LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080624\
Data File : BF138817.D
Acq On : 06 Aug 2024 20:45
Operator : RC/JU
Sample : P3458-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
MLS-15-224-239

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_F\Methods\8270-BF073024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138817.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.134 | 3 | 7 | 13 | rVB | 1865695 | 2793113 | 35.34% | 11.754% |
| 2 | 3.910 | 301 | 309 | 322 | rBB | 724564 | 1152076 | 14.58% | 4.848% |
| 3 | 5.534 | 579 | 585 | 601 | rVB | 214382 | 537129 | 6.80% | 2.260% |
| 4 | 5.857 | 623 | 640 | 645 | rBV | 2488539 | 7902997 | 100.00% | 33.257% |
| 5 | 6.481 | 741 | 746 | 757 | rBV | 259396 | 361497 | 4.57% | 1.521% |
| 6 | 6.840 | 802 | 807 | 812 | rBV | 232437 | 282309 | 3.57% | 1.188% |
| 7 | 7.404 | 896 | 903 | 908 | rBV | 712121 | 982362 | 12.43% | 4.134% |
| 8 | 8.122 | 1019 | 1025 | 1030 | rBV | 287676 | 374420 | 4.74% | 1.576% |
| 9 | 8.339 | 1055 | 1062 | 1064 | rBV | 906023 | 1239648 | 15.69% | 5.217% |
| 10 | 8.369 | 1064 | 1067 | 1076 | rVV | 1085375 | 1480810 | 18.74% | 6.232% |
| 11 | 8.481 | 1083 | 1086 | 1105 | rVB | 41137 | 80568 | 1.02% | 0.339% |
| 12 | 9.192 | 1201 | 1207 | 1212 | rBV | 1398573 | 1811678 | 22.92% | 7.624% |
| 13 | 9.869 | 1317 | 1322 | 1328 | rBV | 338866 | 431375 | 5.46% | 1.815% |
| 14 | 9.969 | 1332 | 1339 | 1353 | rVV | 590968 | 934107 | 11.82% | 3.931% |
| 15 | 10.663 | 1452 | 1457 | 1472 | rBV | 729108 | 961466 | 12.17% | 4.046% |
| 16 | 11.357 | 1570 | 1575 | 1583 | rBV | 357747 | 437837 | 5.54% | 1.843% |
| 17 | 12.445 | 1752 | 1760 | 1766 | rBV | 68639 | 90469 | 1.14% | 0.381% |
| 18 | 12.939 | 1839 | 1844 | 1849 | rBV | 1092916 | 1441520 | 18.24% | 6.066% |
| 19 | 13.998 | 2019 | 2024 | 2031 | rVB | 180854 | 236337 | 2.99% | 0.995% |
| 20 | 15.457 | 2266 | 2272 | 2280 | rBV | 150900 | 231449 | 2.93% | 0.974% |

Sum of corrected areas: 23763167

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080624\
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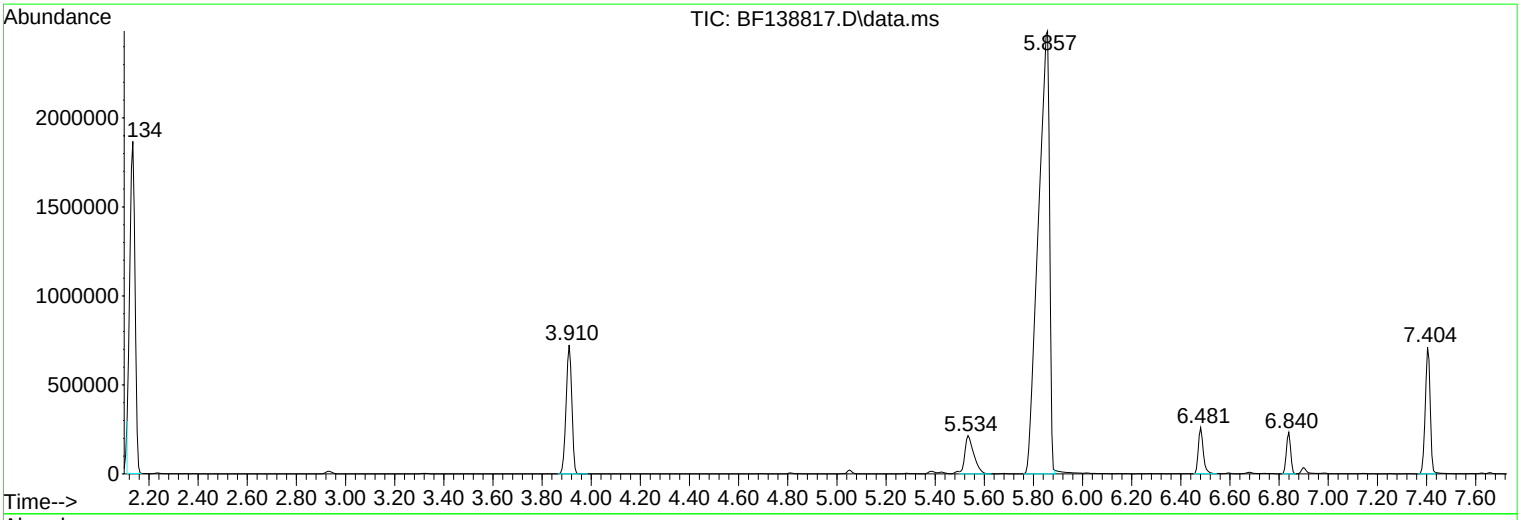
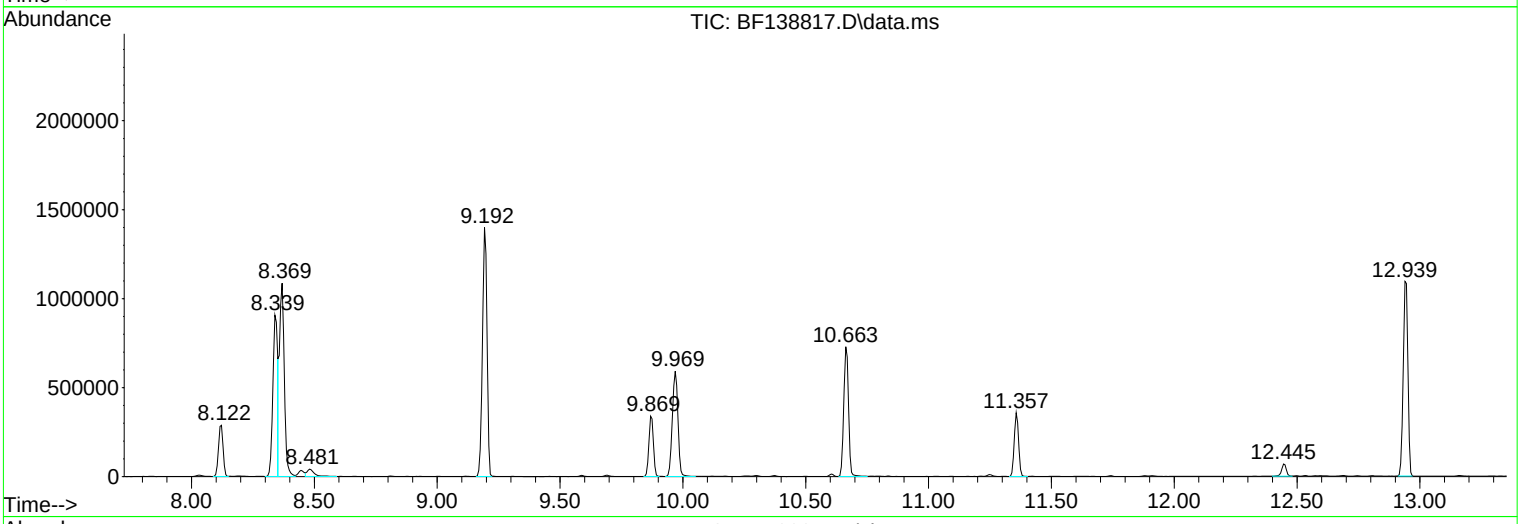
Sample : P3458-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

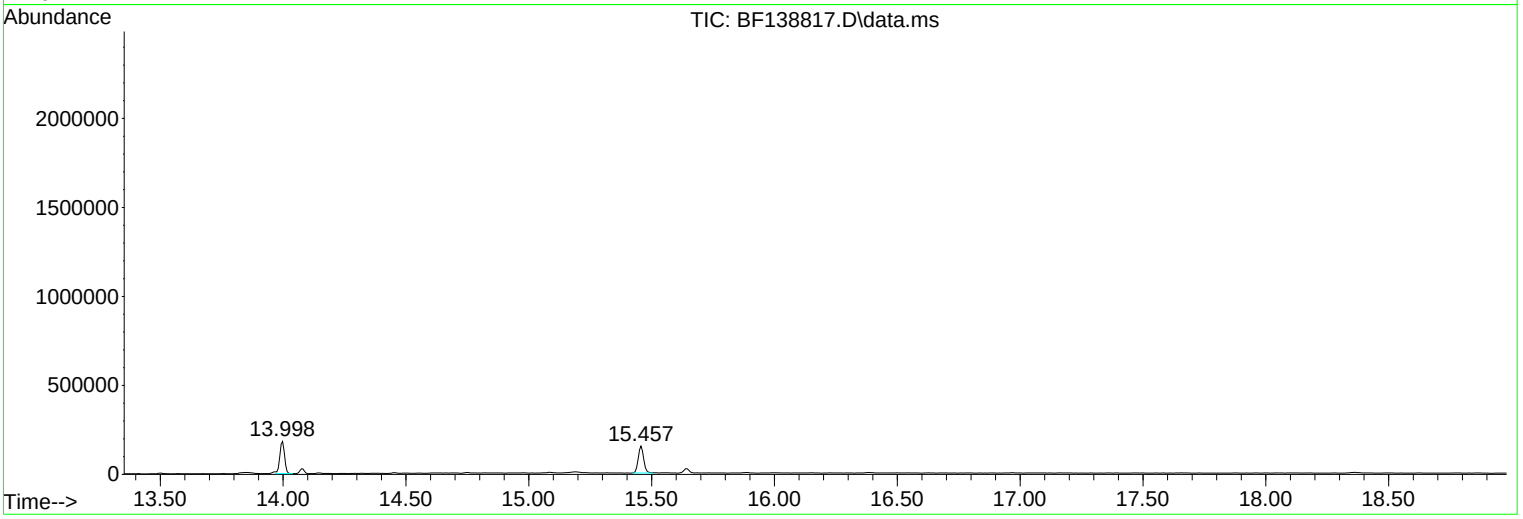
**Instrument :**
BNA_F
**ClientSampleId :**
MLS-15-224-239

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.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 : BF138817.D
Acq On : 06 Aug 2024 20:45
Operator : RC/JU
Sample : P3458-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
MLS-15-224-239

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

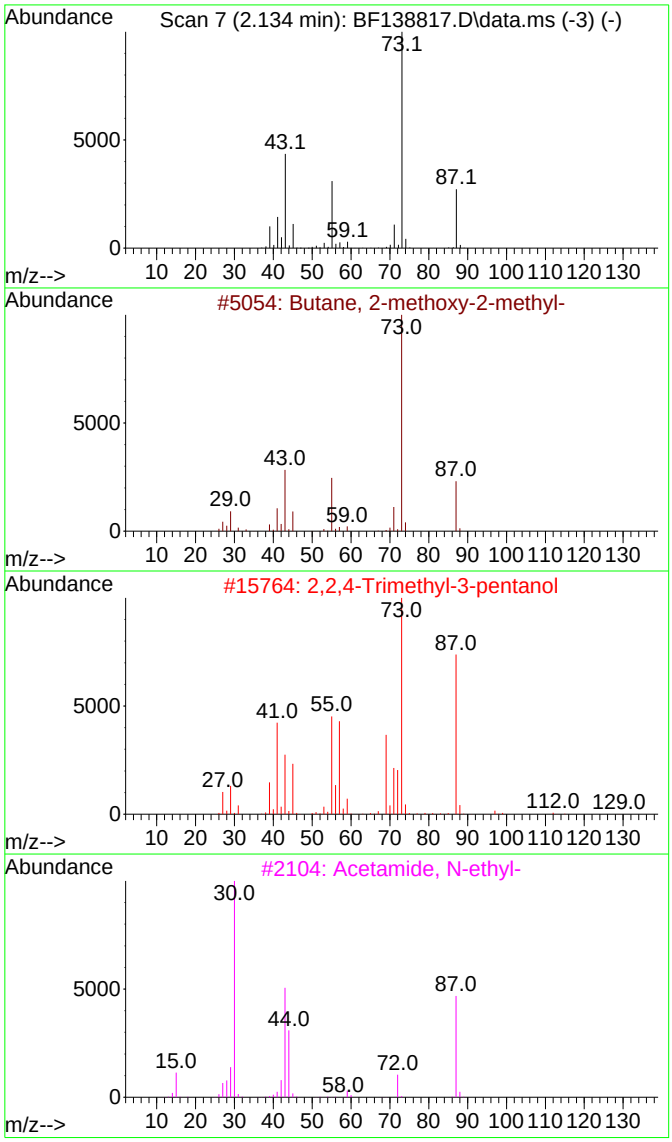
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

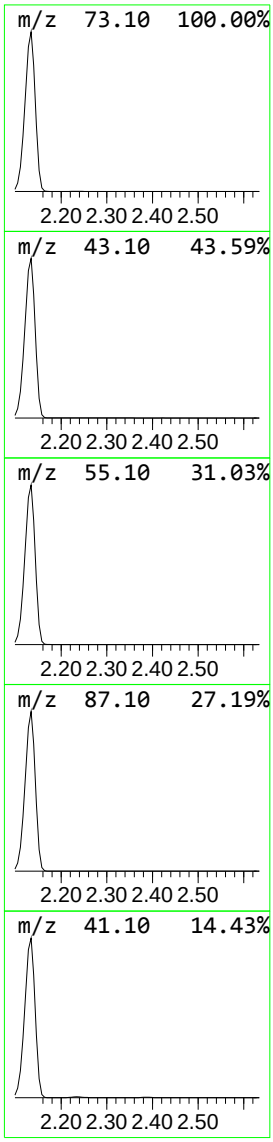
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.134 | 197.88 ng | 2793110 | 1,4-Dichlorobenzene-d4 | 6.840 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 83 |
| 2 | 2,2,4-Trimethyl-3-pentanol | 130 | C8H18O | 005162-48-1 | 39 |
| 3 | Acetamide, N-ethyl- | 87 | C4H9NO | 000625-50-3 | 27 |
| 4 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 12 |
| 5 | Borane, dimethoxy- | 74 | C2H7BO2 | 004542-61-4 | 9 |



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Data File : BF138817.D
Acq On : 06 Aug 2024 20:45
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Sample : P3458-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
MLS-15-224-239

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

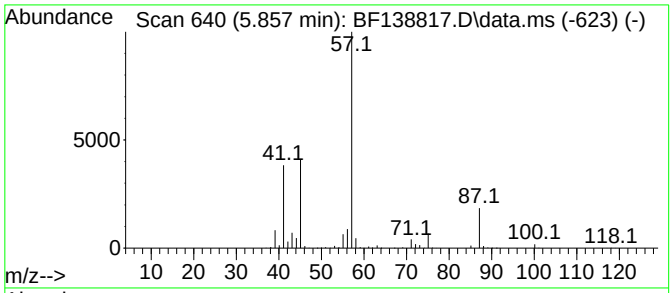
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

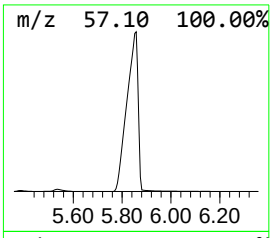
**********

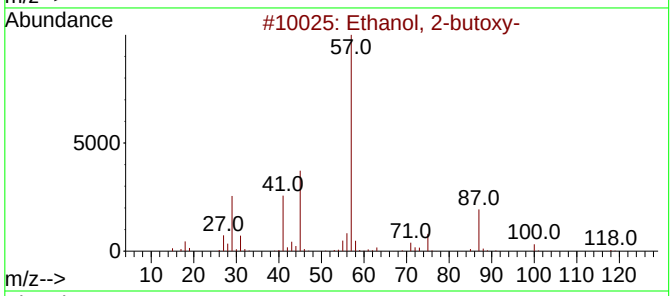
Peak Number 3 Ethanol, 2-butoxy- Concentration Rank 1

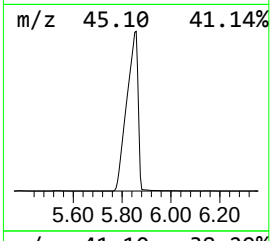
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.857 | 559.88 ng | 7903000 | 1,4-Dichlorobenzene-d4 | 6.840 |

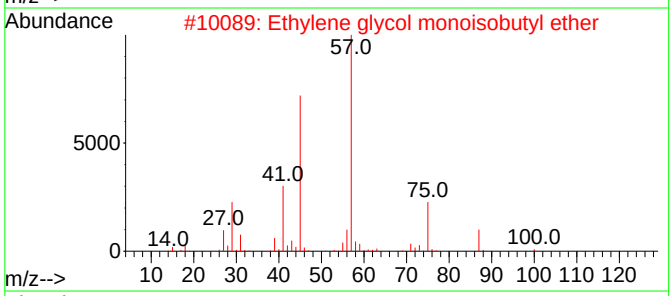
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Ethanol, 2-butoxy- | 118 | C6H14O2 | 000111-76-2 | 91 |
| 2 | Ethylene glycol monoisobutyl ether | 118 | C6H14O2 | 004439-24-1 | 64 |
| 3 | Formic acid, 3,3-dimethylbut-2-y... | 130 | C7H14O2 | 1000368-20-5 | 23 |
| 4 | 1,3-Propanediol, 2-methyl-, dipr... | 202 | C10H18O4 | 054932-83-1 | 17 |
| 5 | Propanoic acid, 2-methylpropyl e... | 130 | C7H14O2 | 000540-42-1 | 17 |

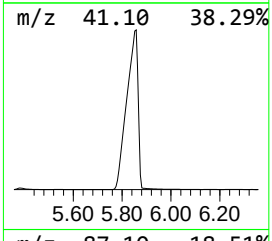


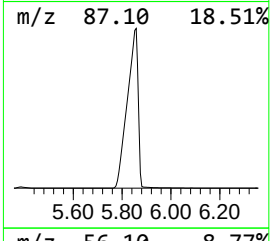



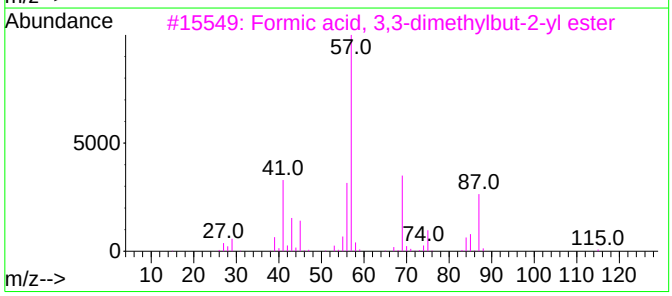



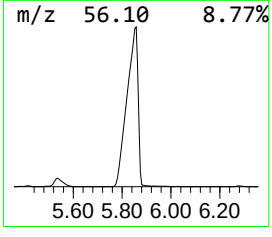



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Acq On : 06 Aug 2024 20:45
Operator : RC/JU
Sample : P3458-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
MLS-15-224-239

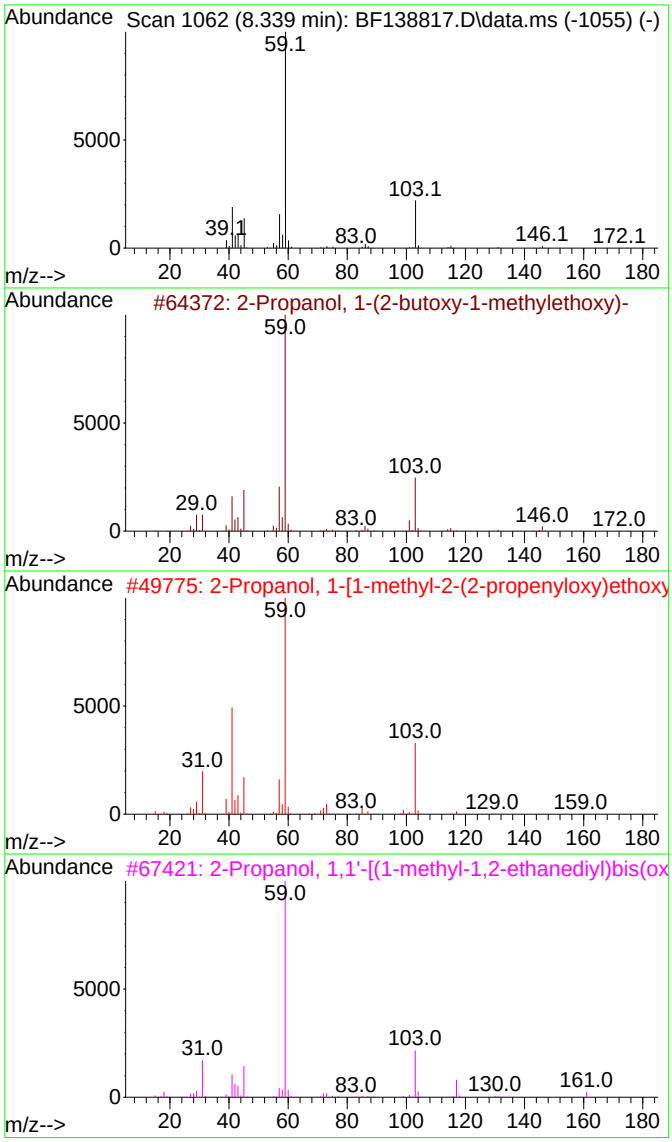
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

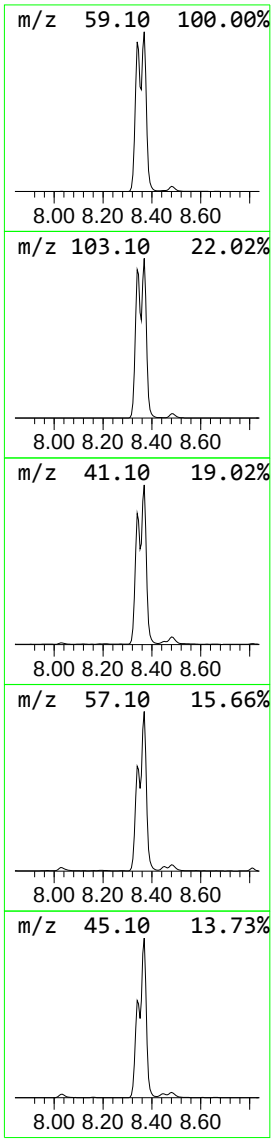
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 4 2-Propanol, 1-(2-butoxy-1-m... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.339 | 66.22 ng | 1239650 | Naphthalene-d8 | 8.122 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Propanol, 1-(2-butoxy-1-methyl... | 190 | C10H22O3 | 029911-28-2 | 83 |
| 2 | 2-Propanol, 1-[1-methyl-2-(2-pro... | 174 | C9H18O3 | 055956-25-7 | 83 |
| 3 | 2-Propanol, 1,1'-[(1-methyl-1,2-... | 192 | C9H20O4 | 001638-16-0 | 78 |
| 4 | 1-Propanol, 2-(2-hydroxypropoxy)- | 134 | C6H14O3 | 000106-62-7 | 78 |
| 5 | Tetraglyme | 222 | C10H22O5 | 000143-24-8 | 72 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080624\
Data File : BF138817.D
Acq On : 06 Aug 2024 20:45
Operator : RC/JU
Sample : P3458-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
MLS-15-224-239

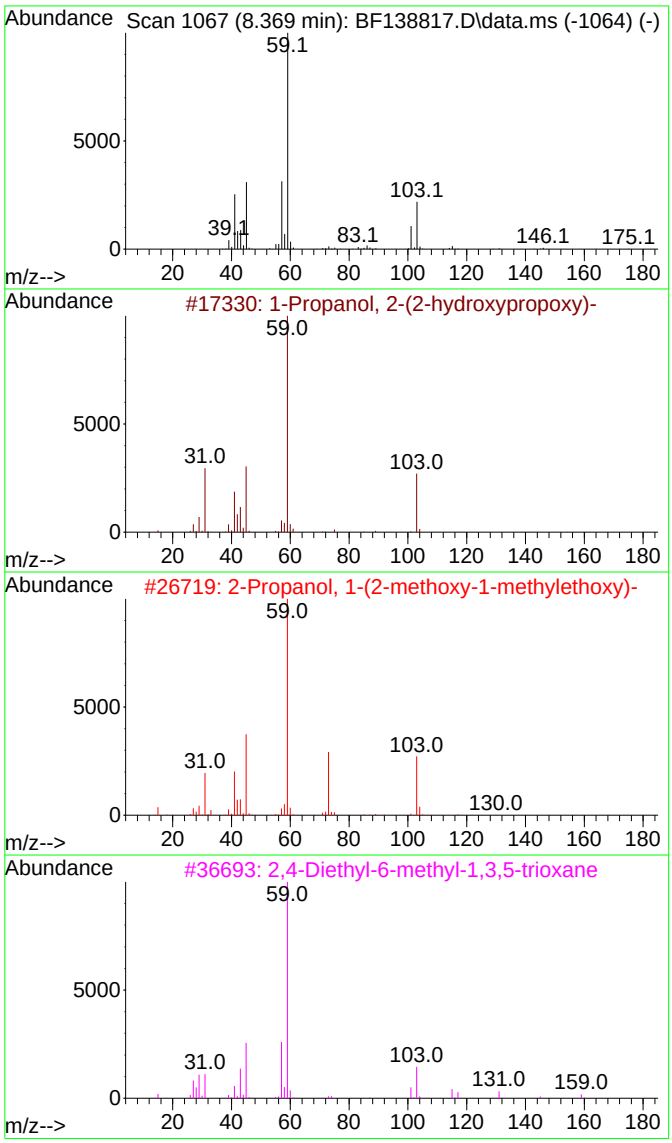
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

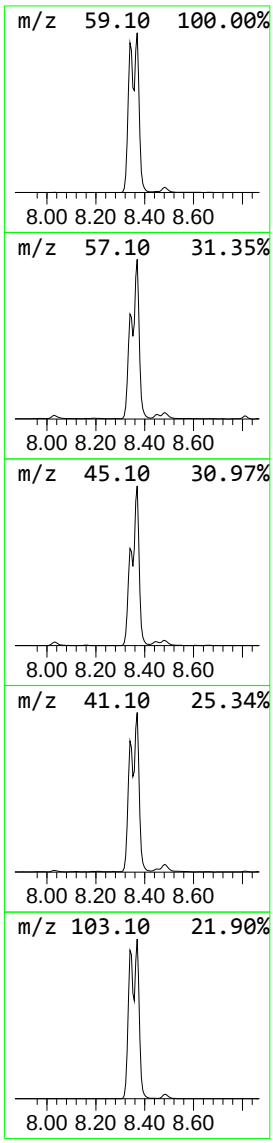
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 5 1-Propanol, 2-(2-hydroxypro... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.369 | 79.10 ng | 1480810 | Naphthalene-d8 | 8.122 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Propanol, 2-(2-hydroxypropoxy)- | 134 | C6H14O3 | 000106-62-7 | 72 |
| 2 | 2-Propanol, 1-(2-methoxy-1-methy... | 148 | C7H16O3 | 020324-32-7 | 72 |
| 3 | 2,4-Diethyl-6-methyl-1,3,5-trioxane | 160 | C8H16O3 | 117888-04-7 | 64 |
| 4 | 1-Propanol, 2,2'-oxybis- | 134 | C6H14O3 | 000108-61-2 | 64 |
| 5 | 2-Propanol, 1-(2-butoxy-1-methyl... | 190 | C10H22O3 | 029911-28-2 | 64 |



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BNA_F
**ClientSampleId :**
MLS-15-224-239

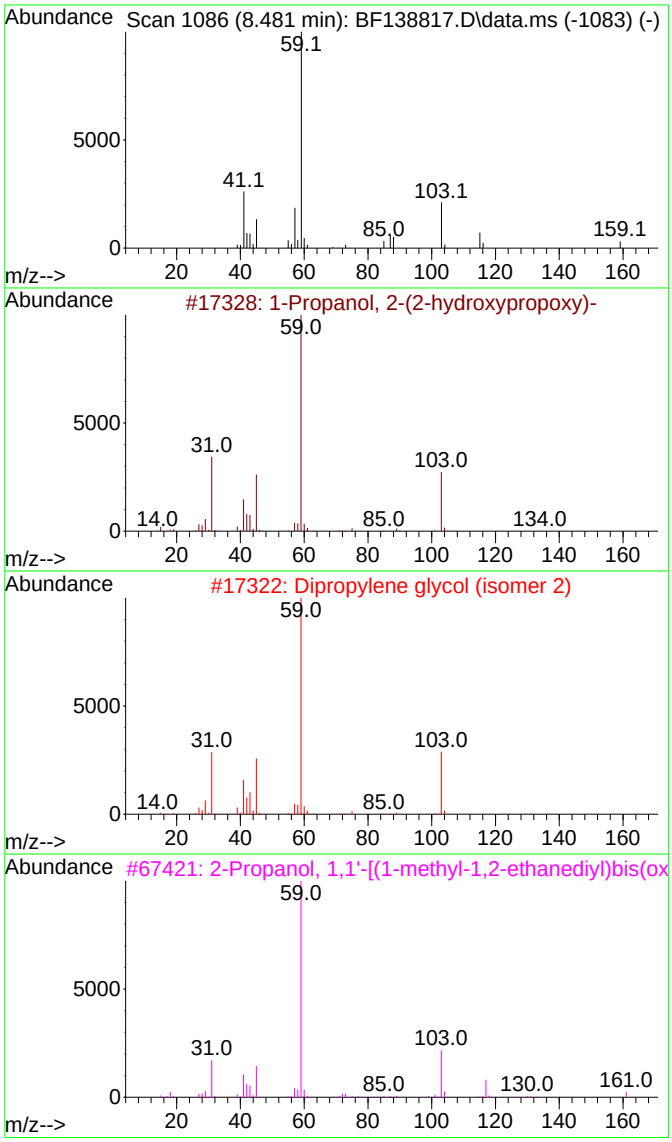
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

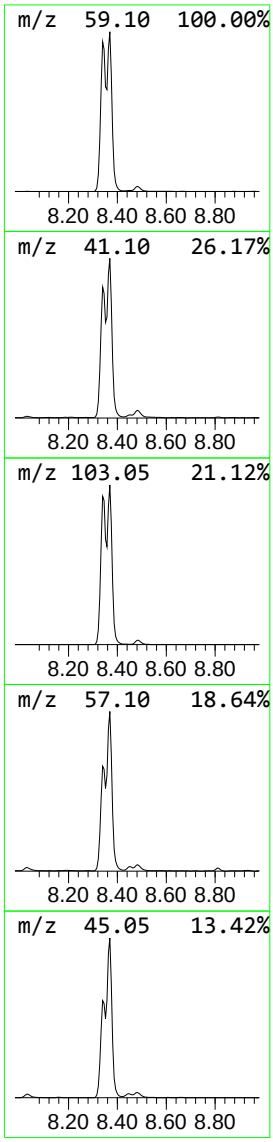
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 6 Dipropylene glycol (isomer 2) Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.481 | 4.30 ng | 80568 | Naphthalene-d8 | 8.122 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Propanol, 2-(2-hydroxypropoxy)- | 134 | C6H14O3 | 000106-62-7 | 64 |
| 2 | Dipropylene glycol (isomer 2) | 134 | C6H14O3 | 1000506-25-4 | 64 |
| 3 | 2-Propanol, 1,1'-[(1-methyl-1,2-... | 192 | C9H20O4 | 001638-16-0 | 64 |
| 4 | Methane, diethoxy- | 104 | C5H12O2 | 000462-95-3 | 64 |
| 5 | 2-Propanol, 1-[1-methyl-2-(2-pro... | 174 | C9H18O3 | 055956-25-7 | 56 |



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Data File : BF138817.D
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Operator : RC/JU
Sample : P3458-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
MLS-15-224-239

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

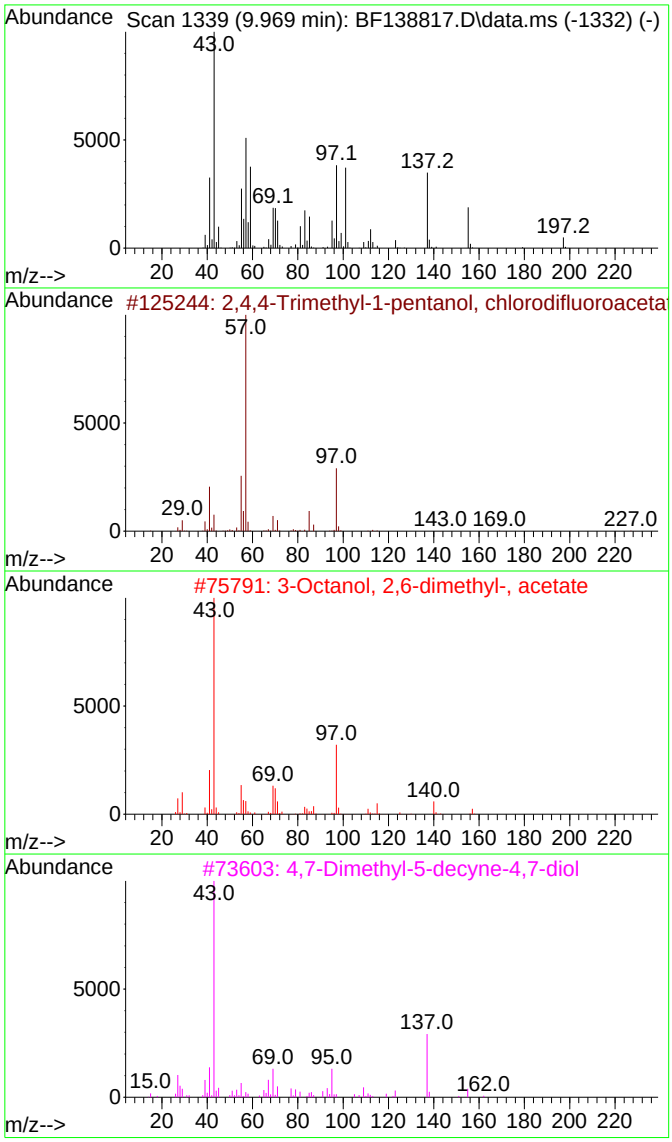
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

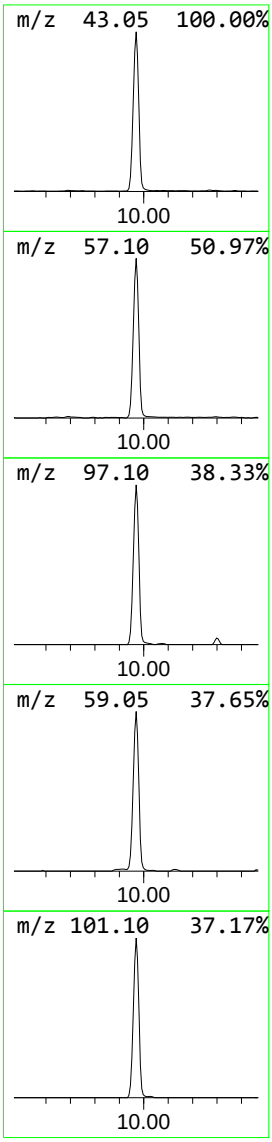
**********

Peak Number 7 unknown9.969 Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.969 | 43.31 ng | 934107 | Acenaphthene-d10 | 9.869 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2,4,4-Trimethyl-1-pentanol, chlo... | 242 | C10H17ClF2O2 | 1000447-27-2 | 22 |
| 2 | 3-Octanol, 2,6-dimethyl-, acetate | 200 | C12H24O2 | 123232-57-5 | 10 |
| 3 | 4,7-Dimethyl-5-decyne-4,7-diol | 198 | C12H22O2 | 000126-87-4 | 10 |
| 4 | Pentadecane, 1-bromo- | 290 | C15H31Br | 000629-72-1 | 10 |
| 5 | 2-Piperidinone, N-[4-bromo-n-but... | 233 | C9H16BrNO | 195194-80-0 | 10 |



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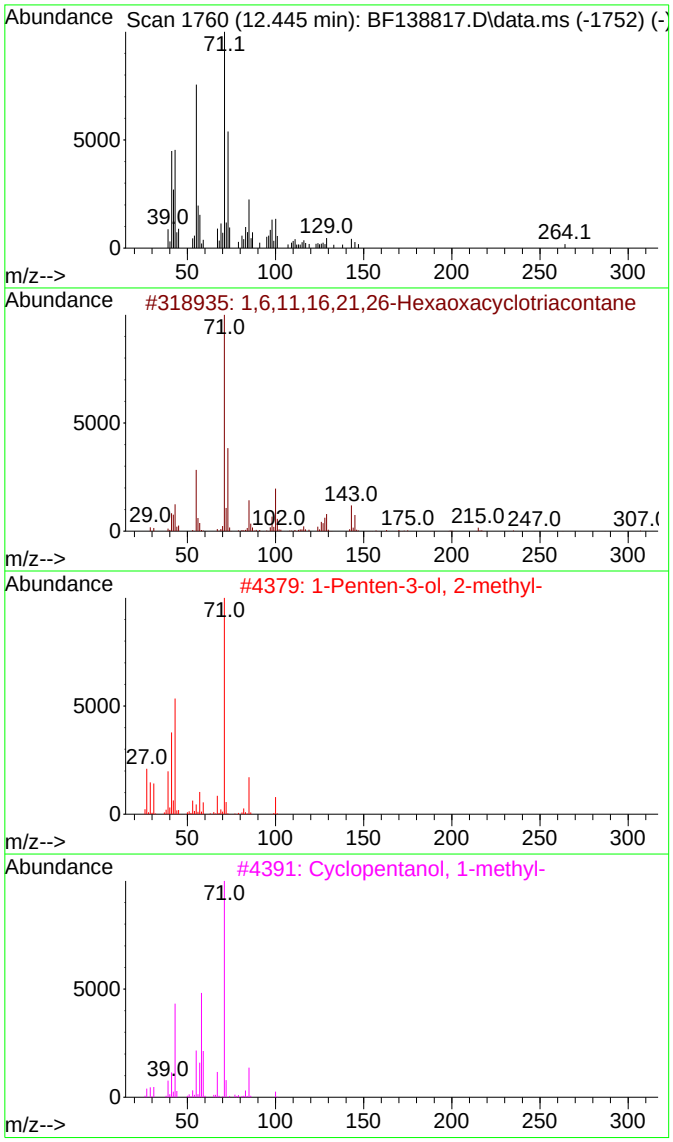
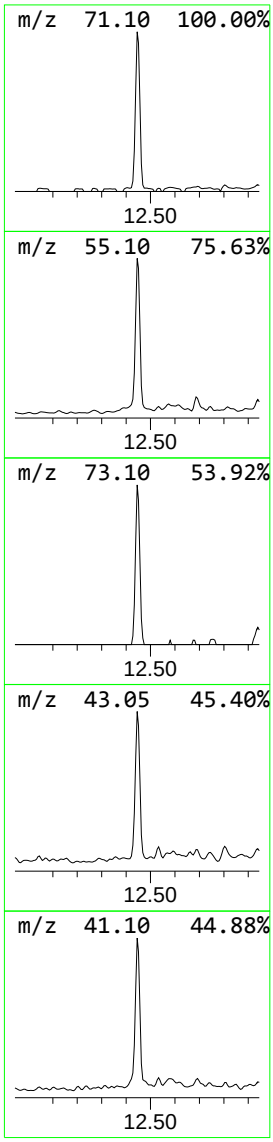
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 8 1,6,11,16,21,26-Hexaoxacycl... Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.445 | 4.13 ng | 90469 | Phenanthrene-d10 | 11.357 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,6,11,16,21,26-Hexaoxacyclotria... | 432 | C24H48O6 | 064001-05-4 | 53 |
| 2 | 1-Penten-3-ol, 2-methyl- | 100 | C6H12O | 002088-07-5 | 52 |
| 3 | Cyclopentanol, 1-methyl- | 100 | C6H12O | 001462-03-9 | 49 |
| 4 | Cis-3-methylpent-3-ene-5-ol | 100 | C6H12O | 030804-75-2 | 43 |
| 5 | 3-Methoxy-1-pentene | 100 | C6H12O | 014092-18-3 | 43 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080624\
Data File : BF138817.D
Acq On : 06 Aug 2024 20:45
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Sample : P3458-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
MLS-15-224-239

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.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... | 2.134 | 197.9 | ng | 2793110 | 1 | 6.840 | 282309 | 20.0 |
| Ethanol, 2-butoxy- | 5.857 | 559.9 | ng | 7903000 | 1 | 6.840 | 282309 | 20.0 |
| 2-Propanol, 1-(... | 8.339 | 66.2 | ng | 1239650 | 2 | 8.122 | 374420 | 20.0 |
| 1-Propanol, 2-(... | 8.369 | 79.1 | ng | 1480810 | 2 | 8.122 | 374420 | 20.0 |
| Dipropylene gly... | 8.481 | 4.3 | ng | 80568 | 2 | 8.122 | 374420 | 20.0 |
| unknown9.969 | 9.969 | 43.3 | ng | 934107 | 3 | 9.869 | 431375 | 20.0 |
| 1,6,11,16,21,26... | 12.445 | 4.1 | ng | 90469 | 4 | 11.357 | 437837 | 20.0 |