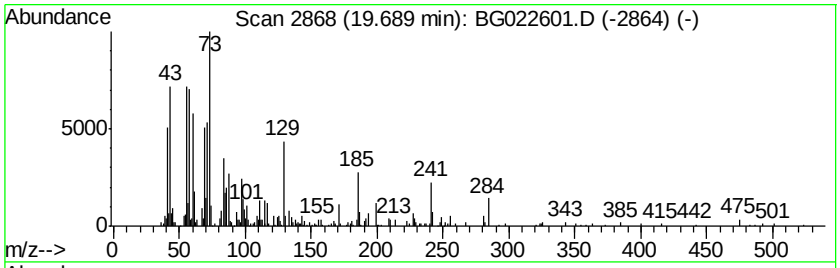
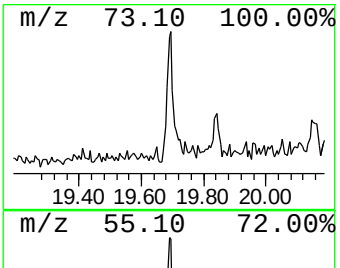
Peak Number 6 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.69	2.42 ng	328515	Phenanthrene-d10	17.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	62
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	30
5	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	27





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Misc :
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Instrument : BNA_G
ClientSampleId : TP-11

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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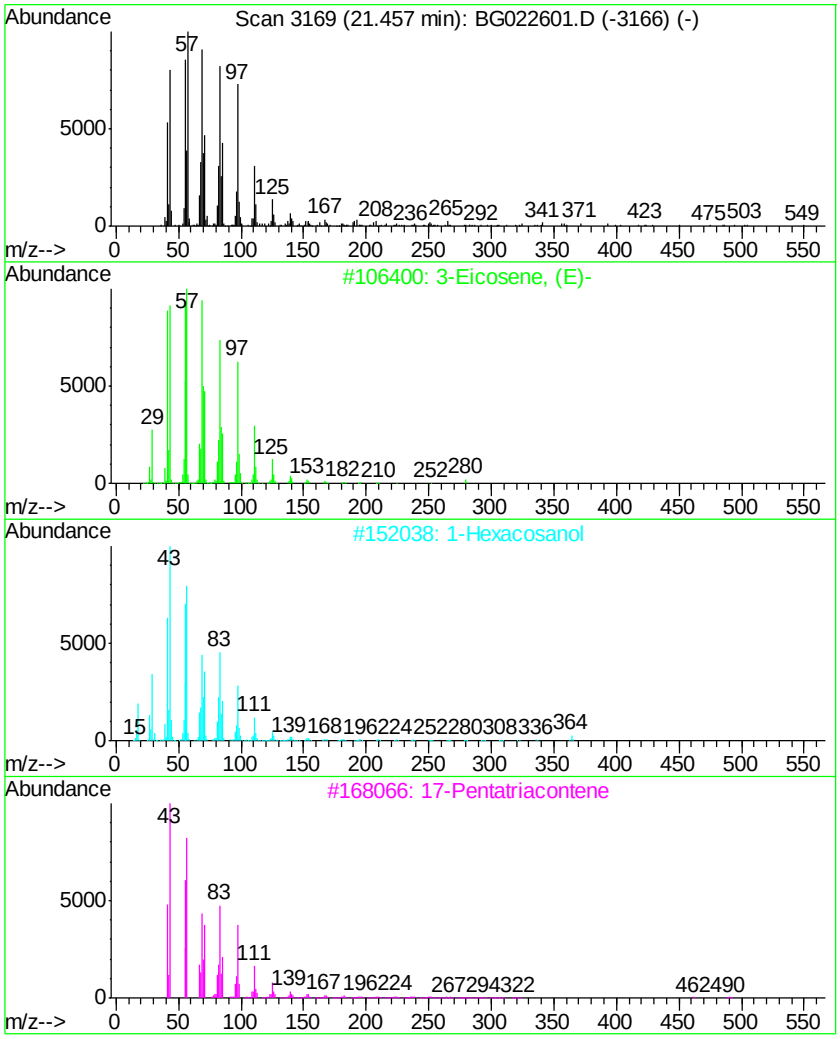
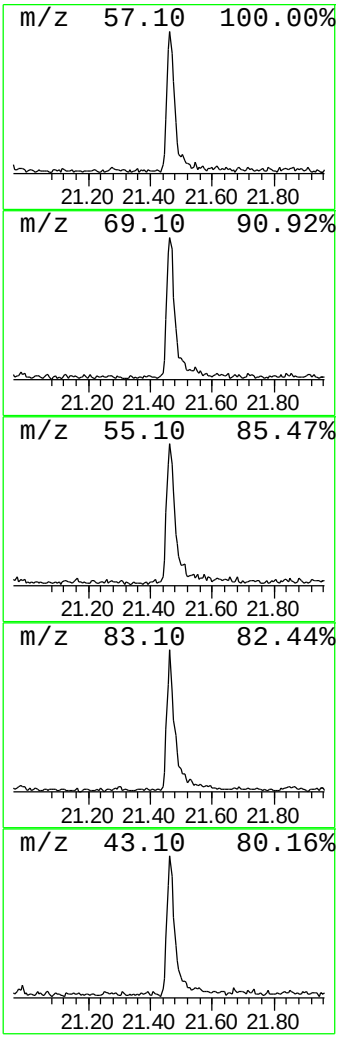
Peak Number 7 3-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.46	5.60 ng	922282	Chrysene-d12	21.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	93
2	1-Hexacosanol	382	C26H54O	000506-52-5	91
3	17-Pentatriacontene	491	C35H70	006971-40-0	91
4	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	68
5	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	68





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ClientSampleId : TP-11

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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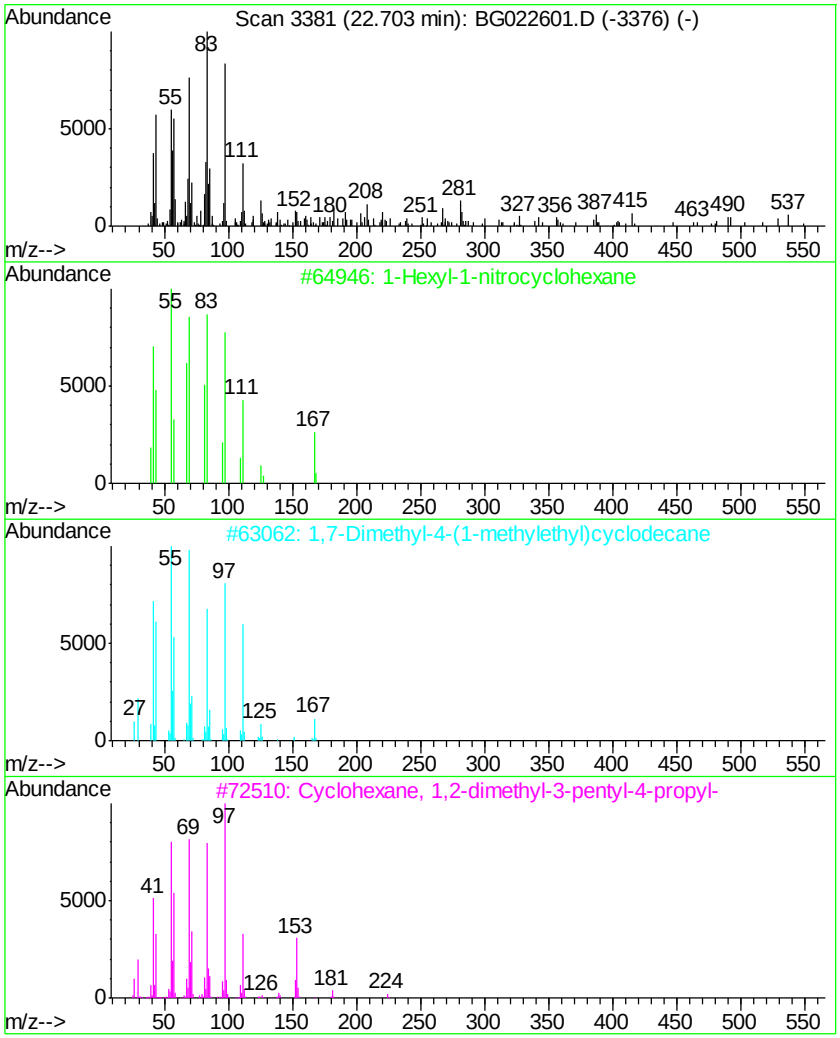
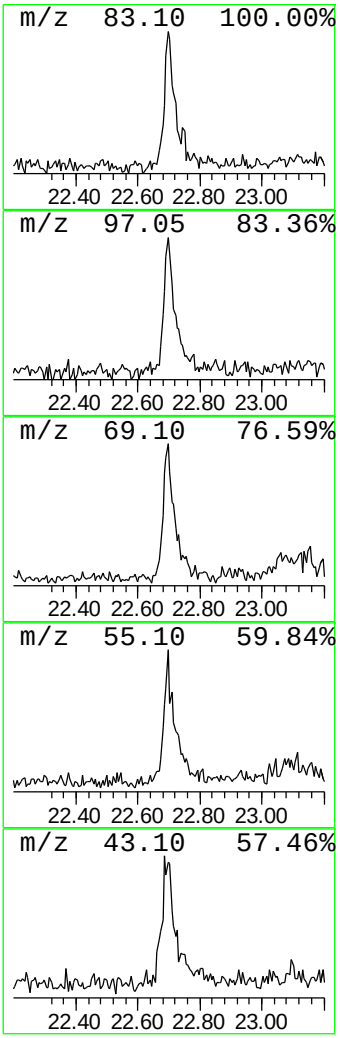
Peak Number 8 1-Hexyl-1-nitrocyclohexane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.70	2.14 ng	351838	Chrysene-d12	21.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexyl-1-nitrocyclohexane	213	C12H23NO2	118252-09-8	72
2	1,7-Dimethyl-4-(1-methylethyl)cy...	210	C15H30	000645-10-3	59
3	Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	50
4	Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	38
5	Cyclooctane, ethyl-	140	C10H20	013152-02-8	30





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062616\
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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
unknown3.06	3.06	186.6	ng	8986970	1	8.16	963025	20.0
2-Pentanone, 4-hy...	5.24	24.1	ng	1159660	1	8.16	963025	20.0
unknown7.69	7.69	112.3	ng	5409880	1	8.16	963025	20.0
n-Hexadecanoic acid	18.43	4.8	ng	648902	4	17.55	2712440	20.0
Octadecanoic acid	19.69	2.4	ng	328515	4	17.55	2712440	20.0
3-Eicosene, (E)-	21.46	5.6	ng	922282	5	21.84	3291220	20.0
1-Hexyl-1-nitrocy...	22.70	2.1	ng	351838	5	21.84	3291220	20.0