LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG032818\
Data File : BG033390.D
Acq On : 28 Mar 2018 17:43
Operator : SJ/JU
Sample : J2072-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C0AB1

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-BG031918.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	3.482	27	33	43	rBV	110689	232403	1.86%	0.884%
2	5.109	305	310	324	rBV2	355025	706548	5.65%	2.686%
3	5.820	417	431	436	rBV	4612567	12515772	100.00%	47.582%
4	6.220	493	499	515	rBV	1474837	2579645	20.61%	9.807%
5	6.713	577	583	587	rBV	1102259	1759321	14.06%	6.688%
6	8.870	942	950	965	rBV4	124771	292303	2.34%	1.111%
7	9.199	998	1006	1017	rBV3	141603	280535	2.24%	1.067%
8	9.545	1059	1065	1075	rVV	154262	278268	2.22%	1.058%
9	10.068	1144	1154	1170	rBV2	131233	334589	2.67%	1.272%
10	11.749	1432	1440	1455	rBV	198807	429600	3.43%	1.633%
11	13.229	1686	1692	1703	rBV	110097	250379	2.00%	0.952%
12	14.111	1835	1842	1860	rBV	435294	765007	6.11%	2.908%
13	14.346	1871	1882	1890	rVB3	232054	630396	5.04%	2.397%
14	15.250	2025	2036	2041	rBV2	73655	132680	1.06%	0.504%
15	15.485	2069	2076	2083	rBV2	368367	648045	5.18%	2.464%
16	15.767	2114	2124	2135	rBV	233674	372502	2.98%	1.416%
17	18.212	2533	2540	2556	rBV	524865	897738	7.17%	3.413%
18	20.732	2963	2969	2980	rBV	703935	981171	7.84%	3.730%
19	22.072	3191	3197	3211	rBV3	85584	185465	1.48%	0.705%
20	22.559	3272	3280	3292	rBV2	510125	1026731	8.20%	3.903%
21	26.326	3908	3921	3935	rBV3	287687	1004754	8.03%	3.820%

Sum of corrected areas: 26303852

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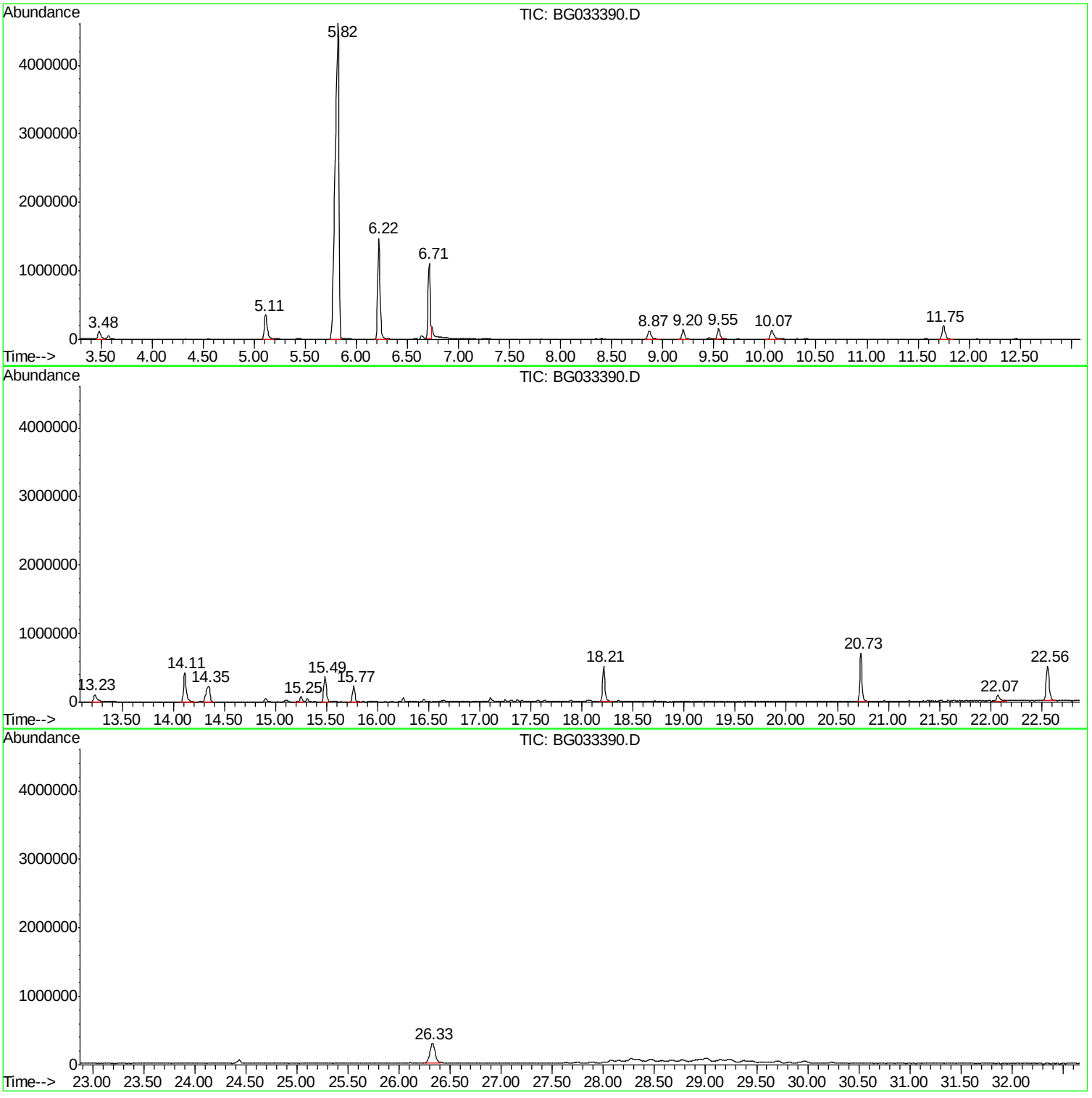
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C0AB1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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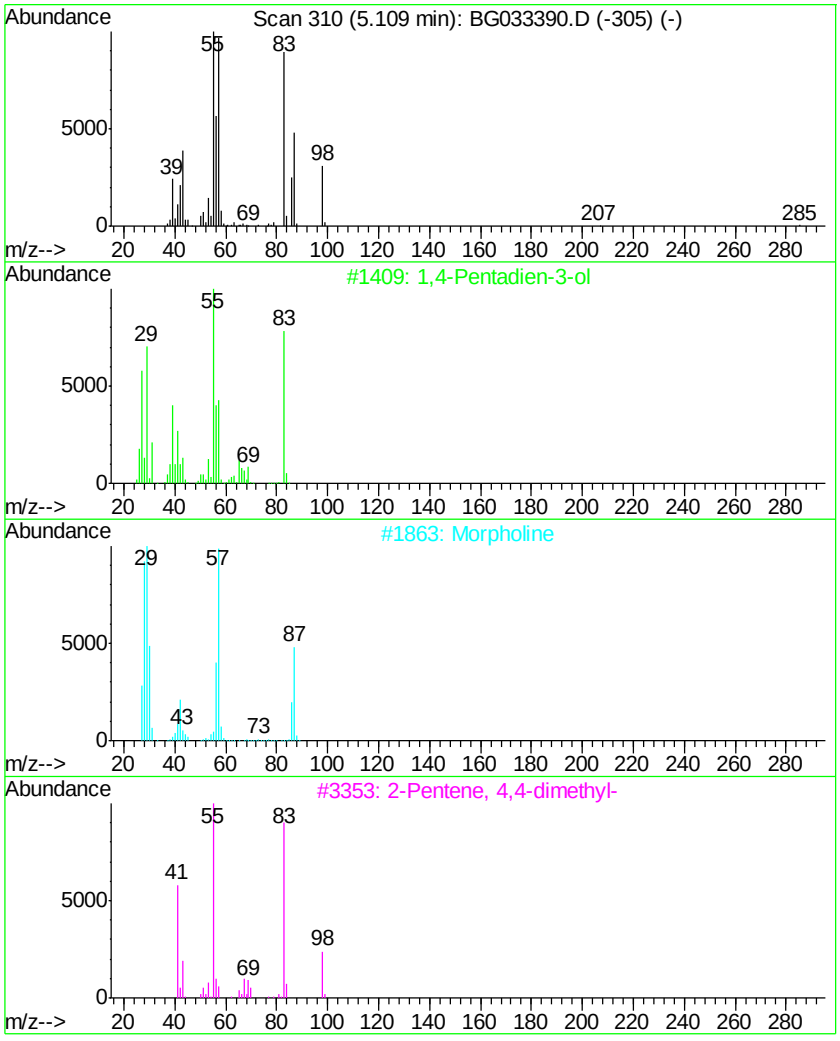
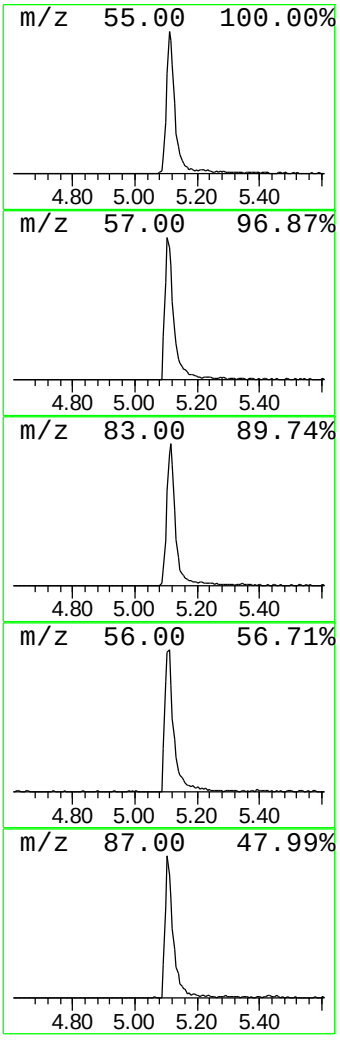
****

Peak Number 2 unknown5.11 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	48.34 ng	706548	1,4-Dichlorobenzene-d4	8.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Pentadien-3-ol	84	C5H8O	000922-65-6	47
2	Morpholine	87	C4H9NO	000110-91-8	45
3	2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	43
4	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	43
5	2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	43





Library Search Compound Report

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Instrument : BNA_G
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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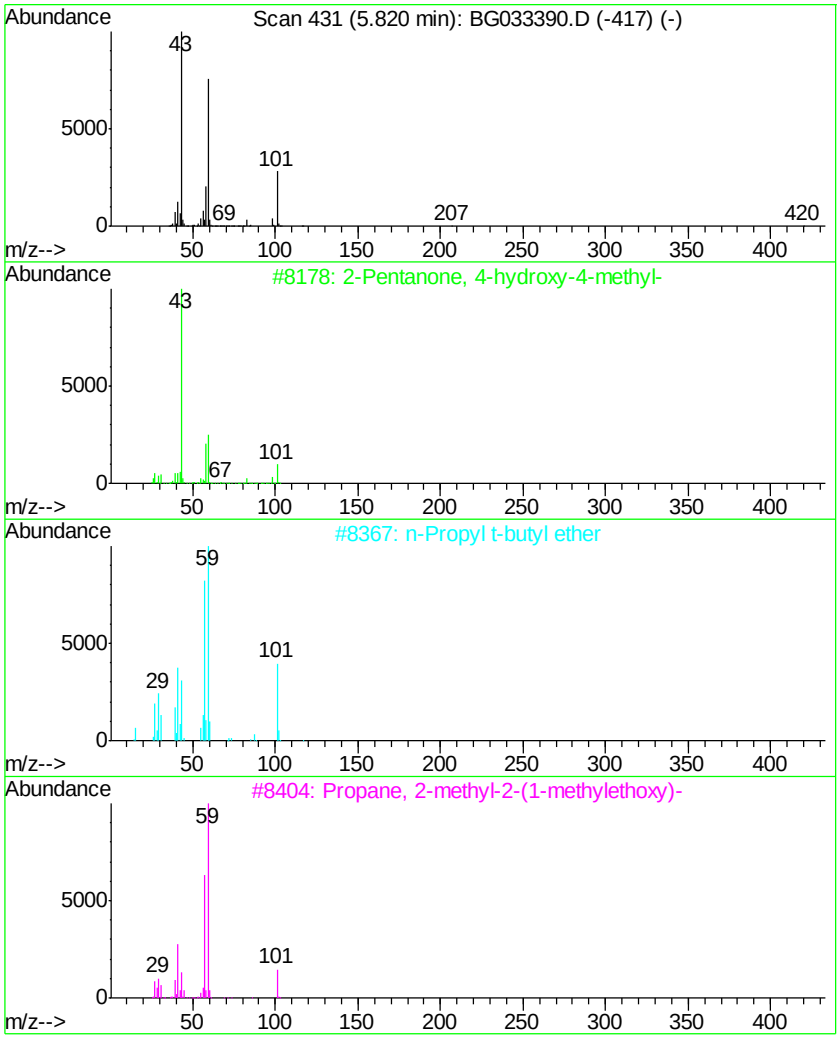
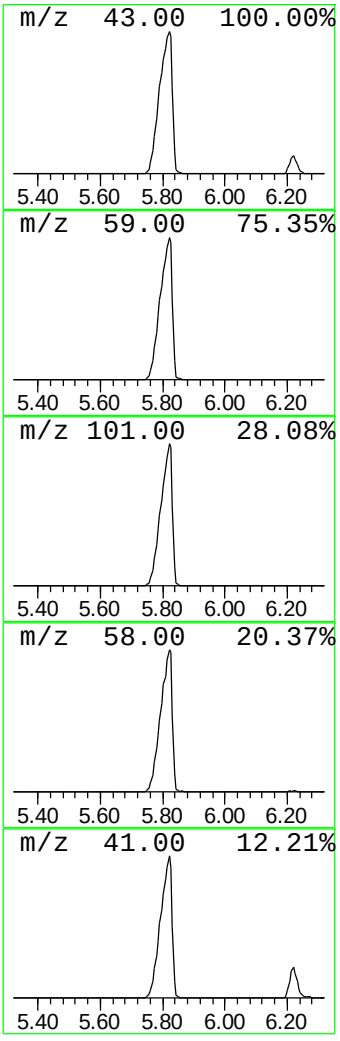
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.82	856.36 ng	12515800	1,4-Dichlorobenzene-d4	8.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	36
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	32
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





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Sample : J2072-02
Misc :
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Instrument : BNA_G
ClientSampleId : C0AB1

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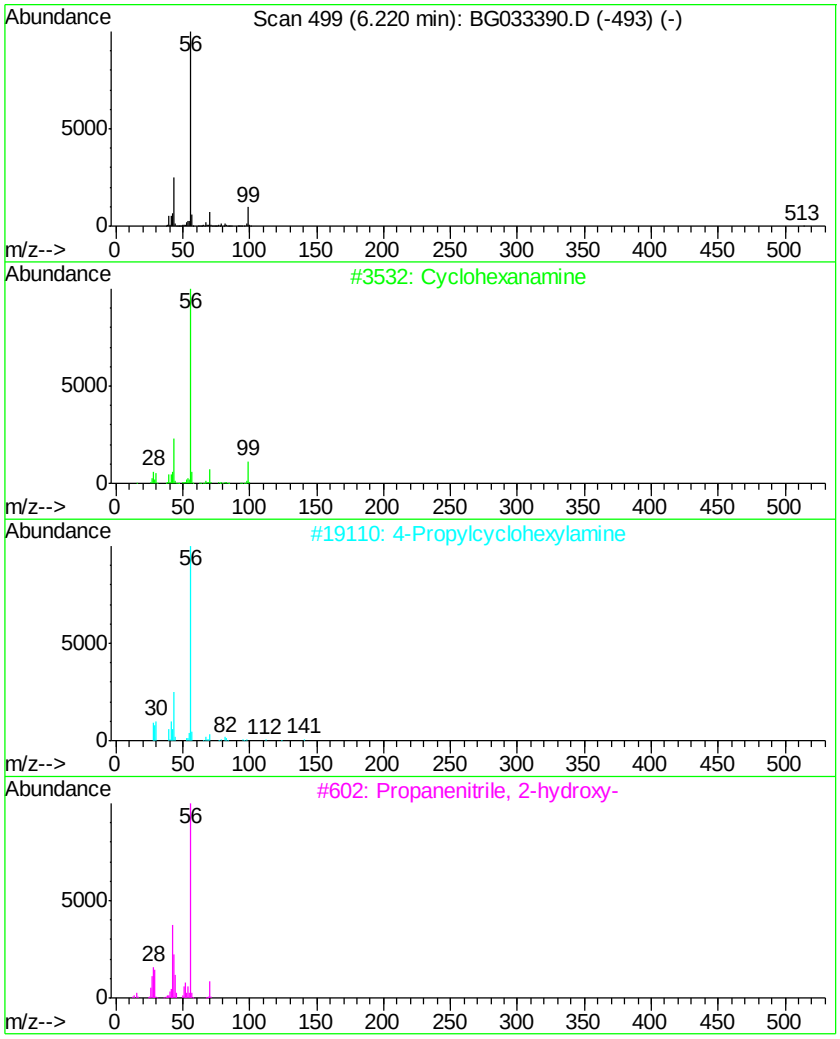
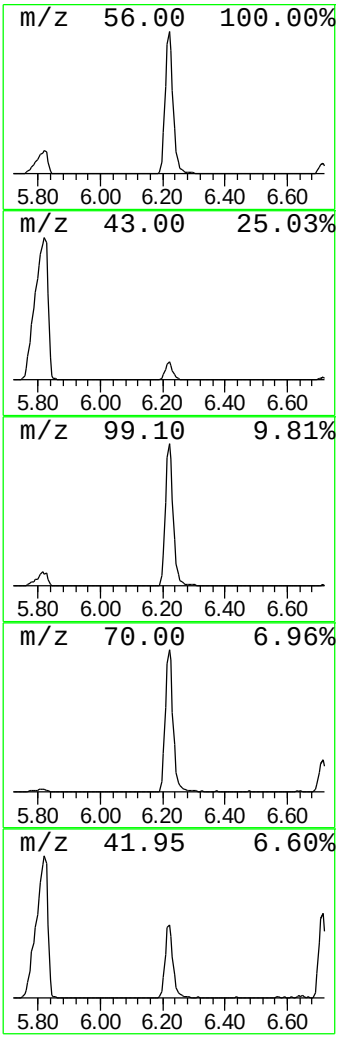
****

Peak Number 4 Cyclohexanamine Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.22	176.51 ng	2579650	1,4-Dichlorobenzene-d4	8.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanamine	99	C6H13N	000108-91-8	90
2	4-Propylcyclohexylamine	141	C9H19N	102653-37-2	50
3	Propanenitrile, 2-hydroxy-	71	C3H5NO	000078-97-7	45
4	Cycloheptylamine	113	C7H15N	005452-35-7	35
5	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	9





Library Search Compound Report

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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C0AB1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
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TIC Library : C:\Database\NIST11.L
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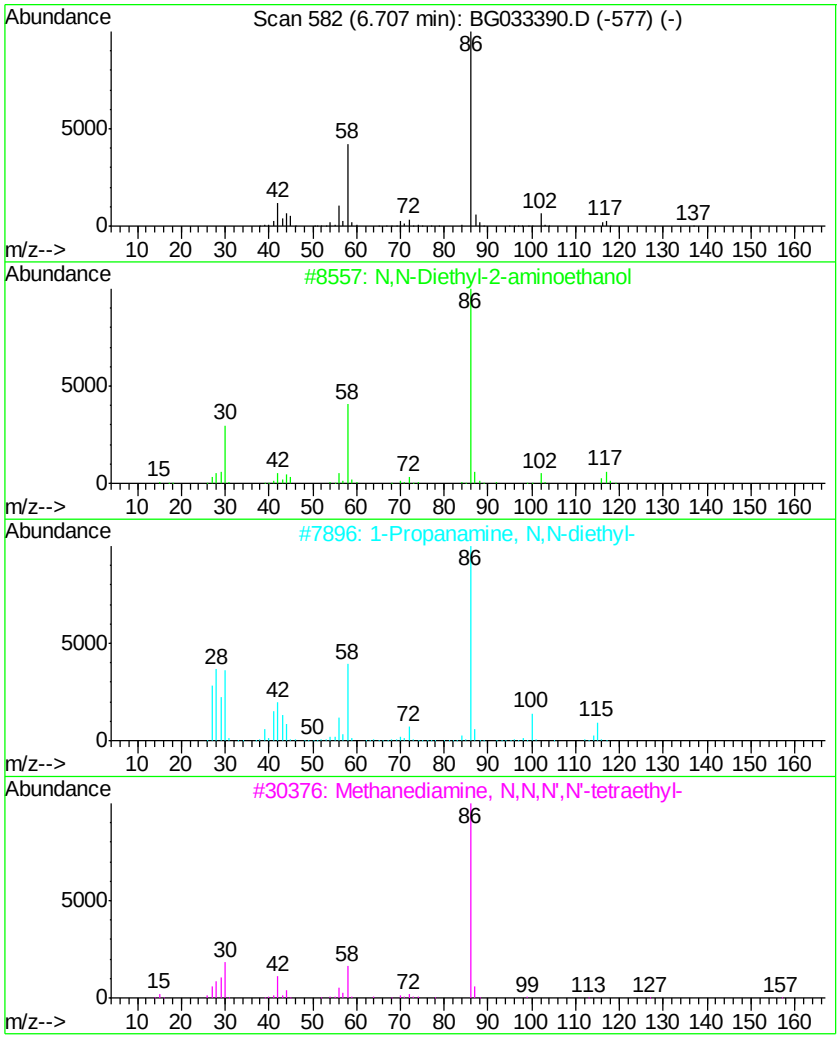
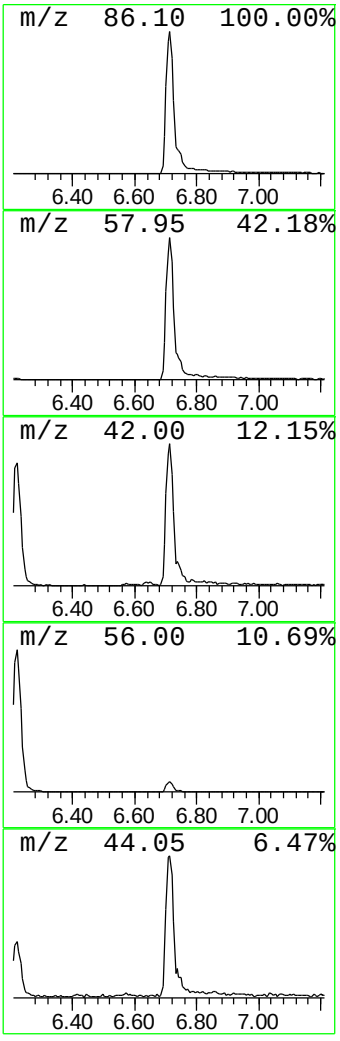
****

Peak Number 5 N,N-Diethyl-2-aminoethanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.71	120.38 ng	1759320	1,4-Dichlorobenzene-d4	8.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N,N-Diethyl-2-aminoethanol	117	C6H15NO	000100-37-8	78
2	1-Propanamine, N,N-diethyl-	115	C7H17N	004458-31-5	78
3	Methanediamine, N,N,N',N'-tetrae...	158	C9H22N2	000102-53-4	64
4	Diethylaminoacetone	129	C7H15NO	001620-14-0	64
5	Oxazolidine, 2-ethyl-3-methyl-	115	C6H13NO	001630-75-7	64





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Sample : J2072-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C0AB1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

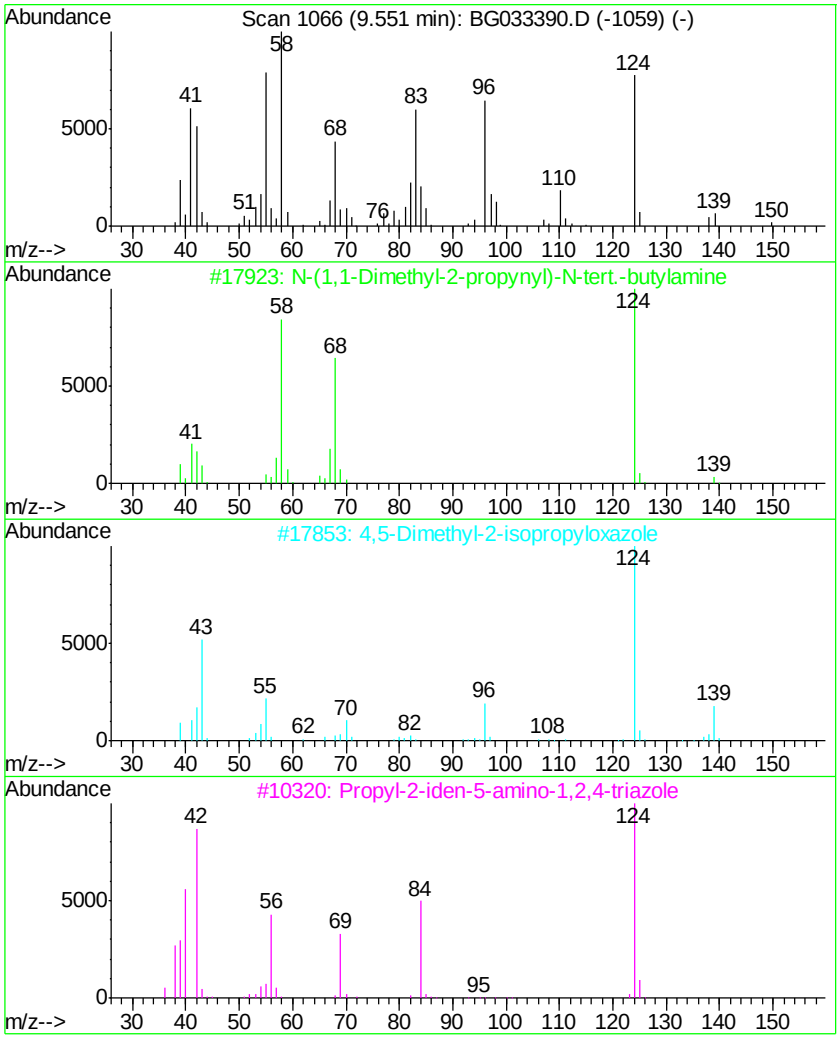
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

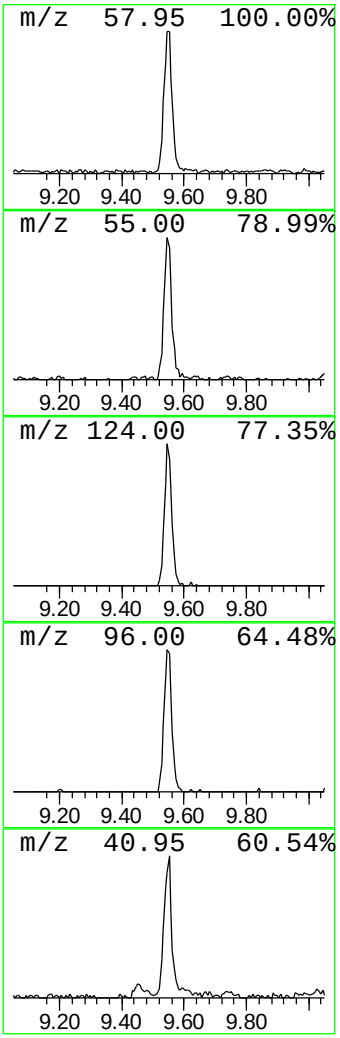
****

Peak Number 7 N-(1,1-Dimethyl-2-propynyl)... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.55	19.04 ng	278268	1,4-Dichlorobenzene-d4	8.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-(1,1-Dimethyl-2-propynyl)-N-te...	139	C9H17N	001118-17-8	60
2	4,5-Dimethyl-2-isopropyloxazole	139	C8H13NO	019519-45-0	27
3	Propyl-2-iden-5-amino-1,2,4-tria...	124	C5H8N4	1000139-49-3	25
4	4(1H)-Pyrimidinone, 2,6-dimethyl-	124	C6H8N2O	006622-92-0	22
5	4-(Bromomethyl)-1-azabicyclo[2.2...	203	C8H14BrN	026458-73-1	22





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Sample : J2072-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C0AB1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
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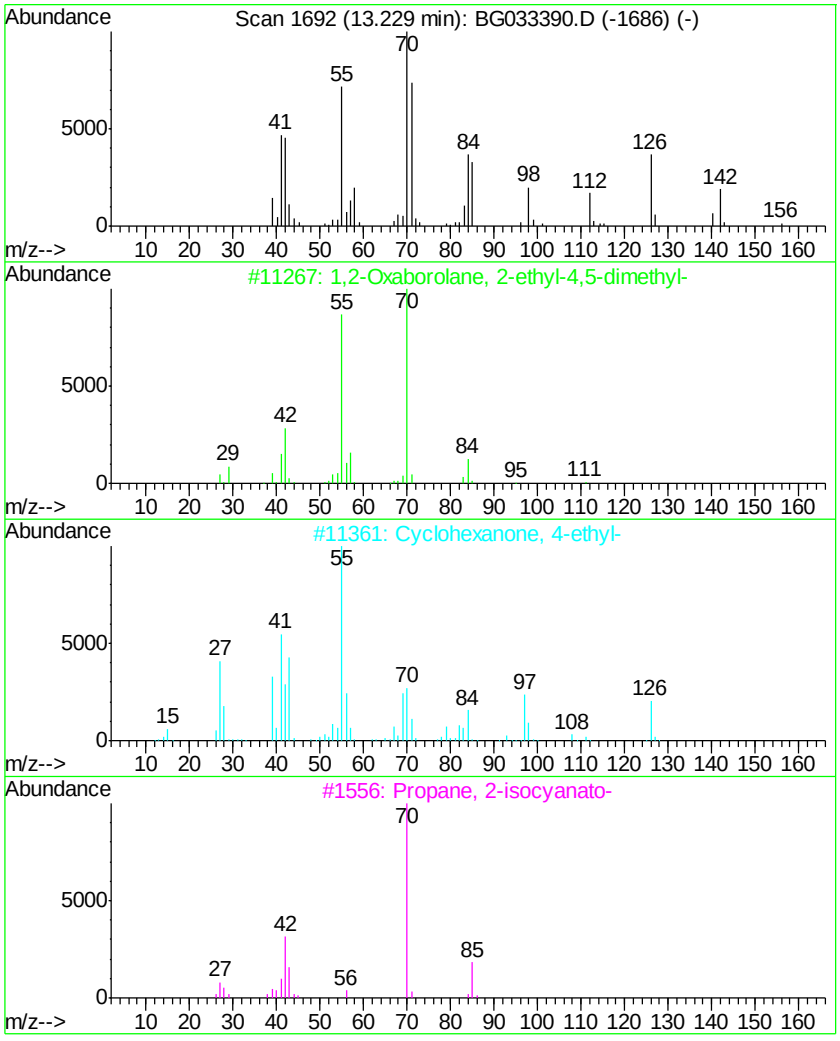
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

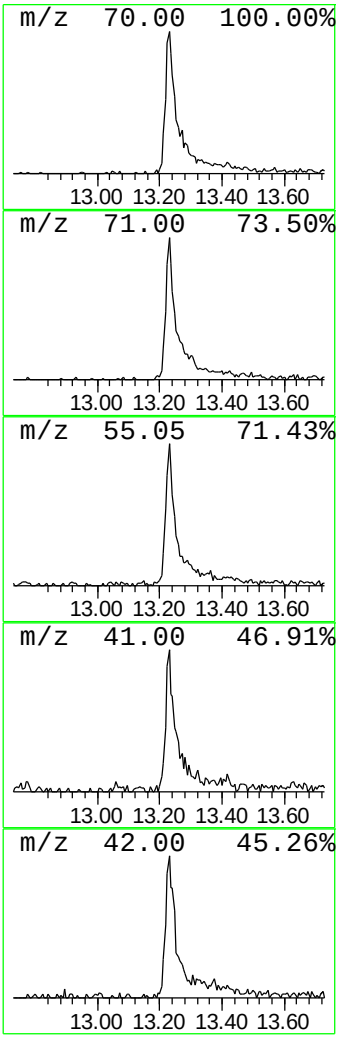
****

Peak Number 8 unknown13.23 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.23	11.66 ng	250379	Naphthalene-d8	11.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Oxaborolane, 2-ethyl-4,5-dim...	126	C7H15BO	074685-45-3	35
2	Cyclohexanone, 4-ethyl-	126	C8H14O	005441-51-0	35
3	Propane, 2-isocyanato-	85	C4H7NO	001795-48-8	35
4	Methylamine, N-(1-butylhexylidene)-	169	C11H23N	018641-76-4	32
5	1,2-Cyclohexanediol, 1-methyl-, ...	130	C7H14O2	019534-08-8	27





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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
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TIC Library : C:\Database\NIST11.L
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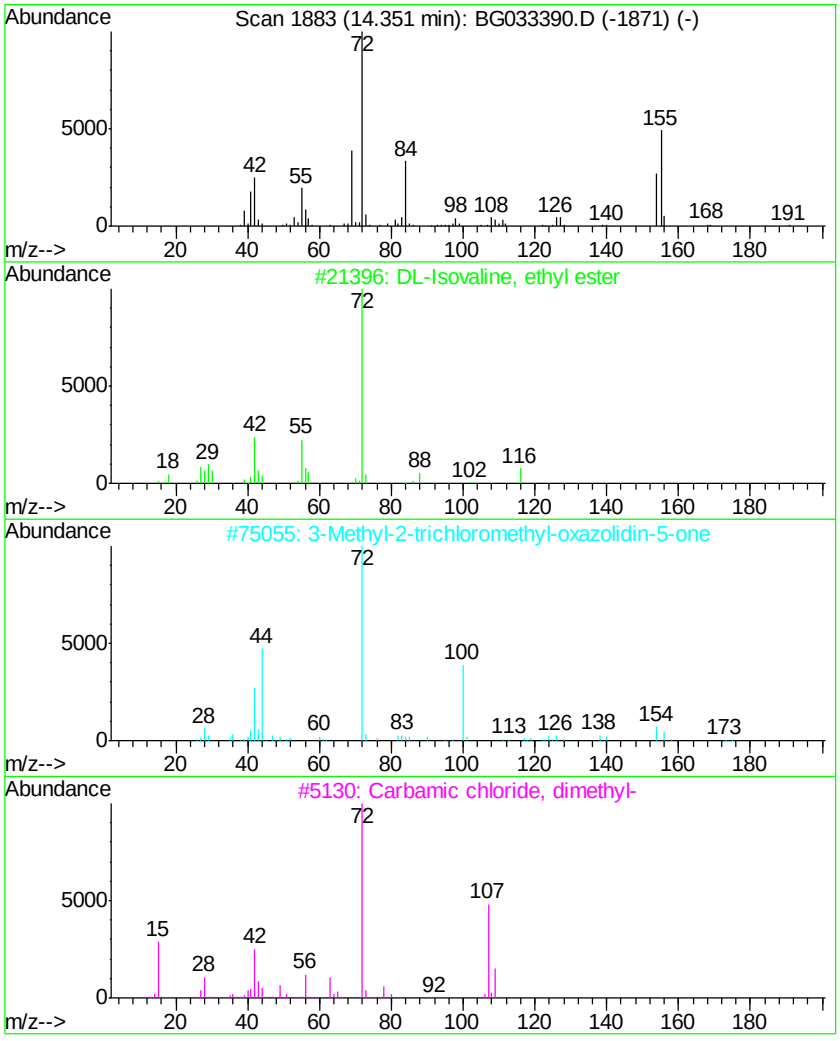
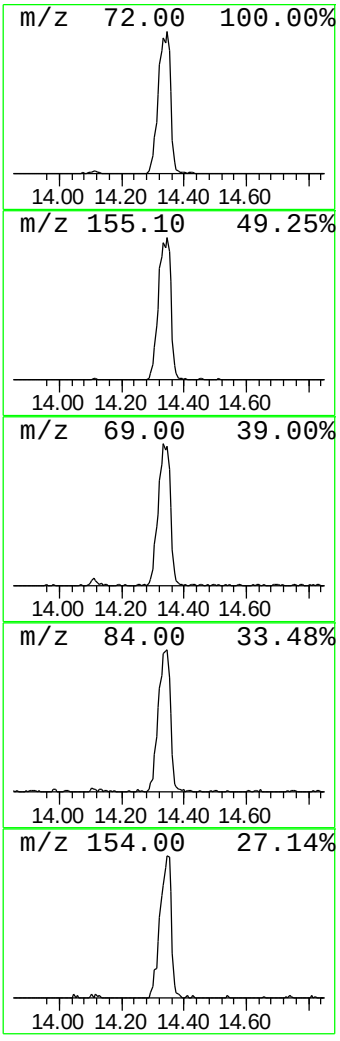
****

Peak Number 9 unknown14.35 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.35	19.46 ng	630396	Acenaphthene-d10	15.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	DL-Isovaline, ethyl ester	145	C7H15NO2	056247-82-6	32
2	3-Methyl-2-trichloromethyl-oxazo...	217	C5H6Cl3NO2	1000188-24-8	25
3	Carbamic chloride, dimethyl-	107	C3H6ClNO	000079-44-7	23
4	3-Buten-1-amine, N-ethyl-N-methyl-	113	C7H15N	061308-10-9	23
5	4-[2-Dimethylaminopropyl]thiosem...	176	C6H16N4S	070619-53-3	23





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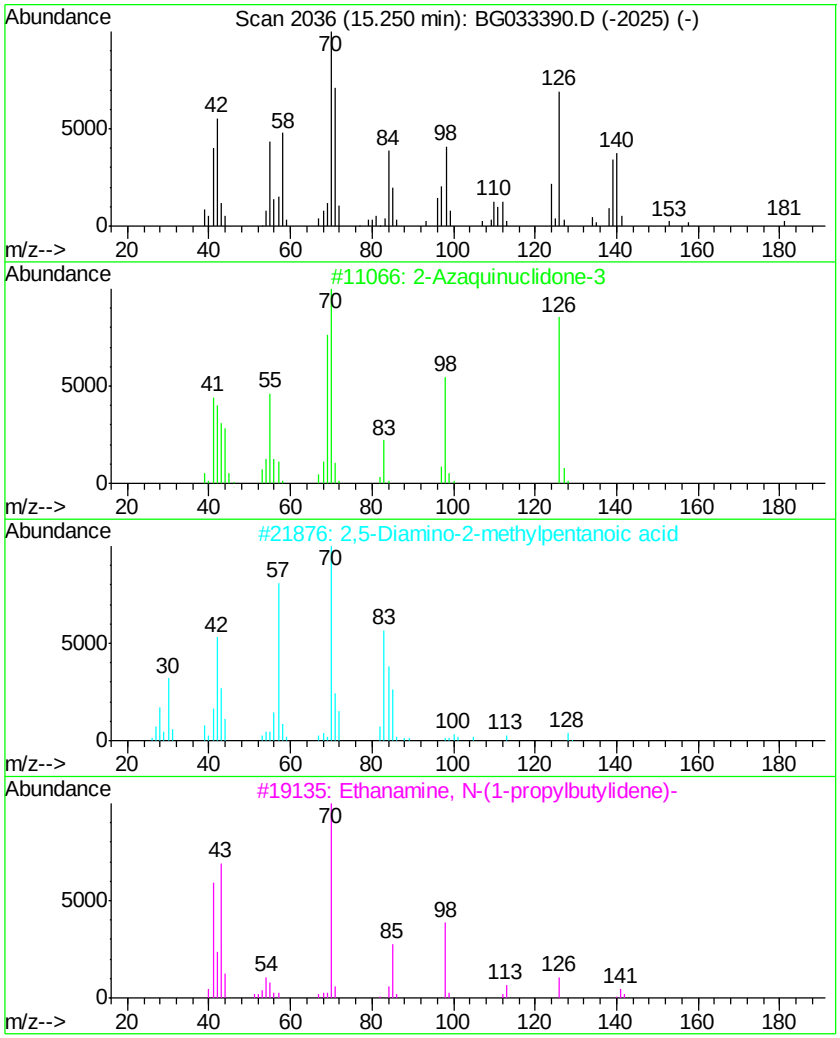
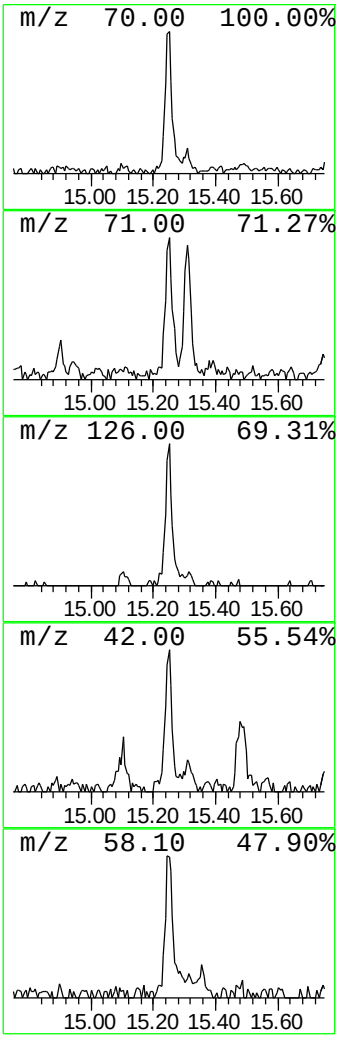
****

Peak Number 10 unknown15.25 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.25	4.09 ng	132680	Acenaphthene-d10	15.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Azaquinuclidone-3	126	C6H10N2O	1000311-41-2	43
2	2,5-Diamino-2-methylpentanoic acid	146	C6H14N2O2	1000191-43-4	25
3	Ethanamine, N-(1-propylbutylidene)-	141	C9H19N	010599-79-8	25
4	1,2,4-Cyclopentanetrione, 3,3-di...	140	C7H8O3	017530-56-2	22
5	4-Piperidinecarboxamide, 1-methyl-	142	C7H14N2O	1000362-58-5	22





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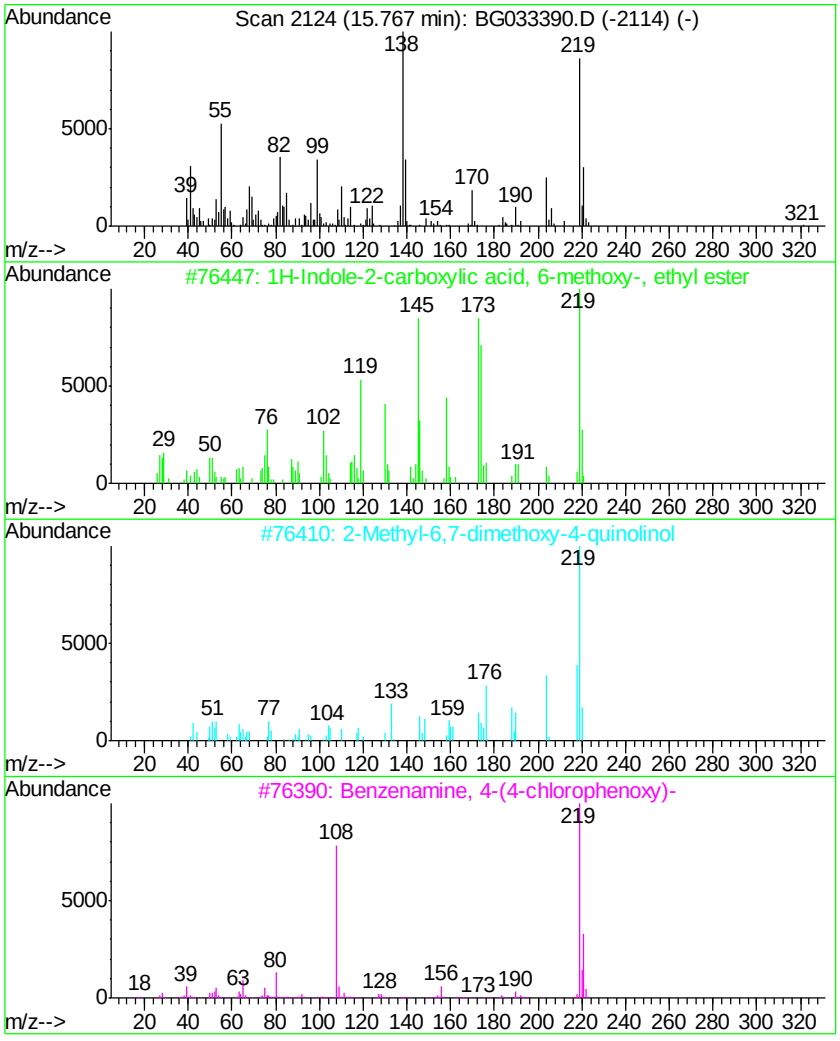
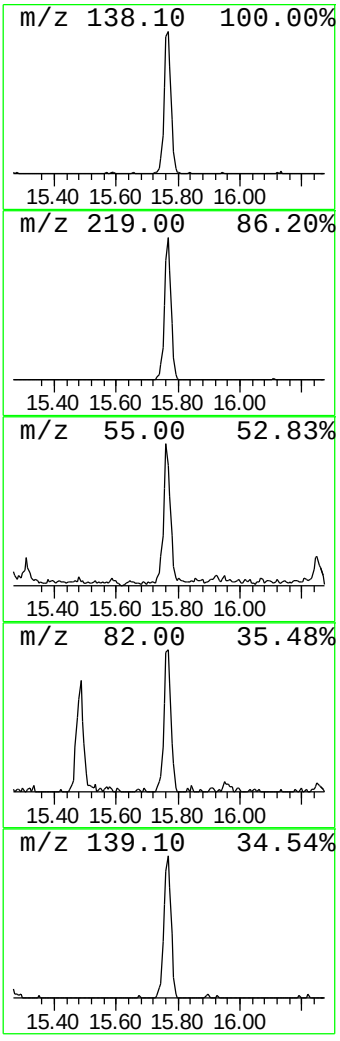
****

Peak Number 11 unknown15.77 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.77	11.50 ng	372502	Acenaphthene-d10	15.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indole-2-carboxylic acid, 6-m...	219	C12H13NO3	015050-04-1	38
2	2-Methyl-6,7-dimethoxy-4-quinolinol	219	C12H13NO3	1000256-04-4	27
3	Benzenamine, 4-(4-chlorophenoxy)-	219	C12H10ClNO	000101-79-1	27
4	Acetamide, N-(4-methoxyphenyl)-2...	219	C9H8F3NO2	000332-34-3	22
5	2H-Pyrimido[1,2-a]pyrimidine, 1,...	139	C7H13N3	005807-14-7	22





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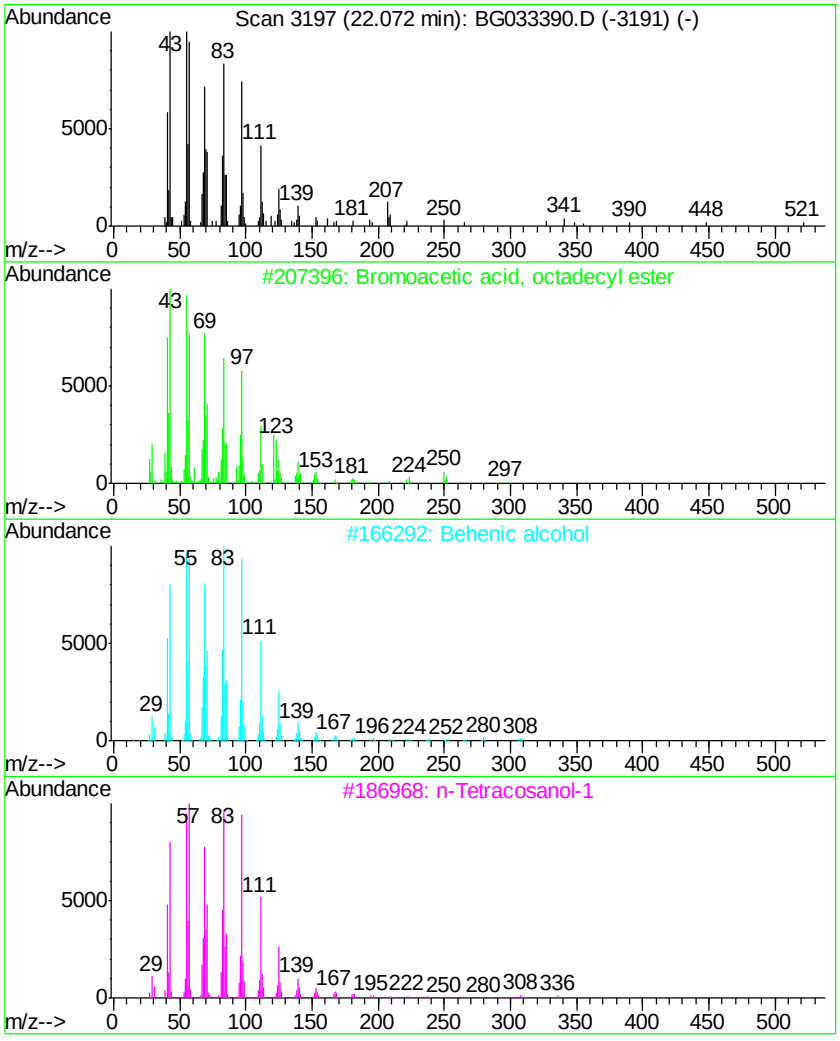
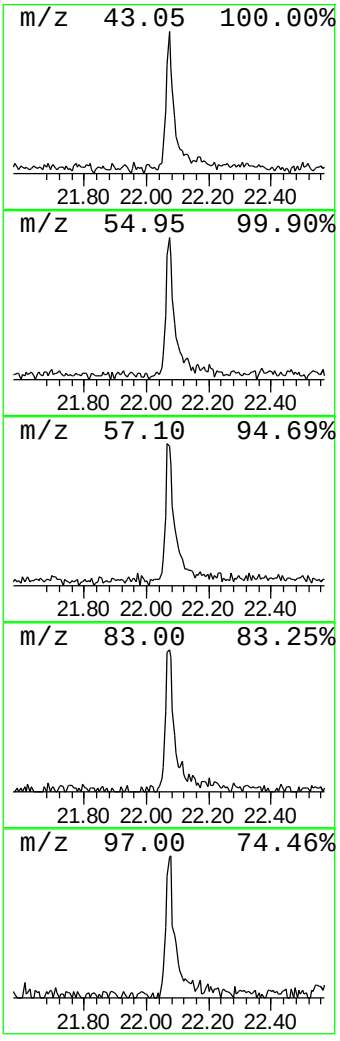
****
Peak Number 12 Bromoacetic acid, octadecyl... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.07	3.61 ng	185465	Chrysene-d12	22.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	94
2	Behenic alcohol	326	C22H46O	000661-19-8	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
4	Octacosanol	410	C28H58O	000557-61-9	93
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG032818\
Data File : BG033390.D
Acq On : 28 Mar 2018 17:43
Operator : SJ/JU
Sample : J2072-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C0AB1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown5.11	5.11	48.3	ng	706548	1	8.87	292303	20.0
2-Pentanone, 4-hy...	5.82	856.4	ng	12515800	1	8.87	292303	20.0
Cyclohexanamine	6.22	176.5	ng	2579650	1	8.87	292303	20.0
N,N-Diethyl-2-ami...	6.71	120.4	ng	1759320	1	8.87	292303	20.0
N-(1,1-Dimethyl-2...	9.55	19.0	ng	278268	1	8.87	292303	20.0
unknown13.23	13.23	11.7	ng	250379	2	11.75	429600	20.0
unknown14.35	14.35	19.5	ng	630396	3	15.48	648045	20.0
unknown15.25	15.25	4.1	ng	132680	3	15.48	648045	20.0
unknown15.77	15.77	11.5	ng	372502	3	15.48	648045	20.0
Bromoacetic acid,...	22.07	3.6	ng	185465	5	22.56	1026730	20.0