LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG091215\
Data File : BG018655.D
Acq On : 12 Sep 2015 1:09
Operator : UM/IZ
Sample : G3640-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MGP210BR48-48.5

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	2.963	16	21	40	rVV	3956402	5334543	100.00%	15.668%
2	3.104	40	45	53	rVV2	45019	86831	1.63%	0.255%
3	3.180	53	58	75	rVB	800419	1090304	20.44%	3.202%
4	5.107	380	386	395	rBV	531186	776098	14.55%	2.279%
5	5.577	459	466	476	rBV	1175985	1817189	34.06%	5.337%
6	7.169	729	737	751	rBV	1197965	1991767	37.34%	5.850%
7	7.540	792	800	812	rVB	1173815	1978338	37.09%	5.810%
8	8.004	872	879	886	rBV	203531	342914	6.43%	1.007%
9	8.327	924	934	941	rBV	843423	1438950	26.97%	4.226%
10	9.161	1069	1076	1087	rVB	683423	1217995	22.83%	3.577%
11	10.806	1349	1356	1361	rBV	280272	504426	9.46%	1.481%
12	10.859	1361	1365	1374	rVB	95620	165489	3.10%	0.486%
13	12.681	1667	1675	1682	rVB	44114	76678	1.44%	0.225%
14	13.256	1765	1773	1780	rBV	1822955	2806802	52.62%	8.244%
15	14.079	1907	1913	1918	rBV	380357	541115	10.14%	1.589%
16	14.631	2000	2007	2016	rBV2	479440	779732	14.62%	2.290%
17	16.118	2252	2260	2269	rBV	1842025	2773833	52.00%	8.147%
18	17.375	2467	2474	2480	rBV2	697309	1083599	20.31%	3.183%
19	18.256	2617	2624	2631	rBV	136201	205866	3.86%	0.605%
20	19.525	2835	2840	2846	rBV5	39217	60947	1.14%	0.179%
21	19.984	2911	2918	2926	rBV	3904155	4904700	91.94%	14.405%
22	21.276	3134	3138	3150	rBV3	68199	148897	2.79%	0.437%
23	21.629	3191	3198	3206	rBV	852035	1338753	25.10%	3.932%
24	22.780	3381	3394	3395	rBV5	73083	198836	3.73%	0.584%
25	22.863	3403	3408	3429	rVB5	141750	572221	10.73%	1.681%
26	23.086	3439	3446	3456	rBV2	171315	382087	7.16%	1.122%
27	23.303	3476	3483	3492	rVB2	49948	91600	1.72%	0.269%
28	24.813	3728	3740	3752	rBV3	463332	1337933	25.08%	3.929%

Sum of corrected areas: 34048443

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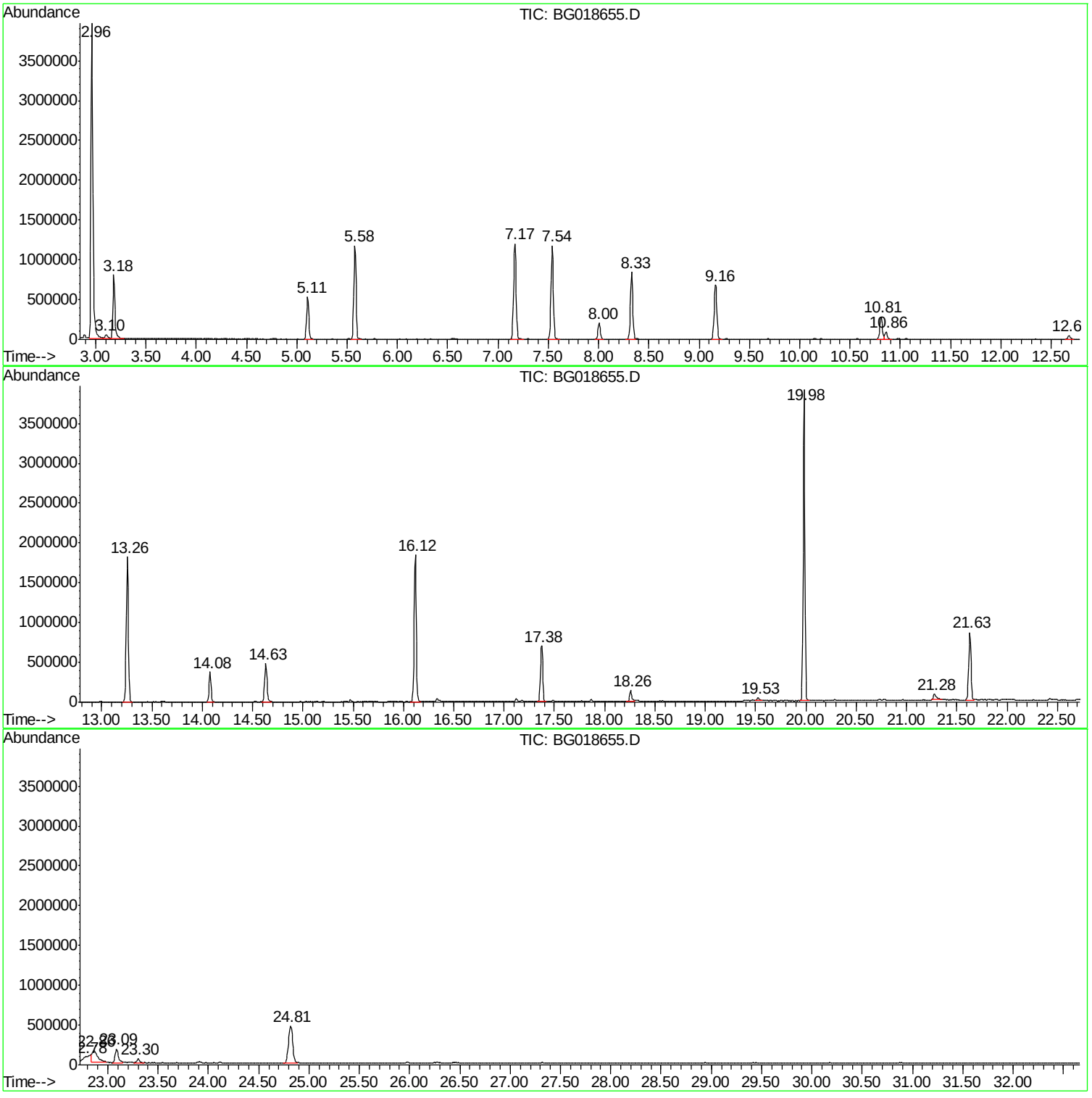
Instrument :
BNA_G
ClientSampleId :
MGP210BR48-48.5

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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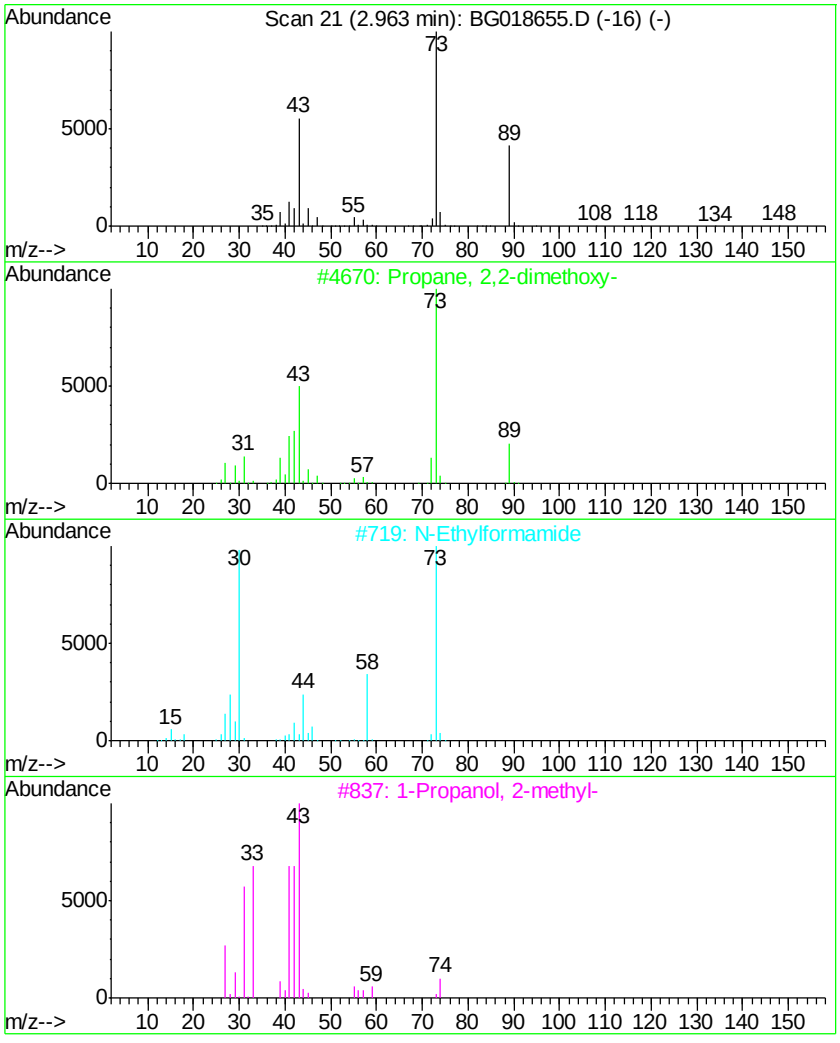
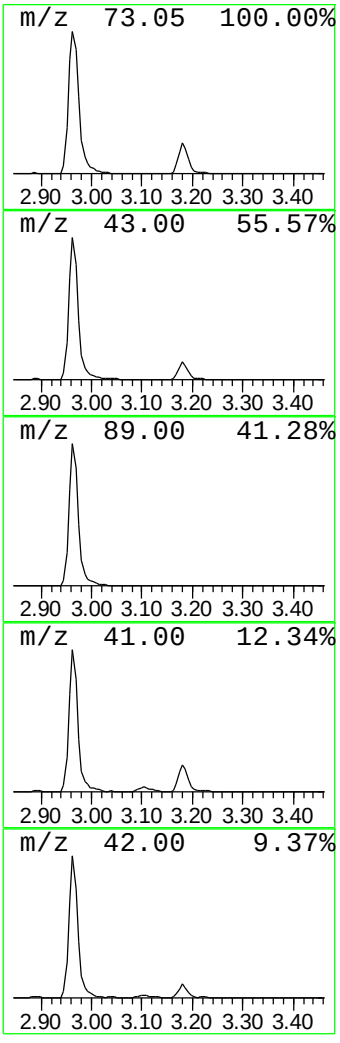
Peak Number 1 unknown2.96 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.96	311.13 ng	5334540	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	40
2	N-Ethylformamide	73	C3H7NO	000627-45-2	25
3	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
4	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
5	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9





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Operator : UM/IZ
Sample : G3640-01
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ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MGP210BR48-48.5

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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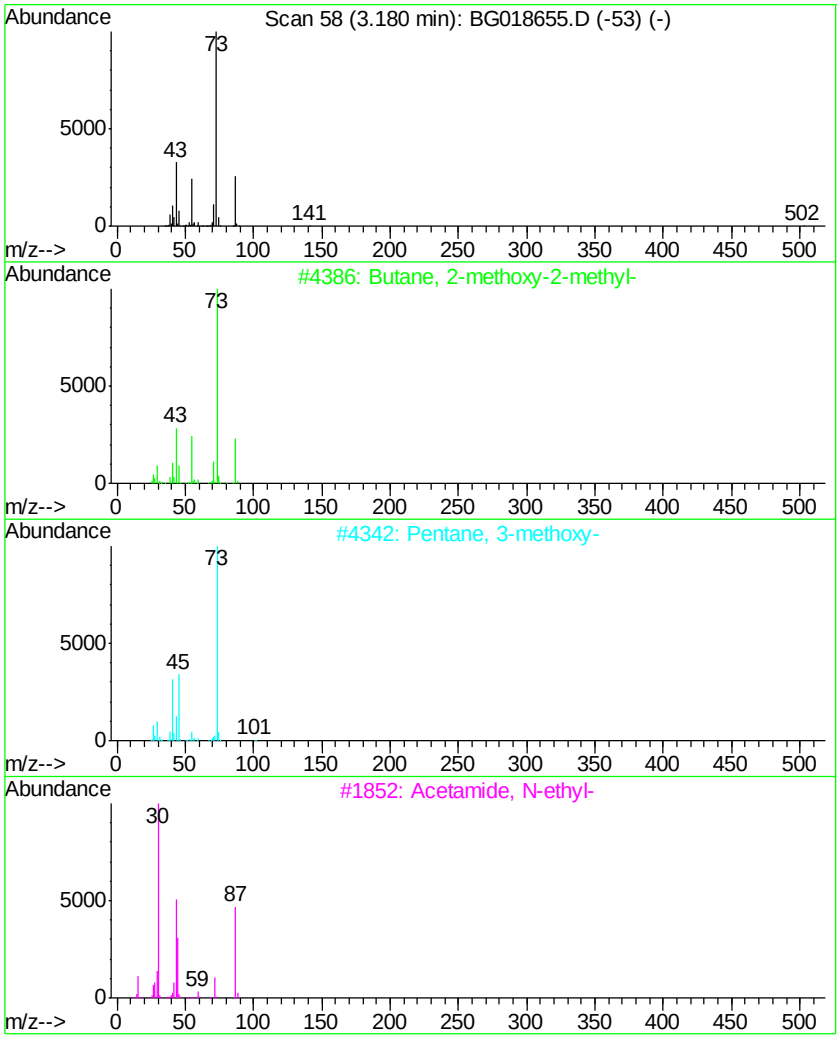
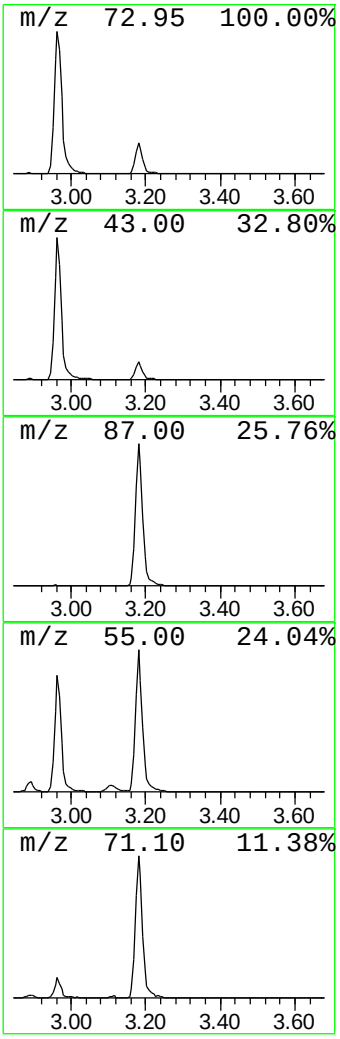
Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	63.59 ng	1090300	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	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	25
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Sample : G3640-01
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ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MGP210BR48-48.5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091115.M
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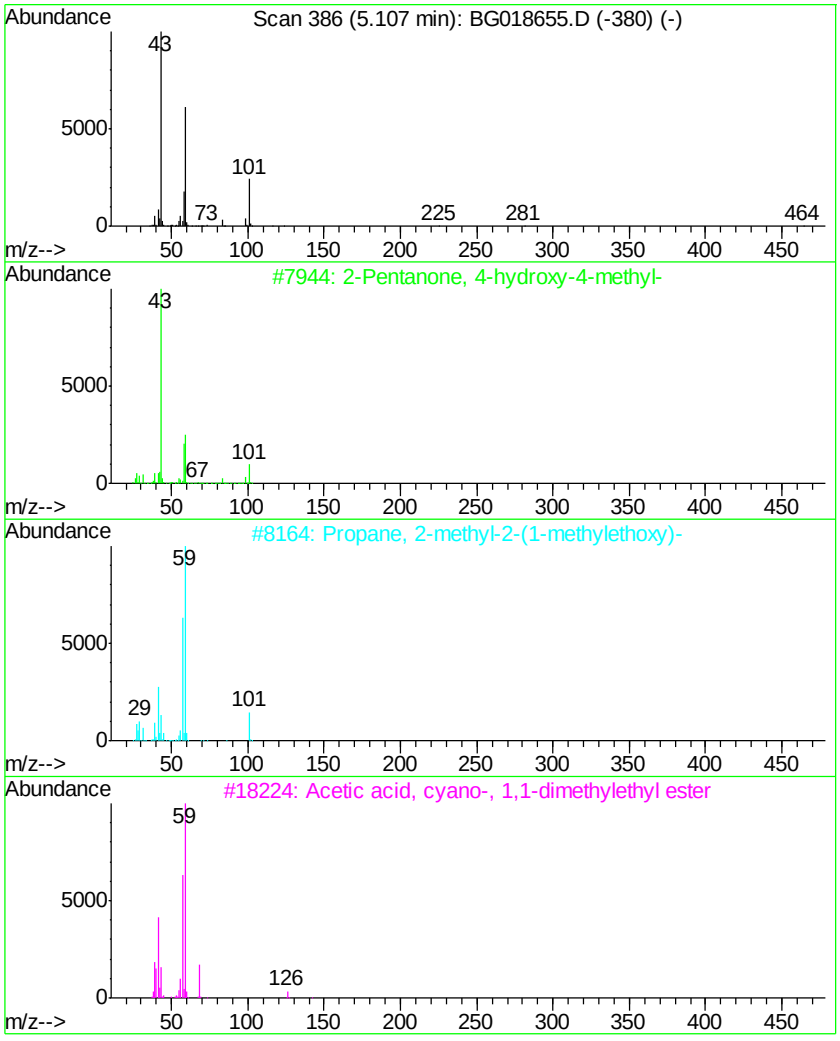
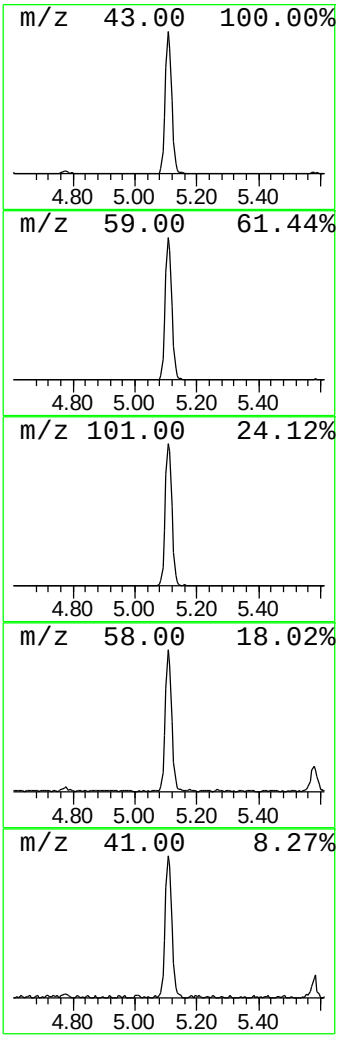
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	45.26 ng	776098	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	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	23
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Instrument : BNA_G
ClientSampleId : MGP210BR48-48.5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091115.M
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TIC Library : C:\DATABASE\NIST02.L
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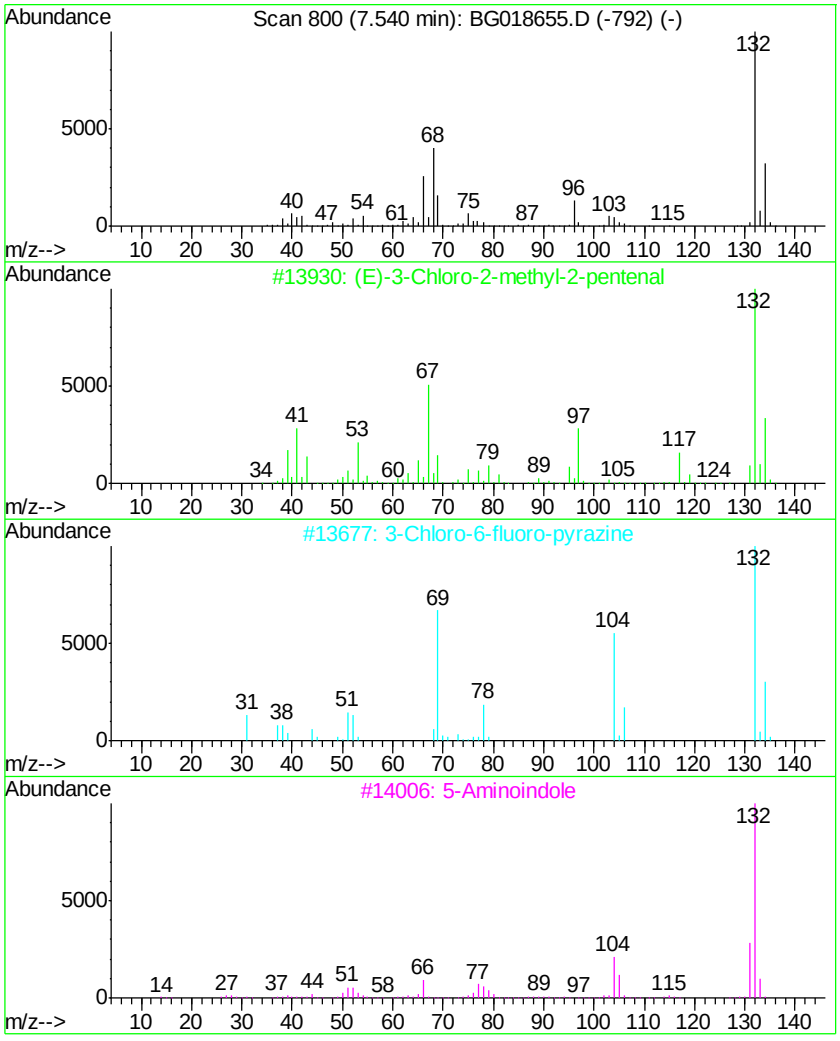
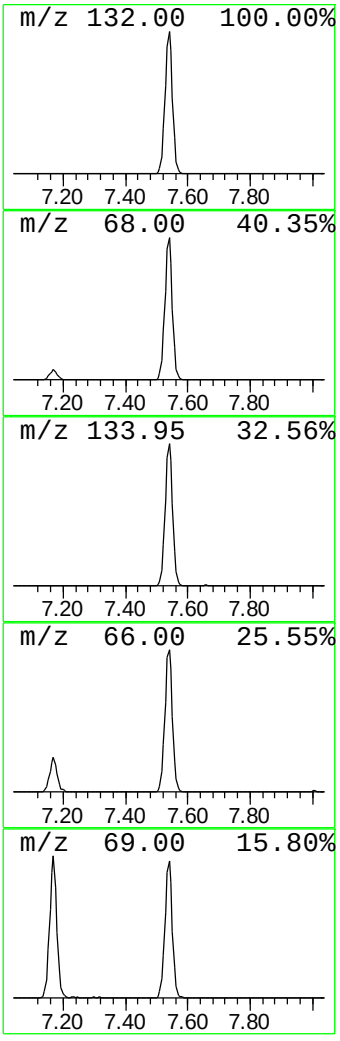
Peak Number 5 unknown7.54 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.54	115.38 ng	1978340	1,4-Dichlorobenzene-d4	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Amphetaminil	250	C17H18N2	017590-01-1	10
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





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Sample : G3640-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MGP210BR48-48.5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091115.M
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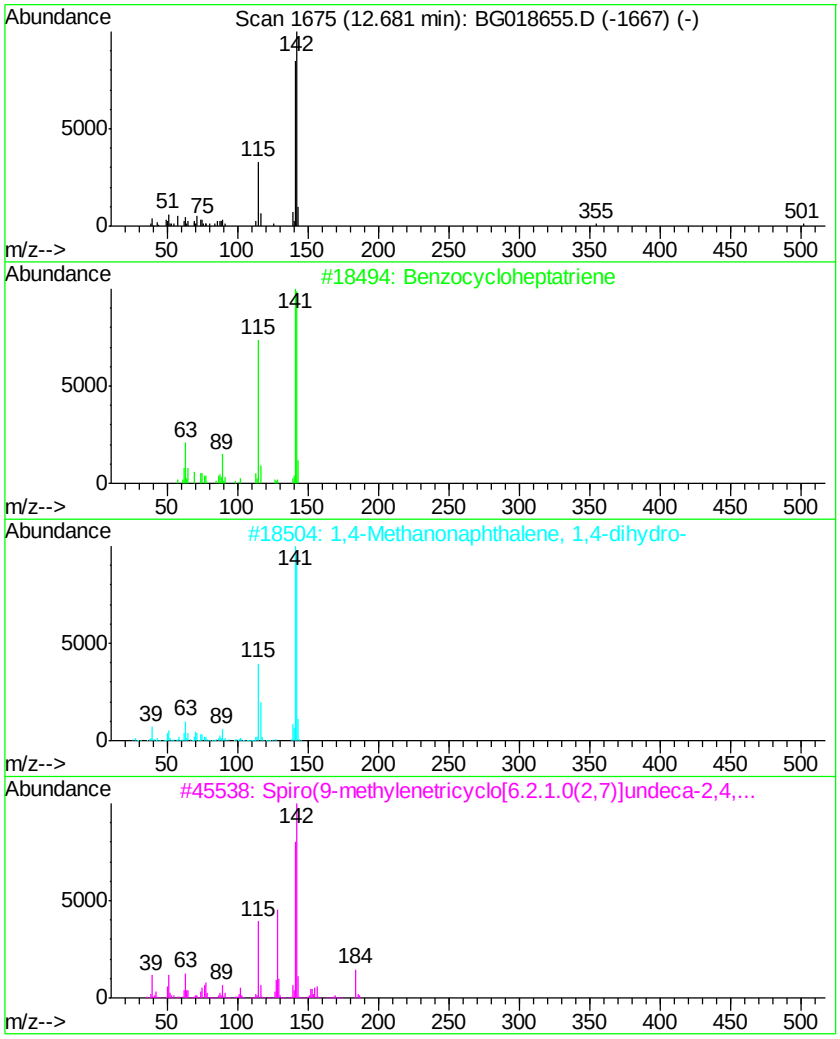
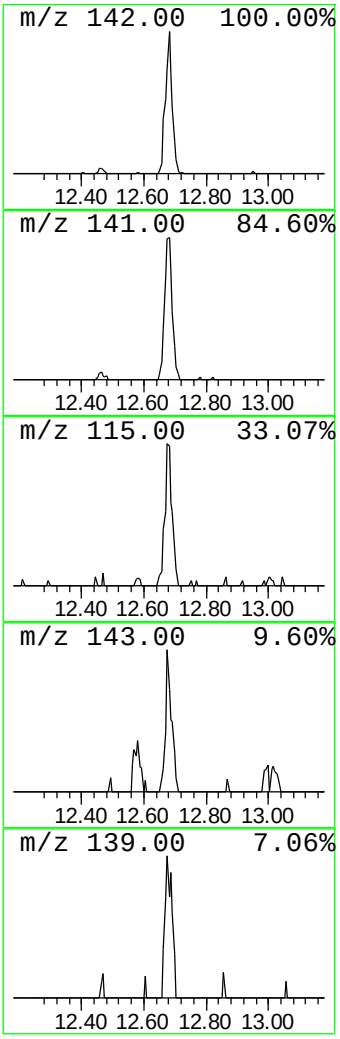
Peak Number 7 Benzocycloheptatriene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.68	3.04 ng	76678	Naphthalene-d8	10.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzocycloheptatriene	142	C11H10	000264-09-5	91
2	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	86
3	Spiro(9-methylenetricyclo[6.2.1....	184	C13H12O	033929-47-4	83
4	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	78
5	Naphthalene, 1-[(2-propenyloxy)m...	198	C14H14O	074685-39-5	74





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Operator : UM/IZ
Sample : G3640-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MGP210BR48-48.5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091115.M
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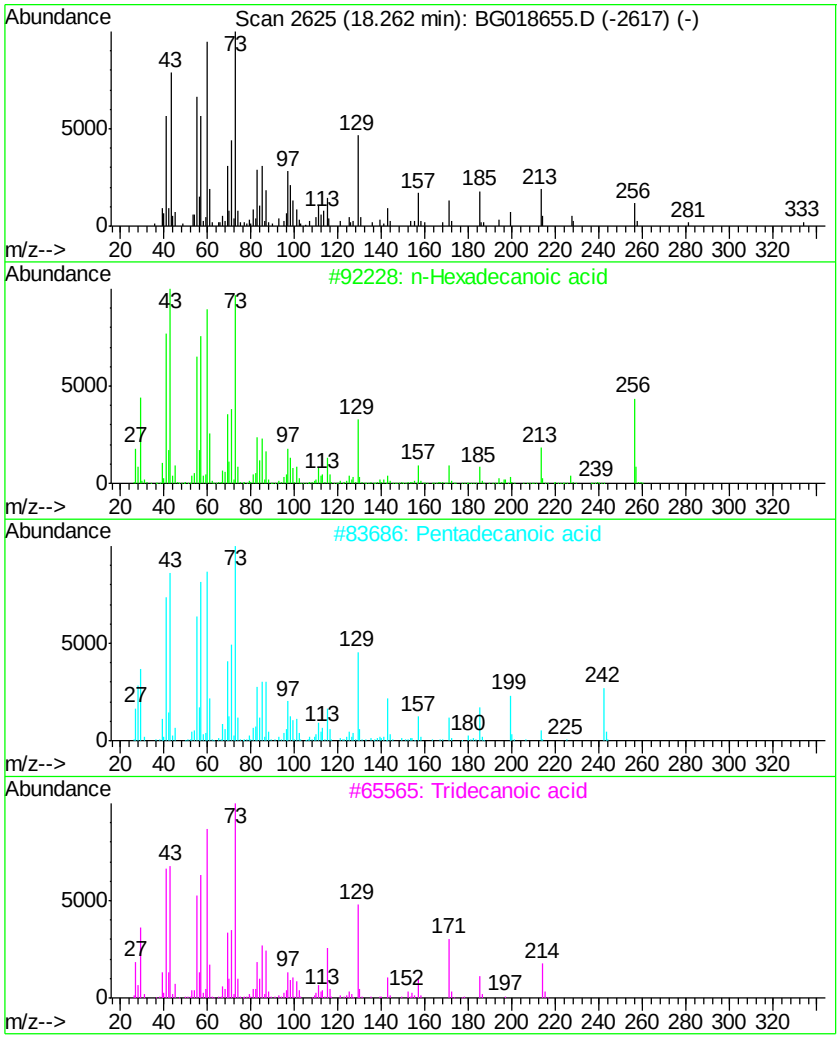
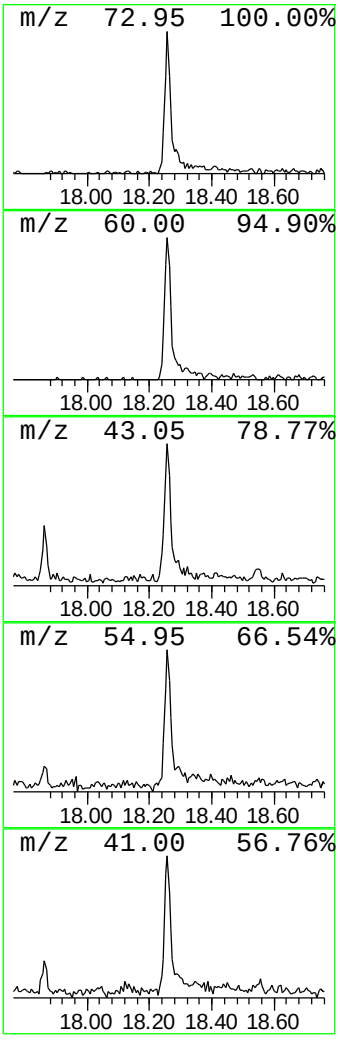
Peak Number 8 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.26	3.80 ng	205866	Phenanthrene-d10	17.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





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Sample : G3640-01
Misc :
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Instrument : BNA_G
ClientSampleId : MGP210BR48-48.5

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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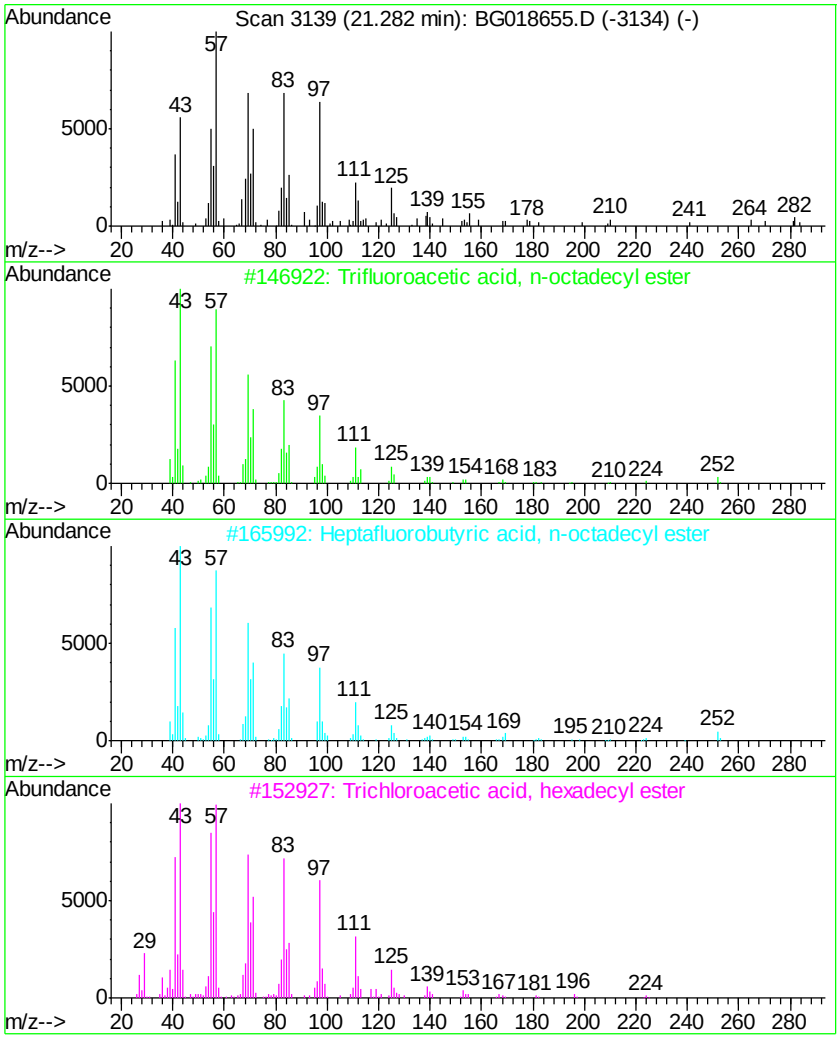
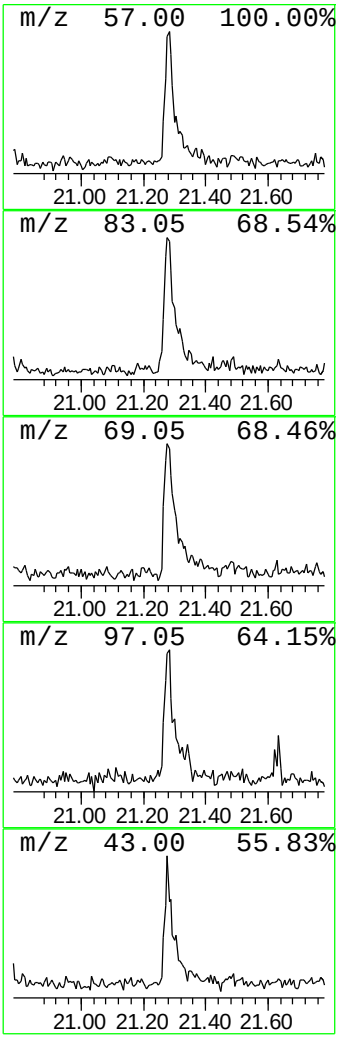
Peak Number 9 Trifluoroacetic acid, n-oct... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.28	2.22 ng	148897	Chrysene-d12	21.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
2	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4	17-Pentatriacontene	491	C35H70	006971-40-0	90
5	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	86





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Sample : G3640-01
Misc :
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Instrument : BNA_G
ClientSampleId : MGP210BR48-48.5

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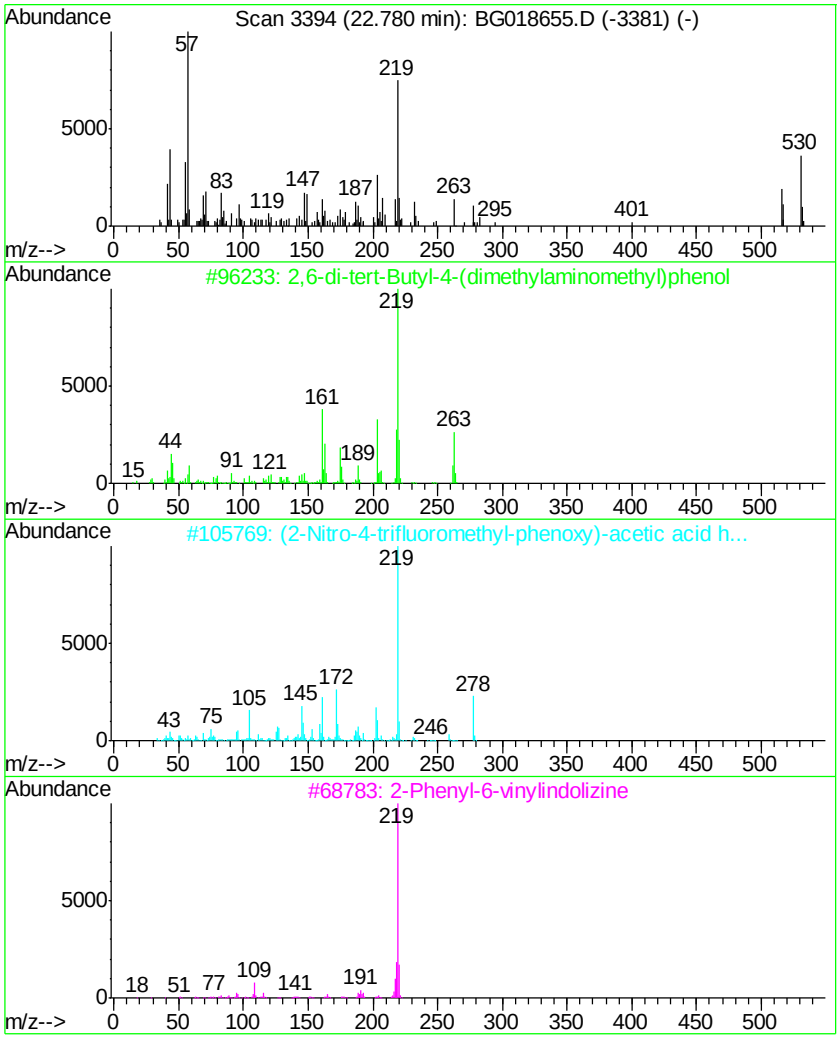
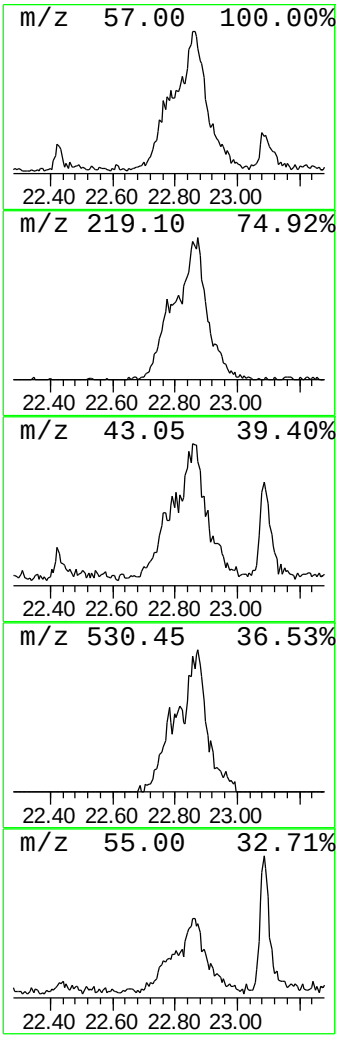
Peak Number 10 2,6-di-tert-Butyl-4-(dimeth... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.78	2.97 ng	198836	Chrysene-d12	21.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-di-tert-Butyl-4-(dimethylami...	263	C17H29NO	000088-27-7	50
2	(2-Nitro-4-trifluoromethyl-pheno...	279	C9H8F3N3O4	1000294-73-1	45
3	2-Phenyl-6-vinylindolizine	219	C16H13N	077652-49-4	38
4	1-Benzylphthalazine	220	C15H12N2	063536-21-0	38
5	2-Amino-6-methoxy-8-nitroquinoline	219	C10H9N3O3	064992-74-1	38





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Sample : G3640-01
Misc :
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Instrument : BNA_G
ClientSampleId : MGP210BR48-48.5

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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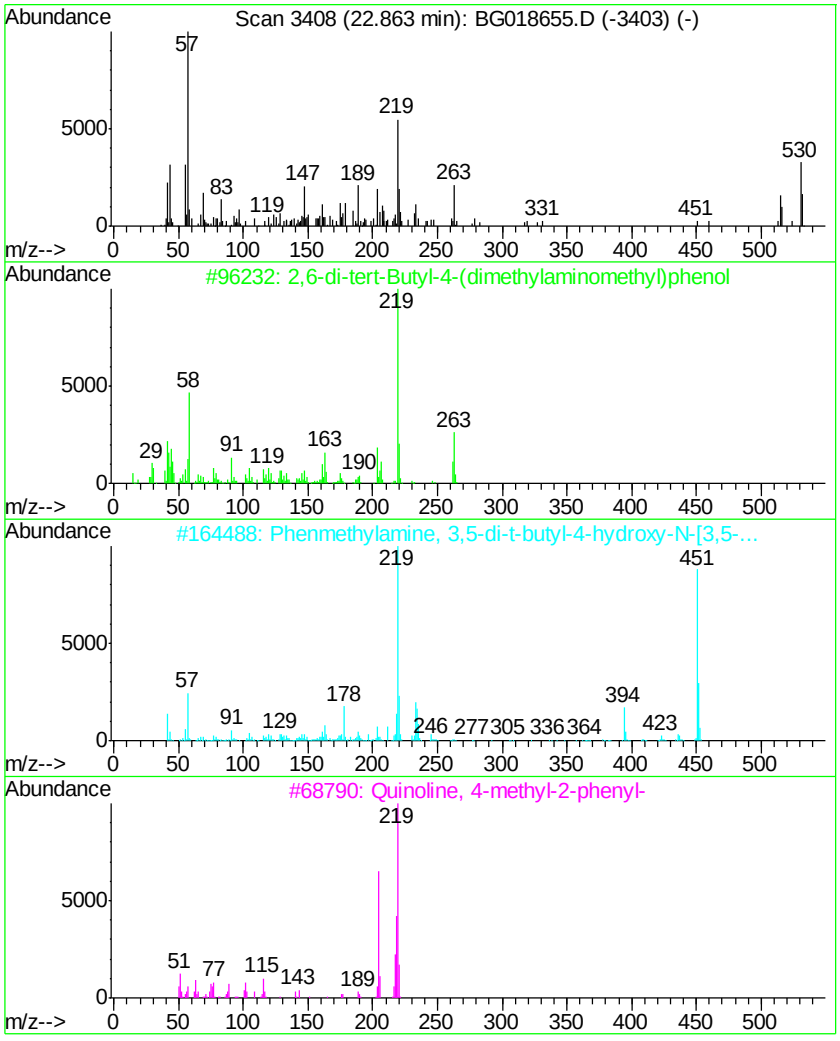
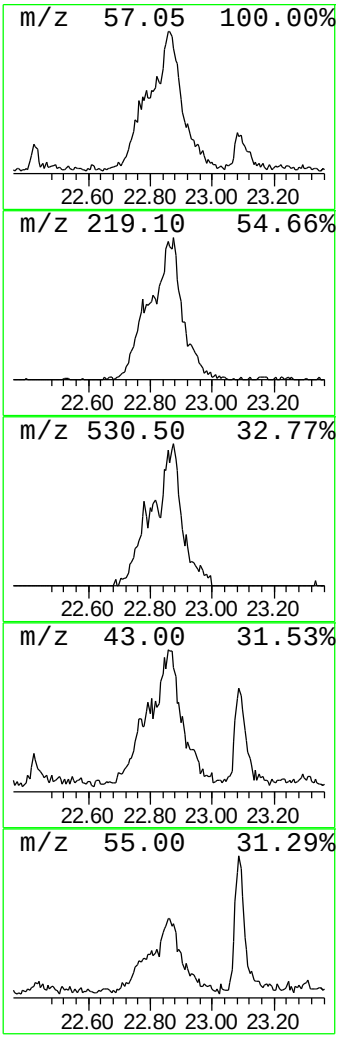
Peak Number 11 unknown22.86 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.86	8.55 ng	572221	Chrysene-d12	21.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-di-tert-Butyl-4-(dimethylami...	263	C17H29NO	000088-27-7	38
2	Phenmethylamine, 3,5-di-t-butyl-...	451	C30H45NO2	1000130-26-1	25
3	Quinoline, 4-methyl-2-phenyl-	219	C16H13N	004789-76-8	22
4	3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	22
5	Benzene, 1-[(4-ethylphenyl)ethyn...	248	C19H20	102225-55-8	16





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Sample : G3640-01
Misc :
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Instrument : BNA_G
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

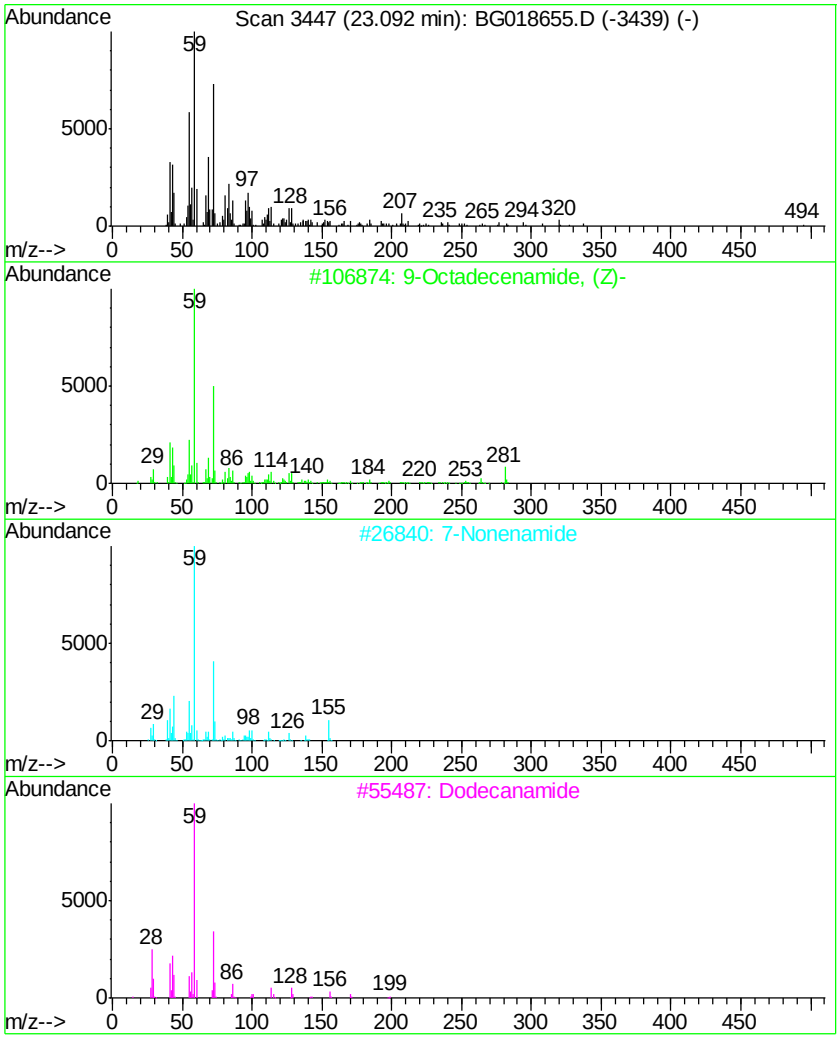
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

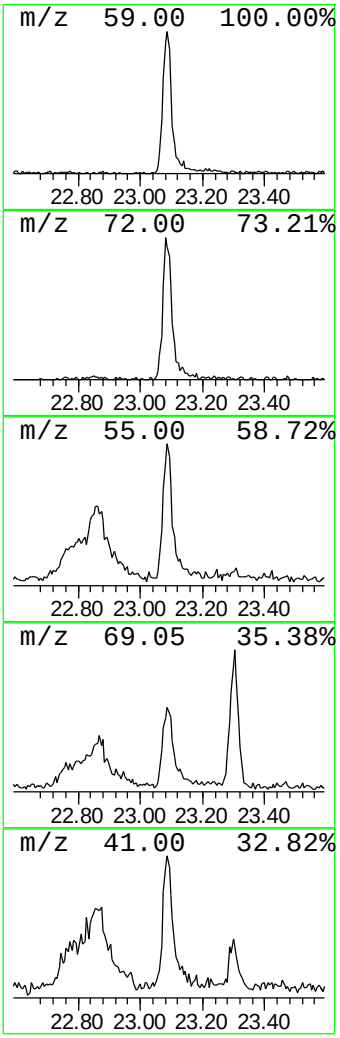
****

Peak Number 12 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.09	5.71 ng	382087	Chrysene-d12	21.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	64
2	7-Nonenamide	155	C9H17NO	090949-53-4	53
3	Dodecanamide	199	C12H25NO	001120-16-7	50
4	Nonanamide	157	C9H19NO	001120-07-6	47
5	Methoxycarbonylsulfenyl chloride	126	C2H3ClO2S	026555-40-8	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG091215\
Data File : BG018655.D
Acq On : 12 Sep 2015 1:09
Operator : UM/IZ
Sample : G3640-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MGP210BR48-48.5

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	311.1	ng	5334540	1	8.00	342914	20.0
Butane, 2-methoxy...	3.18	63.6	ng	1090300	1	8.00	342914	20.0
2-Pentanone, 4-hy...	5.11	45.3	ng	776098	1	8.00	342914	20.0
unknown7.54	7.54	115.4	ng	1978340	1	8.00	342914	20.0
Benzocycloheptatr...	12.68	3.0	ng	76678	2	10.81	504426	20.0
n-Hexadecanoic acid	18.26	3.8	ng	205866	4	17.38	1083600	20.0
Trifluoroacetic a...	21.28	2.2	ng	148897	5	21.63	1338750	20.0
2,6-di-tert-Butyl...	22.78	3.0	ng	198836	5	21.63	1338750	20.0
unknown22.86	22.86	8.6	ng	572221	5	21.63	1338750	20.0
9-Octadecenamide,...	23.09	5.7	ng	382087	5	21.63	1338750	20.0