LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG091215\
Data File : BG018652.D
Acq On : 11 Sep 2015 23:15
Operator : UM/IZ
Sample : G3638-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 091015-EFF-GRAB

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	2.891	5	9	15	rVB	37459	51549	1.00%	0.202%
2	3.109	39	46	53	rBV	96857	177277	3.46%	0.694%
3	3.179	53	58	74	rVB	2254388	3277787	63.90%	12.830%
4	5.106	379	386	393	rBV	43835	66170	1.29%	0.259%
5	5.576	460	466	474	rVB	285132	444874	8.67%	1.741%
6	7.163	727	736	746	rBV	191133	320160	6.24%	1.253%
7	7.539	792	800	806	rBV	511253	873309	17.02%	3.418%
8	8.003	873	879	887	rBV	190818	321288	6.26%	1.258%
9	8.091	887	894	899	rVV	40822	65667	1.28%	0.257%
10	8.326	926	934	943	rBV	745197	1264498	24.65%	4.950%
11	9.161	1068	1076	1083	rBV	576120	1005519	19.60%	3.936%
12	10.806	1348	1356	1365	rBV	257434	469967	9.16%	1.840%
13	13.121	1738	1750	1763	rBV2	118358	227153	4.43%	0.889%
14	13.256	1766	1773	1781	rVB	1853069	2735469	53.33%	10.707%
15	14.078	1907	1913	1917	rBV	115760	166419	3.24%	0.651%
16	14.172	1924	1929	1941	rVB	89777	155668	3.03%	0.609%
17	14.631	2000	2007	2016	rBV2	466076	752124	14.66%	2.944%
18	15.512	2153	2157	2166	rVB	46952	75265	1.47%	0.295%
19	15.718	2186	2192	2195	rBV	949831	1490736	29.06%	5.835%
20	15.812	2203	2208	2216	rVB	201601	359171	7.00%	1.406%
21	16.117	2253	2260	2273	rBV	1017134	1539480	30.01%	6.026%
22	17.163	2433	2438	2441	rBV	262669	381265	7.43%	1.492%
23	17.192	2441	2443	2453	rVB	159664	203308	3.96%	0.796%
24	17.374	2467	2474	2481	rBV2	720711	1102245	21.49%	4.314%
25	18.262	2619	2625	2633	rBV4	80916	177969	3.47%	0.697%
26	19.525	2836	2840	2844	rBV4	39235	60048	1.17%	0.235%
27	19.983	2911	2918	2925	rBV	3974667	5129786	100.00%	20.079%
28	21.628	3192	3198	3208	rVB	807659	1335064	26.03%	5.226%
29	24.819	3730	3741	3756	rBV2	464207	1318313	25.70%	5.160%

Sum of corrected areas: 25547548

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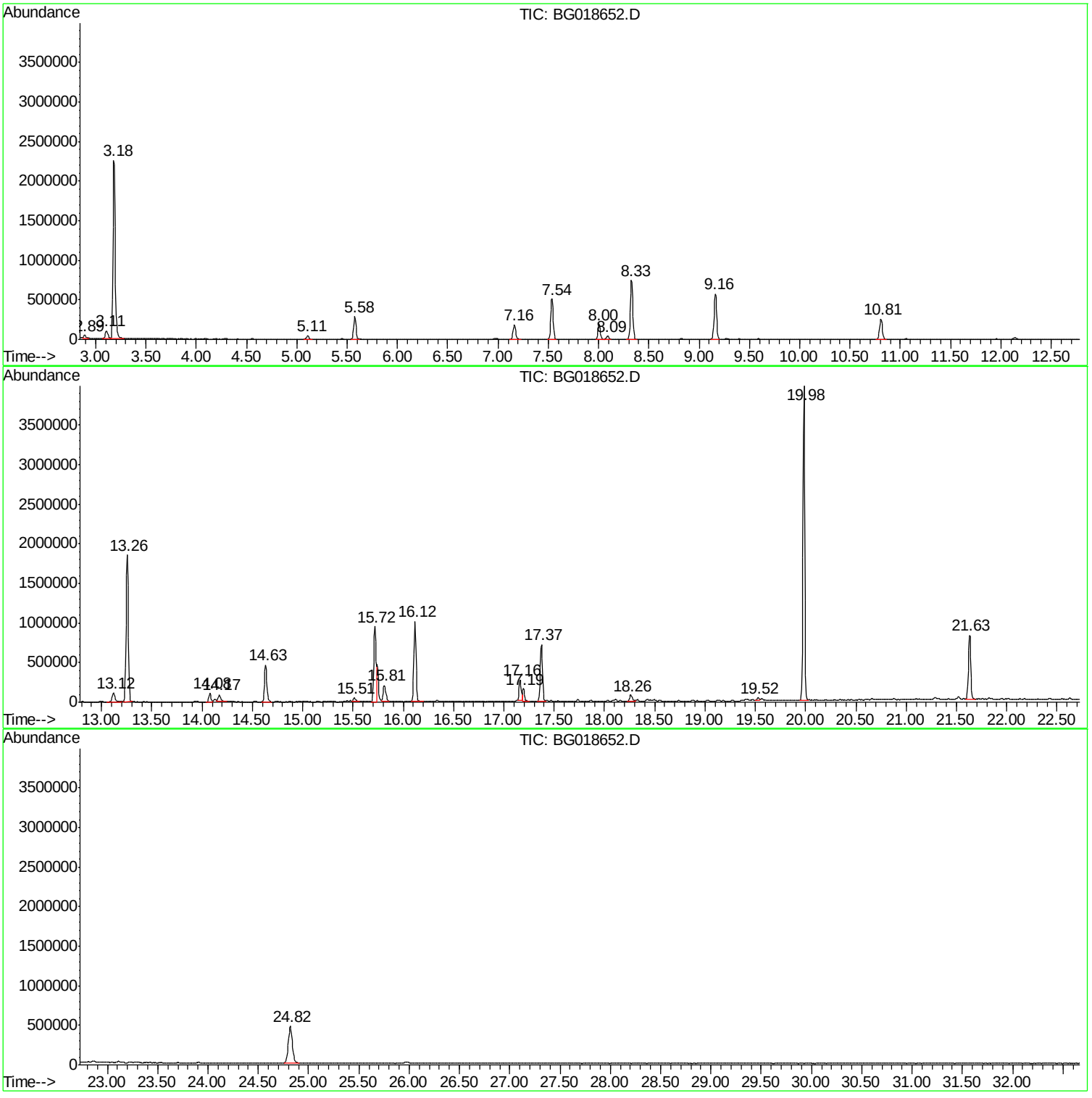
Instrument : BNA_G
ClientSampleId : 091015-EFF-GRAB

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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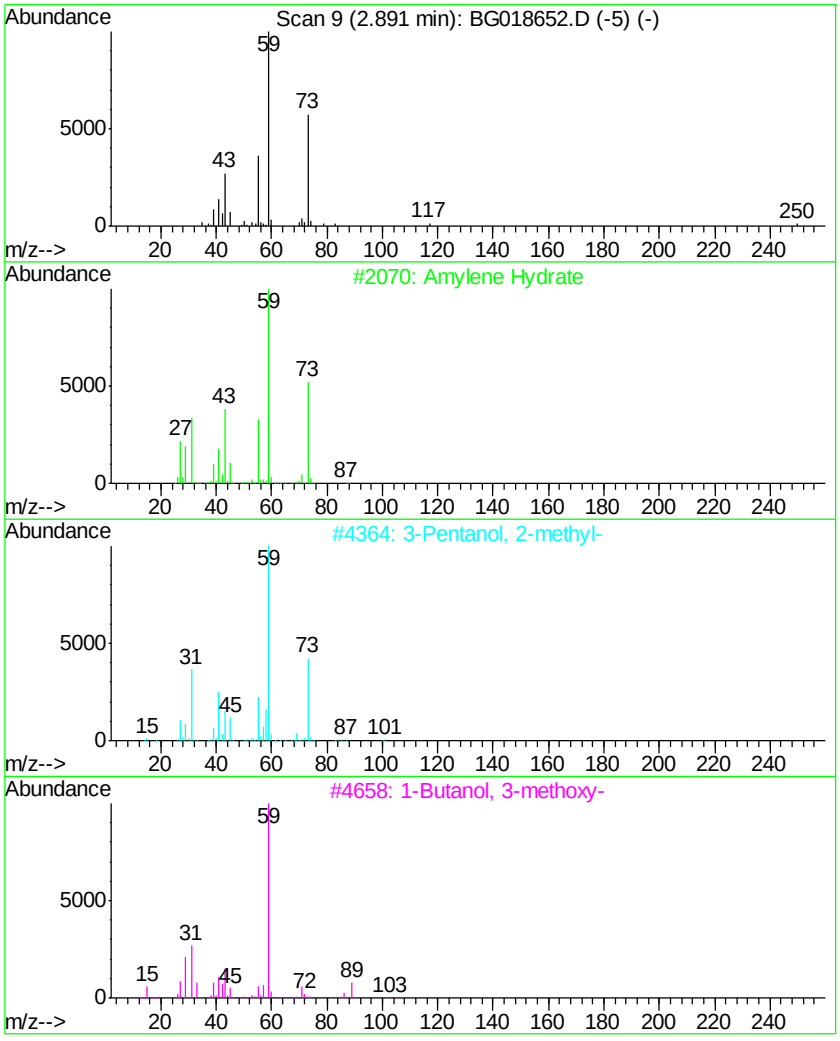
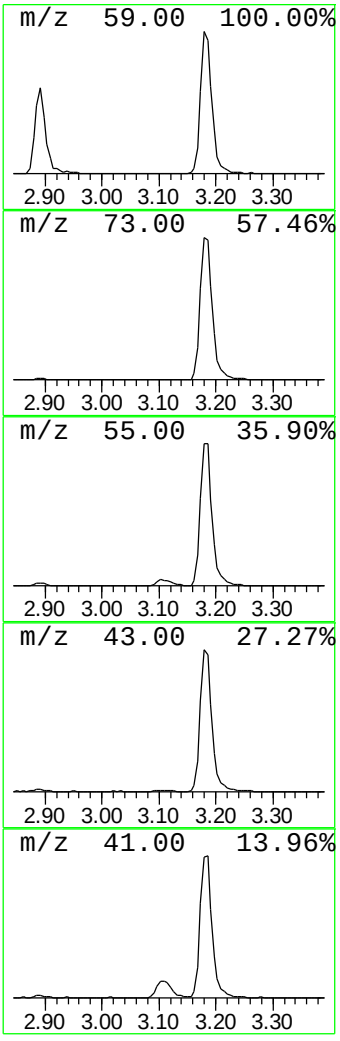
Peak Number 1 Amylene Hydrate Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.89	3.21 ng	51549	1,4-Dichlorobenzene-d4	8.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Amylene Hydrate	88	C5H12O	000075-85-4	64
2	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	56
3	1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	50
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	42
5	3-Hexanol	102	C6H14O	000623-37-0	39





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Instrument : BNA_G
ClientSampleId : 091015-EFF-GRAB

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091115.M
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TIC Integration Parameters: LSCINT.P

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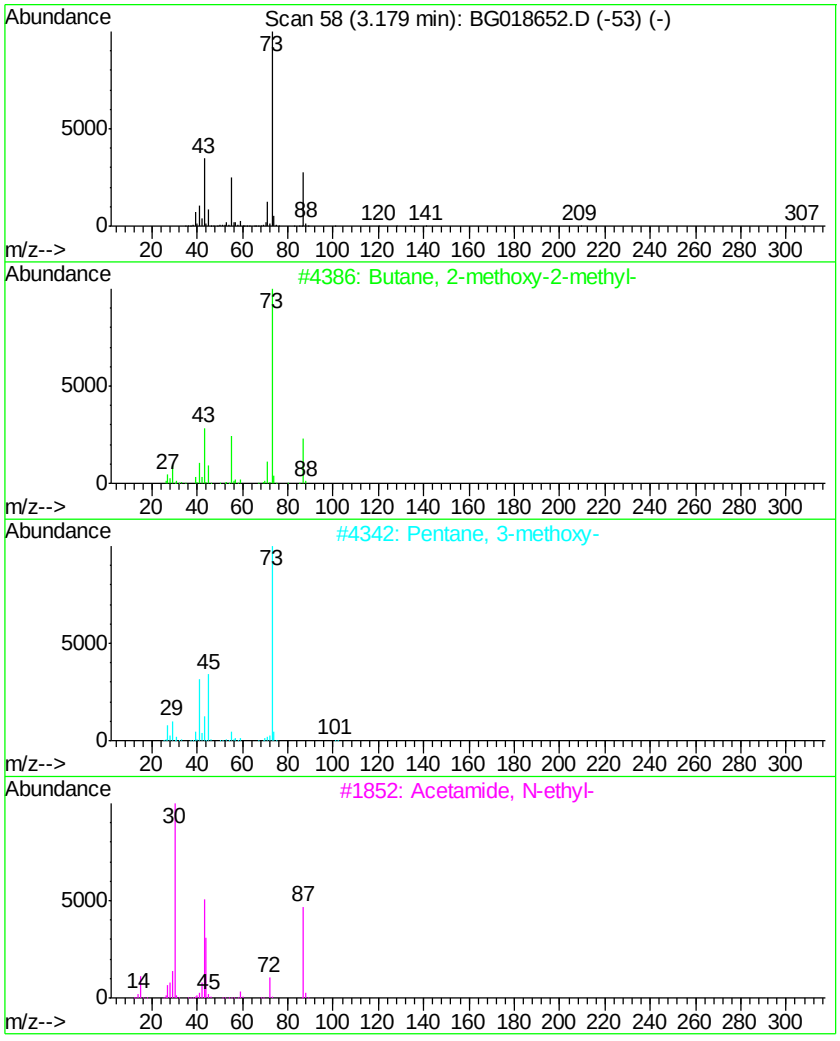
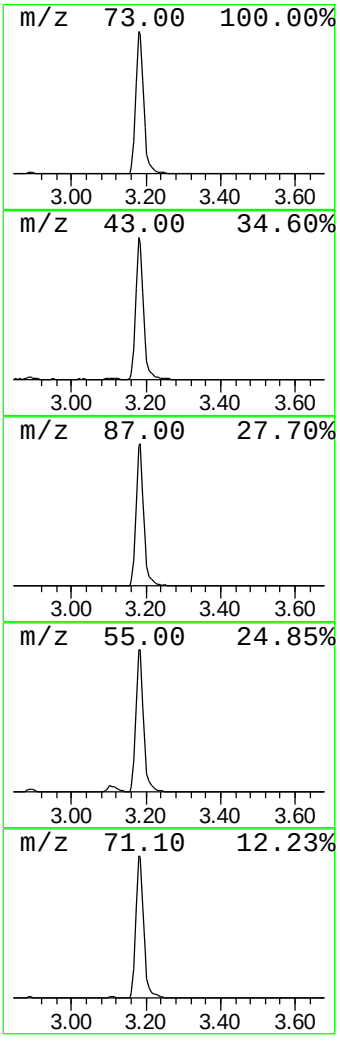
Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	204.04 ng	3277790	1,4-Dichlorobenzene-d4	8.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
4	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





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Instrument : BNA_G
ClientSampleId : 091015-EFF-GRAB

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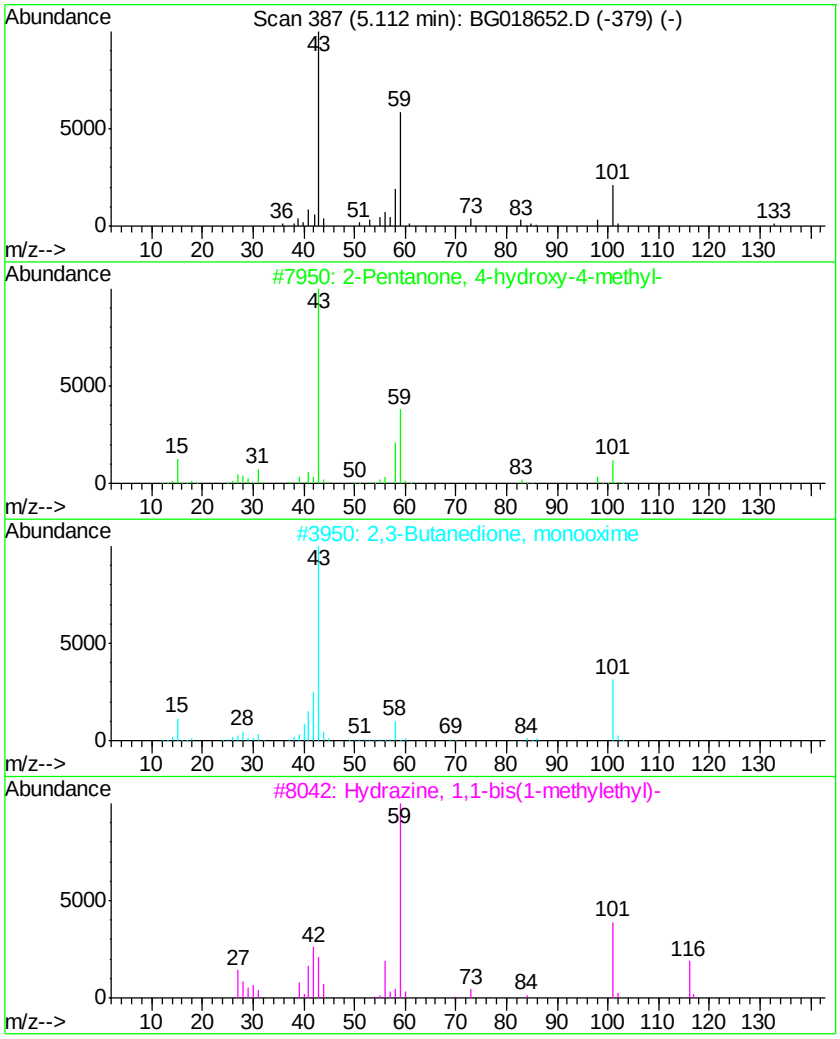
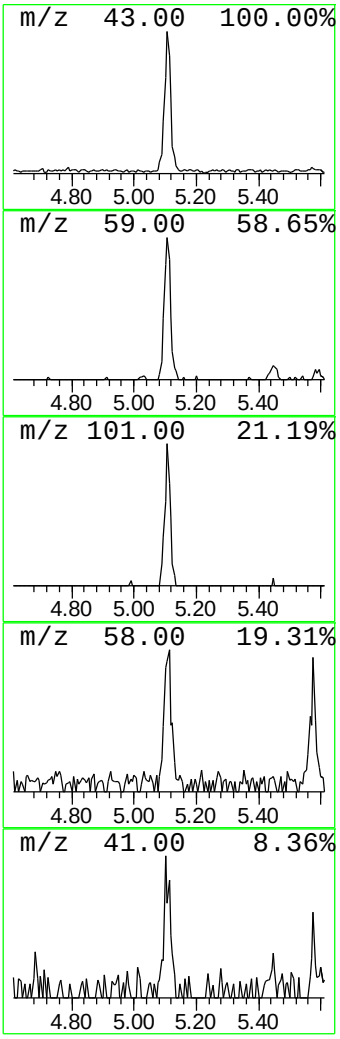
Peak Number 4 unknown5.11 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	4.12 ng	66170	1,4-Dichlorobenzene-d4	8.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	32
3	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Instrument : BNA_G
ClientSampleId : 091015-EFF-GRAB

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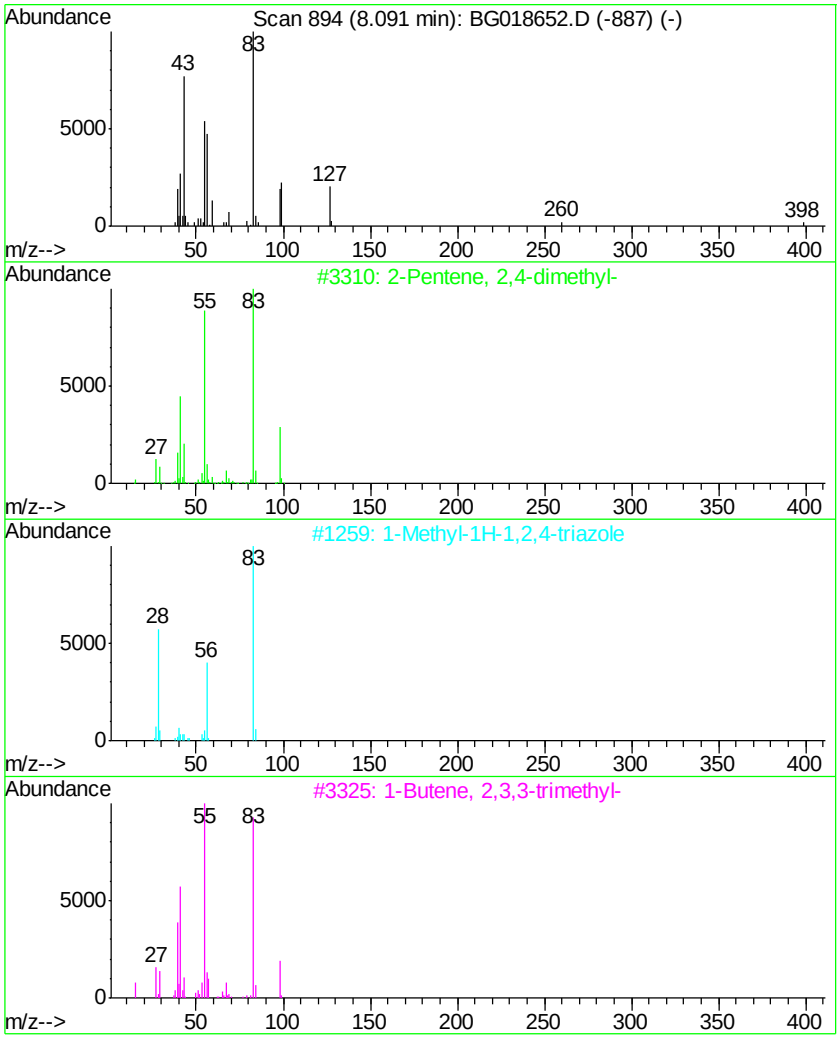
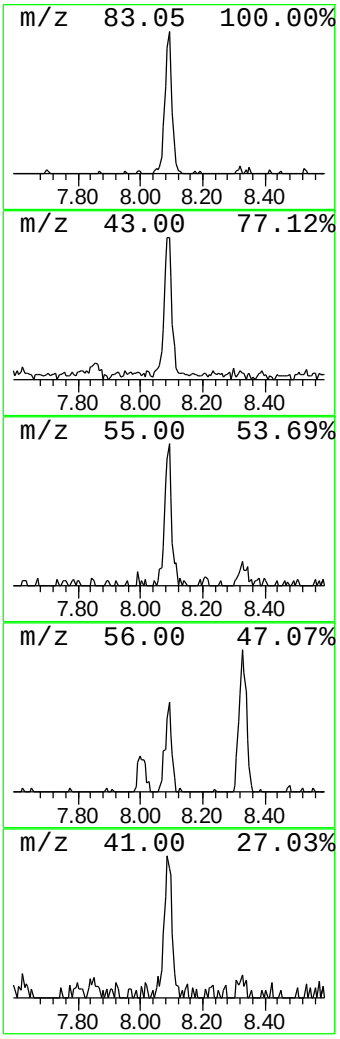
Peak Number 6 unknown8.09 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.09	4.09 ng	65667	1,4-Dichlorobenzene-d4	8.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	47
2	1-Methyl-1H-1,2,4-triazole	83	C3H5N3	006086-21-1	47
3	1-Butene, 2,3,3-trimethyl-	98	C7H14	000594-56-9	43
4	Cyclopropane, 1,1,2,2-tetramethyl-	98	C7H14	004127-47-3	43
5	3-Hexen-2-one	98	C6H10O	000763-93-9	43





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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 091015-EFF-GRAB

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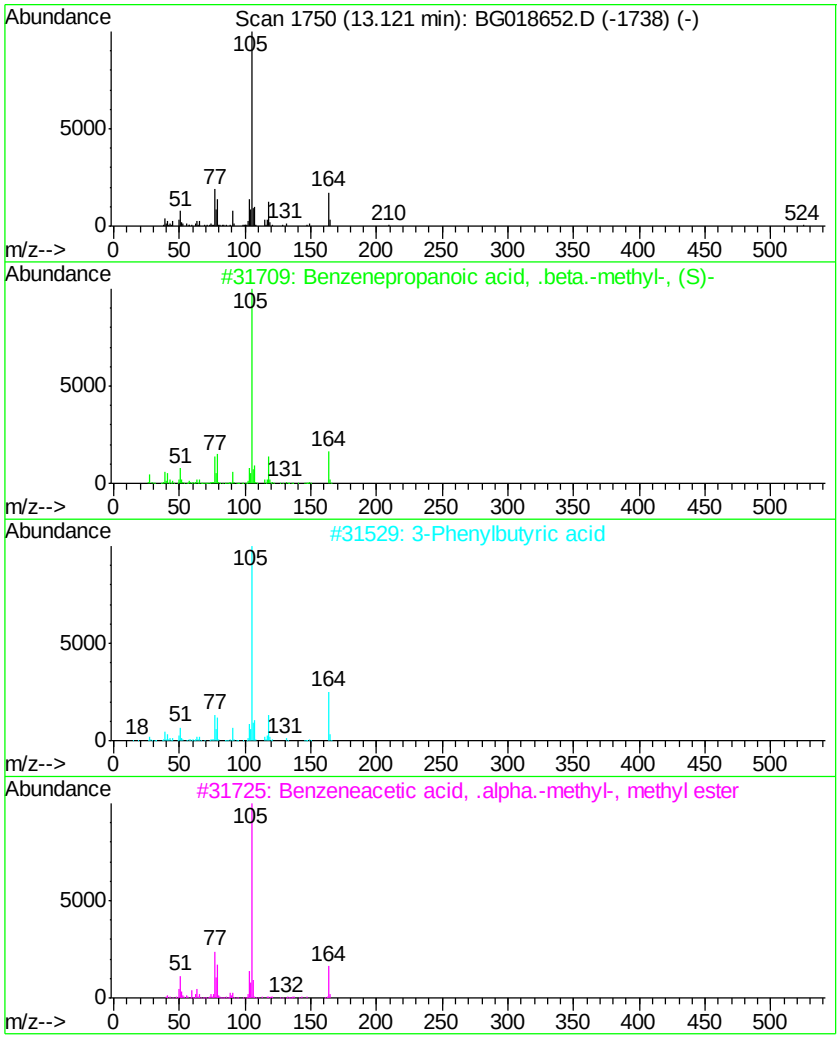
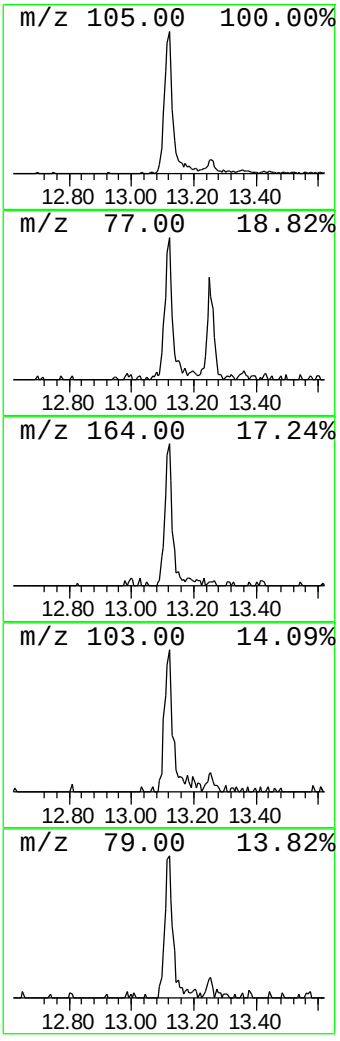
****

Peak Number 8 Benzenepropanoic acid, .bet... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.12	6.04 ng	227153	Acenaphthene-d10	14.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenepropanoic acid, .beta.-me...	164	C10H12O2	000772-15-6	91
2	3-Phenylbutyric acid	164	C10H12O2	004593-90-2	90
3	Benzeneacetic acid, .alpha.-meth...	164	C10H12O2	031508-44-8	58
4	3-(2-Methylphenyl)propionic acid	164	C10H12O2	022084-89-5	47
5	2-(p-Tolyl)ethylamine	135	C9H13N	003261-62-9	47





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Instrument : BNA_G
ClientSampleId : 091015-EFF-GRAB

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091115.M
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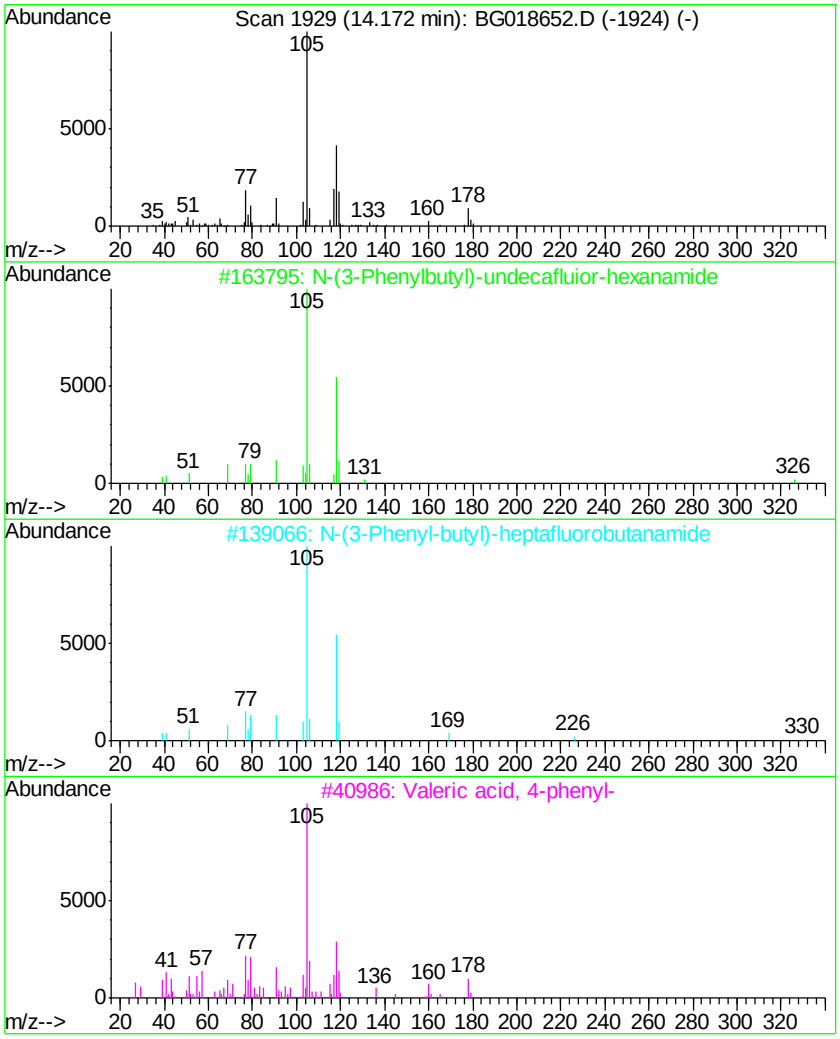
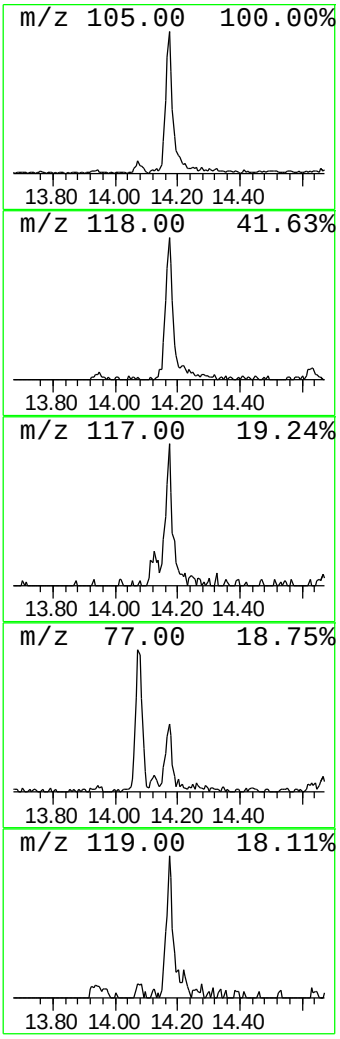
Peak Number 9 N-(3-Phenylbutyl)-undecaflu... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.17	4.14 ng	155668	Acenaphthene-d10	14.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-(3-Phenylbutyl)-undecafluior-h...	445	C16H14F11NO	077970-70-8	59
2	N-(3-Phenyl-butyl)-heptafluorobu...	345	C14H14F7NO	077970-69-5	47
3	Valeric acid, 4-phenyl-	178	C11H14O2	016433-43-5	38
4	Ethyl o-tolylacetate	178	C11H14O2	040291-39-2	35
5	Benzene, (3-chloro-1-methylpropyl)-	168	C10H13Cl	013556-61-1	27





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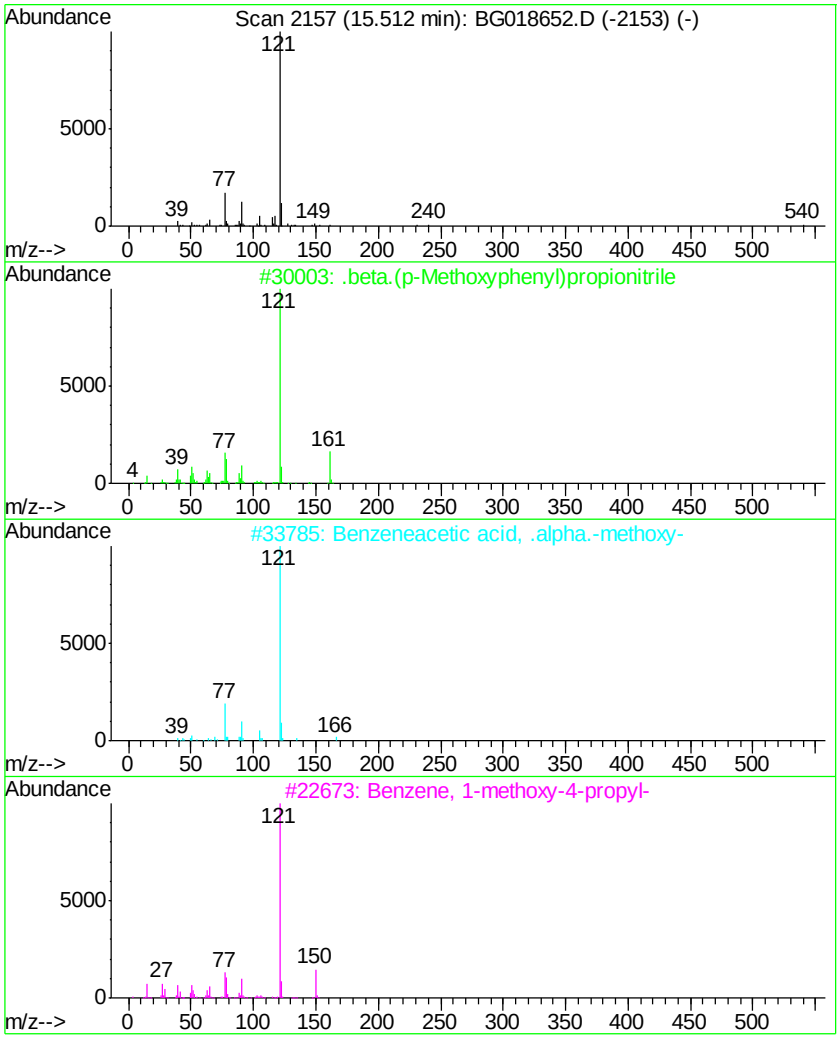
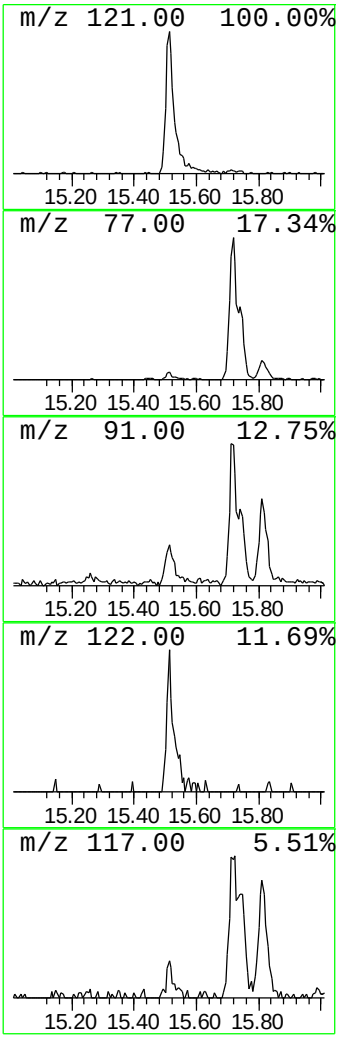
Peak Number 10 .beta.(p-Methoxyphenyl)prop... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.51	2.00 ng	75265	Acenaphthene-d10	14.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.(p-Methoxyphenyl)propionit...	161	C10H11NO	022442-48-4	72
2	Benzeneacetic acid, .alpha.-meth...	166	C9H10O3	001701-77-5	72
3	Benzene, 1-methoxy-4-propyl-	150	C10H14O	000104-45-0	72
4	Benzene, (1,2-dimethoxyethyl)-	166	C10H14O2	004013-37-0	72
5	Benzeneacetic acid, .alpha.-meth...	180	C10H12O3	056143-21-6	72





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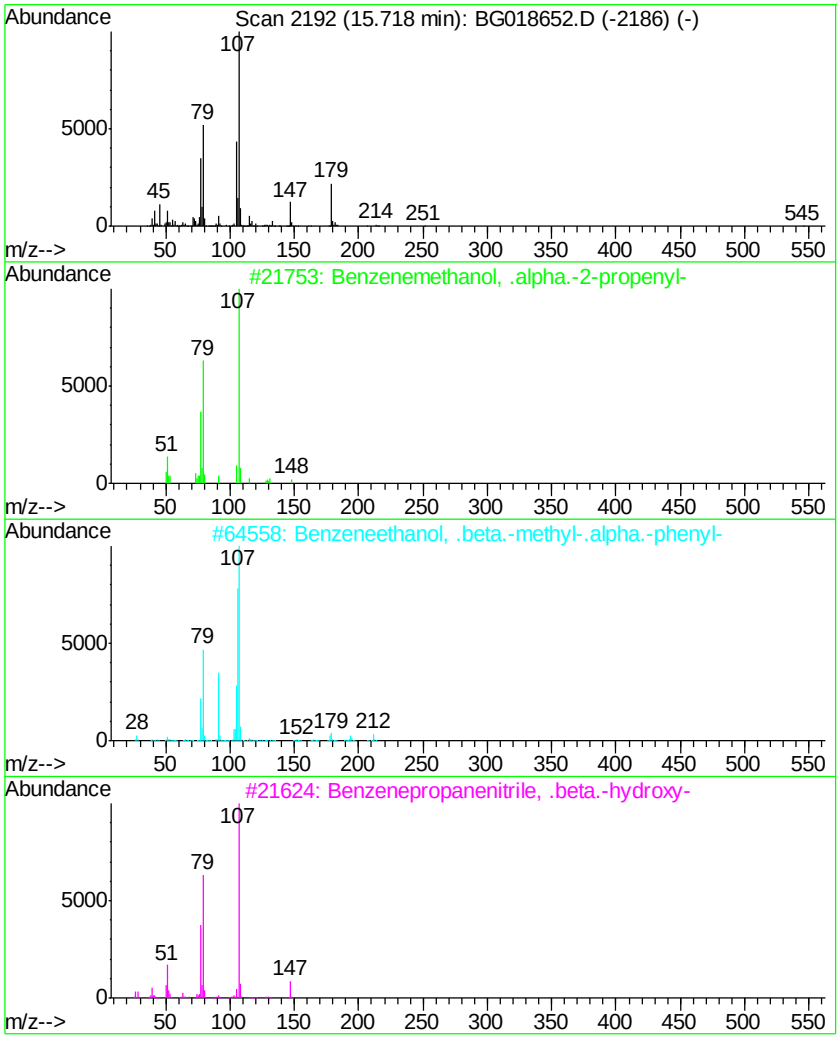
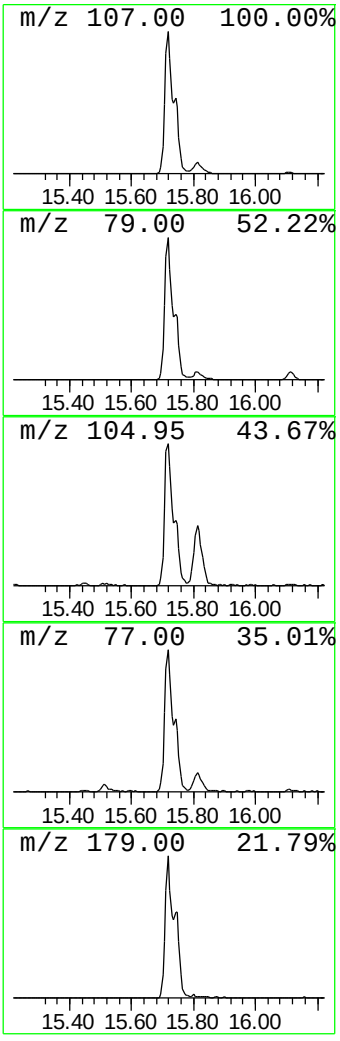
Peak Number 11 Benzenemethanol, .alpha.-2-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	39.64 ng	1490740	Acenaphthene-d10	14.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenemethanol, .alpha.-2-prope...	148	C10H12O	000936-58-3	72
2	Benzeneethanol, .beta.-methyl-.a...	212	C15H16O	028795-94-0	72
3	Benzenepropanenitrile, .beta.-hy...	147	C9H9NO	017190-29-3	72
4	Benzenemethanol, .alpha.-propyl-	150	C10H14O	000614-14-2	64
5	Ethyl dl-mandelate	180	C10H12O3	004358-88-7	64





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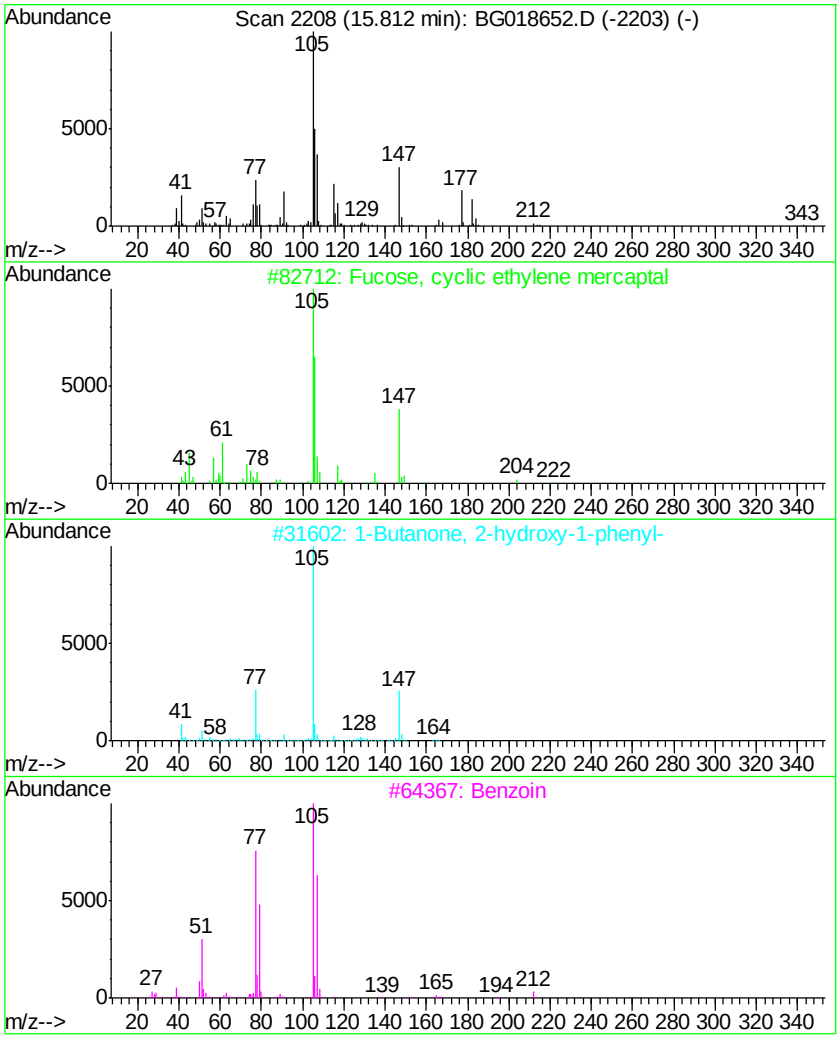
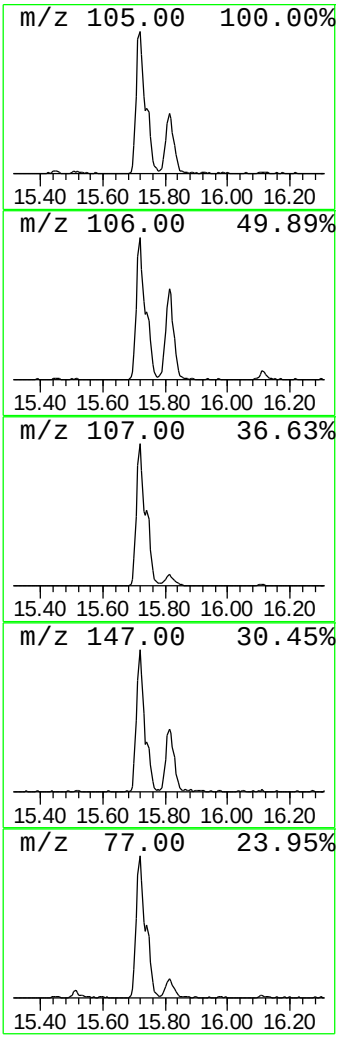
Peak Number 12 unknown15.81 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.81	9.55 ng	359171	Acenaphthene-d10	14.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fucose, cyclic ethylene mercaptal	240	C8H16O4S2	003650-70-2	43
2	1-Butanone, 2-hydroxy-1-phenyl-	164	C10H12O2	016183-46-3	22
3	Benzoin	212	C14H12O2	000579-44-2	12
4	Ethanone, 2-(acetyloxy)-1,2-diph...	254	C16H14O3	000574-06-1	12
5	(1H)Pyrrole-2-carbonitrile, 5-me...	106	C6H6N2	026173-92-2	12





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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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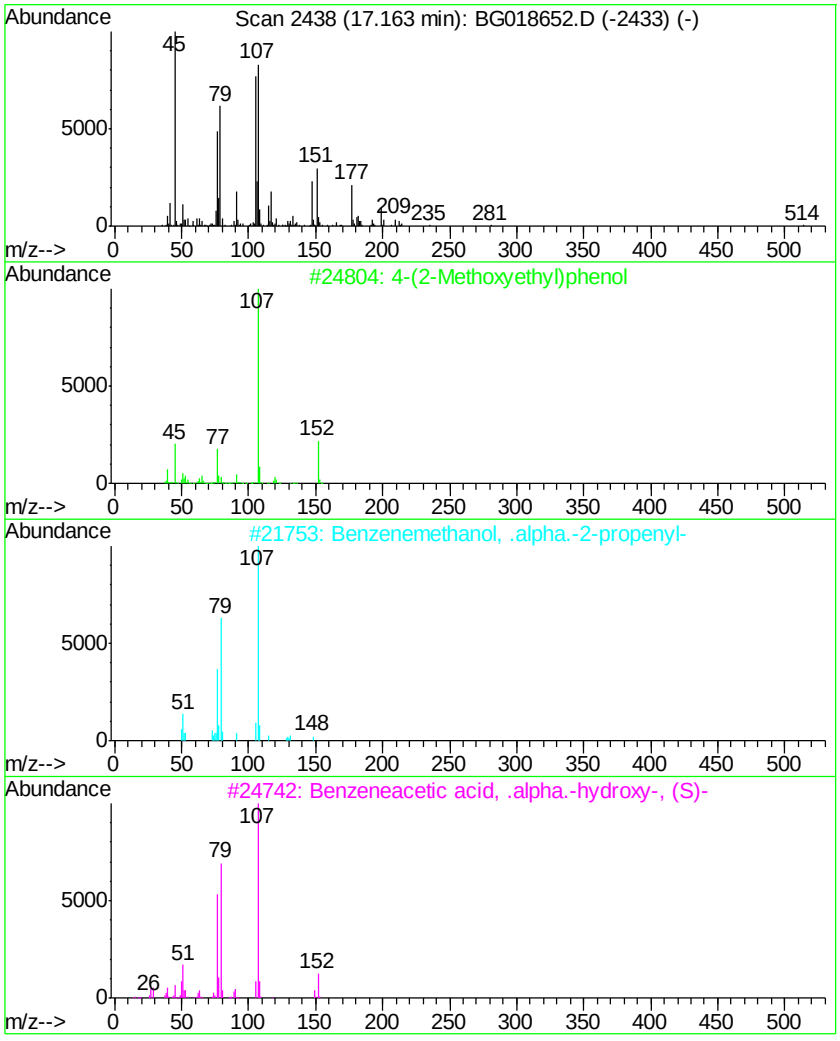
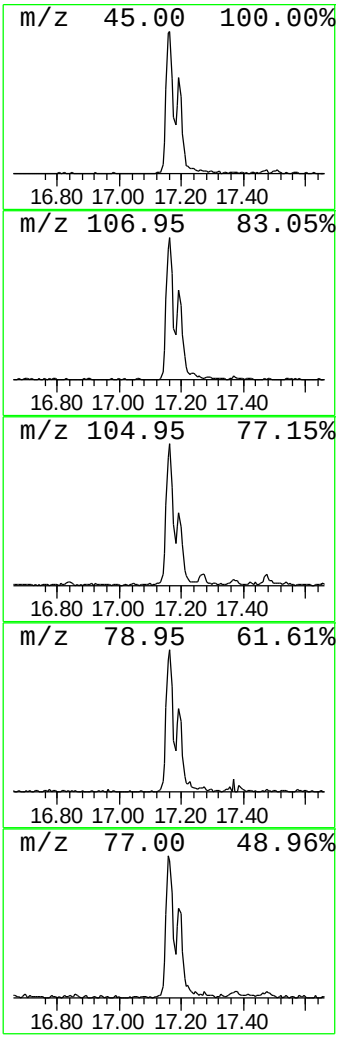
Peak Number 13 unknown17.16 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.16	6.92 ng	381265	Phenanthrene-d10	17.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-(2-Methoxyethyl)phenol	152	C9H12O2	056718-71-9	47
2	Benzenemethanol, .alpha.-2-prope...	148	C10H12O	000936-58-3	46
3	Benzeneacetic acid, .alpha.-hydr...	152	C8H8O3	017199-29-0	46
4	Benzeneacetic acid, .alpha.-hydr...	152	C8H8O3	000611-72-3	45
5	1-Phenylpropane-1,3-diol	152	C9H12O2	004850-49-1	43





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG091215\
Data File : BG018652.D
Acq On : 11 Sep 2015 23:15
Operator : UM/IZ
Sample : G3638-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 091015-EFF-GRAB

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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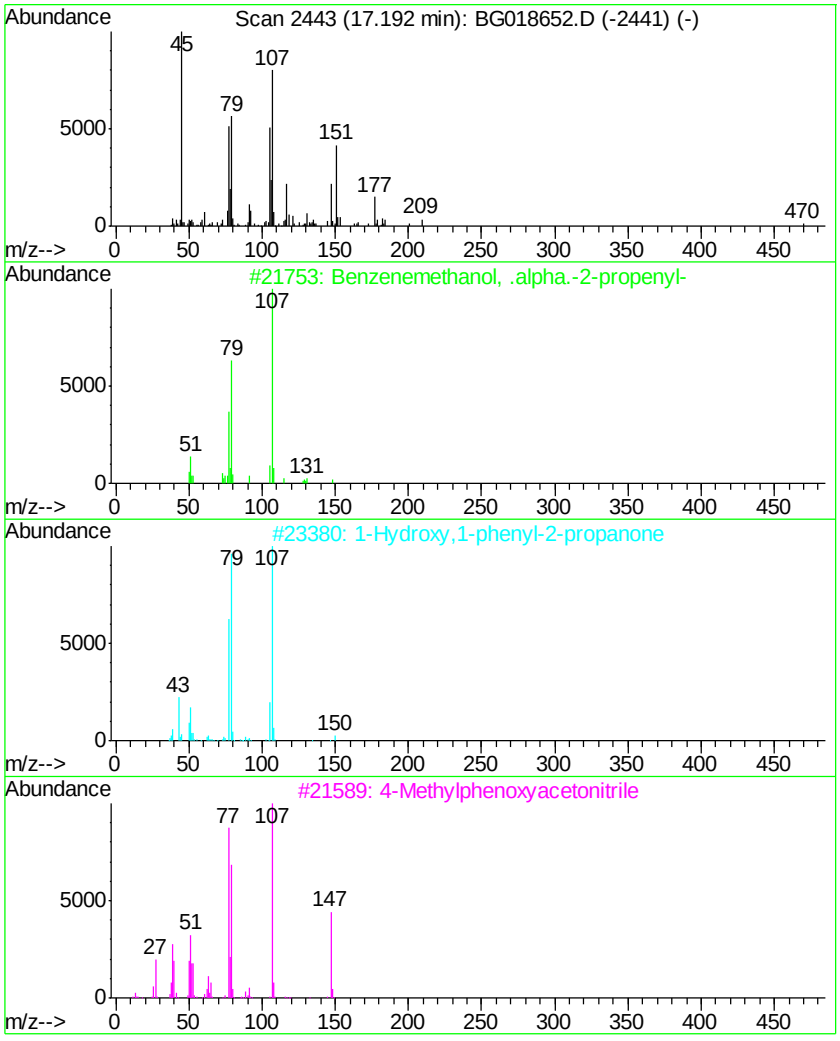
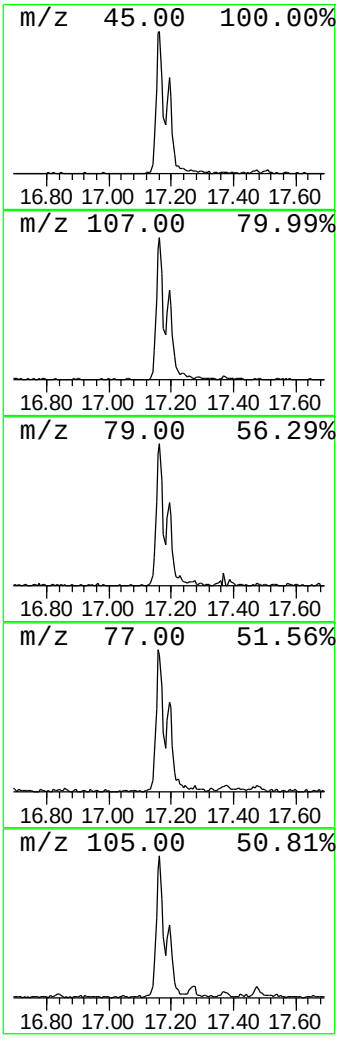
Peak Number 14 unknown17.19 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.19	3.69 ng	203308	Phenanthrene-d10	17.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenemethanol, .alpha.-2-prope...	148	C10H12O	000936-58-3	43
2	1-Hydroxy,1-phenyl-2-propanone	150	C9H10O2	1000222-86-8	35
3	4-Methylphenoxyacetonitrile	147	C9H9NO	033901-44-9	35
4	Benzenemethanol, .alpha.-pentyl-	178	C12H18O	004471-05-0	35
5	3-Nitrobenzylamine	152	C7H8N2O2	007409-18-9	35





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG091215\
Data File : BG018652.D
Acq On : 11 Sep 2015 23:15
Operator : UM/IZ
Sample : G3638-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 091015-EFF-GRAB

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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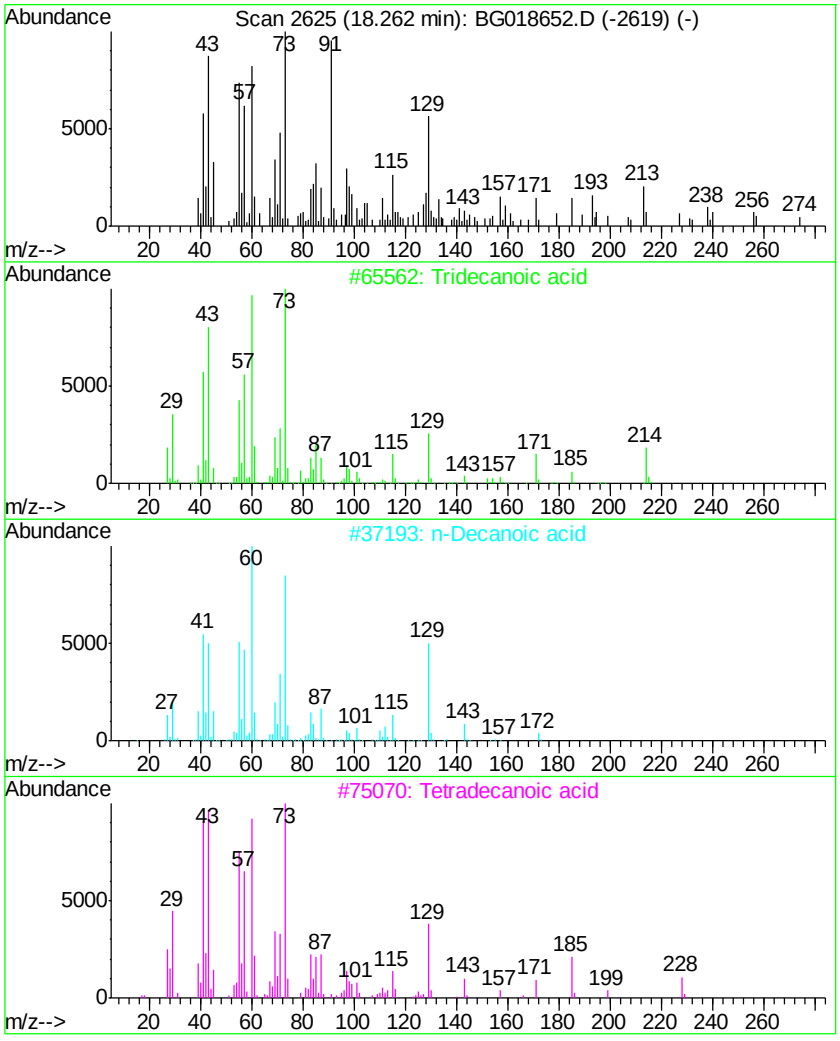
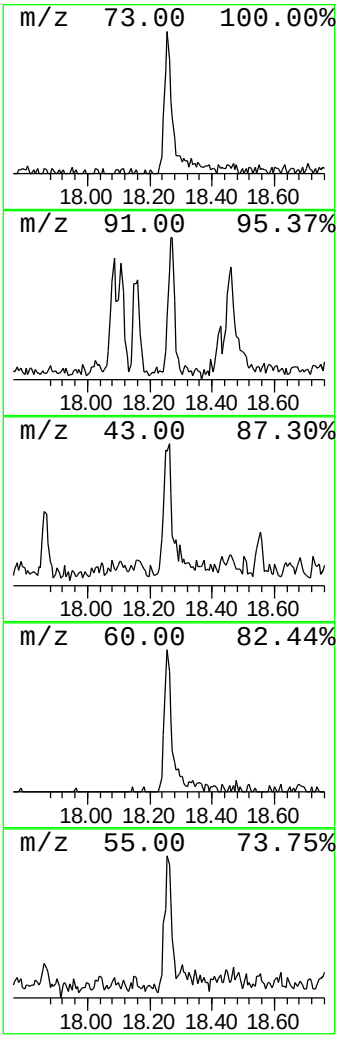
Peak Number 15 Tridecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.26	3.23 ng	177969	Phenanthrene-d10	17.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	89
2	n-Decanoic acid	172	C10H20O2	000334-48-5	53
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	49
4	Nonanoic acid	158	C9H18O2	000112-05-0	45
5	Octanoic Acid	144	C8H16O2	000124-07-2	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG091215\
Data File : BG018652.D
Acq On : 11 Sep 2015 23:15
Operator : UM/IZ
Sample : G3638-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 091015-EFF-GRAB

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
Amylene Hydrate	2.89	3.2	ng	51549	1	8.01	321288	20.0
Butane, 2-methoxy...	3.18	204.0	ng	3277790	1	8.01	321288	20.0
unknown5.11	5.11	4.1	ng	66170	1	8.01	321288	20.0
unknown8.09	8.09	4.1	ng	65667	1	8.01	321288	20.0
Benzenepropanoic ...	13.12	6.0	ng	227153	3	14.63	752124	20.0
N-(3-Phenylbutyl)...	14.17	4.1	ng	155668	3	14.63	752124	20.0
.beta.(p-Methoxyp...	15.51	2.0	ng	75265	3	14.63	752124	20.0
Benzenemethanol, ...	15.72	39.6	ng	1490740	3	14.63	752124	20.0
unknown15.81	15.81	9.6	ng	359171	3	14.63	752124	20.0
unknown17.16	17.16	6.9	ng	381265	4	17.37	1102250	20.0
unknown17.19	17.19	3.7	ng	203308	4	17.37	1102250	20.0
Tridecanoic acid	18.26	3.2	ng	177969	4	17.37	1102250	20.0