LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG091715\
Data File : BG018718.D
Acq On : 16 Sep 2015 22:50
Operator : TP
Sample : G3651-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CPS043034

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	2.961	16	21	40	rVB	1960865	2560566	59.90%	11.473%
2	3.102	40	45	53	rVV	56792	98436	2.30%	0.441%
3	3.178	53	58	76	rVB	1297222	1785339	41.76%	7.999%
4	5.105	380	386	392	rBV	90640	132375	3.10%	0.593%
5	5.575	456	466	476	rVB	297317	465290	10.88%	2.085%
6	7.162	730	736	746	rBV	188040	315621	7.38%	1.414%
7	7.532	792	799	807	rBV	572488	981869	22.97%	4.399%
8	8.002	871	879	885	rBV	129951	221129	5.17%	0.991%
9	8.325	926	934	941	rBV	563781	935200	21.88%	4.190%
10	9.160	1069	1076	1085	rVB	464991	799527	18.70%	3.582%
11	10.570	1307	1316	1325	rBV4	22854	46450	1.09%	0.208%
12	10.805	1349	1356	1363	rBV	191233	342217	8.01%	1.533%
13	11.451	1459	1466	1476	rVB	55821	106002	2.48%	0.475%
14	12.984	1722	1727	1733	rBV	29963	50792	1.19%	0.228%
15	13.255	1761	1773	1779	rBV	1540168	2414652	56.48%	10.819%
16	14.071	1906	1912	1918	rBV	72554	103378	2.42%	0.463%
17	14.630	2000	2007	2014	rVB2	359770	588346	13.76%	2.636%
18	15.435	2137	2144	2155	rBV	254174	363669	8.51%	1.629%
19	16.116	2252	2260	2271	rBV	1298015	1996389	46.70%	8.945%
20	17.368	2467	2473	2480	rBV2	567563	837814	19.60%	3.754%
21	17.644	2513	2520	2528	rVB	368307	462869	10.83%	2.074%
22	18.031	2581	2586	2591	rBV2	128318	167616	3.92%	0.751%
23	18.325	2631	2636	2643	rVB	44114	54746	1.28%	0.245%
24	19.976	2911	2917	2929	rBV	3201692	4275014	100.00%	19.155%
25	21.510	3174	3178	3185	rVB	68217	95599	2.24%	0.428%
26	21.627	3191	3198	3206	rBV	629699	1020802	23.88%	4.574%
27	23.079	3440	3445	3457	rBV6	29214	73038	1.71%	0.327%
28	24.812	3729	3740	3751	rBV2	364680	1023391	23.94%	4.585%

Sum of corrected areas: 22318136

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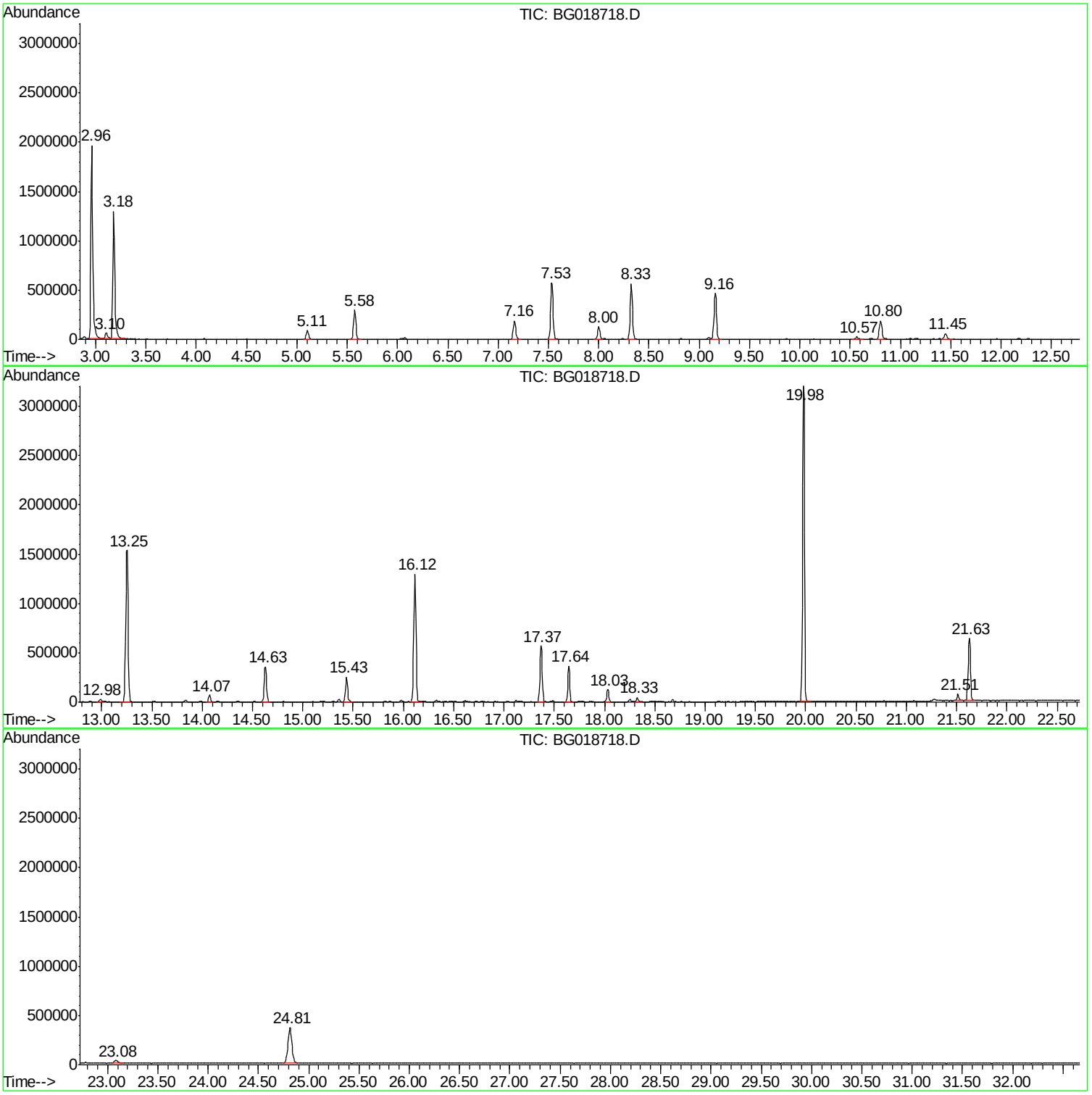
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CPS043034

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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

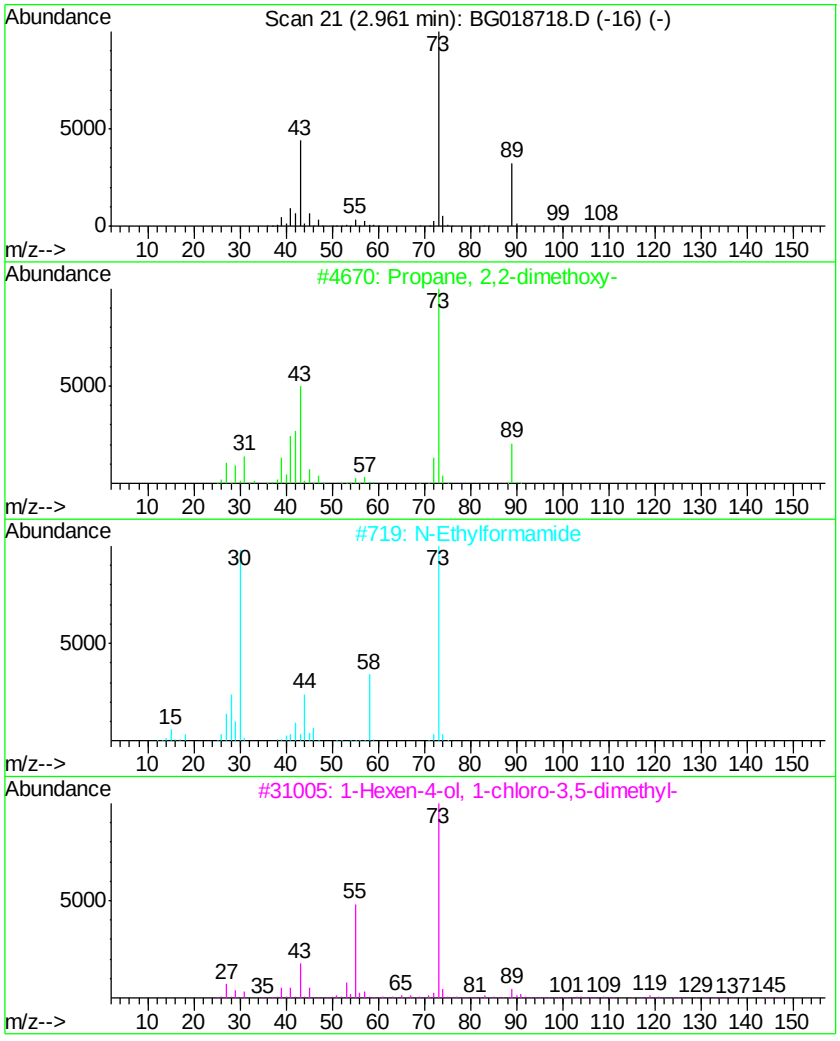
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

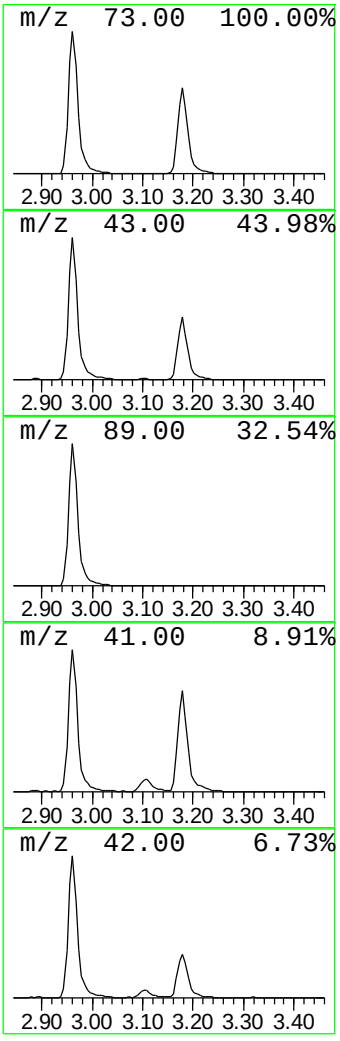
****

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.96	231.59 ng	2560570	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	56
2	N-Ethylformamide	73	C3H7NO	000627-45-2	9
3	1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
4	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
5	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9





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Data File : BG018718.D
Acq On : 16 Sep 2015 22:50
Operator : TP
Sample : G3651-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CPS043034

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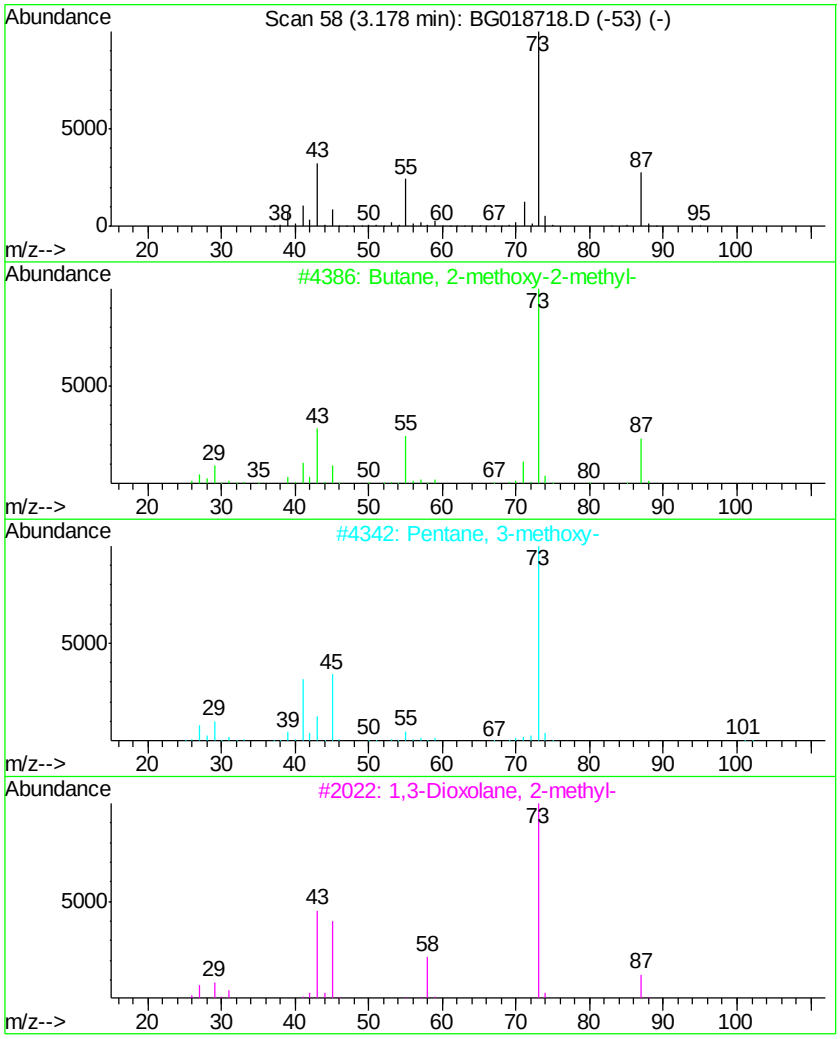
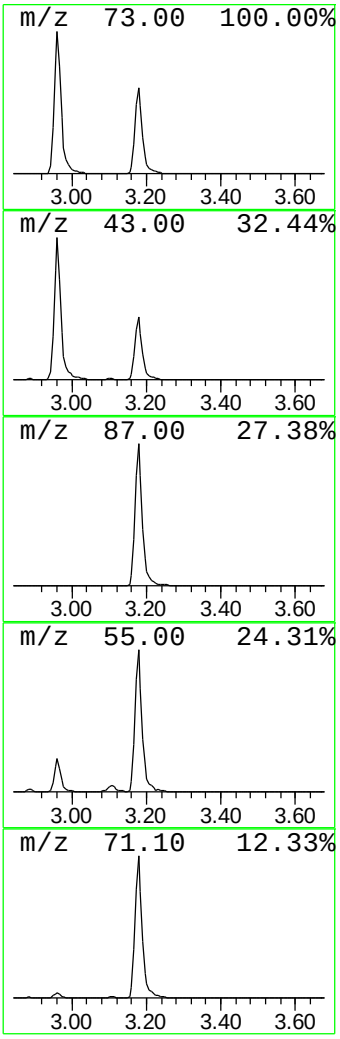
Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	161.48 ng	1785340	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	78
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





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Data File : BG018718.D
Acq On : 16 Sep 2015 22:50
Operator : TP
Sample : G3651-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CPS043034

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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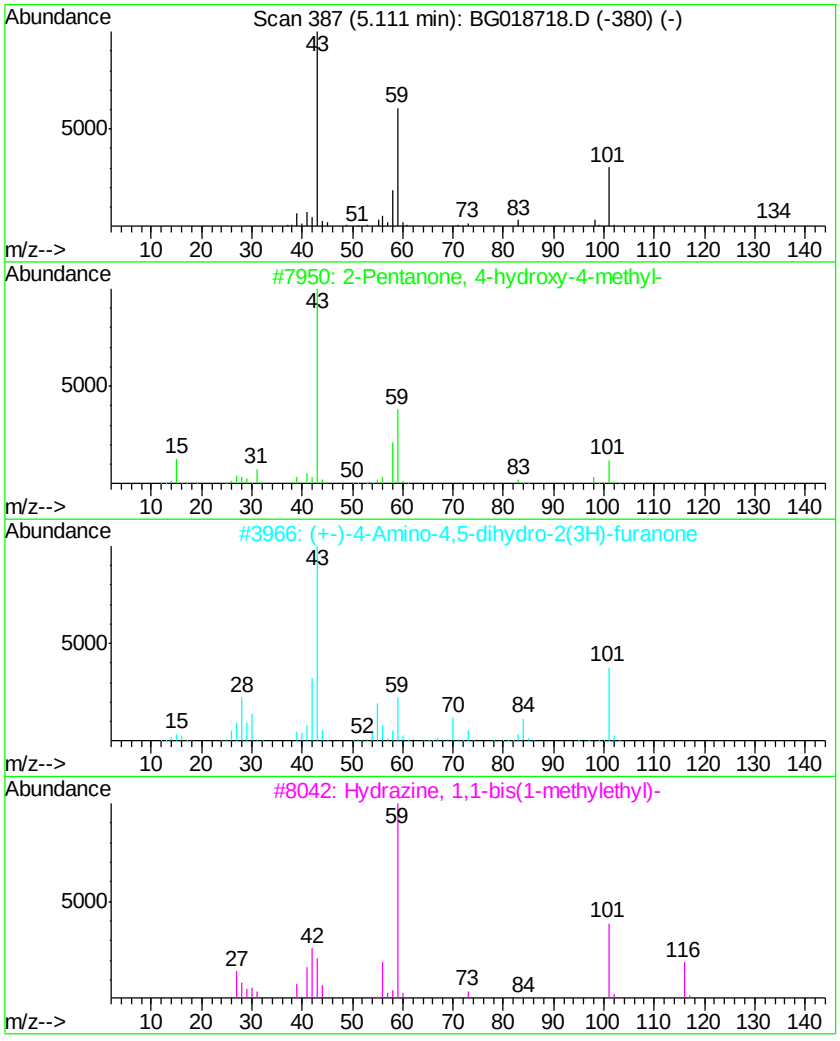
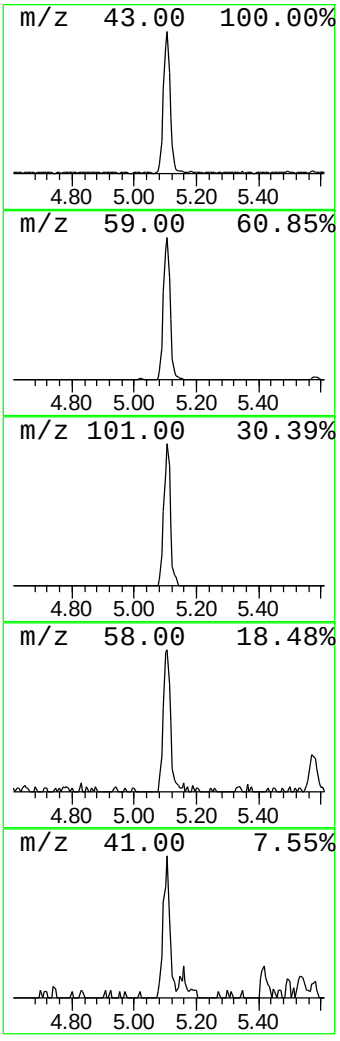
Peak Number 4 unknown5.11 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	11.97 ng	132375	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	45
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	43
3	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
4	2,5,8,11,14-Pentaoxapentadecane	222	C10H22O5	000143-24-8	25
5	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25





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Acq On : 16 Sep 2015 22:50
Operator : TP
Sample : G3651-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CPS043034

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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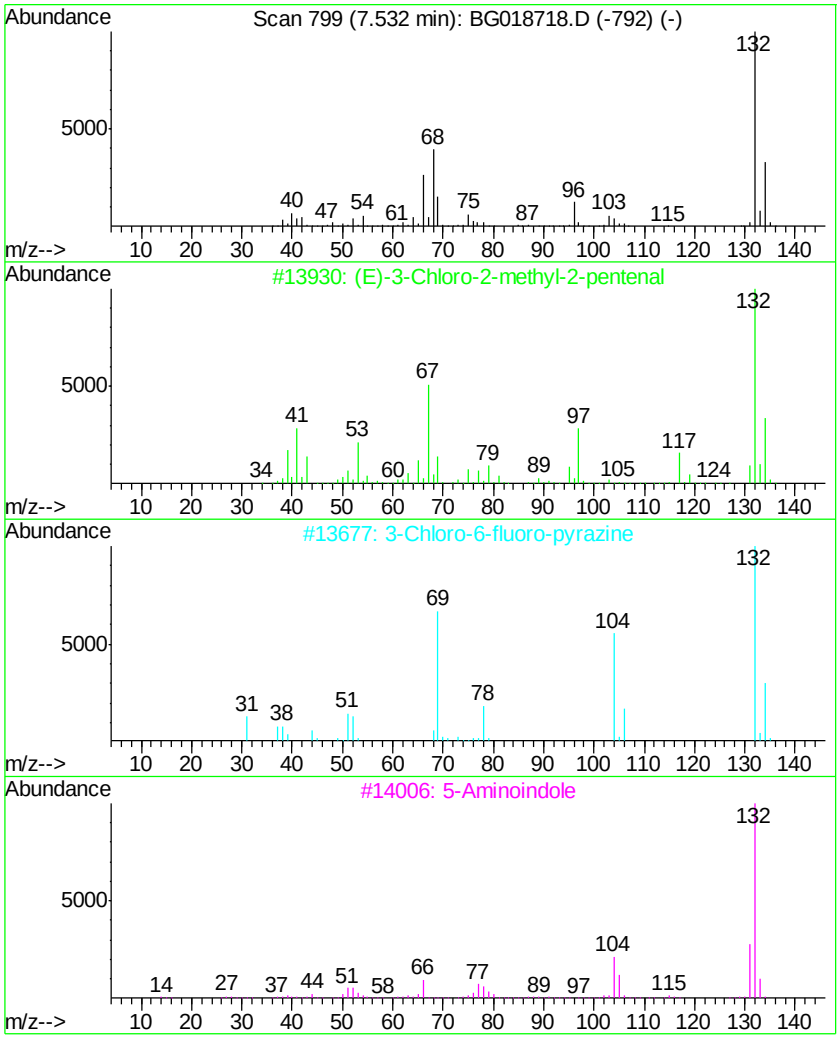
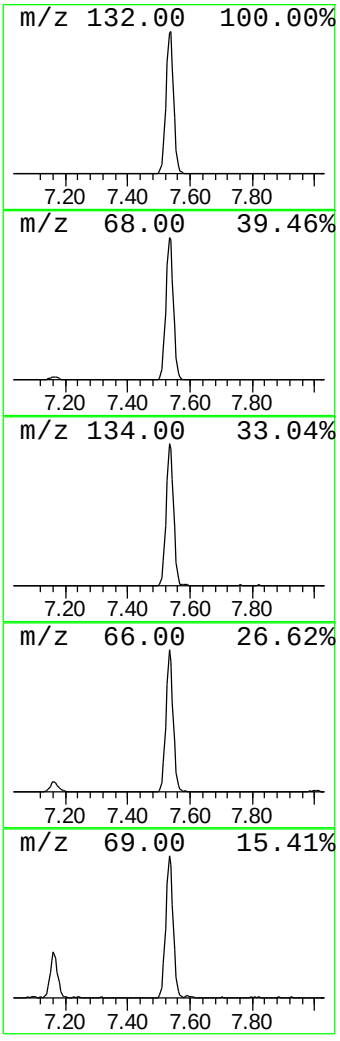
Peak Number 5 unknown7.53 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.53	88.81 ng	981869	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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG091715\
Data File : BG018718.D
Acq On : 16 Sep 2015 22:50
Operator : TP
Sample : G3651-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CPS043034

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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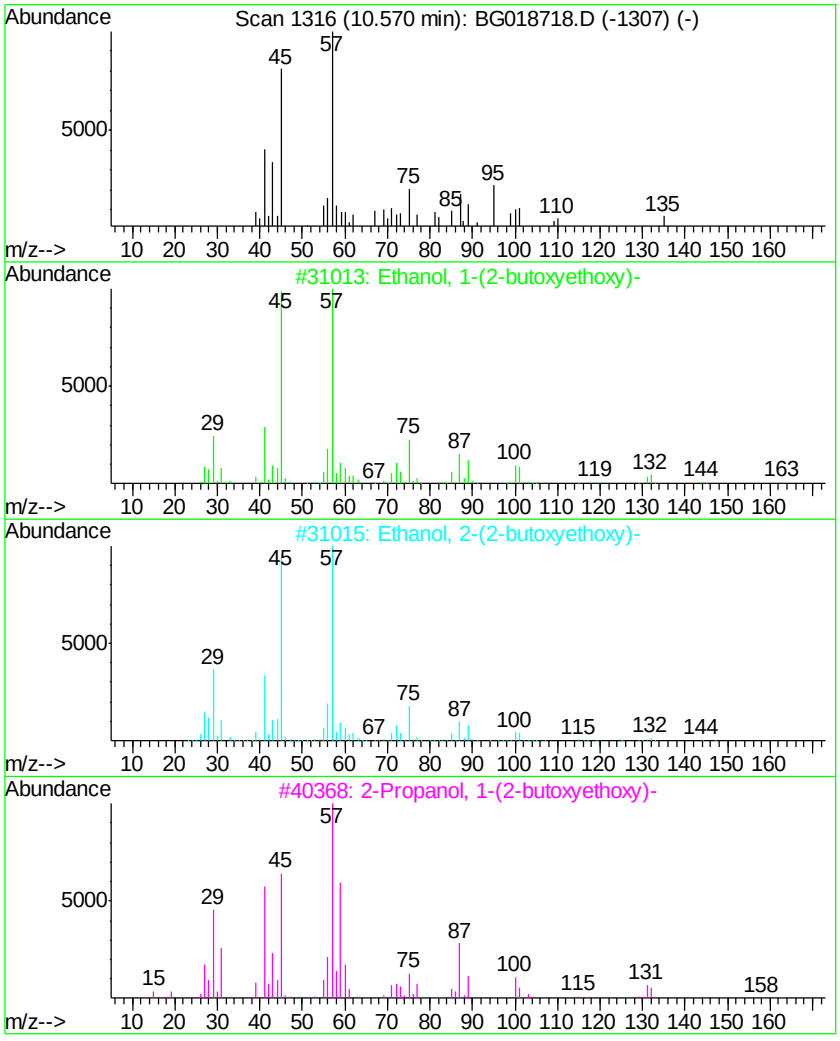
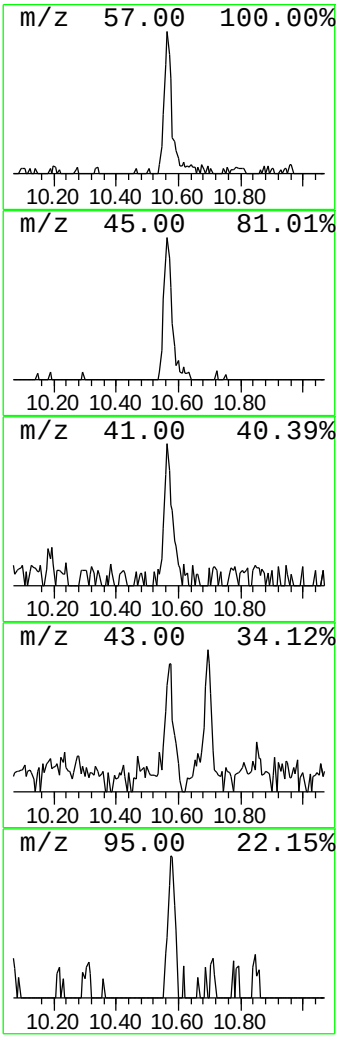
Peak Number 7 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.57	2.71 ng	46450	Naphthalene-d8	10.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	72
2	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	72
3	2-Propanol, 1-(2-butoxyethoxy)-	176	C9H20O3	000124-16-3	45
4	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	43
5	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	42





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Operator : TP
Sample : G3651-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CPS043034

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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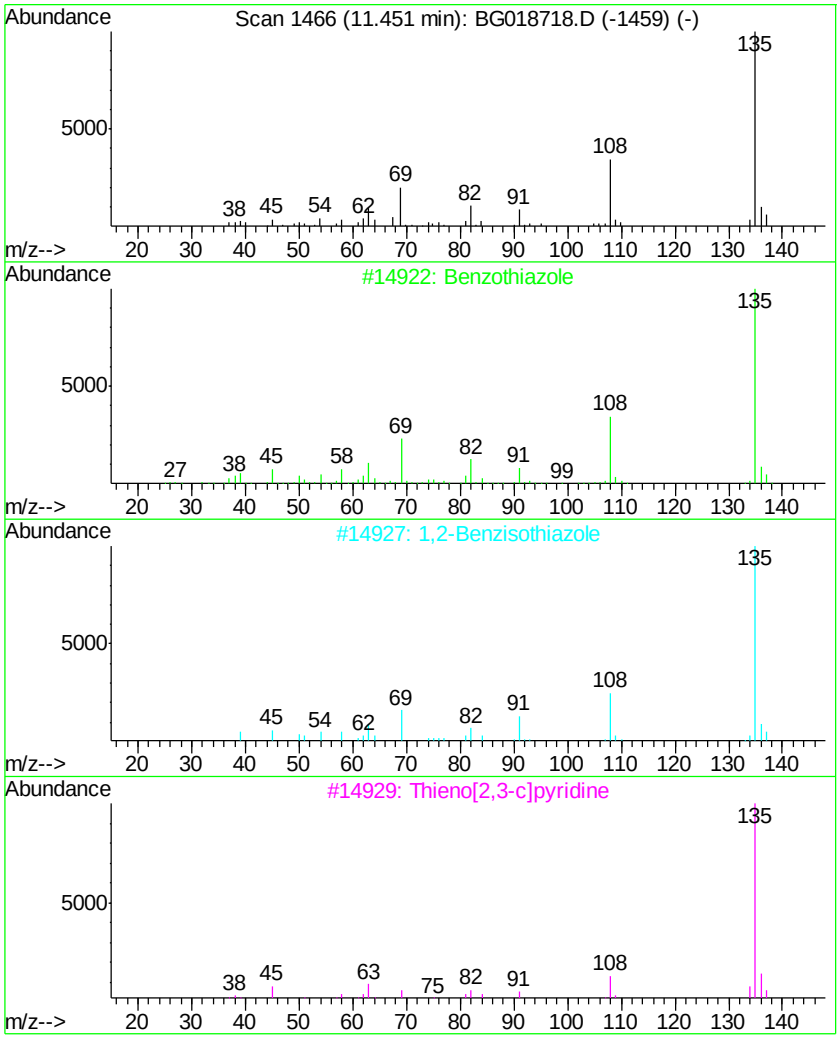
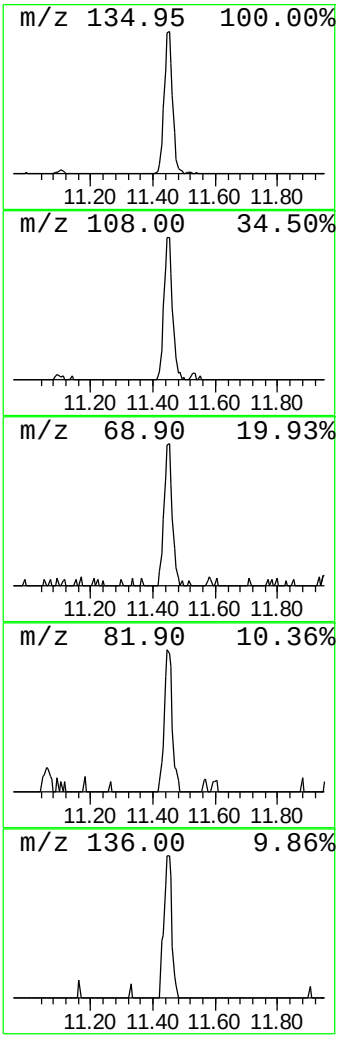
Peak Number 8 Benzothiazole Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.45	6.20 ng	106002	Naphthalene-d8	10.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzothiazole	135	C7H5NS	000095-16-9	95
2	1,2-Benzisothiazole	135	C7H5NS	000272-16-2	91
3	Thieno[2,3-c]pyridine	135	C7H5NS	000272-12-8	83
4	3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	78
5	1H-Pyrazolo[3,4-d]pyrimidin-4-amine	135	C5H5N5	002380-63-4	59





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Sample : G3651-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CPS043034

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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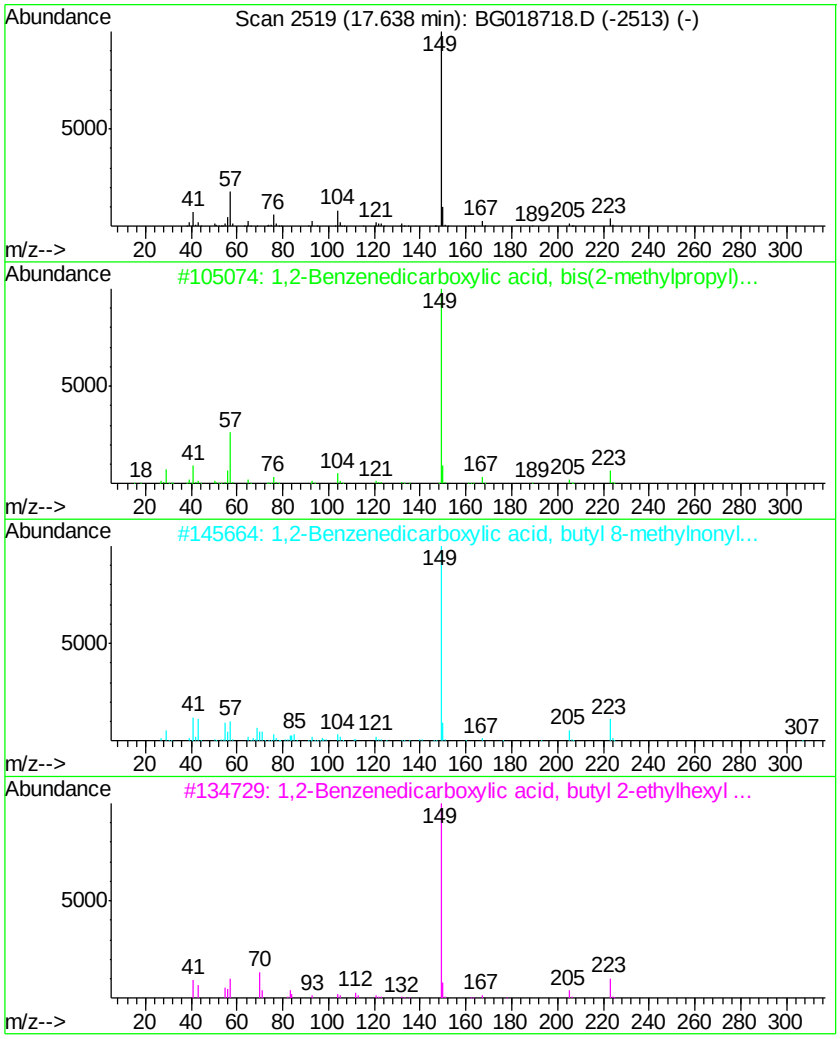
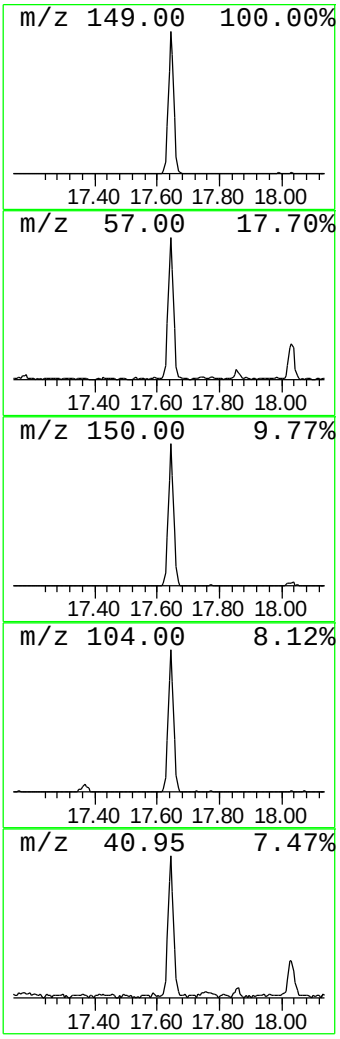
Peak Number 9 1,2-Benzenedicarboxylic aci... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.64	11.05 ng	462869	Phenanthrene-d10	17.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	83
2	1,2-Benzenedicarboxylic acid, bu...	362	C22H34O4	000089-18-9	72
3	1,2-Benzenedicarboxylic acid, bu...	334	C20H30O4	000085-69-8	72
4	Dibutyl phthalate	278	C16H22O4	000084-74-2	72
5	1,2-Benzenedicarboxylic acid, bu...	304	C18H24O4	000084-64-0	72





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ALS Vial : 10 Sample Multiplier: 1

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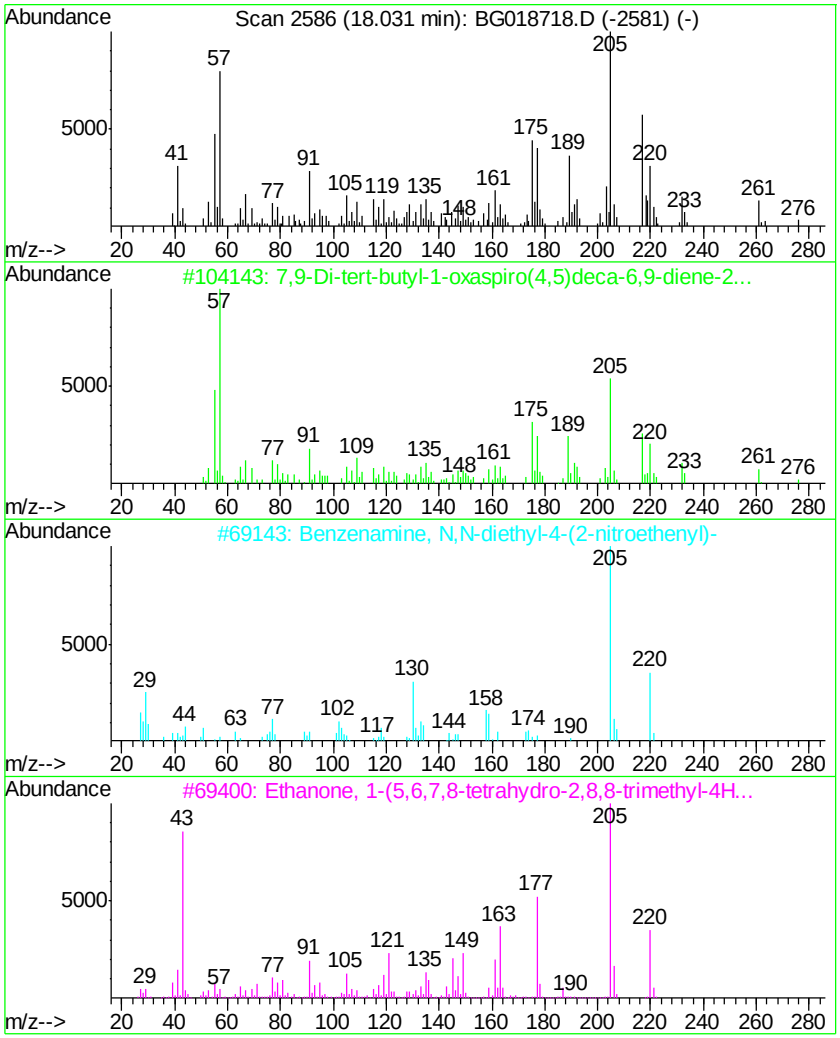
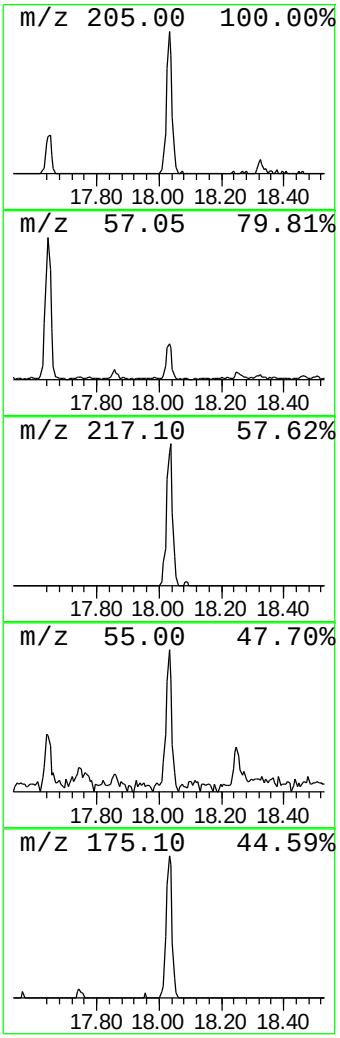
****

Peak Number 10 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.03	4.00 ng	167616	Phenanthrene-d10	17.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	97
2	Benzenamine, N,N-diethyl-4-(2-ni...	220	C12H16N2O2	064462-51-7	38
3	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	38
4	3H-Cyclopenta[1,3]cyclopropa[1,2...	220	C14H20O2	066708-18-7	35
5	2,5-Cyclohexadien-1-one, 2,6-bis...	232	C16H24O	006738-27-8	30





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG091715\
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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
Propane, 2,2-dime...	2.96	231.6	ng	2560570	1	8.00	221129	20.0
Butane, 2-methoxy...	3.18	161.5	ng	1785340	1	8.00	221129	20.0
unknown5.11	5.11	12.0	ng	132375	1	8.00	221129	20.0
unknown7.53	7.53	88.8	ng	981869	1	8.00	221129	20.0
Ethanol, 1-(2-but...	10.57	2.7	ng	46450	2	10.80	342217	20.0
Benzothiazole	11.45	6.2	ng	106002	2	10.80	342217	20.0
1,2-Benzenedicarb...	17.64	11.1	ng	462869	4	17.37	837814	20.0
7,9-Di-tert-butyl...	18.03	4.0	ng	167616	4	17.37	837814	20.0