LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081022\
Data File : BG054595.D
Acq On : 10 Aug 2022 19:35
Operator : CG/JU
Sample : N3971-23
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
GES-2R

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: BG054595.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 | 11 | 17 | 31 | rVB | 222126 | 395694 | 22.98% | 6.215% |
| 2 | 4.404 | 235 | 241 | 252 | rBV | 46116 | 81391 | 4.73% | 1.278% |
| 3 | 5.050 | 346 | 351 | 358 | rVB3 | 14918 | 24531 | 1.42% | 0.385% |
| 4 | 5.561 | 429 | 438 | 456 | rVB | 110196 | 199227 | 11.57% | 3.129% |
| 5 | 6.601 | 609 | 615 | 623 | rBV | 19223 | 32024 | 1.86% | 0.503% |
| 6 | 7.177 | 707 | 713 | 726 | rBV | 70163 | 131460 | 7.64% | 2.065% |
| 7 | 7.970 | 841 | 848 | 854 | rBV | 51364 | 86795 | 5.04% | 1.363% |
| 8 | 8.029 | 854 | 858 | 865 | rVB | 24664 | 39853 | 2.31% | 0.626% |
| 9 | 9.139 | 1040 | 1047 | 1058 | rBV | 166747 | 309980 | 18.00% | 4.869% |
| 10 | 9.704 | 1135 | 1143 | 1149 | rBB | 10323 | 17983 | 1.04% | 0.282% |
| 11 | 10.779 | 1319 | 1326 | 1334 | rBV | 65230 | 125227 | 7.27% | 1.967% |
| 12 | 11.707 | 1475 | 1484 | 1496 | rBV2 | 20653 | 46640 | 2.71% | 0.733% |
| 13 | 13.229 | 1736 | 1743 | 1752 | rBV | 527834 | 855666 | 49.70% | 13.440% |
| 14 | 13.464 | 1776 | 1783 | 1794 | rBV | 169254 | 261718 | 15.20% | 4.111% |
| 15 | 14.610 | 1972 | 1978 | 1985 | rBV | 131177 | 202695 | 11.77% | 3.184% |
| 16 | 16.108 | 2227 | 2233 | 2248 | rBV | 486800 | 781563 | 45.39% | 12.276% |
| 17 | 16.689 | 2326 | 2332 | 2338 | rVB | 11675 | 17277 | 1.00% | 0.271% |
| 18 | 17.359 | 2440 | 2446 | 2455 | rVB | 180472 | 277352 | 16.11% | 4.356% |
| 19 | 18.011 | 2550 | 2557 | 2562 | rBV3 | 18674 | 23722 | 1.38% | 0.373% |
| 20 | 19.968 | 2884 | 2890 | 2898 | rBV | 1265318 | 1721775 | 100.00% | 27.043% |
| 21 | 21.625 | 3166 | 3172 | 3179 | rBV | 213151 | 361628 | 21.00% | 5.680% |
| 22 | 24.833 | 3708 | 3718 | 3730 | rVB2 | 131578 | 372489 | 21.63% | 5.851% |

Sum of corrected areas: 6366690

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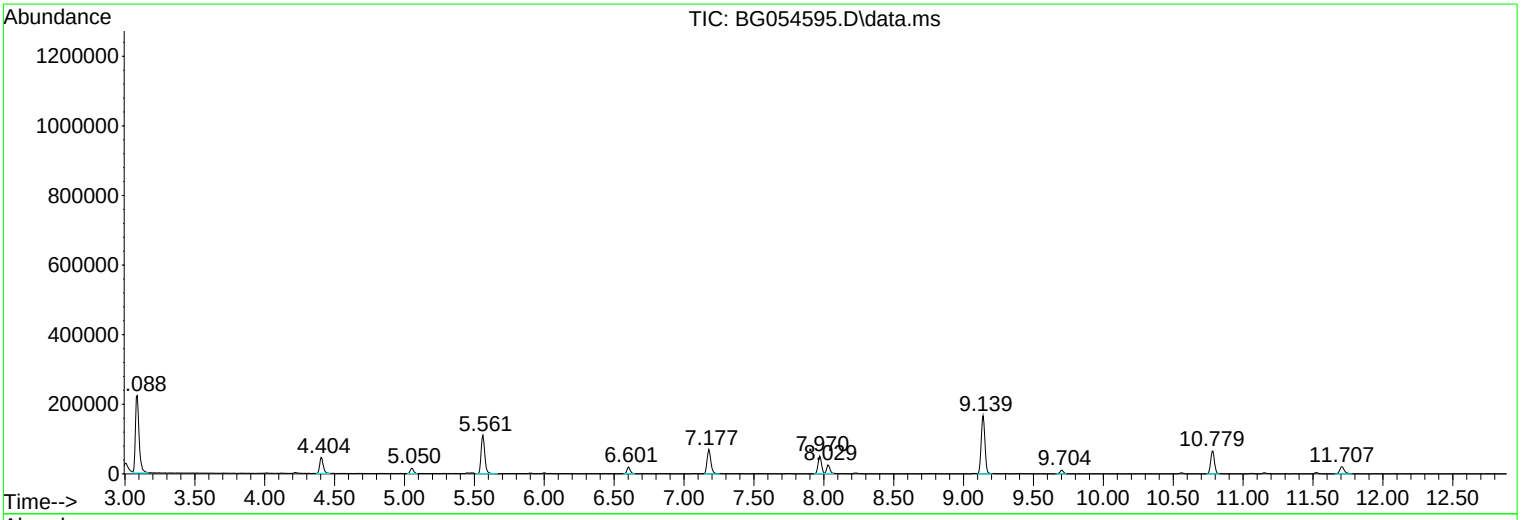
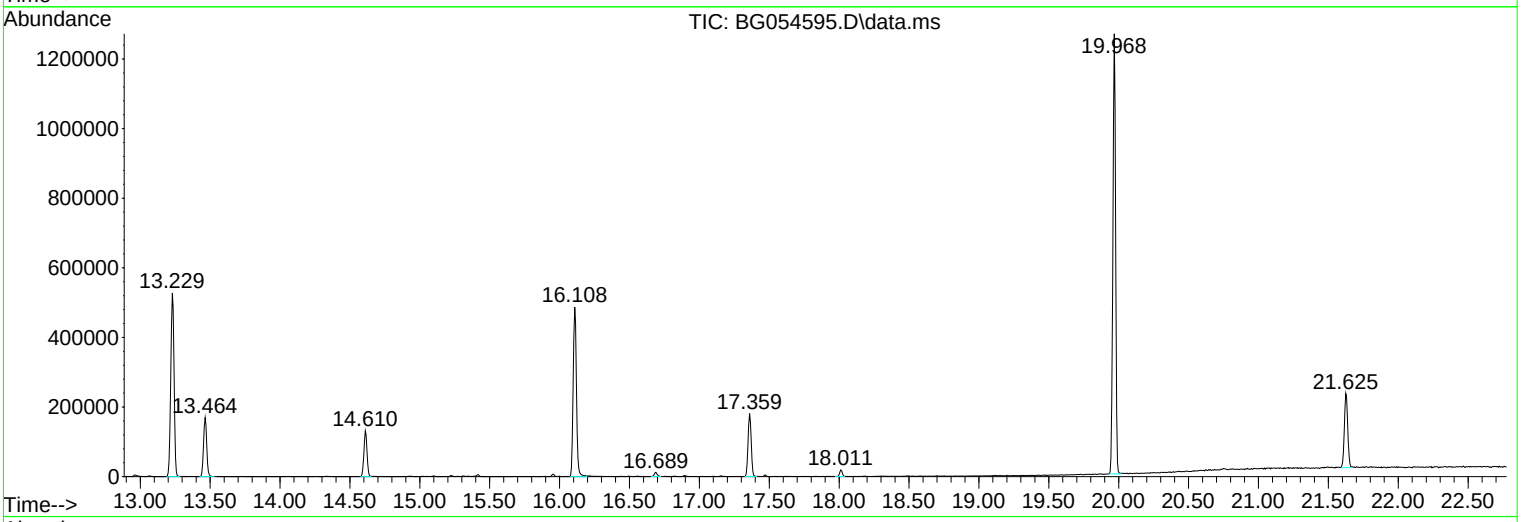
Misc :
ALS Vial : 16 Sample Multiplier: 1

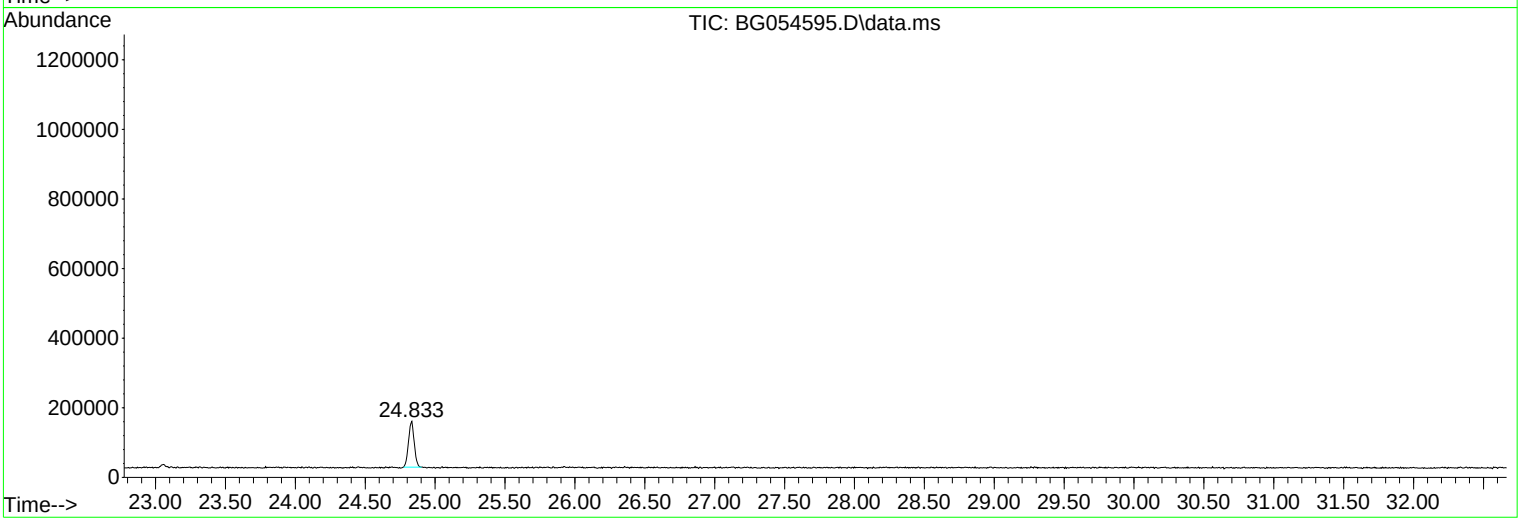
**Instrument :**
BNA_G
**ClientSampleId :**
GES-2R

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 : BG054595.D
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Operator : CG/JU
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Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
GES-2R

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

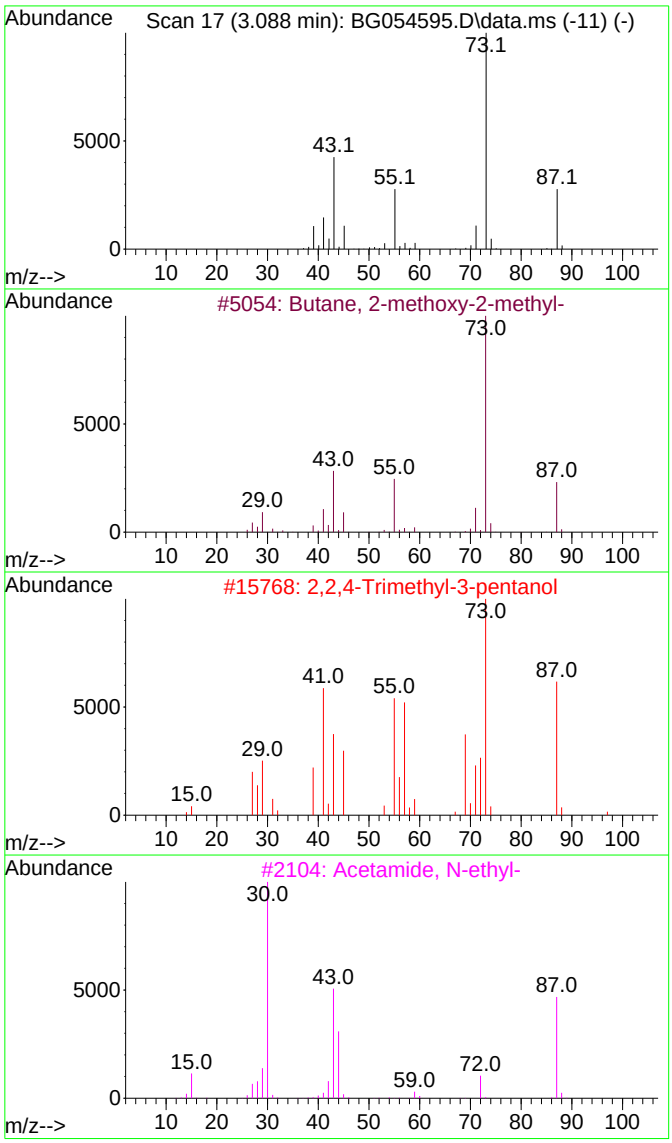
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

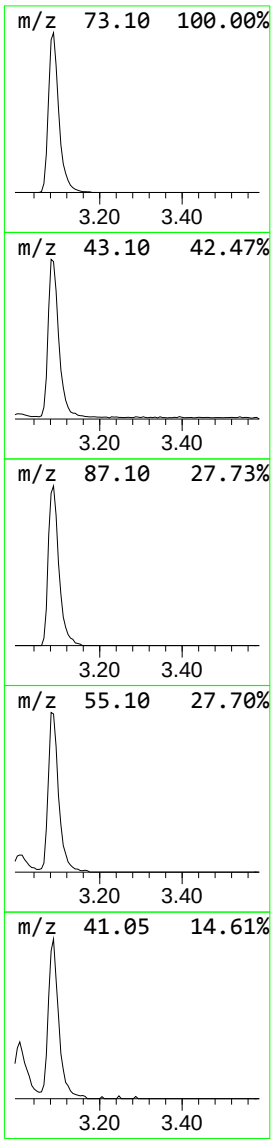
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.088 | 91.18 ng | 395694 | 1,4-Dichlorobenzene-d4 | 7.970 |

| 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 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 9 |
| 5 | N-Ethylformamide | 73 | C3H7NO | 000627-45-2 | 9 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081022\
Data File : BG054595.D
Acq On : 10 Aug 2022 19:35
Operator : CG/JU
Sample : N3971-23
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
GES-2R

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

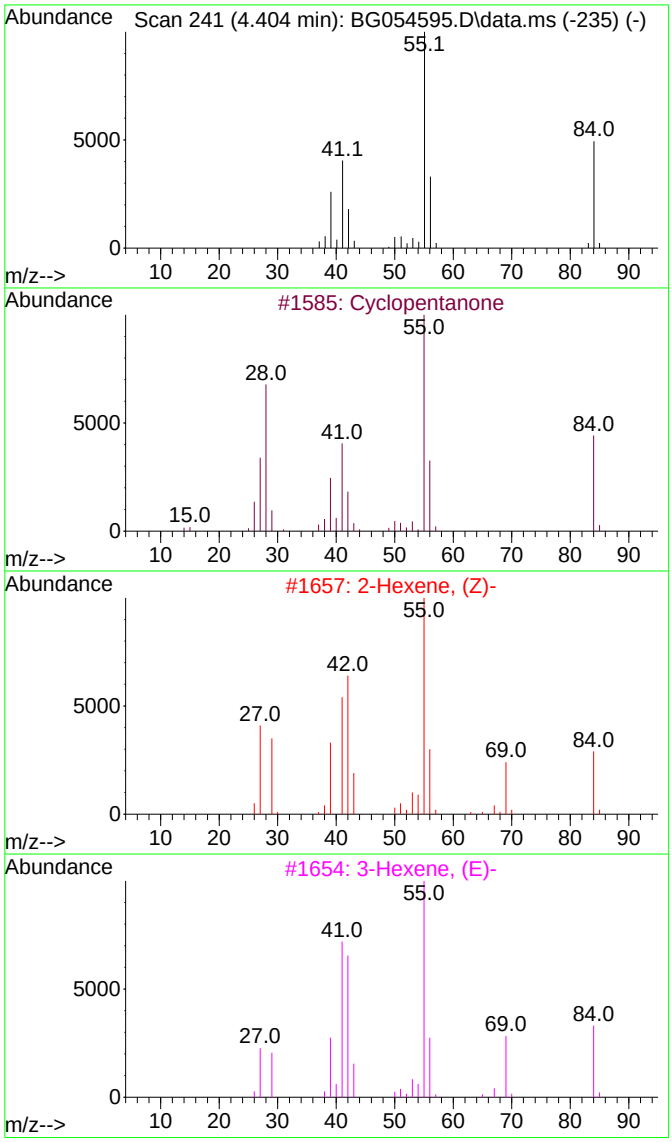
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

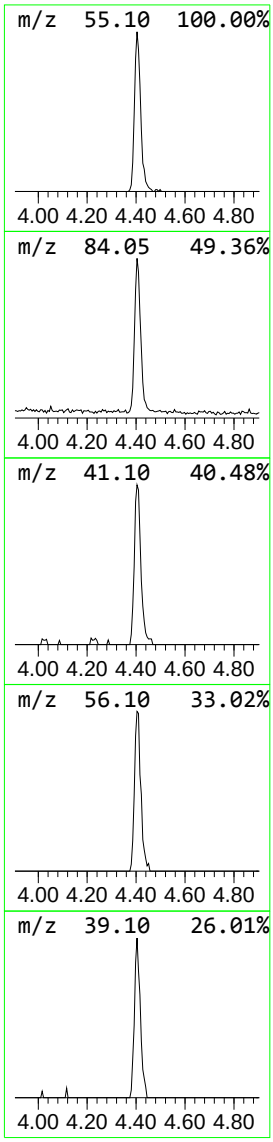
**********

Peak Number 2 Cyclopentanone Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.404 | 18.75 ng | 81391 | 1,4-Dichlorobenzene-d4 | 7.970 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclopentanone | 84 | C5H8O | 000120-92-3 | 91 |
| 2 | 2-Hexene, (Z)- | 84 | C6H12 | 007688-21-3 | 72 |
| 3 | 3-Hexene, (E)- | 84 | C6H12 | 013269-52-8 | 72 |
| 4 | 2-Hexene | 84 | C6H12 | 000592-43-8 | 64 |
| 5 | 2-Hexene, (E)- | 84 | C6H12 | 004050-45-7 | 64 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081022\
Data File : BG054595.D
Acq On : 10 Aug 2022 19:35
Operator : CG/JU
Sample : N3971-23
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
GES-2R

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

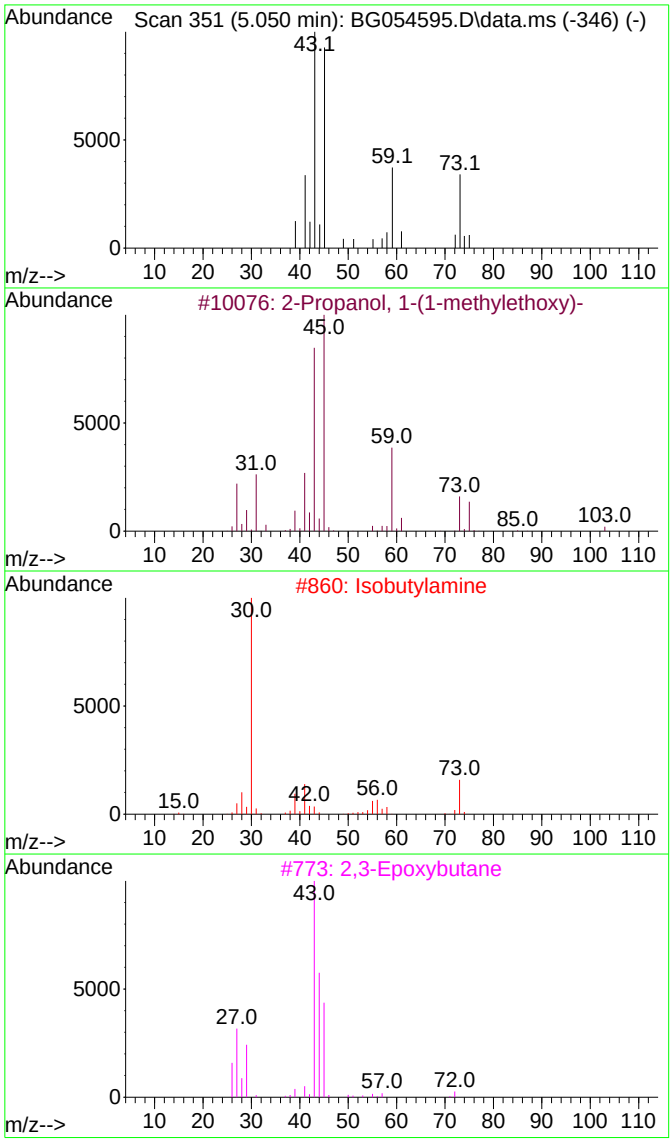
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

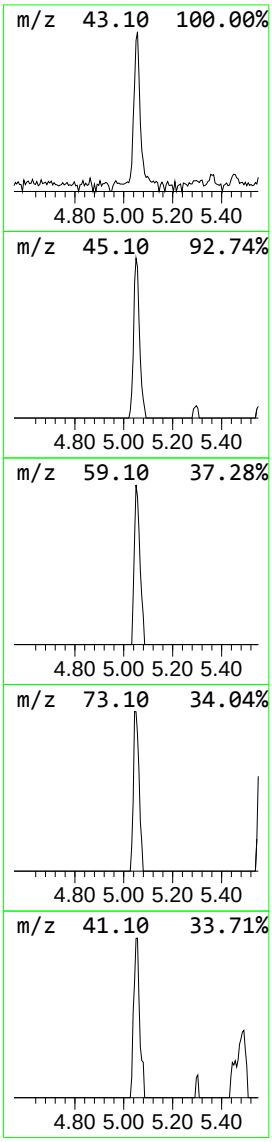
**********

Peak Number 3 unknown5.050 Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.050 | 5.65 ng | 24531 | 1,4-Dichlorobenzene-d4 | 7.970 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Propanol, 1-(1-methylethoxy)- | 118 | C6H14O2 | 003944-36-3 | 39 |
| 2 | Isobutylamine | 73 | C4H11N | 000078-81-9 | 9 |
| 3 | 2,3-Epoxybutane | 72 | C4H8O | 003266-23-7 | 9 |
| 4 | 1-Butanamine | 73 | C4H11N | 000109-73-9 | 9 |
| 5 | Acetamide, N-methyl- | 73 | C3H7NO | 000079-16-3 | 9 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081022\
Data File : BG054595.D
Acq On : 10 Aug 2022 19:35
Operator : CG/JU
Sample : N3971-23
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
GES-2R

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

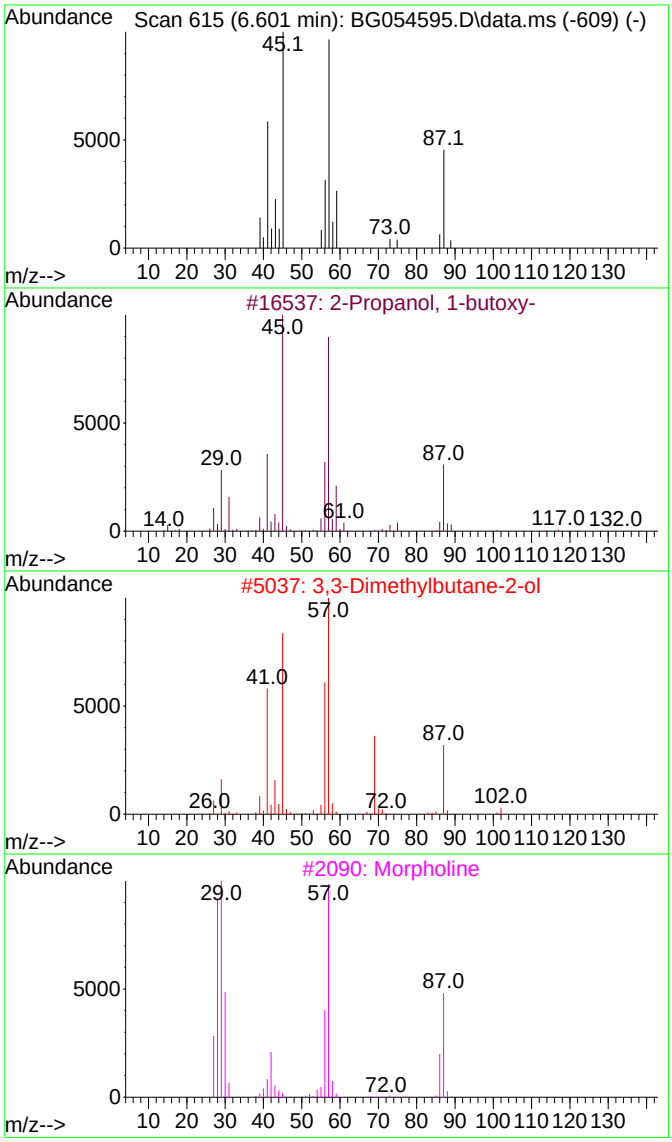
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

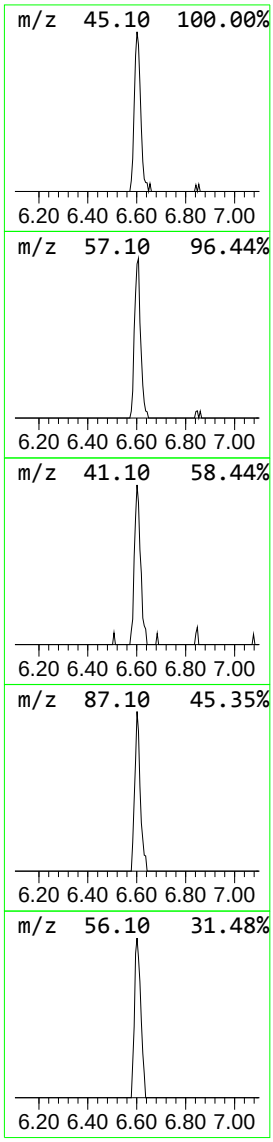
**********

Peak Number 4 2-Propanol, 1-butoxy- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.601 | 7.38 ng | 32024 | 1,4-Dichlorobenzene-d4 | 7.970 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Propanol, 1-butoxy- | 132 | C7H16O2 | 005131-66-8 | 78 |
| 2 | 3,3-Dimethylbutane-2-ol | 102 | C6H14O | 000464-07-3 | 36 |
| 3 | Morpholine | 87 | C4H9NO | 000110-91-8 | 35 |
| 4 | Formic acid, 1-methylpropyl ester | 102 | C5H10O2 | 000589-40-2 | 28 |
| 5 | Acetaldehyde, O-ethyloxime- | 87 | C4H9NO | 1000288-34-6 | 10 |



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Data File : BG054595.D
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Operator : CG/JU
Sample : N3971-23
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
GES-2R

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

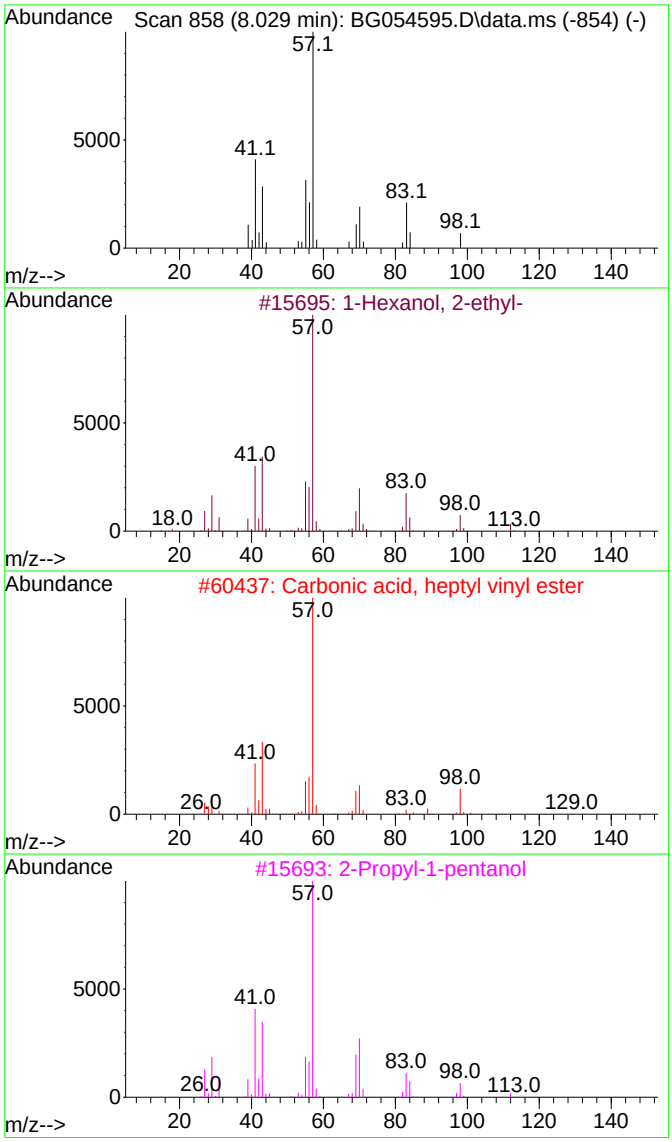
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

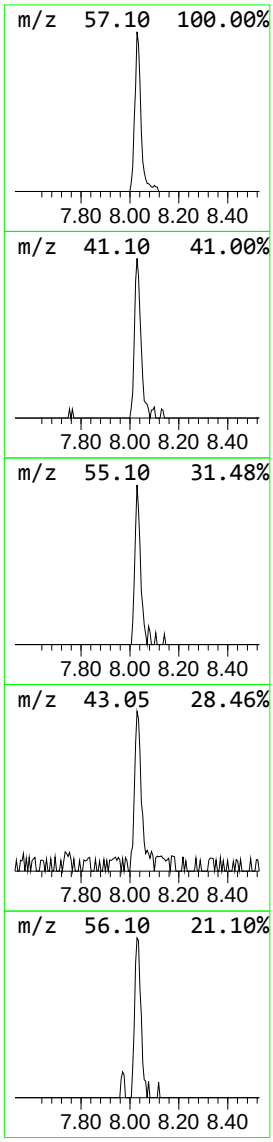
**********

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.029 | 9.18 ng | 39853 | 1,4-Dichlorobenzene-d4 | 7.970 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Hexanol, 2-ethyl- | 130 | C8H18O | 000104-76-7 | 83 |
| 2 | Carbonic acid, heptyl vinyl ester | 186 | C10H18O3 | 1010383-25-4 | 42 |
| 3 | 2-Propyl-1-pentanol | 130 | C8H18O | 058175-57-8 | 40 |
| 4 | Carbonic acid, heptyl prop-1-en-... | 200 | C11H20O3 | 1000382-54-1 | 40 |
| 5 | 1-Pentanol, 2-ethyl-4-methyl- | 130 | C8H18O | 000106-67-2 | 38 |



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Operator : CG/JU
Sample : N3971-23
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
GES-2R

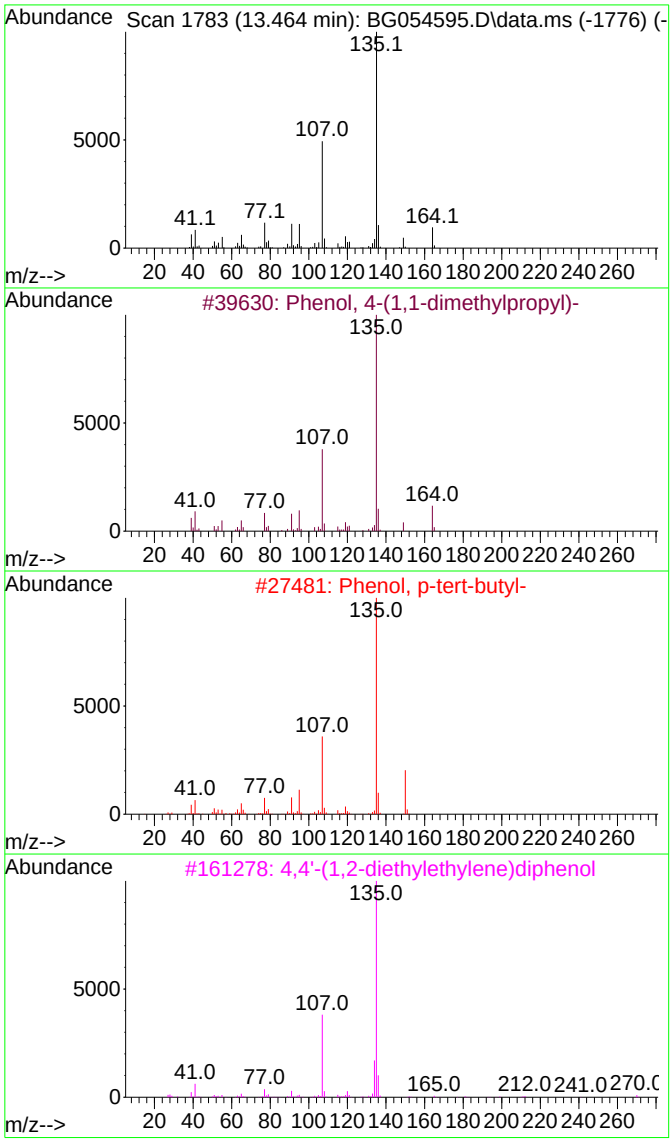
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

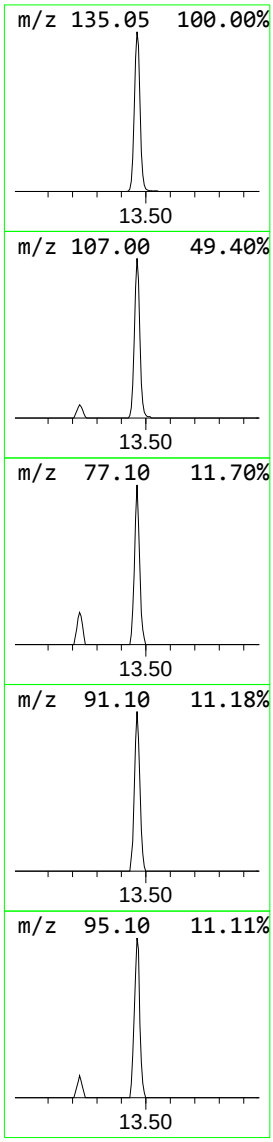
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.464 | 25.82 ng | 261718 | Acenaphthene-d10 | 14.610 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Phenol, 4-(1,1-dimethylpropyl)- | 164 | C11H16O | 000080-46-6 | 96 |
| 2 | Phenol, p-tert-butyl- | 150 | C10H14O | 000098-54-4 | 78 |
| 3 | 4,4'-(1,2-diethylethylene)diphenol | 270 | C18H22O2 | 005635-50-7 | 64 |
| 4 | Imidazo[1,2-c]pyrimidin-5-ol | 135 | C6H5N3O | 055662-66-3 | 64 |
| 5 | Phenol, 4-(1,1,3,3-tetramethylbu... | 206 | C14H22O | 000140-66-9 | 64 |



Tentatively Identified Compound (LSC) summary

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Acq On : 10 Aug 2022 19:35
Operator : CG/JU
Sample : N3971-23
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :**
BNA_G
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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 | 91.2 | ng | 395694 | 1 | 7.970 | 86795 | 20.0 |
| Cyclopentanone | 4.404 | 18.8 | ng | 81391 | 1 | 7.970 | 86795 | 20.0 |
| unknown5.050 | 5.050 | 5.7 | ng | 24531 | 1 | 7.970 | 86795 | 20.0 |
| 2-Propanol, 1-b... | 6.601 | 7.4 | ng | 32024 | 1 | 7.970 | 86795 | 20.0 |
| 1-Hexanol, 2-et... | 8.029 | 9.2 | ng | 39853 | 1 | 7.970 | 86795 | 20.0 |
| Phenol, 4-(1,1-... | 13.464 | 25.8 | ng | 261718 | 3 | 14.610 | 202695 | 20.0 |