LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081122\
Data File : BG054604.D
Acq On : 11 Aug 2022 14:26
Operator : CG/JU
Sample : N3971-17
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-25R

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:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054604.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.088	12	17	34	rVB	217613	371488	20.88%	6.287%
2	4.404	235	241	253	rVB	59004	99330	5.58%	1.681%
3	5.051	347	351	359	rVB2	15324	24539	1.38%	0.415%
4	5.556	432	437	448	rBV	95047	170241	9.57%	2.881%
5	6.602	610	615	622	rBV2	14383	23332	1.31%	0.395%
6	7.172	707	712	723	rBV	58624	114627	6.44%	1.940%
7	7.971	840	848	853	rBV	41892	72797	4.09%	1.232%
8	8.030	854	858	866	rVB2	13600	21390	1.20%	0.362%
9	9.140	1039	1047	1059	rBV	137045	254867	14.33%	4.314%
10	10.779	1319	1326	1333	rBV	53876	100160	5.63%	1.695%
11	11.719	1481	1486	1496	rVB4	8035	20468	1.15%	0.346%
12	13.229	1736	1743	1755	rBV	448984	718829	40.41%	12.166%
13	13.464	1776	1783	1794	rBV	147475	233006	13.10%	3.944%
14	14.610	1972	1978	1985	rBV	108240	170274	9.57%	2.882%
15	16.108	2227	2233	2248	rBV	456737	731228	41.10%	12.376%
16	17.360	2439	2446	2454	rBV	167967	263908	14.83%	4.467%
17	18.012	2553	2557	2564	rVB2	16578	19654	1.10%	0.333%
18	19.969	2884	2890	2898	rBV	1390042	1779012	100.00%	30.109%
19	21.625	3166	3172	3181	rVB2	208216	357479	20.09%	6.050%
20	24.833	3708	3718	3730	rVB2	123931	361910	20.34%	6.125%

Sum of corrected areas: 5908539

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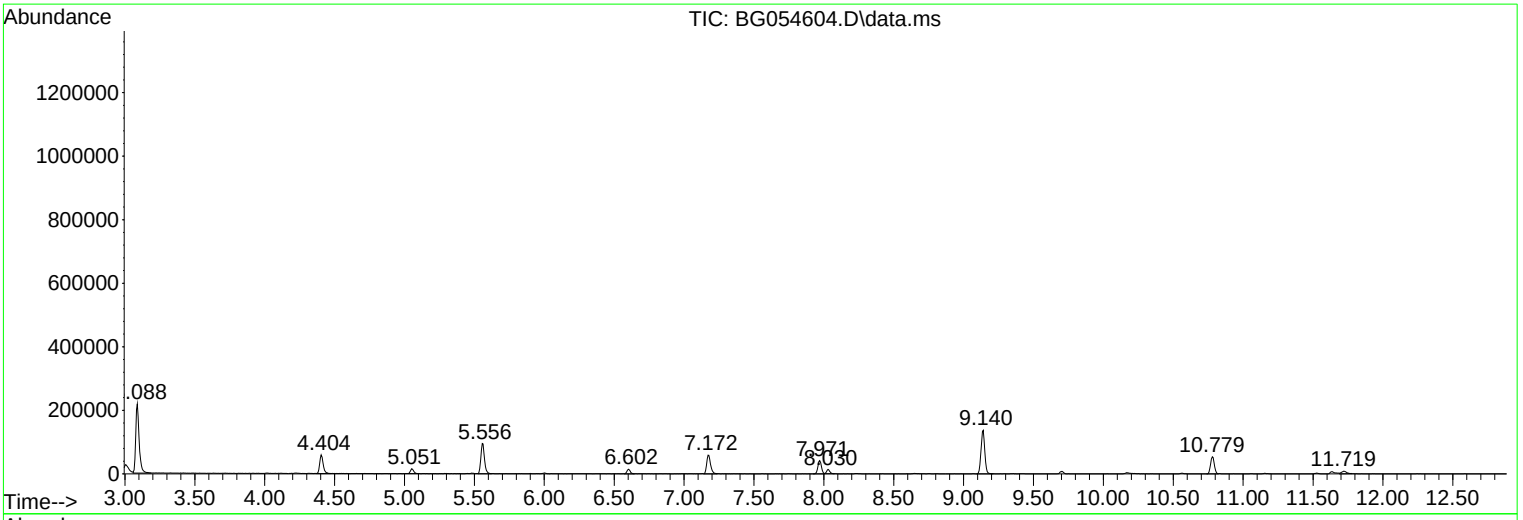
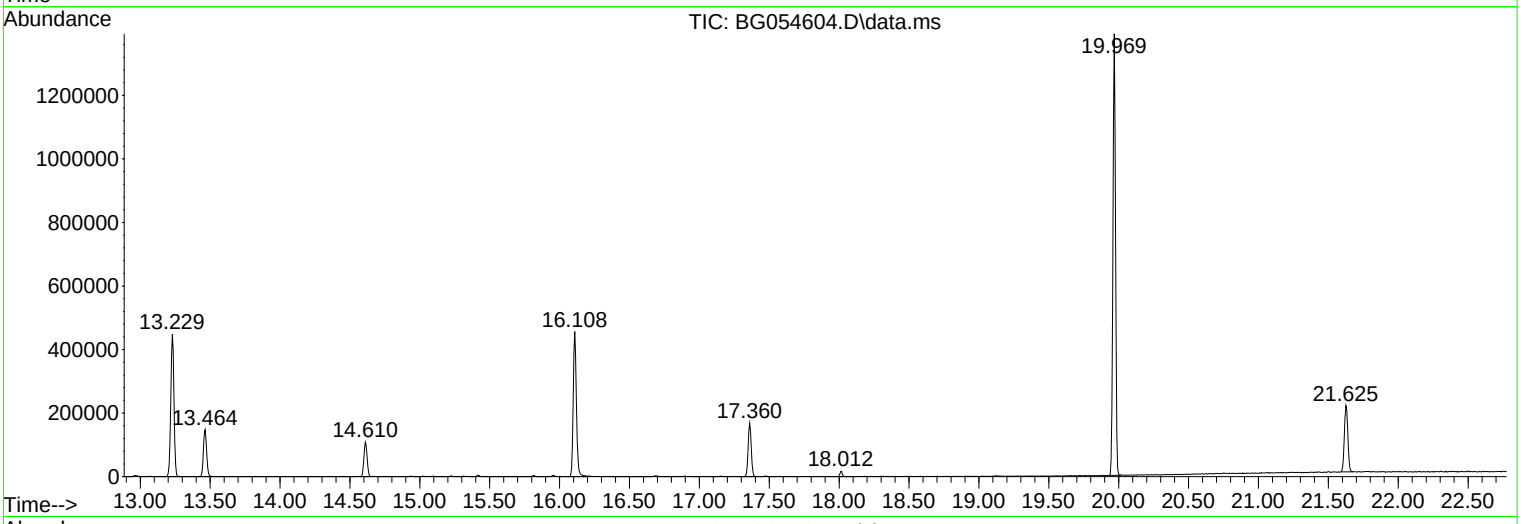
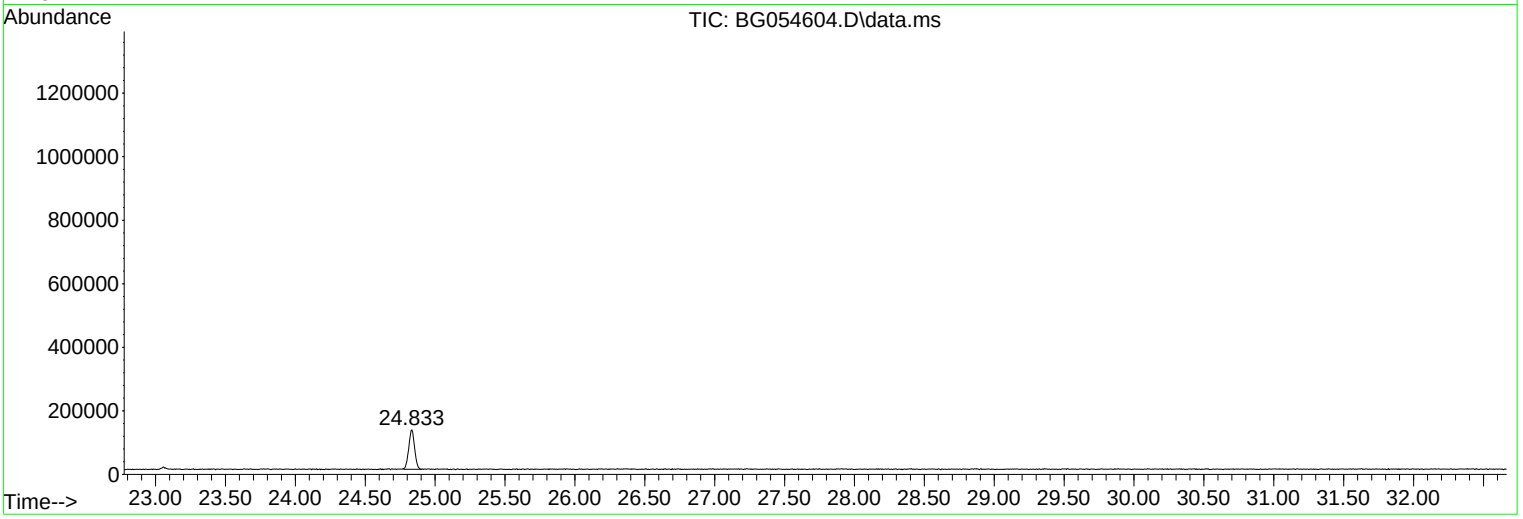
Instrument :
BNA_G
ClientSampleId :
MW-25R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







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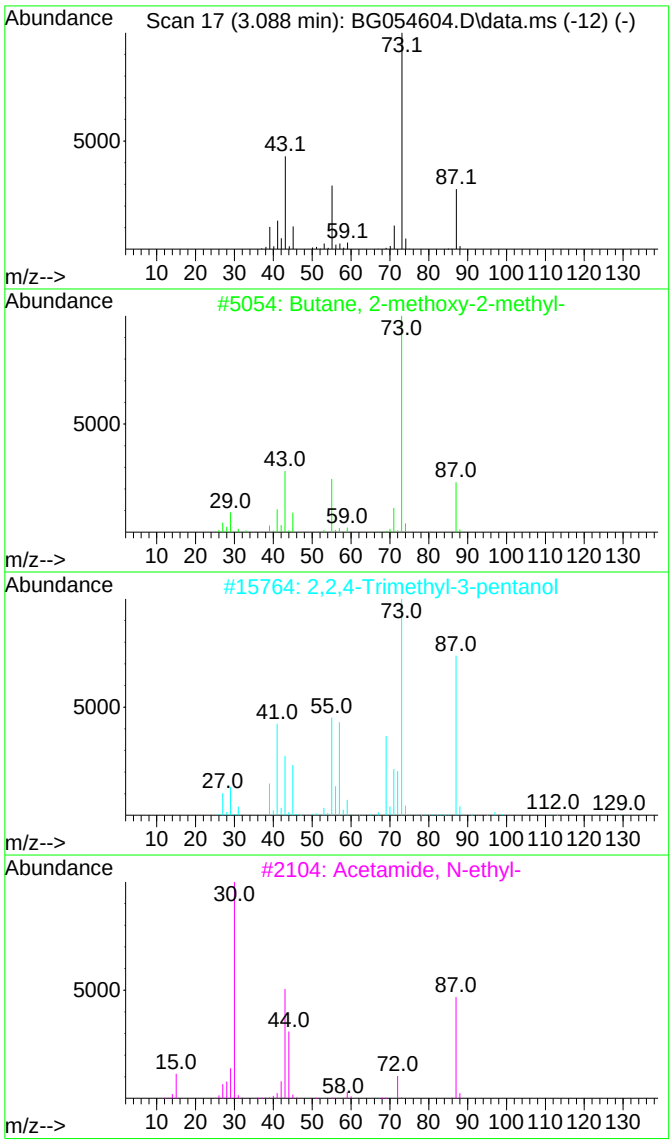
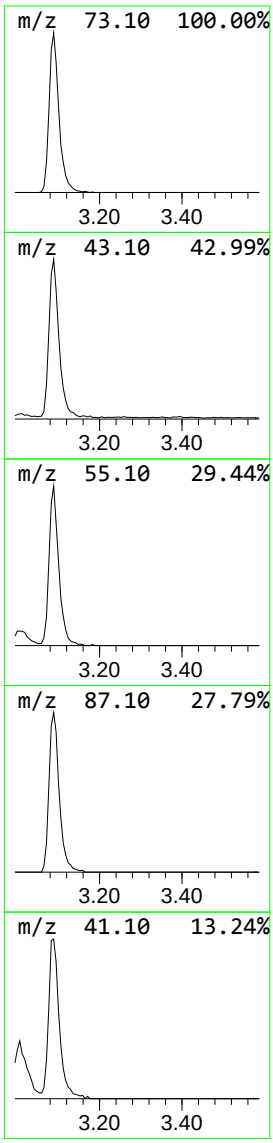
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.088	102.06 ng	371488	1,4-Dichlorobenzene-d4	7.971

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	25
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9





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Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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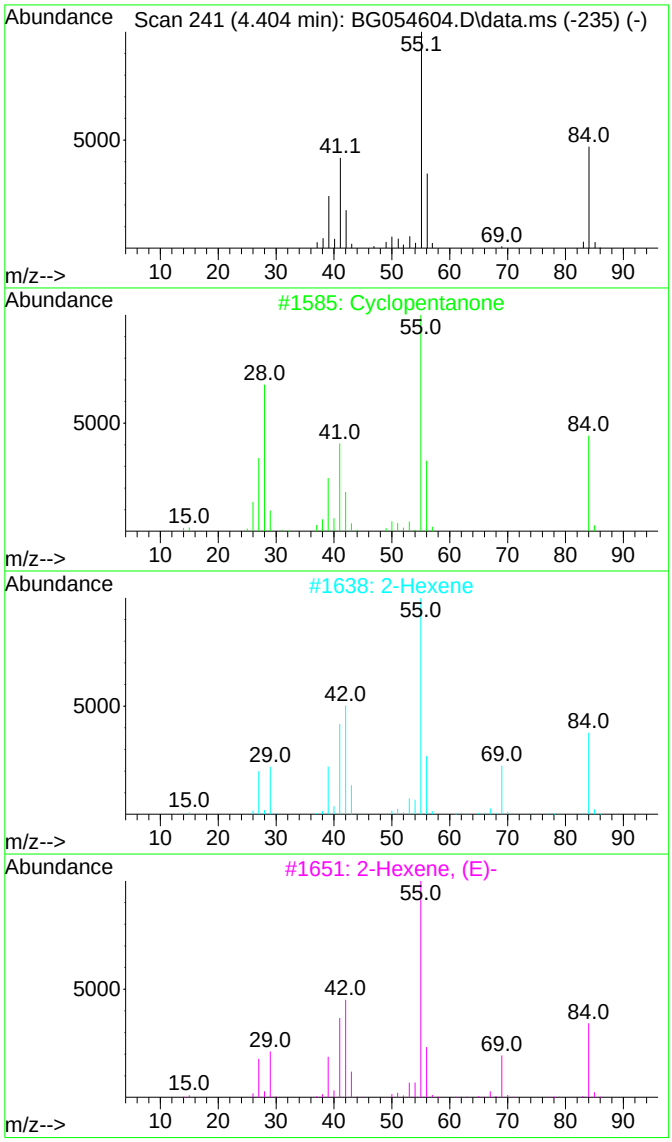
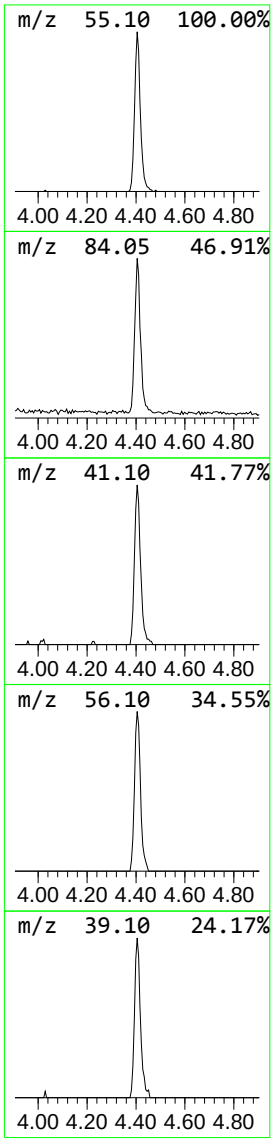
Peak Number 2 Cyclopentanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.404	27.29 ng	99330	1,4-Dichlorobenzene-d4	7.971

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanone	84	C5H8O	000120-92-3	91
2	2-Hexene	84	C6H12	000592-43-8	72
3	2-Hexene, (E)-	84	C6H12	004050-45-7	64
4	3-Hexene, (E)-	84	C6H12	013269-52-8	59
5	2-Ethylacrolein	84	C5H8O	000922-63-4	59





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Operator : CG/JU
Sample : N3971-17
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-25R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
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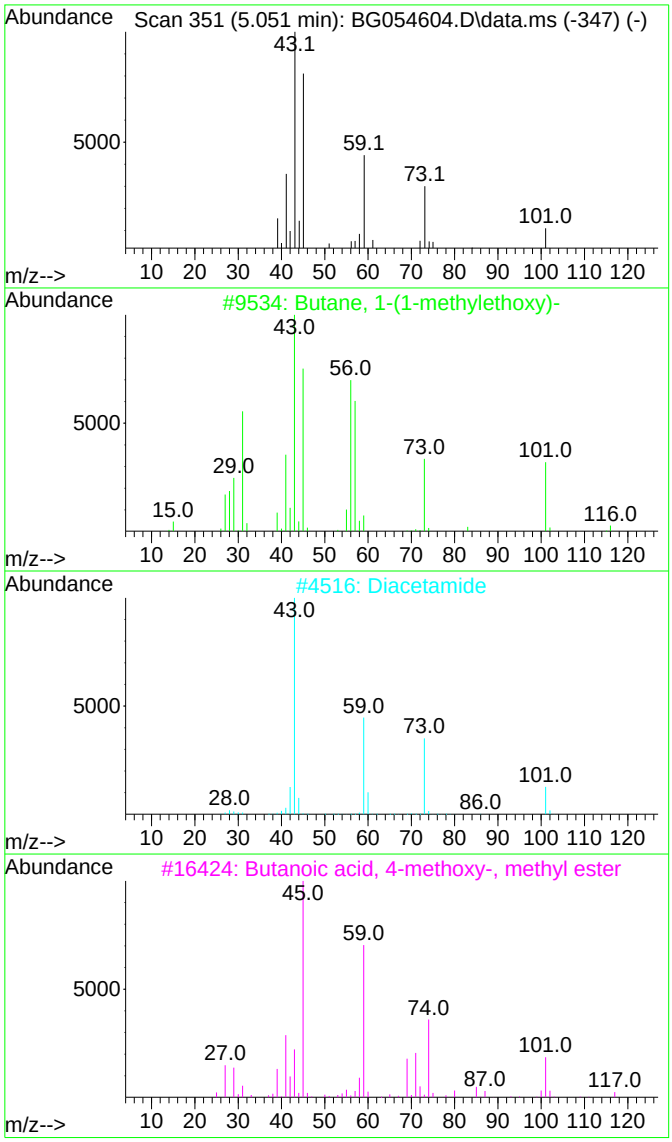
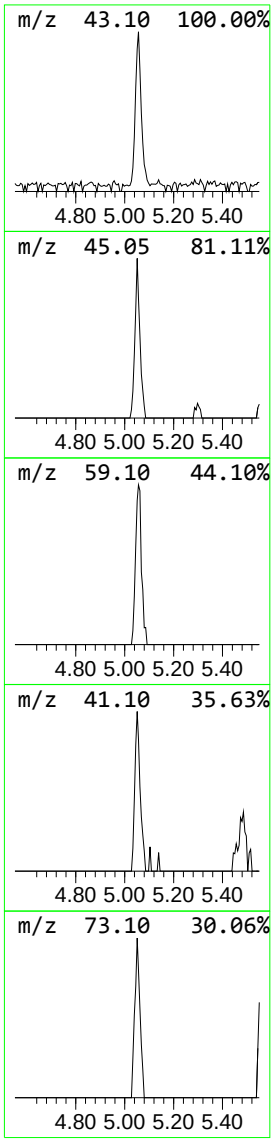
Peak Number 3 unknown5.051 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.051	6.74 ng	24539	1,4-Dichlorobenzene-d4	7.971

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 1-(1-methylethoxy)-	116	C7H16O	001860-27-1	45
2	Diacetamide	101	C4H7NO2	000625-77-4	43
3	Butanoic acid, 4-methoxy-, methy...	132	C6H12O3	029006-01-7	42
4	Oxirane-2-carboxylic acid, methy...	102	C4H6O3	004538-50-5	38
5	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	38





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Misc :
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Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
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TIC Library : C:\Database\NIST20.L
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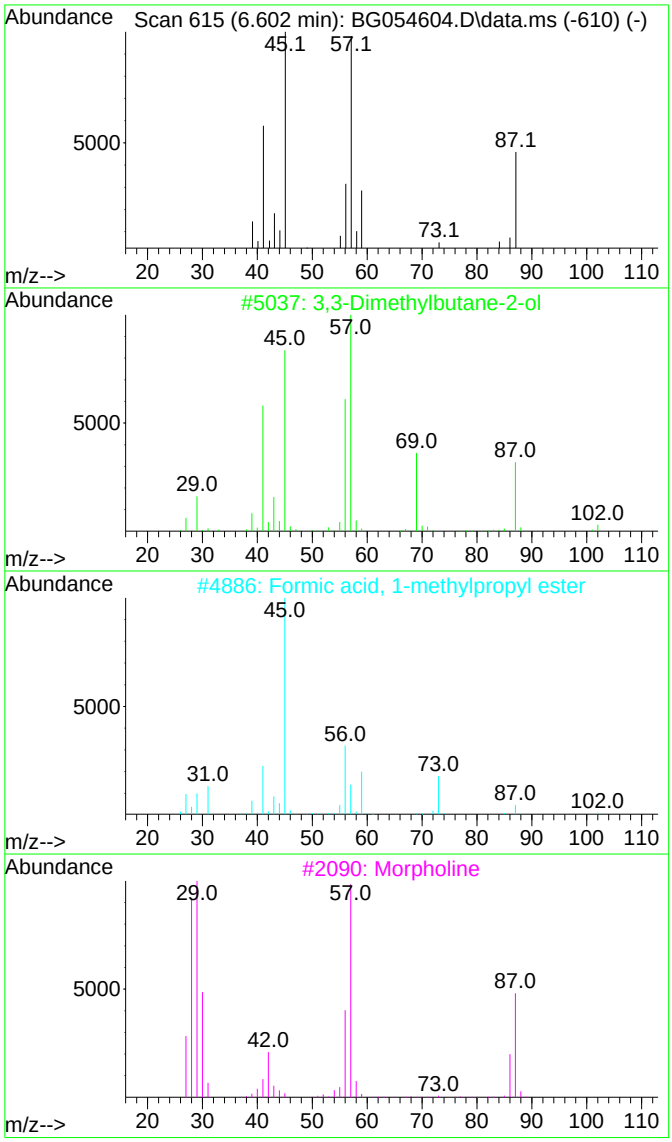
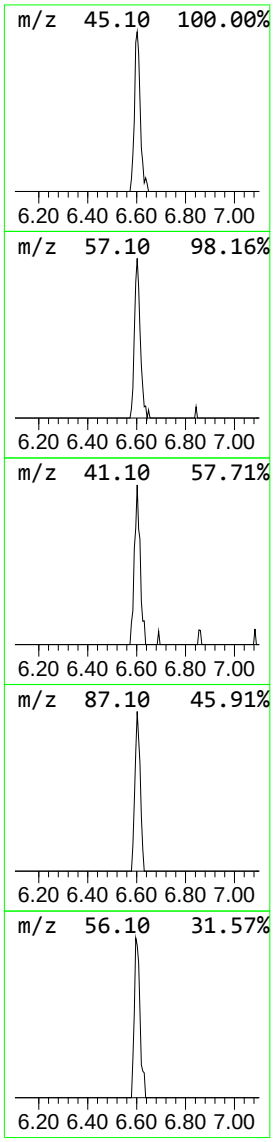
Peak Number 4 unknown6.602 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.602	6.41 ng	23332	1,4-Dichlorobenzene-d4	7.971

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	36
2	Formic acid, 1-methylpropyl ester	102	C5H10O2	000589-40-2	33
3	Morpholine	87	C4H9NO	000110-91-8	17
4	Cyclopentanol	86	C5H10O	000096-41-3	9
5	Borinic acid, diethyl-	86	C4H11BO	004426-31-7	9





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BNA_G
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TIC Library : C:\Database\NIST20.L
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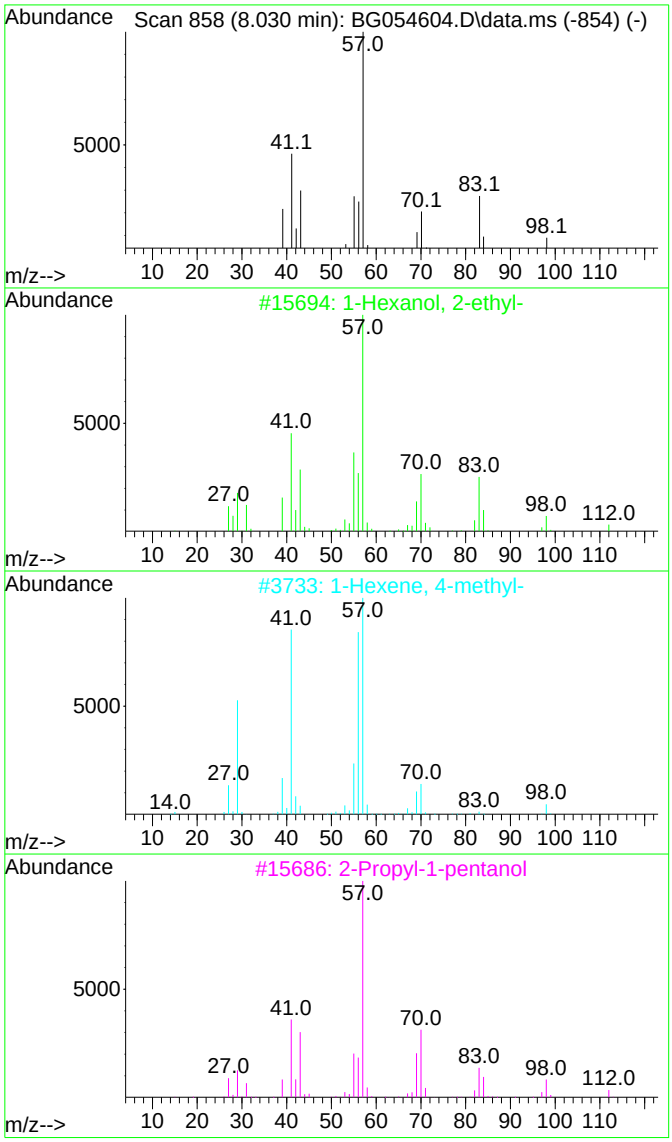
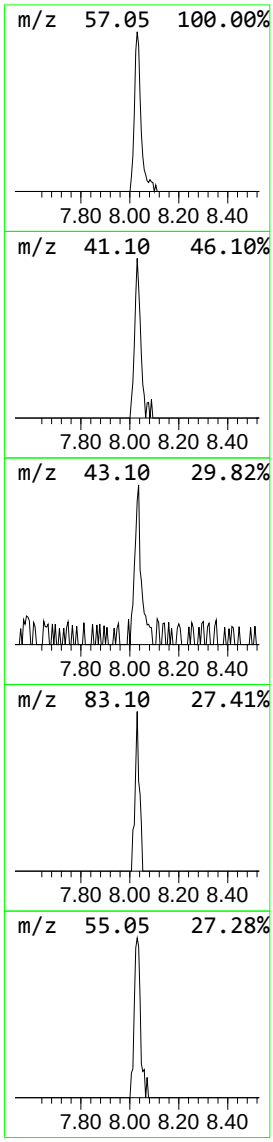
****

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.030	5.88 ng	21390	1,4-Dichlorobenzene-d4	7.971

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	1-Hexene, 4-methyl-	98	C7H14	003769-23-1	43
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	40
4	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	40
5	Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	38





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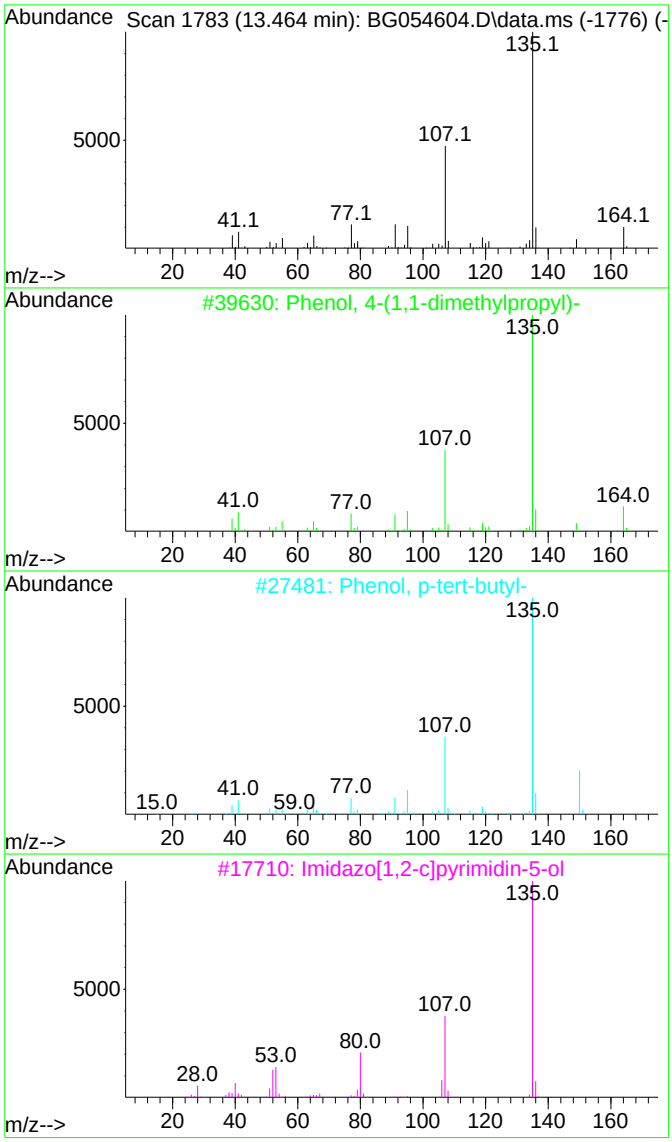
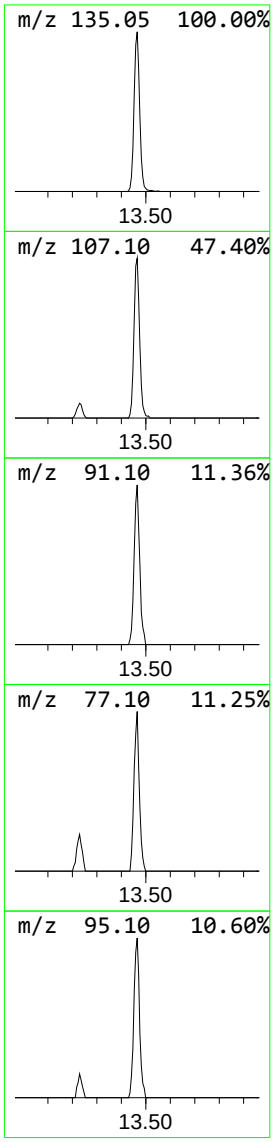
****

Peak Number 6 Phenol, 4-(1,1-dimethylprop... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.464	27.37 ng	233006	Acenaphthene-d10	14.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	95
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	72
3	Imidazo[1,2-c]pyrimidin-5-ol	135	C6H5N3O	055662-66-3	64
4	1,5,6,7-Tetrahydro-4-indolone	135	C8H9NO	013754-86-4	59
5	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	59





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.088	102.1	ng	371488	1	7.971	72797	20.0
Cyclopentanone	4.404	27.3	ng	99330	1	7.971	72797	20.0
unknown5.051	5.051	6.7	ng	24539	1	7.971	72797	20.0
unknown6.602	6.602	6.4	ng	23332	1	7.971	72797	20.0
1-Hexanol, 2-et...	8.030	5.9	ng	21390	1	7.971	72797	20.0
Phenol, 4-(1,1-...	13.464	27.4	ng	233006	3	14.610	170274	20.0