LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062723\
Data File : BG057879.D
Acq On : 27 Jun 2023 23:28
Operator : CG/JU
Sample : 03339-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW-13

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-BG062723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057879.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 5.024 | 324 | 329 | 336 | rVB | 43767 | 64096 | 1.75% | 0.520% |
| 2 | 5.494 | 402 | 409 | 417 | rBV | 358328 | 549211 | 14.97% | 4.457% |
| 3 | 7.080 | 672 | 679 | 687 | rBV | 232598 | 384255 | 10.48% | 3.118% |
| 4 | 7.920 | 816 | 822 | 827 | rBV | 105817 | 172291 | 4.70% | 1.398% |
| 5 | 7.979 | 827 | 832 | 837 | rVB | 64873 | 96930 | 2.64% | 0.787% |
| 6 | 9.084 | 1012 | 1020 | 1028 | rBV | 441173 | 766982 | 20.91% | 6.224% |
| 7 | 9.207 | 1034 | 1041 | 1050 | rBV | 51593 | 100666 | 2.74% | 0.817% |
| 8 | 10.488 | 1252 | 1259 | 1266 | rBV | 23648 | 40231 | 1.10% | 0.326% |
| 9 | 10.723 | 1293 | 1299 | 1306 | rBV | 150389 | 261251 | 7.12% | 2.120% |
| 10 | 12.021 | 1513 | 1520 | 1527 | rBV | 100187 | 158684 | 4.33% | 1.288% |
| 11 | 13.179 | 1710 | 1717 | 1725 | rVB | 1129314 | 1735248 | 47.31% | 14.082% |
| 12 | 14.554 | 1946 | 1951 | 1965 | rVB | 263164 | 425636 | 11.60% | 3.454% |
| 13 | 16.040 | 2197 | 2204 | 2213 | rBV | 1121784 | 1764137 | 48.09% | 14.316% |
| 14 | 17.298 | 2412 | 2418 | 2425 | rBV | 404972 | 597050 | 16.28% | 4.845% |
| 15 | 18.185 | 2564 | 2569 | 2575 | rBV4 | 26814 | 43562 | 1.19% | 0.354% |
| 16 | 19.918 | 2857 | 2864 | 2869 | rBV | 2781817 | 3668162 | 100.00% | 29.767% |
| 17 | 21.287 | 3093 | 3097 | 3103 | rBV | 28479 | 37600 | 1.03% | 0.305% |
| 18 | 21.551 | 3136 | 3142 | 3150 | rVB | 437337 | 696907 | 19.00% | 5.655% |
| 19 | 24.701 | 3668 | 3678 | 3691 | rVB | 270074 | 759828 | 20.71% | 6.166% |

Sum of corrected areas: 12322727

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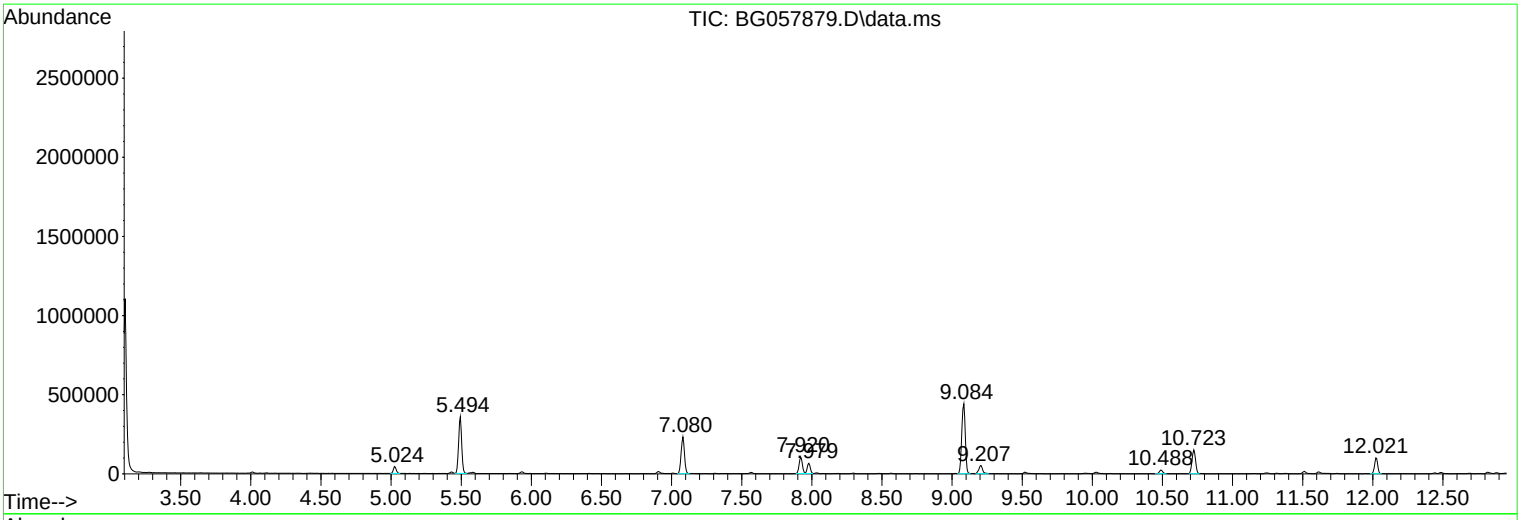
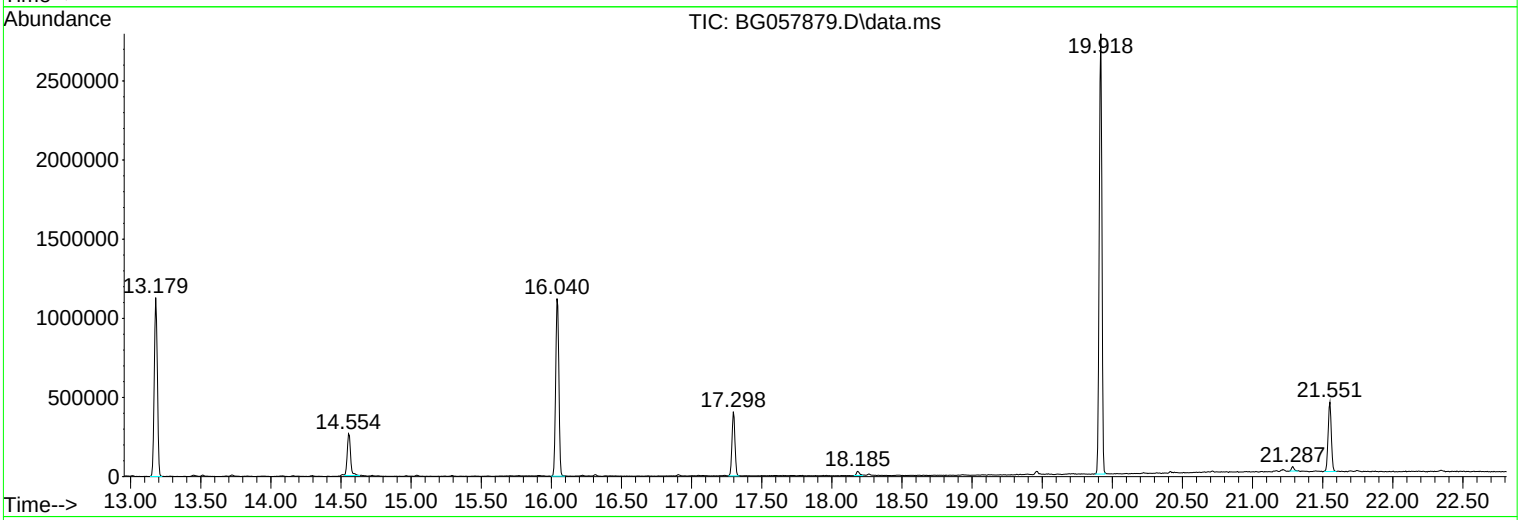
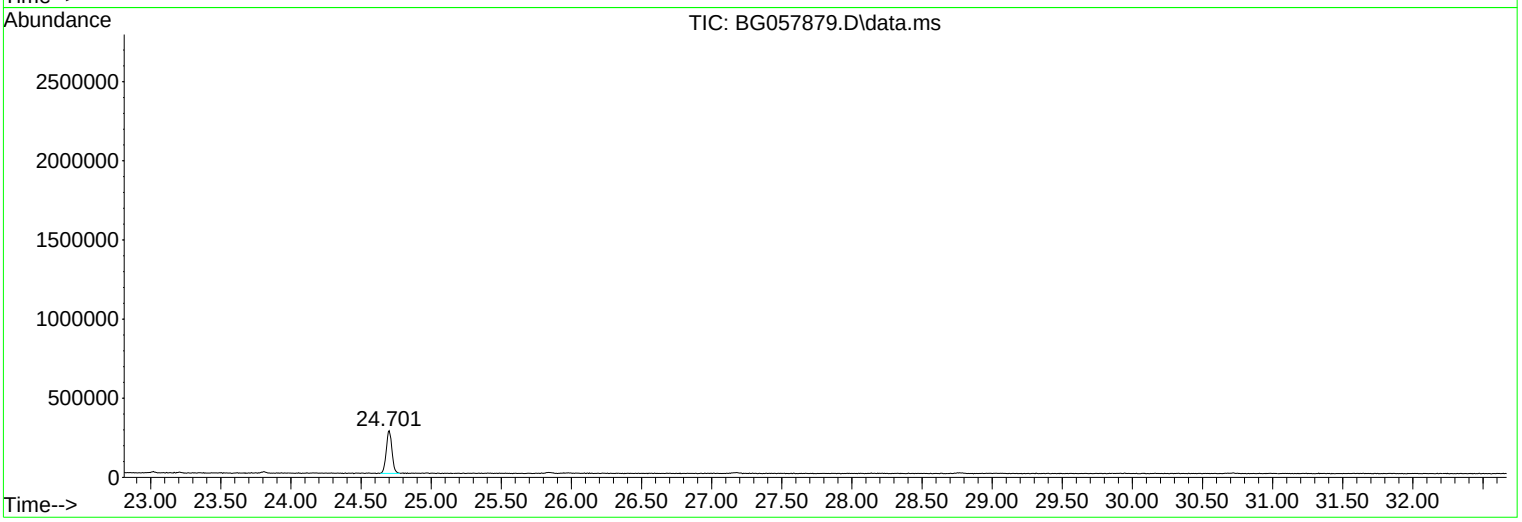
**Instrument :**
BNA_G
**ClientSampleId :**
MW-13

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.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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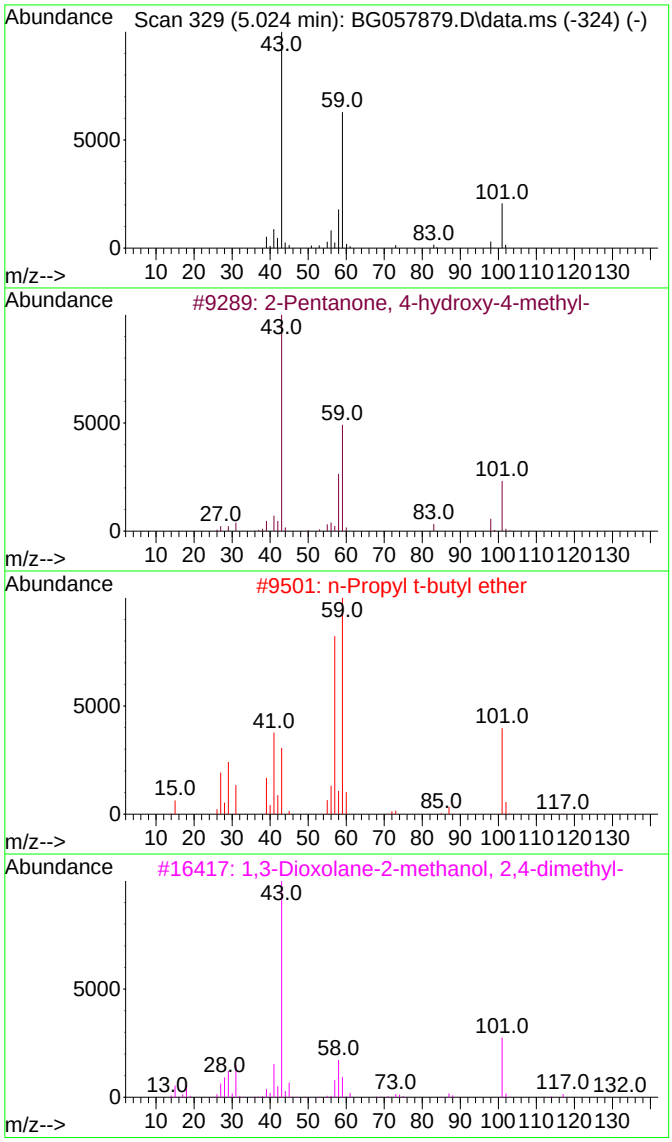
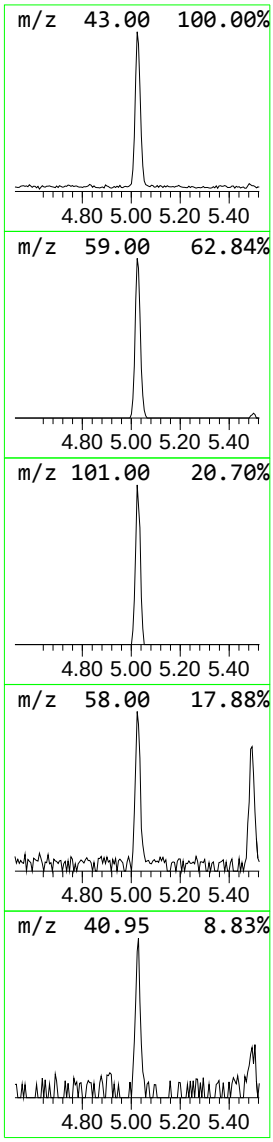
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.024 | 7.44 ng | 64096 | 1,4-Dichlorobenzene-d4 | 7.920 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 72 |
| 2 | n-Propyl t-butyl ether | 116 | C7H16O | 1000334-81-9 | 36 |
| 3 | 1,3-Dioxolane-2-methanol, 2,4-di... | 132 | C6H12O3 | 053951-43-2 | 28 |
| 4 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23 |
| 5 | Formamide, N,N-diethyl- | 101 | C5H11NO | 000617-84-5 | 9 |



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**Instrument :**
BNA_G
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

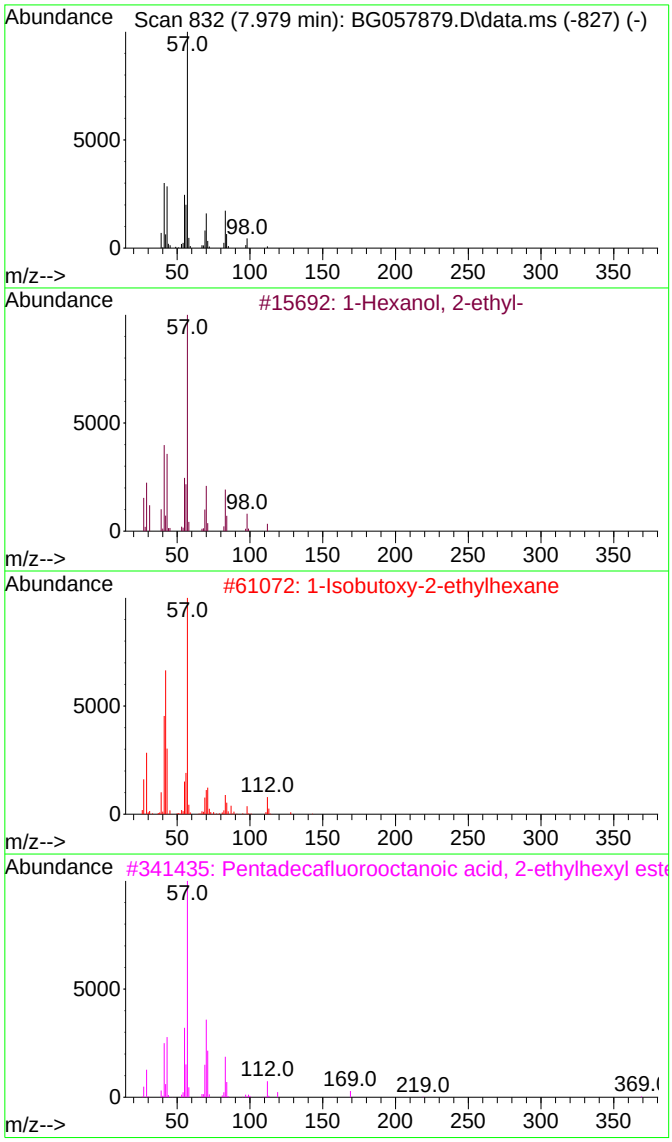
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

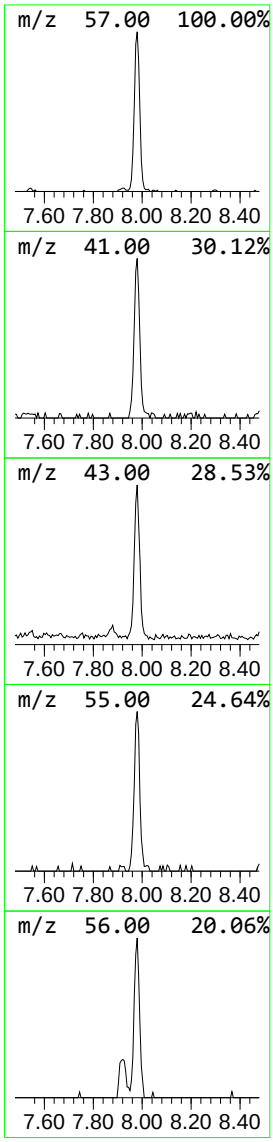
**********

Peak Number 2 1-Hexanol, 2-ethyl- Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.979 | 11.25 ng | 96930 | 1,4-Dichlorobenzene-d4 | 7.920 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Hexanol, 2-ethyl- | 130 | C8H18O | 000104-76-7 | 83 |
| 2 | 1-Isobutoxy-2-ethylhexane | 186 | C12H26O | 1000139-90-3 | 56 |
| 3 | Pentadecafluorooctanoic acid, 2-... | 526 | C16H17F15O2 | 1000406-80-9 | 53 |
| 4 | 2-Decene, 5-methyl-, (Z)- | 154 | C11H22 | 074645-86-6 | 50 |
| 5 | Carbonic acid, heptyl vinyl ester | 186 | C10H18O3 | 1010383-25-4 | 50 |



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**Instrument :**
BNA_G
**ClientSampleId :**
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

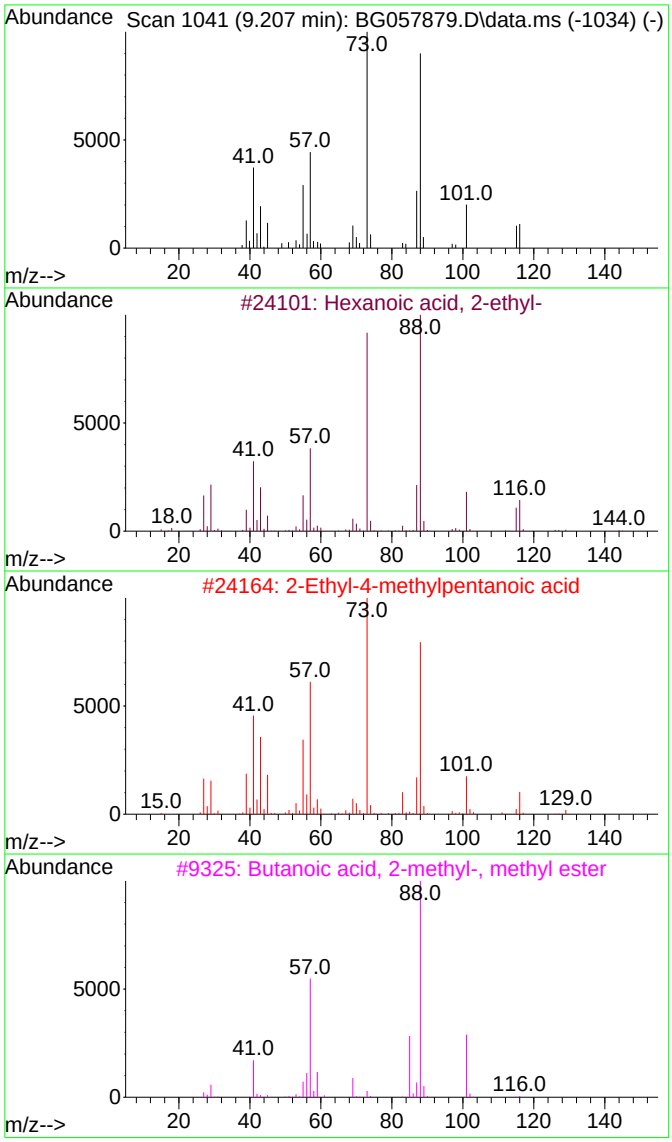
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

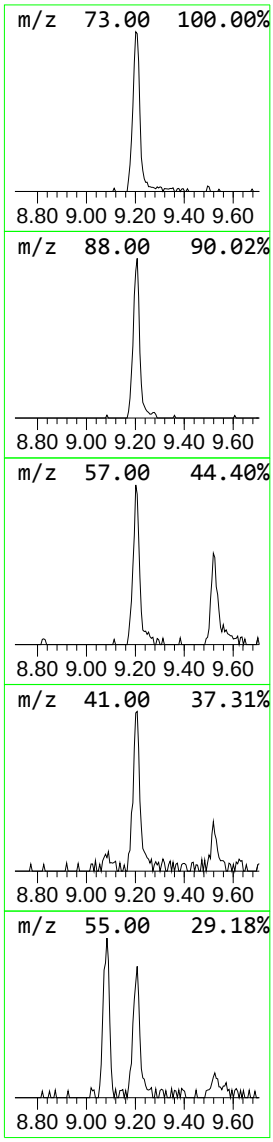
**********

Peak Number 3 Hexanoic acid, 2-ethyl- Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.207 | 11.69 ng | 100666 | 1,4-Dichlorobenzene-d4 | 7.920 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexanoic acid, 2-ethyl- | 144 | C8H16O2 | 000149-57-5 | 78 |
| 2 | 2-Ethyl-4-methylpentanoic acid | 144 | C8H16O2 | 000108-81-6 | 56 |
| 3 | Butanoic acid, 2-methyl-, methyl... | 116 | C6H12O2 | 000868-57-5 | 53 |
| 4 | Heptanoic acid, 2-ethyl- | 158 | C9H18O2 | 003274-29-1 | 40 |
| 5 | Butanoic acid, 2-ethyl-, 1,2,3-p... | 386 | C21H38O6 | 056554-54-2 | 38 |



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ALS Vial : 16 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
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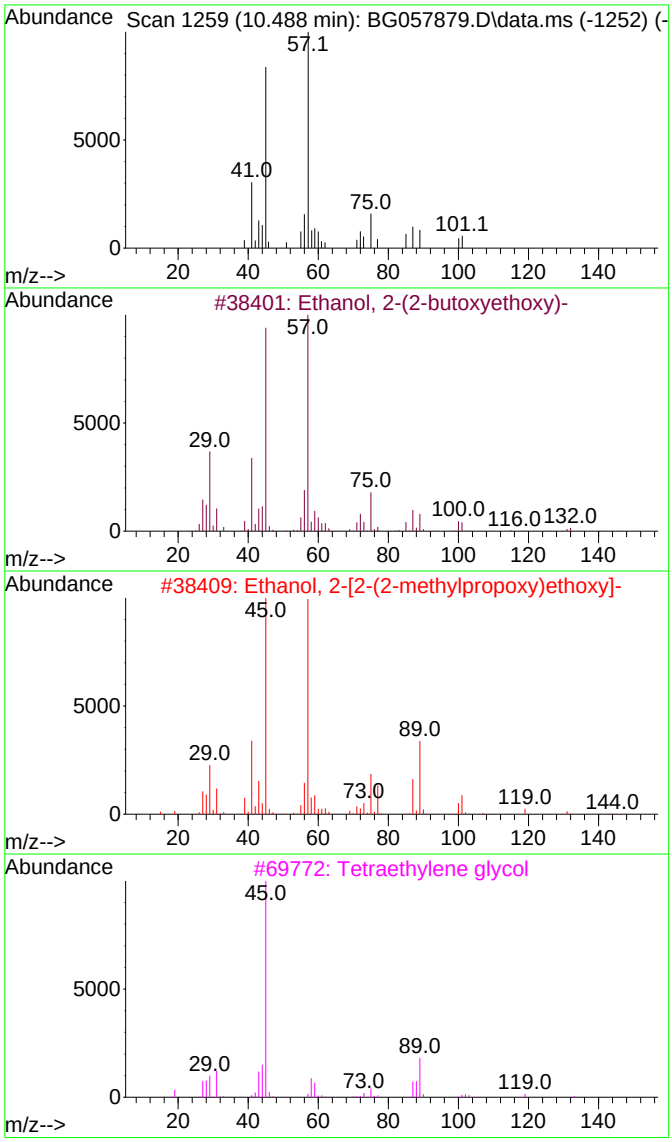
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

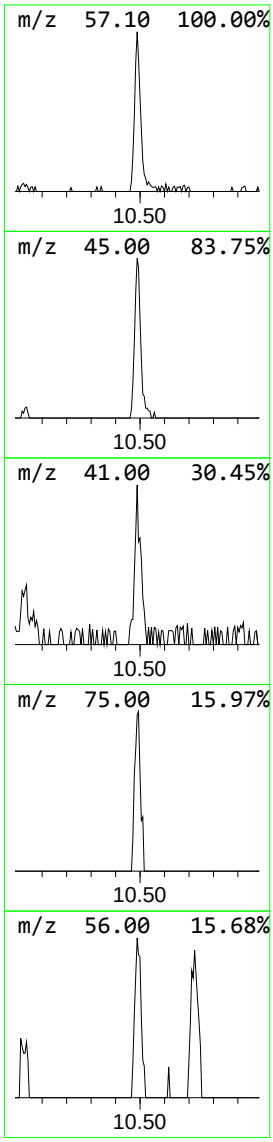
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.488 | 3.08 ng | 40231 | Naphthalene-d8 | 10.723 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Ethanol, 2-(2-butoxyethoxy)- | 162 | C8H18O3 | 000112-34-5 | 90 |
| 2 | Ethanol, 2-[2-(2-methylpropoxy)e... | 162 | C8H18O3 | 018912-80-6 | 56 |
| 3 | Tetraethylene glycol | 194 | C8H18O5 | 000112-60-7 | 53 |
| 4 | Butane, 1,1'-[oxybis(2,1-ethaned... | 218 | C12H26O3 | 000112-73-2 | 50 |
| 5 | Ethylene glycol monoisobutyl ether | 118 | C6H14O2 | 004439-24-1 | 45 |



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Sample : 03339-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
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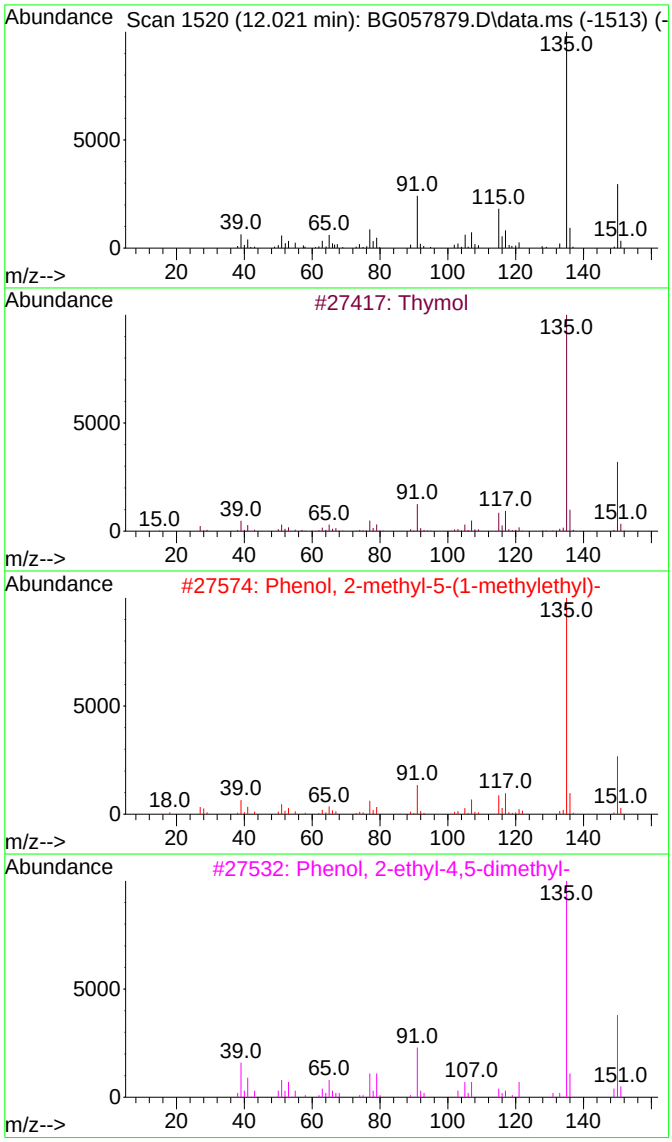
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

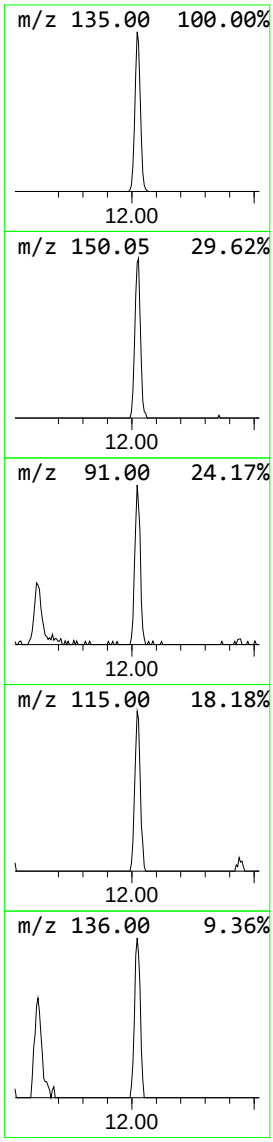
**********

Peak Number 5 Thymol Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.021 | 12.15 ng | 158684 | Naphthalene-d8 | 10.723 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Thymol | 150 | C10H14O | 000089-83-8 | 90 |
| 2 | Phenol, 2-methyl-5-(1-methylethyl)- | 150 | C10H14O | 000499-75-2 | 87 |
| 3 | Phenol, 2-ethyl-4,5-dimethyl- | 150 | C10H14O | 002219-78-5 | 80 |
| 4 | ortho-Methoxyacetophenone | 150 | C9H10O2 | 000579-74-8 | 72 |
| 5 | Phenol, 2-(1,1-dimethylethyl)- | 150 | C10H14O | 000088-18-6 | 72 |



Tentatively Identified Compound (LSC) summary

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

| | | | | | --Internal Standard--- | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 2-Pentanone, 4-... | 5.024 | 7.4 | ng | 64096 | 1 | 7.920 | 172291 | 20.0 |
| 1-Hexanol, 2-et... | 7.979 | 11.3 | ng | 96930 | 1 | 7.920 | 172291 | 20.0 |
| Hexanoic acid, ... | 9.207 | 11.7 | ng | 100666 | 1 | 7.920 | 172291 | 20.0 |
| Ethanol, 2-(2-b... | 10.488 | 3.1 | ng | 40231 | 2 | 10.723 | 261251 | 20.0 |
| Thymol | 12.021 | 12.2 | ng | 158684 | 2 | 10.723 | 261251 | 20.0 |