LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG091215\
Data File : BG018657.D
Acq On : 12 Sep 2015 2:25
Operator : UM/IZ
Sample : G3620-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-14(7-9.5)

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-BG091115.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	2.964	16	21	40	rVV	3249070	4391897	89.49%	14.601%
2	3.105	40	45	53	rVV3	37516	73169	1.49%	0.243%
3	3.181	53	58	63	rVV	536779	709205	14.45%	2.358%
4	3.222	63	65	75	rVB2	55063	71946	1.47%	0.239%
5	5.108	378	386	395	rBV	487321	709442	14.46%	2.358%
6	5.578	458	466	479	rBV	1056197	1613644	32.88%	5.364%
7	7.170	729	737	746	rBV	1031474	1771683	36.10%	5.890%
8	7.541	791	800	810	rBV	1057923	1781078	36.29%	5.921%
9	8.005	871	879	888	rVB	200994	337068	6.87%	1.121%
10	8.328	925	934	942	rBV	742495	1262214	25.72%	4.196%
11	9.162	1067	1076	1086	rBV	625566	1087381	22.16%	3.615%
12	10.807	1349	1356	1366	rVB	267408	484596	9.87%	1.611%
13	13.257	1763	1773	1780	rBV	1779616	2729931	55.63%	9.075%
14	14.074	1906	1912	1919	rBV	324256	470174	9.58%	1.563%
15	14.632	1998	2007	2017	rVB2	469191	755008	15.38%	2.510%
16	16.119	2252	2260	2270	rBV	1662478	2481482	50.57%	8.250%
17	17.376	2467	2474	2482	rBV	688680	1064517	21.69%	3.539%
18	18.257	2619	2624	2634	rBV2	197262	308162	6.28%	1.024%
19	19.527	2836	2840	2848	rBV3	41715	71559	1.46%	0.238%
20	19.985	2911	2918	2930	rBV	3626246	4907504	100.00%	16.315%
21	21.277	3133	3138	3147	rBV3	116584	242534	4.94%	0.806%
22	21.630	3192	3198	3206	rBV	795692	1308377	26.66%	4.350%
23	23.299	3475	3482	3489	rBV	65286	130751	2.66%	0.435%
24	24.820	3730	3741	3754	rVB2	472764	1317038	26.84%	4.378%

Sum of corrected areas: 30080360

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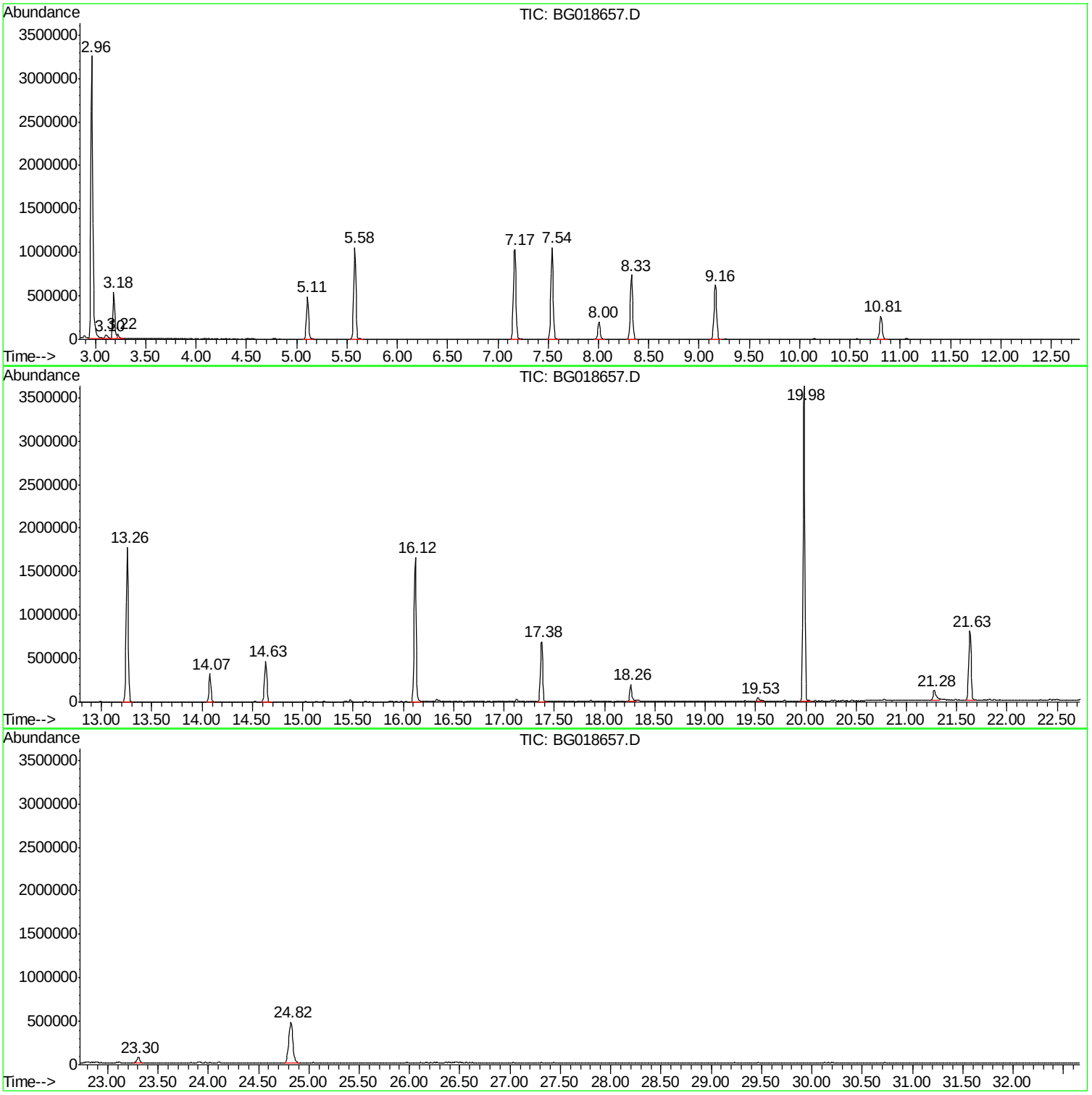
Instrument :
BNA_G
ClientSampleId :
SB-14(7-9.5)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091115.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\BG091215\
Data File : BG018657.D
Acq On : 12 Sep 2015 2:25
Operator : UM/IZ
Sample : G3620-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-14(7-9.5)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

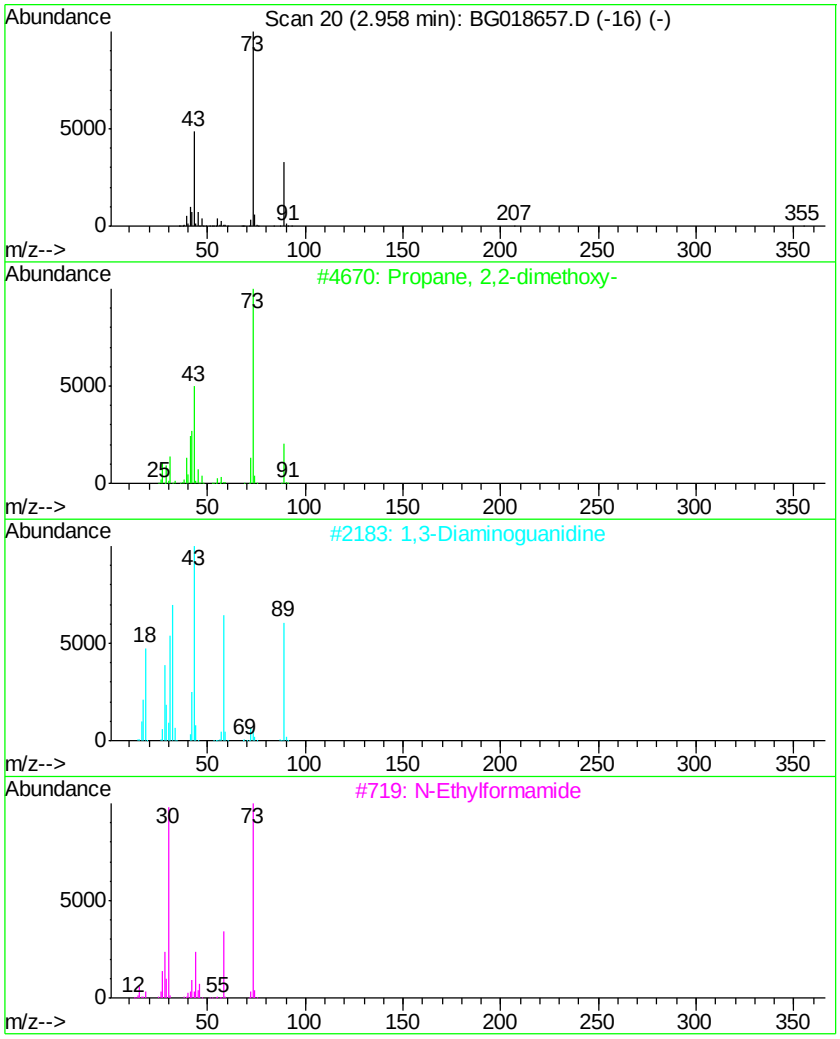
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

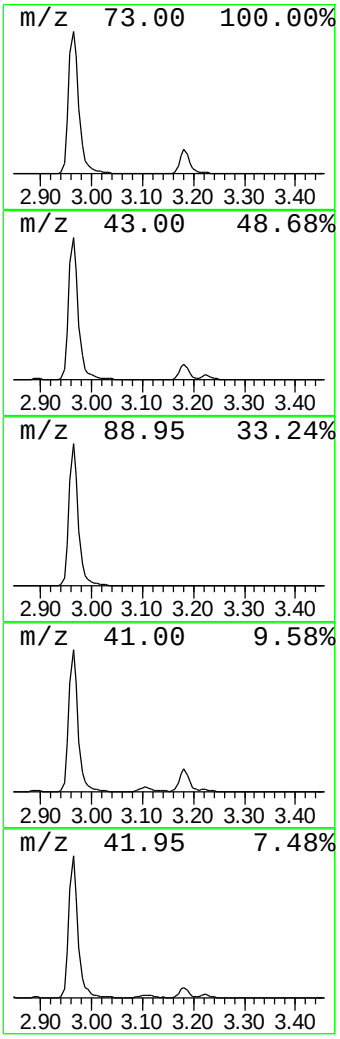
****

Peak Number 1 unknown2.96 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.96	260.59 ng	4391900	1,4-Dichlorobenzene-d4	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	28
2	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	25
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
5	1,3-Dioxolane, 2-(3-bromo-5,5,5-...	352	C10H16BrCl3O2	1000115-31-4	9





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Acq On : 12 Sep 2015 2:25
Operator : UM/IZ
Sample : G3620-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-14(7-9.5)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091115.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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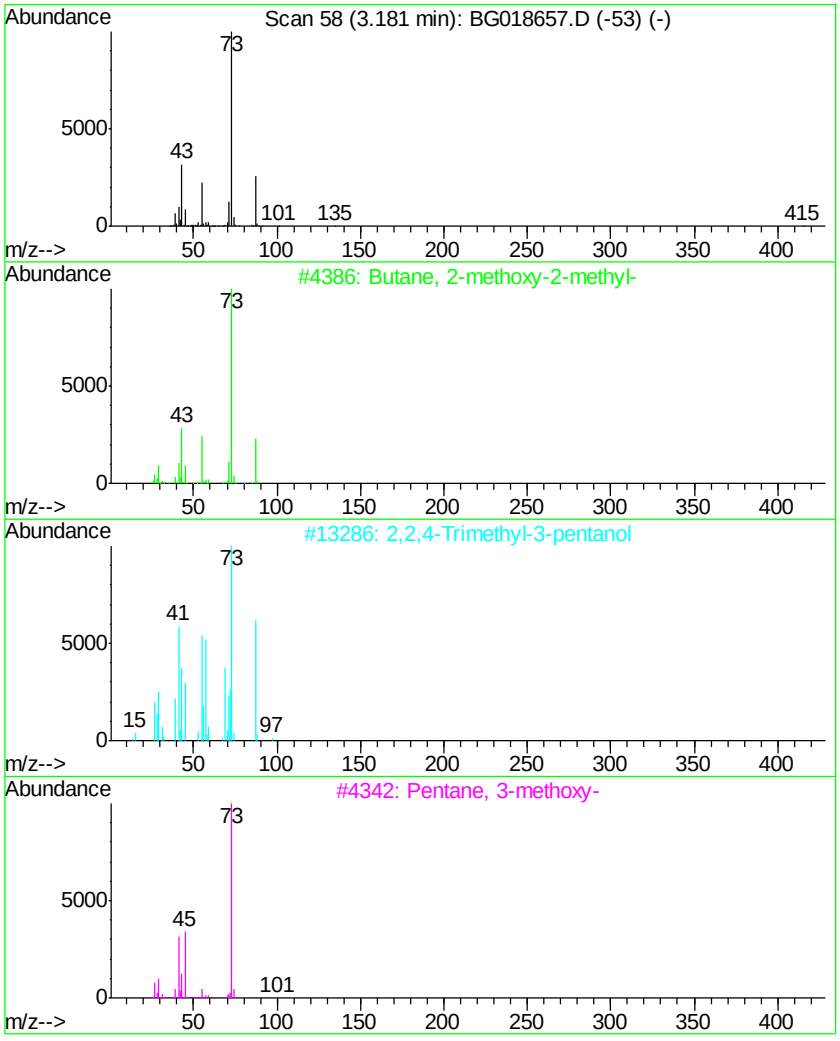
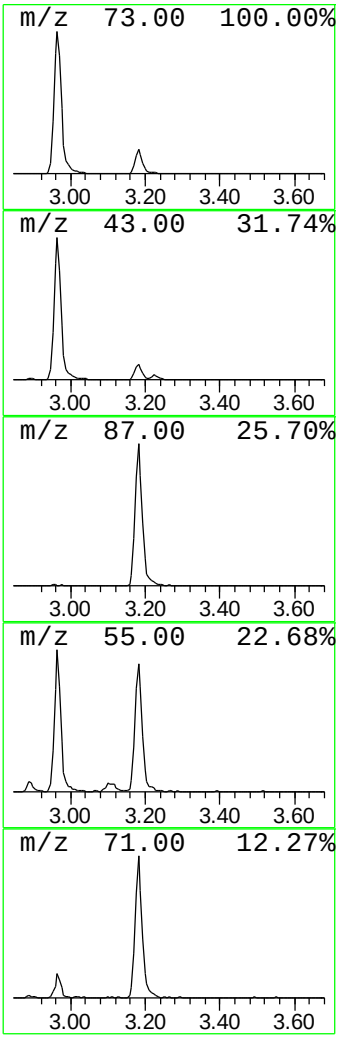
Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	42.08 ng	709205	1,4-Dichlorobenzene-d4	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	86
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	56
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG091215\
Data File : BG018657.D
Acq On : 12 Sep 2015 2:25
Operator : UM/IZ
Sample : G3620-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-14(7-9.5)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091115.M
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TIC Library : C:\DATABASE\NIST02.L
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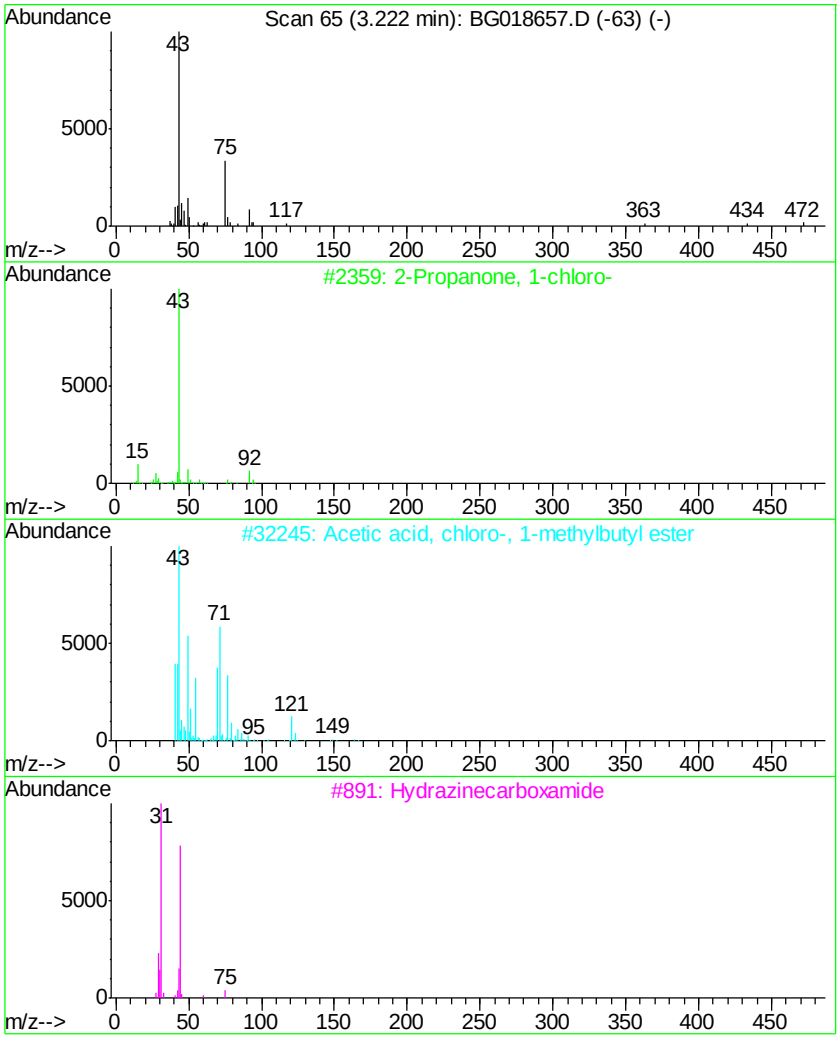
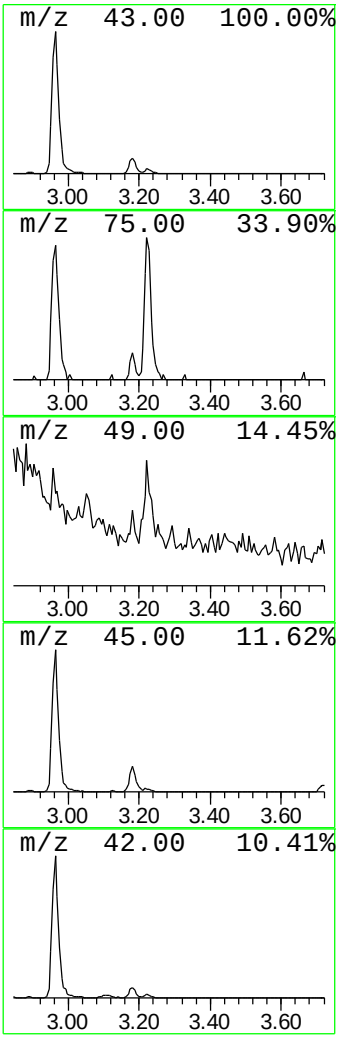
Peak Number 4 unknown3.22 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.22	4.27 ng	71946	1,4-Dichlorobenzene-d4	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanone, 1-chloro-	92	C3H5ClO	000078-95-5	35
2	Acetic acid, chloro-, 1-methylbu...	164	C7H13ClO2	090380-52-2	9
3	Hydrazinecarboxamide	75	CH5N3O	000057-56-7	4
4	Glycine	75	C2H5NO2	000056-40-6	4
5	1-Propionylethyl acetate	144	C7H12O3	002983-05-3	4





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Operator : UM/IZ
Sample : G3620-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-14(7-9.5)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091115.M
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TIC Library : C:\DATABASE\NIST02.L
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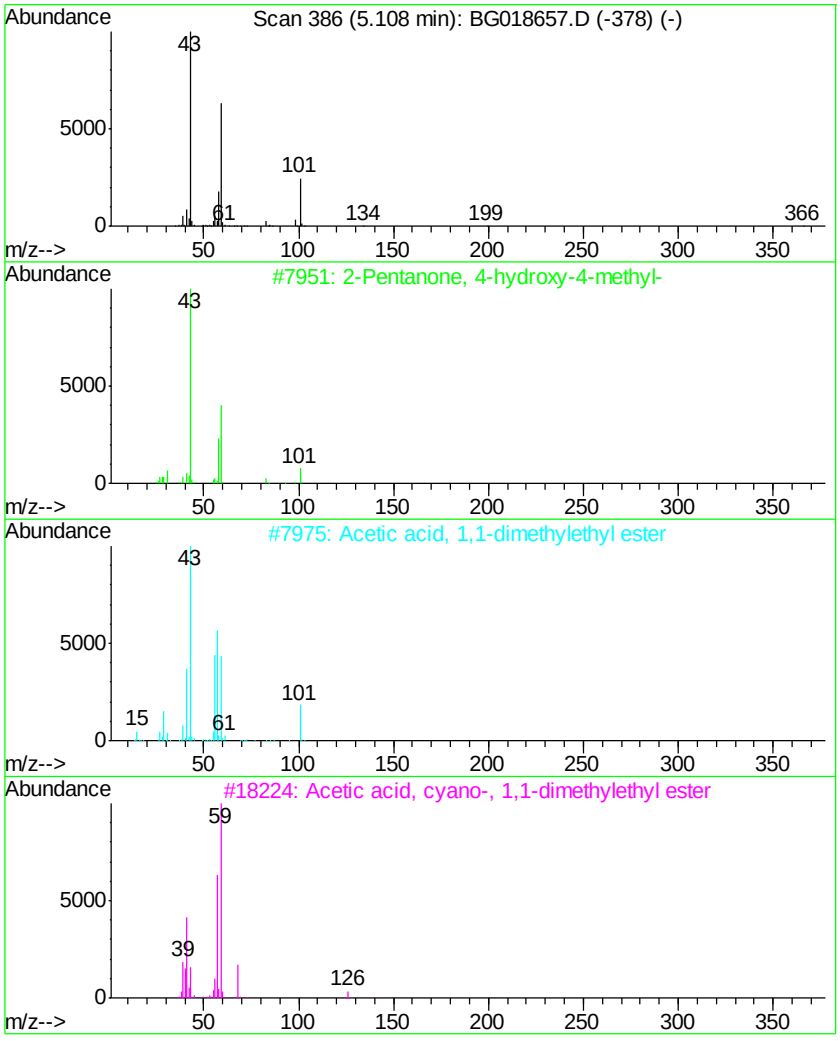
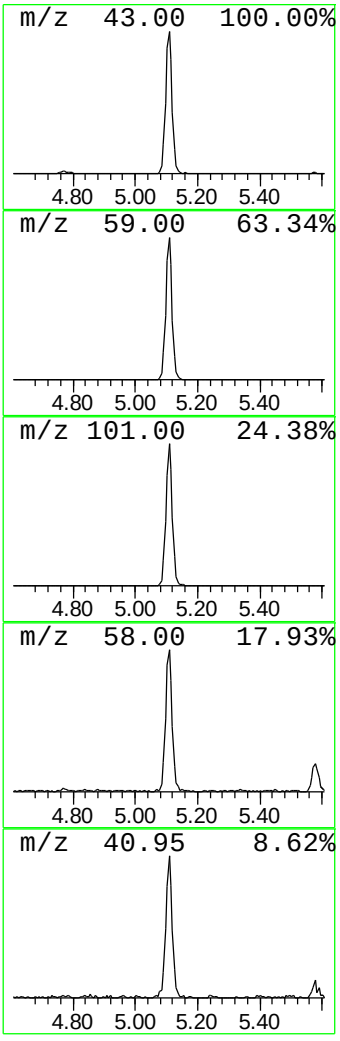
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	42.09 ng	709442	1,4-Dichlorobenzene-d4	8.00

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	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Guanidine	59	CH5N3	000113-00-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Acq On : 12 Sep 2015 2:25
Operator : UM/IZ
Sample : G3620-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-14(7-9.5)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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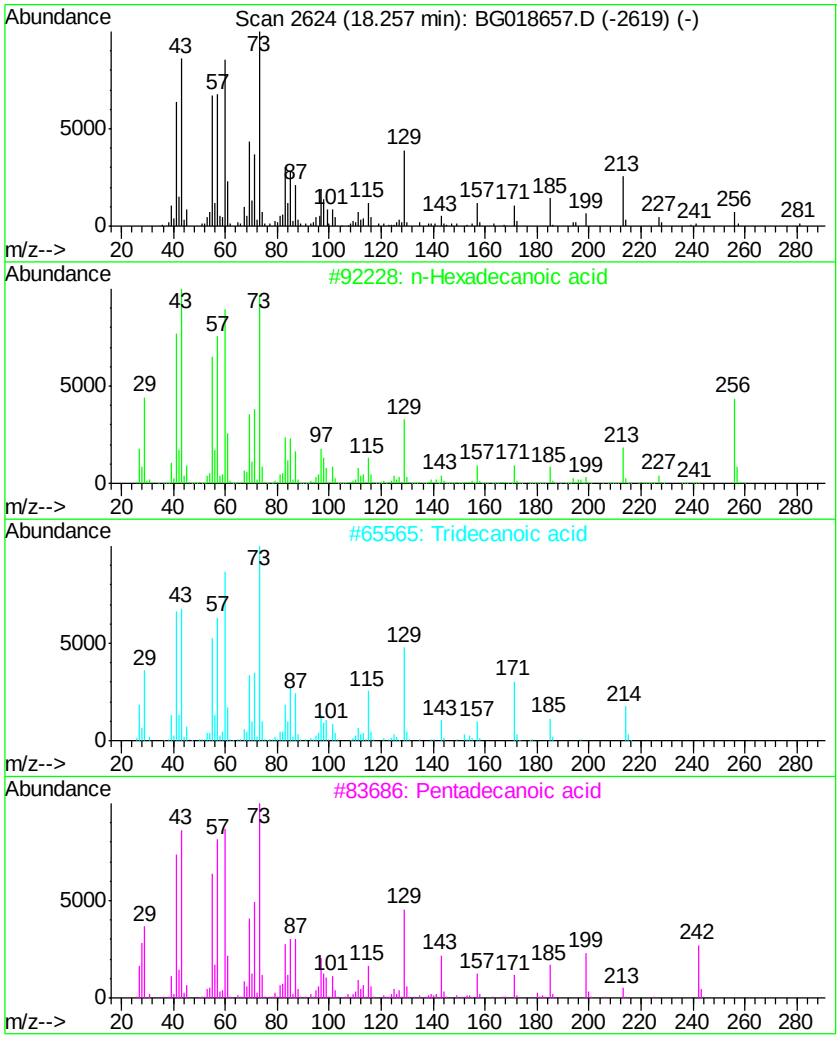
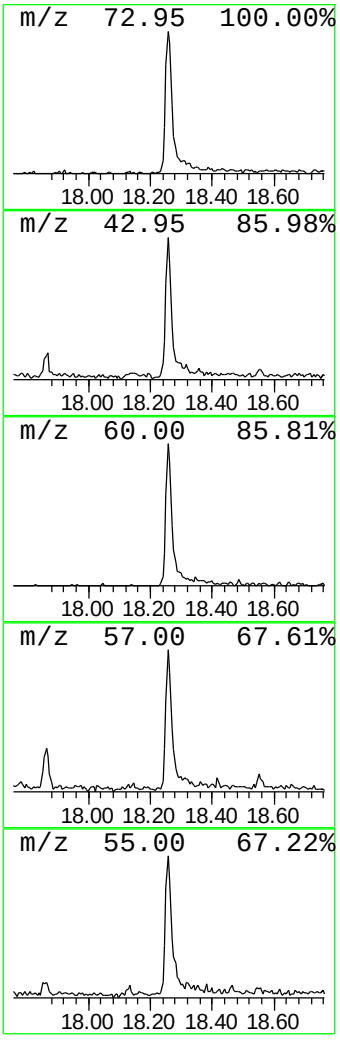
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.26	5.79 ng	308162	Phenanthrene-d10	17.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58





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Sample : G3620-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-14(7-9.5)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091115.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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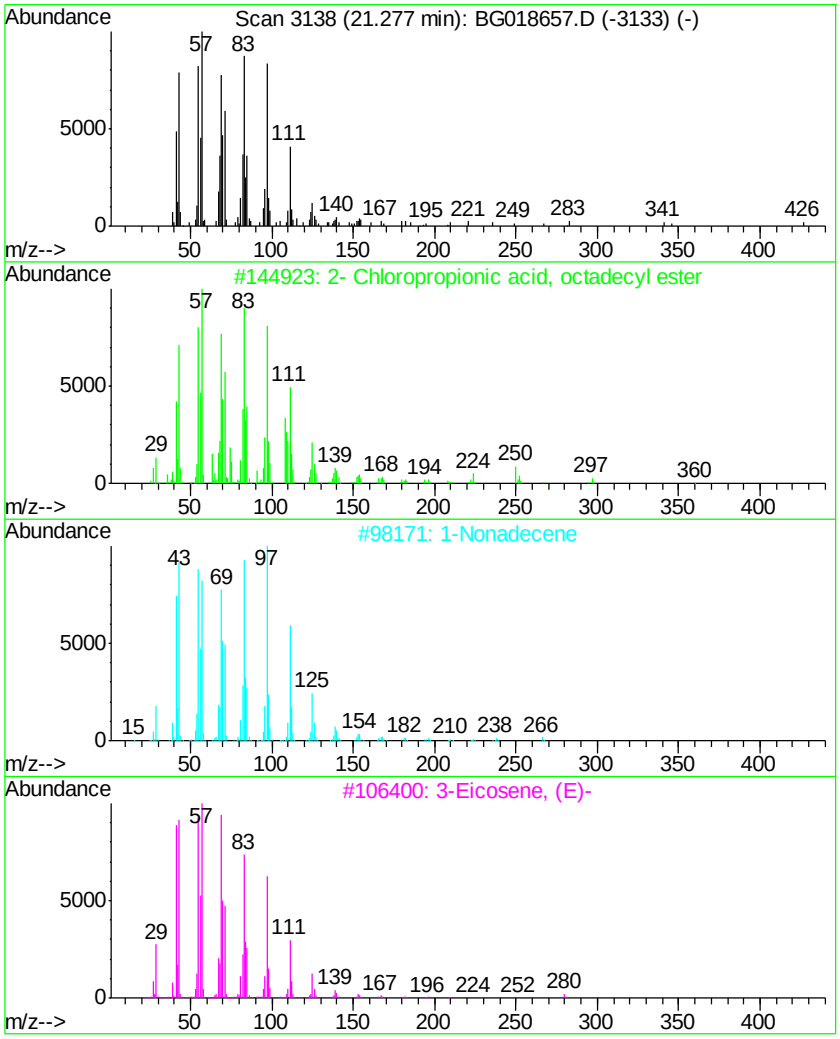
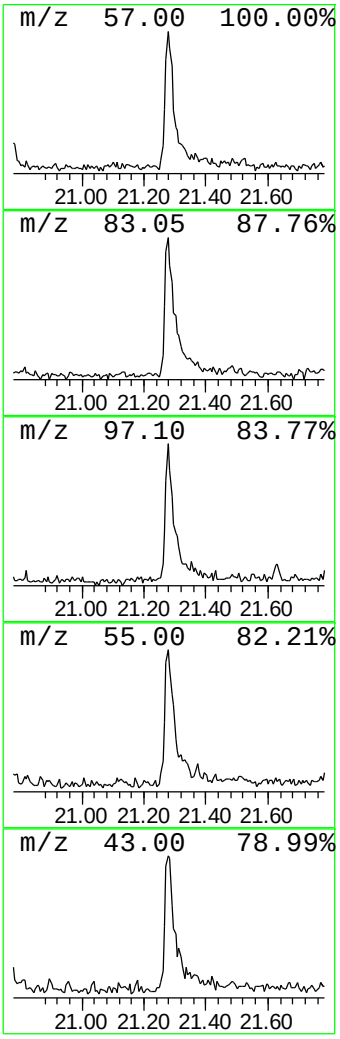
Peak Number 9 2- Chloropropionic acid, oc... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.28	3.71 ng	242534	Chrysene-d12	21.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	90
2	1-Nonadecene	266	C19H38	018435-45-5	87
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	83
4	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	74
5	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	74





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_G
ClientSampleId : SB-14(7-9.5)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091115.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
unknown2.96	2.96	260.6	ng	4391900	1	8.00	337068	20.0
Butane, 2-methoxy...	3.18	42.1	ng	709205	1	8.00	337068	20.0
unknown3.22	3.22	4.3	ng	71946	1	8.00	337068	20.0
2-Pentanone, 4-hy...	5.11	42.1	ng	709442	1	8.00	337068	20.0
n-Hexadecanoic acid	18.26	5.8	ng	308162	4	17.38	1064520	20.0
2- Chloropropioni...	21.28	3.7	ng	242534	5	21.63	1308380	20.0