LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081022\
Data File : BG054594.D
Acq On : 10 Aug 2022 18:53
Operator : CG/JU
Sample : N3971-22
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GES-1

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: BG054594.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	37	rVB	224502	435585	25.98%	6.576%
2	4.410	236	242	252	rBV	44197	78770	4.70%	1.189%
3	5.056	346	352	362	rBV	19527	33900	2.02%	0.512%
4	5.562	432	438	453	rVB	127936	229927	13.71%	3.471%
5	6.602	608	615	626	rBV	23677	38571	2.30%	0.582%
6	7.177	707	713	724	rVB	81446	150775	8.99%	2.276%
7	7.971	841	848	854	rBV	60716	105513	6.29%	1.593%
8	9.140	1040	1047	1057	rVB	189105	344349	20.54%	5.198%
9	9.704	1137	1143	1149	rVB2	11745	19908	1.19%	0.301%
10	10.168	1216	1222	1232	rBV3	9398	21860	1.30%	0.330%
11	10.785	1320	1327	1334	rBV	79348	147165	8.78%	2.222%
12	11.631	1466	1471	1477	rBV2	8855	18908	1.13%	0.285%
13	11.719	1480	1486	1497	rVB4	11387	29719	1.77%	0.449%
14	12.965	1691	1698	1709	rBV2	10394	18755	1.12%	0.283%
15	13.229	1733	1743	1754	rBV	584717	946833	56.47%	14.293%
16	13.464	1776	1783	1795	rBB	152812	239902	14.31%	3.622%
17	14.610	1972	1978	1985	rBV	144329	229611	13.69%	3.466%
18	16.108	2227	2233	2245	rBV	483992	791200	47.19%	11.944%
19	17.360	2440	2446	2455	rBV	187392	289117	17.24%	4.365%
20	18.012	2553	2557	2563	rVB2	16265	18411	1.10%	0.278%
21	19.968	2884	2890	2897	rBV	1249214	1676770	100.00%	25.313%
22	21.625	3166	3172	3180	rVB	220524	368037	21.95%	5.556%
23	24.833	3708	3718	3730	rVB3	127455	390642	23.30%	5.897%

Sum of corrected areas: 6624228

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081022\
Data File : BG054594.D
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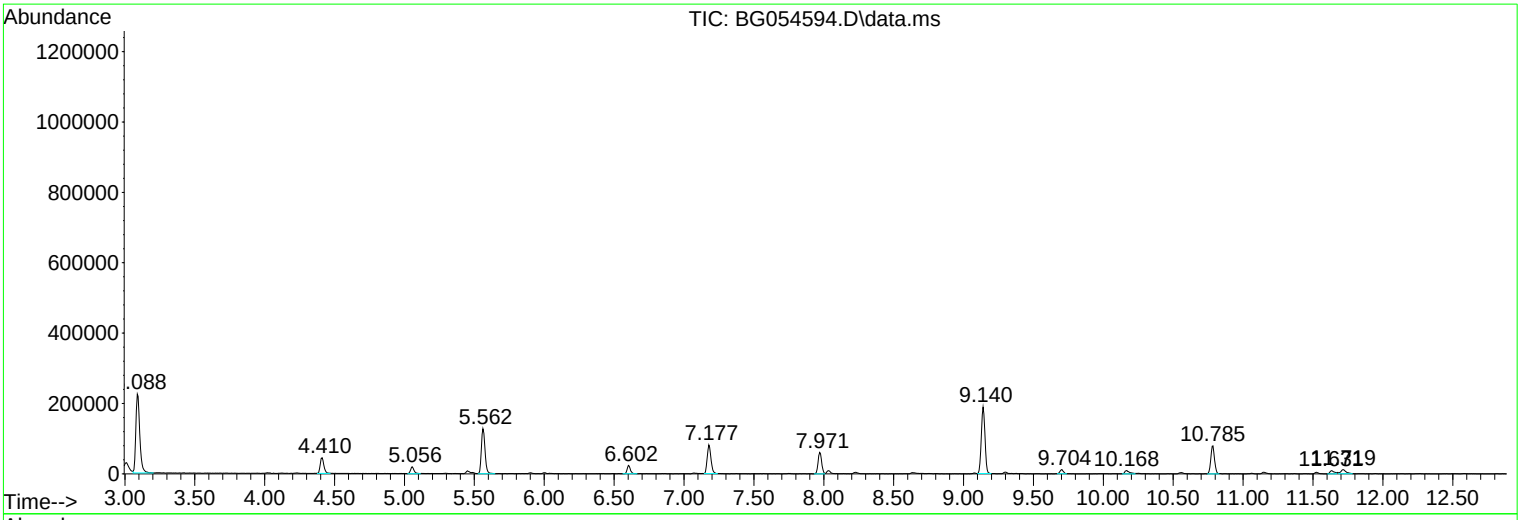
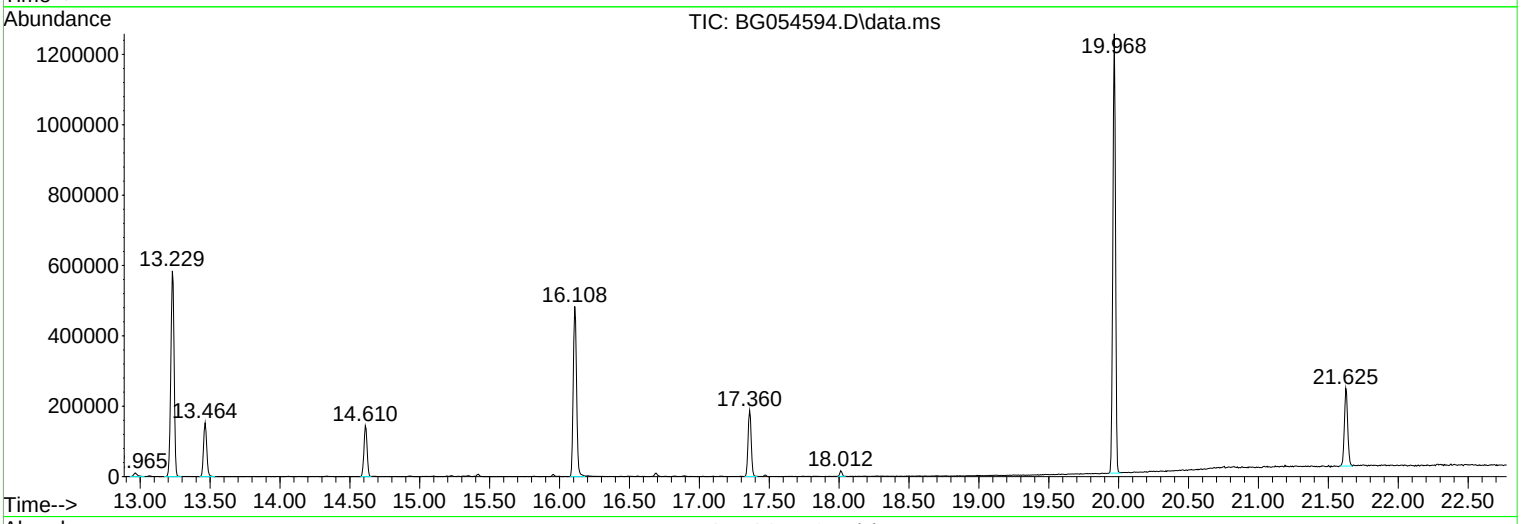
Operator : CG/JU
Sample : N3971-22
Misc :
ALS Vial : 15 Sample Multiplier: 1

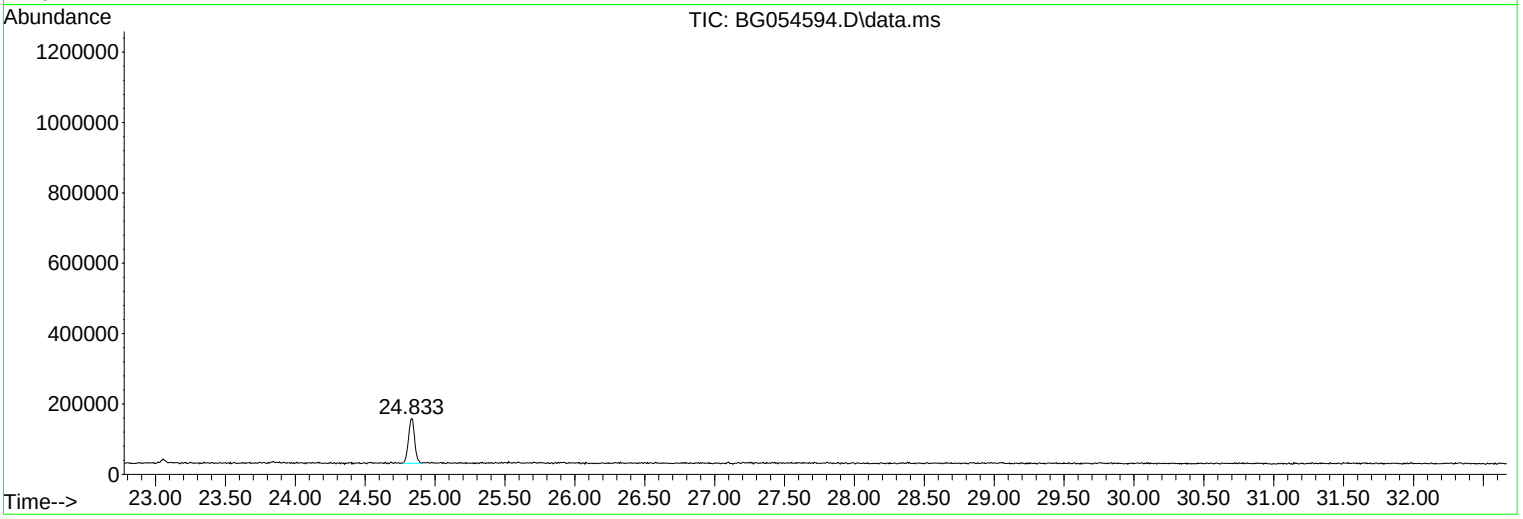
Instrument :
BNA_G
ClientSampleId :
GES-1

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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Data File : BG054594.D
Acq On : 10 Aug 2022 18:53
Operator : CG/JU
Sample : N3971-22
Misc :
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Instrument :
BNA_G
ClientSampleId :
GES-1

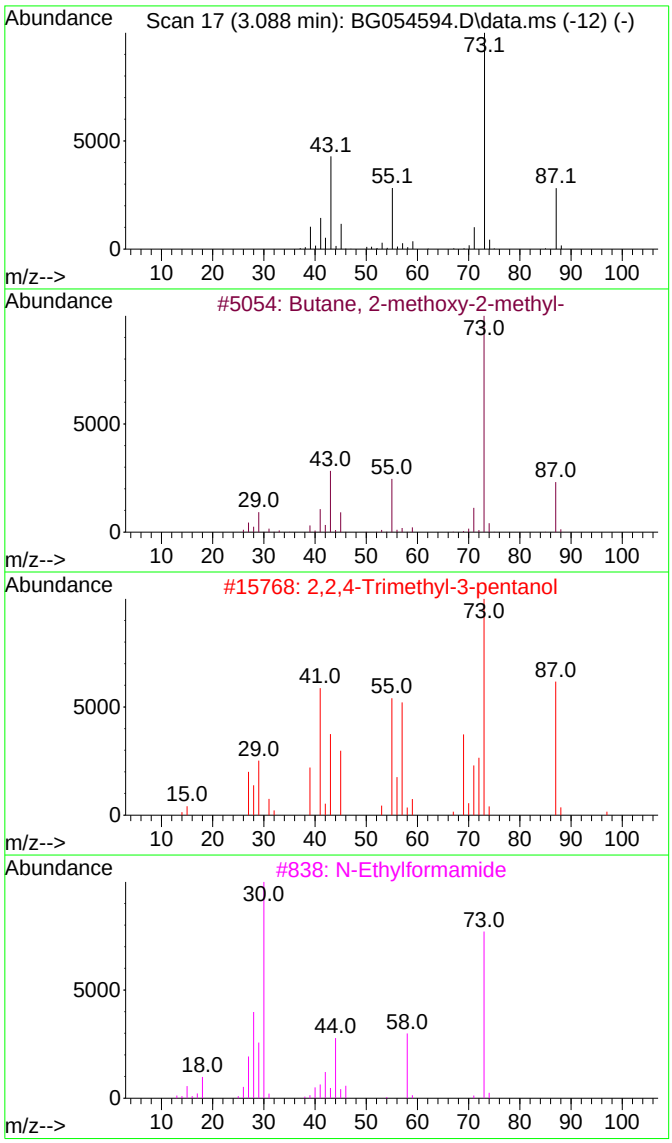
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

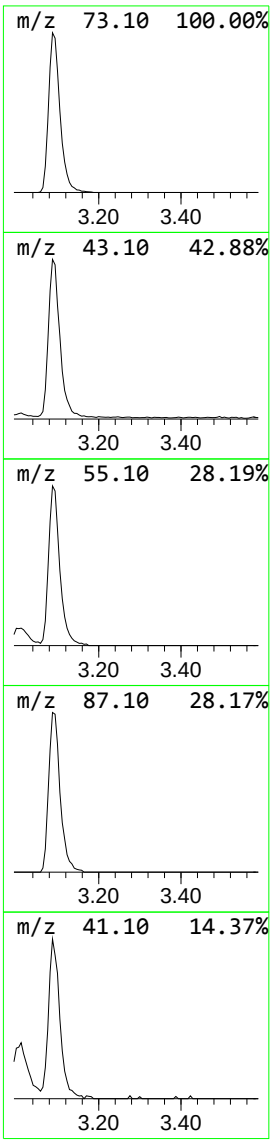
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.088	82.57 ng	435585	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	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081022\
Data File : BG054594.D
Acq On : 10 Aug 2022 18:53
Operator : CG/JU
Sample : N3971-22
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GES-1

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

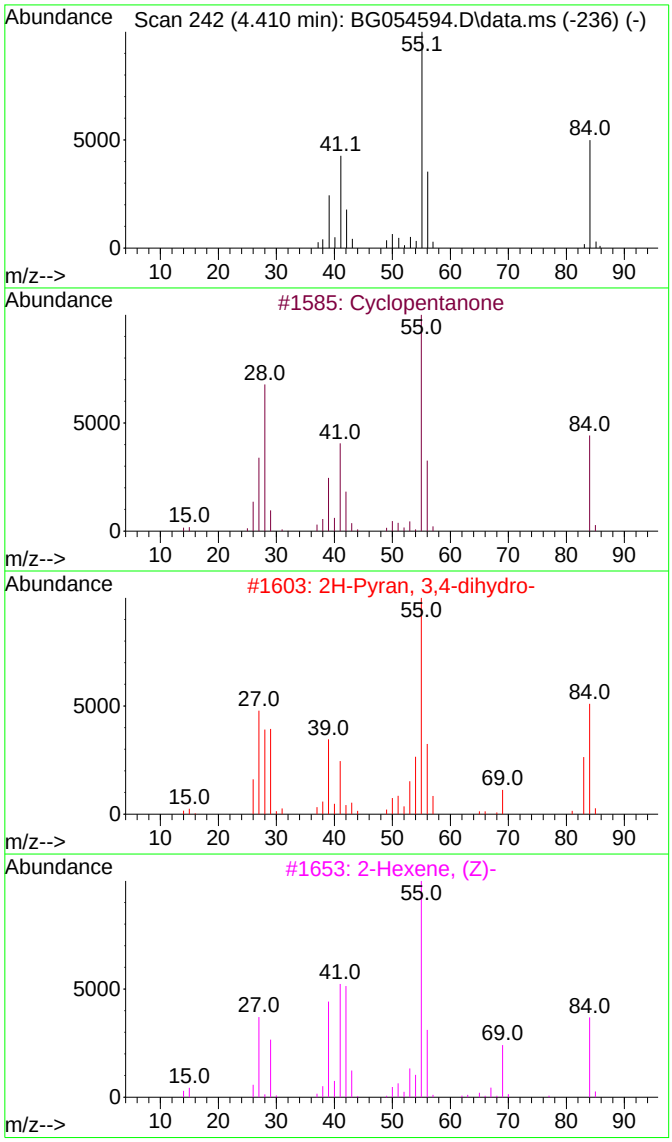
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

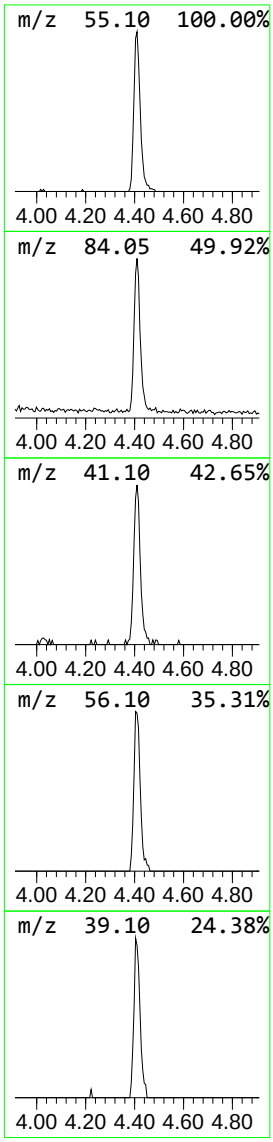
****

Peak Number 2 Cyclopentanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.410	14.93 ng	78770	1,4-Dichlorobenzene-d4	7.971

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanone	84	C5H8O	000120-92-3	91
2	2H-Pyran, 3,4-dihydro-	84	C5H8O	000110-87-2	64
3	2-Hexene, (Z)-	84	C6H12	007688-21-3	64
4	2-Hexene	84	C6H12	000592-43-8	59
5	Formamide, N-(cyanomethyl)-	84	C3H4N2O	005018-27-9	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081022\
Data File : BG054594.D
Acq On : 10 Aug 2022 18:53
Operator : CG/JU
Sample : N3971-22
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GES-1

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

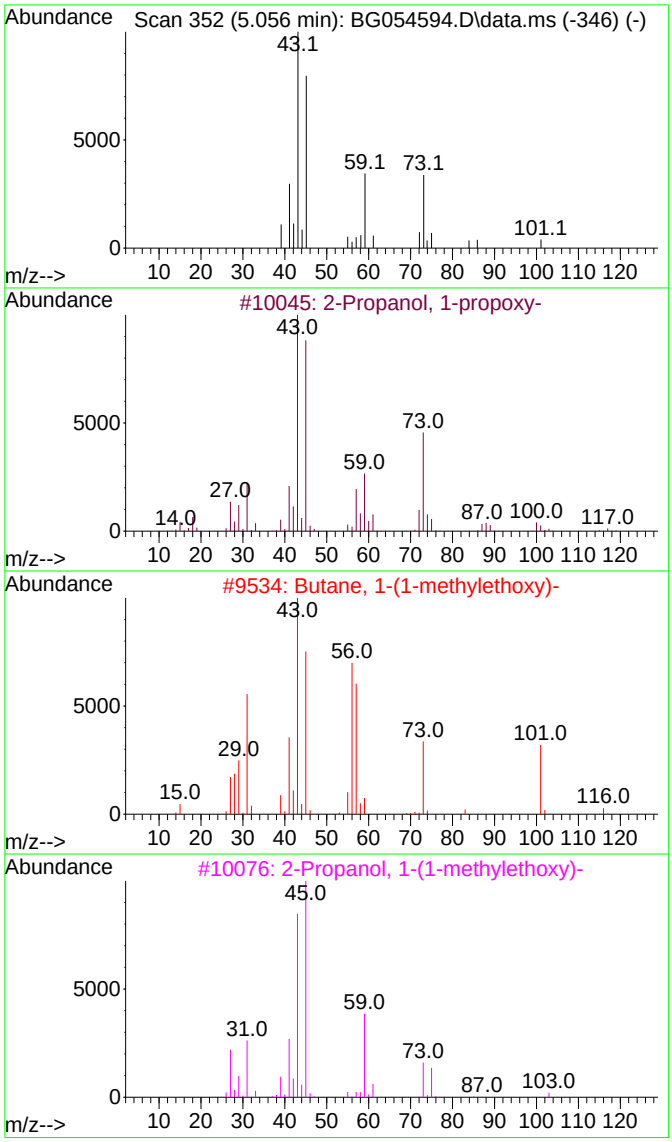
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

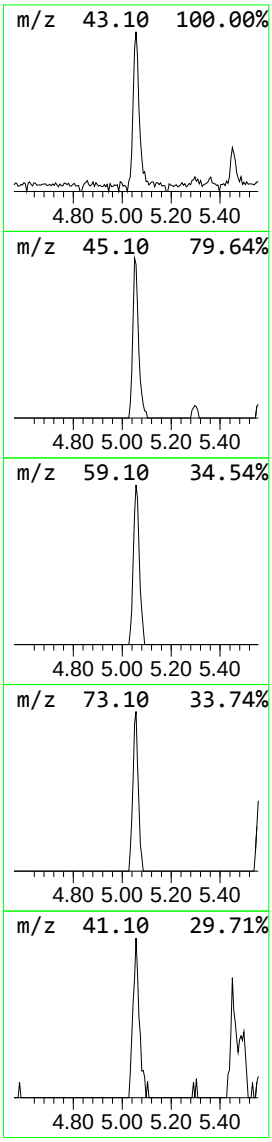
****

Peak Number 3 2-Propanol, 1-propoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.056	6.43 ng	33900	1,4-Dichlorobenzene-d4	7.971

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-propoxy-	118	C6H14O2	001569-01-3	64
2	Butane, 1-(1-methylethoxy)-	116	C7H16O	001860-27-1	45
3	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	38
4	Ethanol, 2-propoxy-	104	C5H12O2	002807-30-9	38
5	1-Butaneboronic acid	102	C4H11BO2	004426-47-5	33





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081022\
Data File : BG054594.D
Acq On : 10 Aug 2022 18:53
Operator : CG/JU
Sample : N3971-22
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GES-1

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

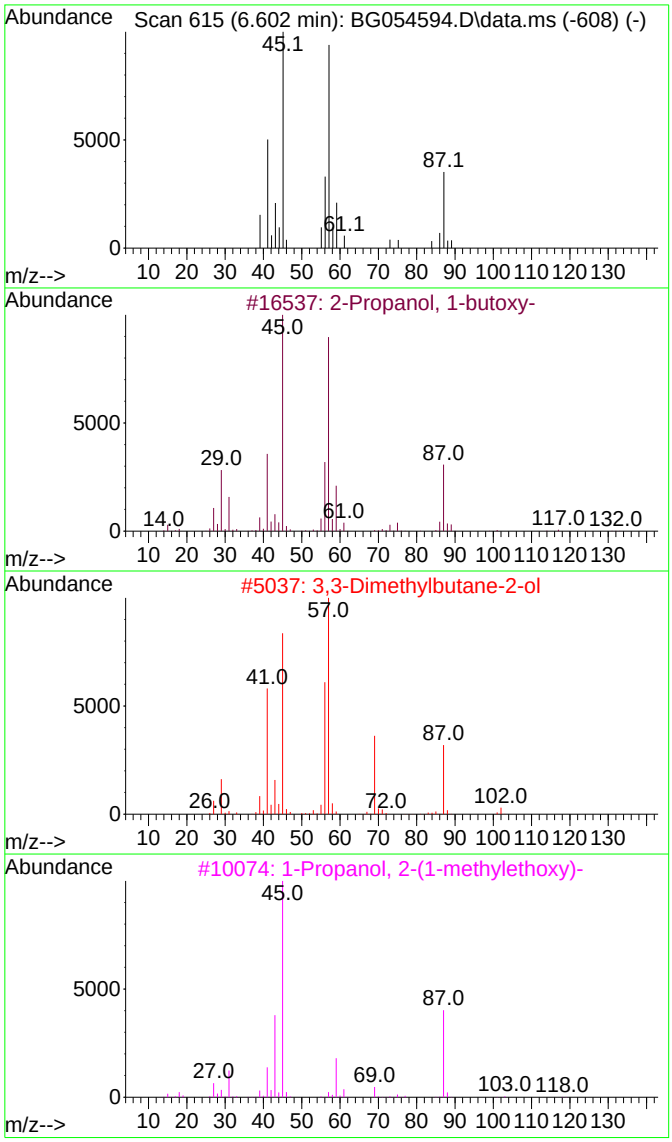
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

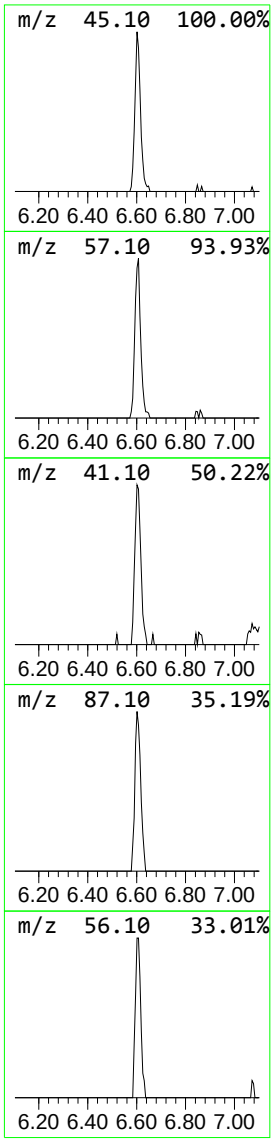
****

Peak Number 4 2-Propanol, 1-butoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.602	7.31 ng	38571	1,4-Dichlorobenzene-d4	7.971

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	90
2	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
3	1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	42
4	Formic acid, 1-methylpropyl ester	102	C5H10O2	000589-40-2	38
5	2-Hydroxy-3-pentanone	102	C5H10O2	005704-20-1	33





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081022\
Data File : BG054594.D
Acq On : 10 Aug 2022 18:53
Operator : CG/JU
Sample : N3971-22
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GES-1

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

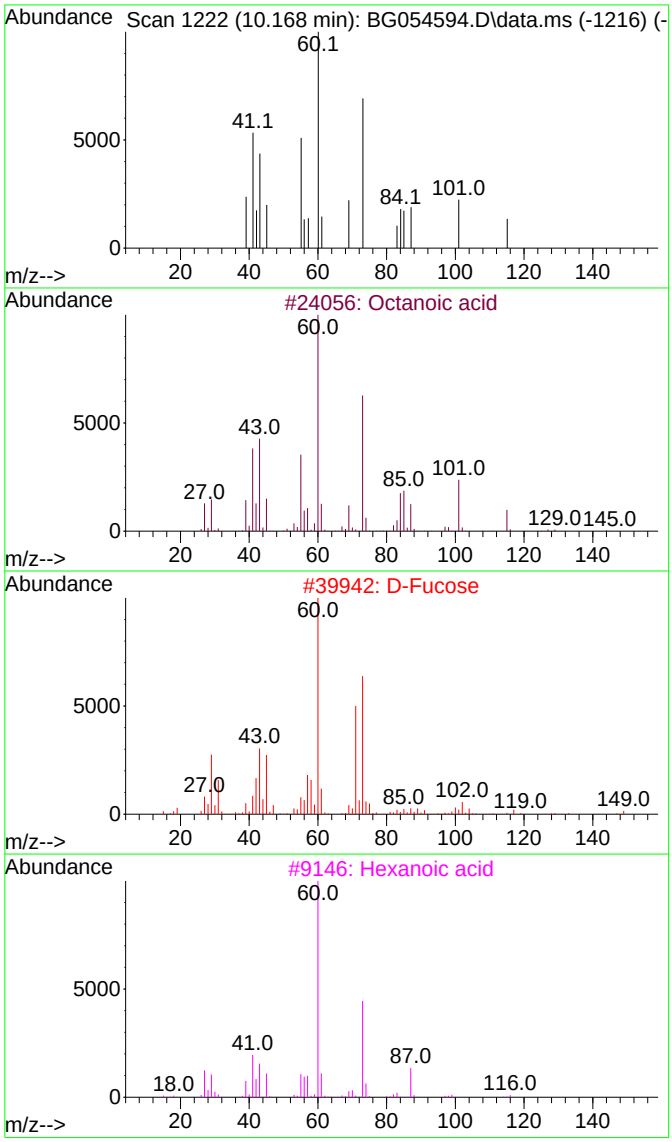
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

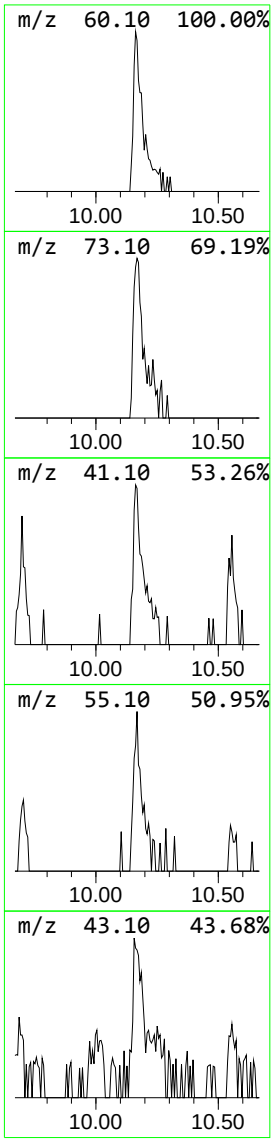
****

Peak Number 5 Octanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.168	2.97 ng	21860	Naphthalene-d8	10.779

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic acid	144	C8H16O2	000124-07-2	90
2	D-Fucose	164	C6H12O5	003615-37-0	47
3	Hexanoic acid	116	C6H12O2	000142-62-1	47
4	Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	33
5	Rhamnose	164	C6H12O5	003615-41-6	28





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Sample : N3971-22
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GES-1

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

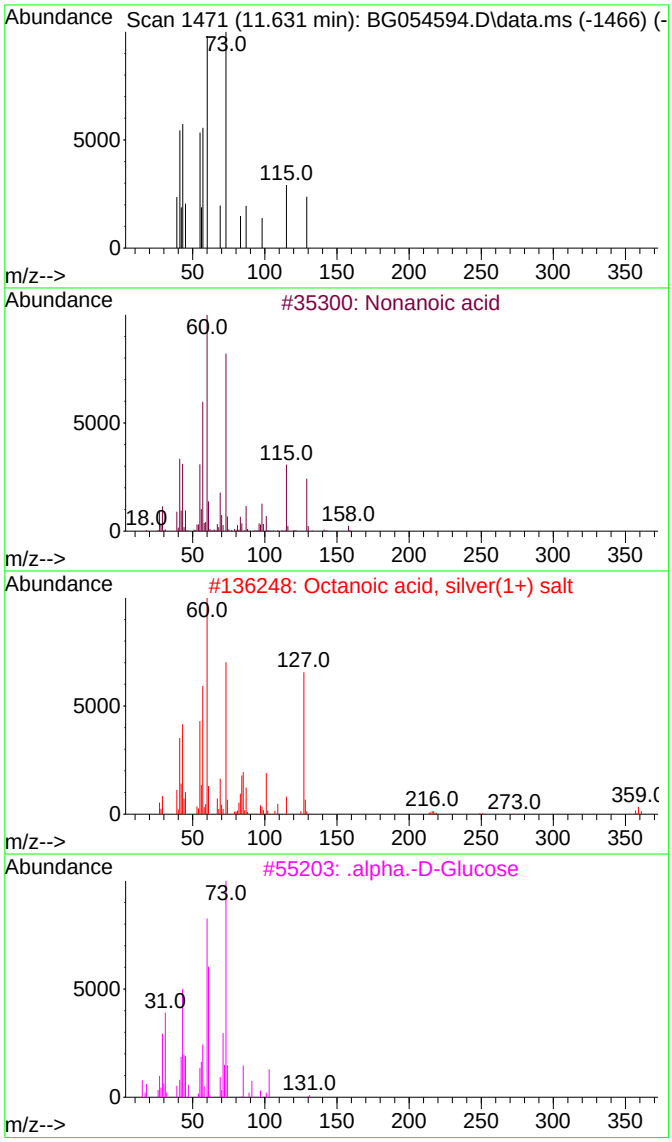
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

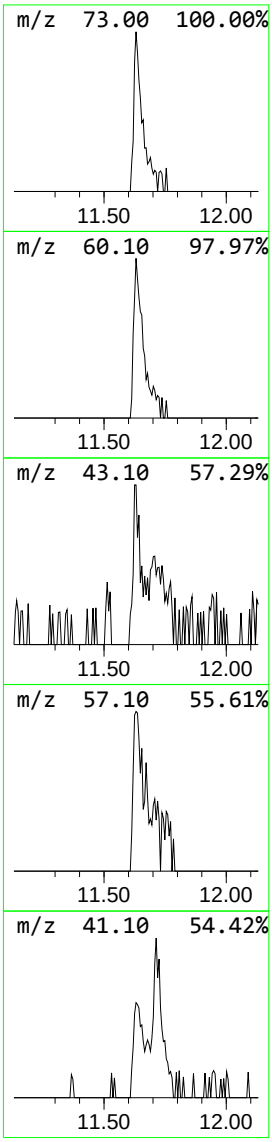
****

Peak Number 6 Nonanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.631	2.57 ng	18908	Naphthalene-d8	10.779

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanoic acid	158	C9H18O2	000112-05-0	64
2	Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	38
3	.alpha.-D-Glucose	180	C6H12O6	000492-62-6	38
4	1,2,3,4-Cyclopentanetetrol, (1.a...	134	C5H10O4	014003-71-5	38
5	3,4-Altrosan	162	C6H10O5	1000129-76-4	37





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Acq On : 10 Aug 2022 18:53
Operator : CG/JU
Sample : N3971-22
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GES-1

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

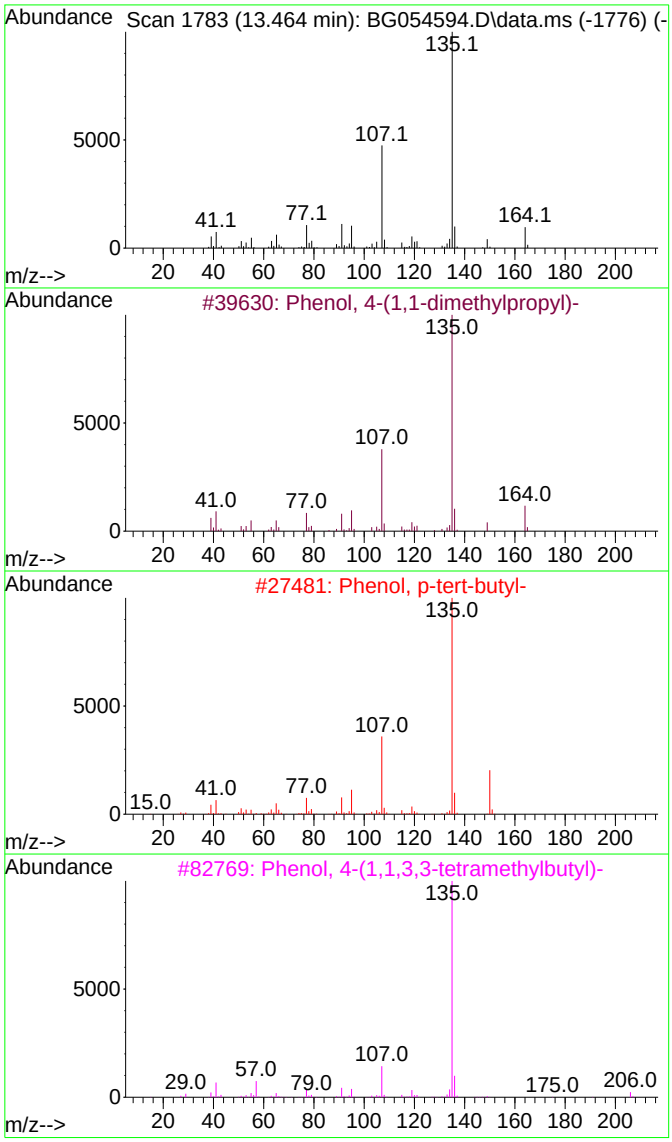
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

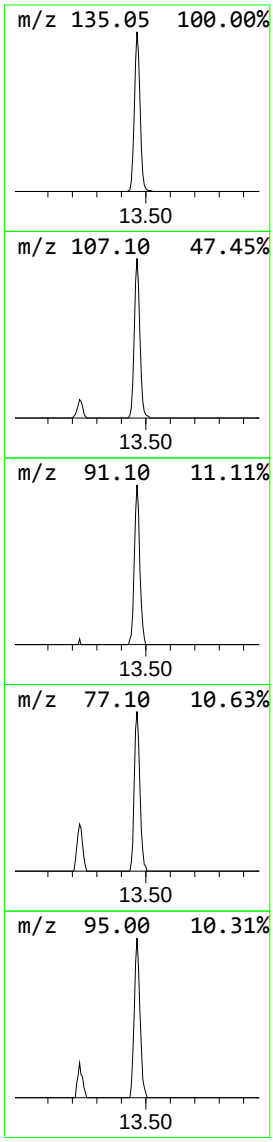
****

Peak Number 7 Phenol, 4-(1,1-dimethylprop... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.464	20.90 ng	239902	Acenaphthene-d10	14.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	94
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	78
3	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	64
4	4,4'-(1,2-diethylethylene)diphenol	270	C18H22O2	005635-50-7	64
5	Phenol, 2-(1,1,3,3-tetramethylbu...	206	C14H22O	003884-95-5	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081022\
Data File : BG054594.D
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BNA_G
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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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.088	82.6	ng	435585	1	7.971	105513	20.0
Cyclopentanone	4.410	14.9	ng	78770	1	7.971	105513	20.0
2-Propanol, 1-p...	5.056	6.4	ng	33900	1	7.971	105513	20.0
2-Propanol, 1-b...	6.602	7.3	ng	38571	1	7.971	105513	20.0
Octanoic acid	10.168	3.0	ng	21860	2	10.779	147165	20.0
Nonanoic acid	11.631	2.6	ng	18908	2	10.779	147165	20.0
Phenol, 4-(1,1-...	13.464	20.9	ng	239902	3	14.610	229611	20.0