LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071516\
Data File : BG023133.D
Acq On : 16 Jul 2016 5:36
Operator : UM/SJ
Sample : H4016-14
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** C5-16

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:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.893 | 6 | 9 | 20 | rVB2 | 118987 | 246747 | 3.87% | 0.525% |
| 2 | 3.040 | 29 | 34 | 48 | rVB | 1208786 | 1635709 | 25.64% | 3.481% |
| 3 | 3.187 | 54 | 59 | 70 | rVB3 | 98510 | 199096 | 3.12% | 0.424% |
| 4 | 3.304 | 75 | 79 | 87 | rVB3 | 39441 | 71060 | 1.11% | 0.151% |
| 5 | 5.220 | 399 | 405 | 412 | rBV | 260413 | 403617 | 6.33% | 0.859% |
| 6 | 5.696 | 479 | 486 | 498 | rBV | 1886596 | 3067723 | 48.08% | 6.529% |
| 7 | 7.305 | 752 | 760 | 777 | rBV | 2192054 | 3895959 | 61.07% | 8.292% |
| 8 | 7.681 | 816 | 824 | 832 | rBV | 1931918 | 3420942 | 53.62% | 7.281% |
| 9 | 8.152 | 895 | 904 | 914 | rBV2 | 357034 | 642321 | 10.07% | 1.367% |
| 10 | 8.475 | 949 | 959 | 968 | rVB | 1297261 | 2281493 | 35.76% | 4.856% |
| 11 | 9.327 | 1095 | 1104 | 1112 | rBV | 1311413 | 2423724 | 37.99% | 5.158% |
| 12 | 9.427 | 1116 | 1121 | 1127 | rBV3 | 50543 | 90464 | 1.42% | 0.193% |
| 13 | 10.978 | 1375 | 1385 | 1392 | rBV | 551746 | 1013220 | 15.88% | 2.156% |
| 14 | 13.416 | 1791 | 1800 | 1812 | rBV | 3137643 | 4934835 | 77.35% | 10.503% |
| 15 | 14.239 | 1932 | 1940 | 1956 | rBV | 1140269 | 1715406 | 26.89% | 3.651% |
| 16 | 14.797 | 2028 | 2035 | 2043 | rBV2 | 996987 | 1659541 | 26.01% | 3.532% |
| 17 | 16.289 | 2282 | 2289 | 2302 | rBV | 3194192 | 4983618 | 78.11% | 10.607% |
| 18 | 16.477 | 2317 | 2321 | 2325 | rBV3 | 47388 | 71887 | 1.13% | 0.153% |
| 19 | 17.276 | 2454 | 2457 | 2460 | rBV2 | 71291 | 84375 | 1.32% | 0.180% |
| 20 | 17.552 | 2497 | 2504 | 2518 | rBV | 1316755 | 2062527 | 32.33% | 4.390% |
| 21 | 18.016 | 2579 | 2583 | 2588 | rBV3 | 52787 | 69953 | 1.10% | 0.149% |
| 22 | 18.416 | 2646 | 2651 | 2664 | rBV2 | 182999 | 298710 | 4.68% | 0.636% |
| 23 | 19.679 | 2862 | 2866 | 2872 | rBV8 | 43150 | 76010 | 1.19% | 0.162% |
| 24 | 20.149 | 2940 | 2946 | 2953 | rBV | 4929063 | 6379883 | 100.00% | 13.578% |
| 25 | 21.477 | 3165 | 3172 | 3174 | rBV6 | 113759 | 203187 | 3.18% | 0.432% |
| 26 | 21.859 | 3229 | 3237 | 3243 | rBV2 | 1322431 | 2295823 | 35.99% | 4.886% |
| 27 | 22.729 | 3377 | 3385 | 3388 | rBV10 | 75471 | 164106 | 2.57% | 0.349% |
| 28 | 25.232 | 3801 | 3811 | 3831 | rVB2 | 650256 | 2155252 | 33.78% | 4.587% |
| 29 | 29.591 | 4546 | 4553 | 4555 | rBV8 | 70360 | 146693 | 2.30% | 0.312% |
| 30 | 30.014 | 4619 | 4625 | 4637 | rVB8 | 82286 | 291544 | 4.57% | 0.620% |

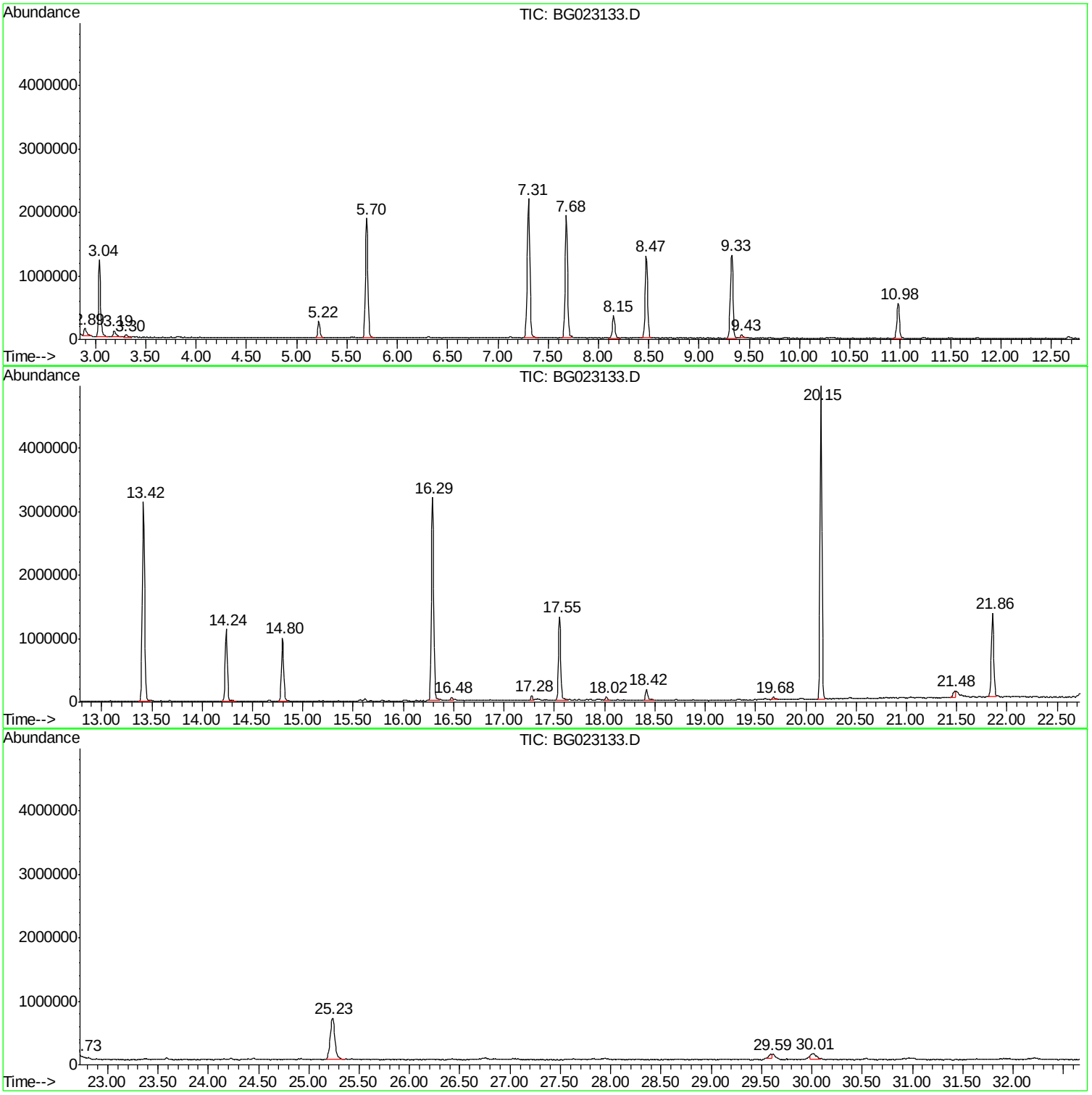
Sum of corrected areas: 46985425

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071516\
Data File : BG023133.D
Acq On : 16 Jul 2016 5:36
Operator : UM/SJ
Sample : H4016-14
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
C5-16

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

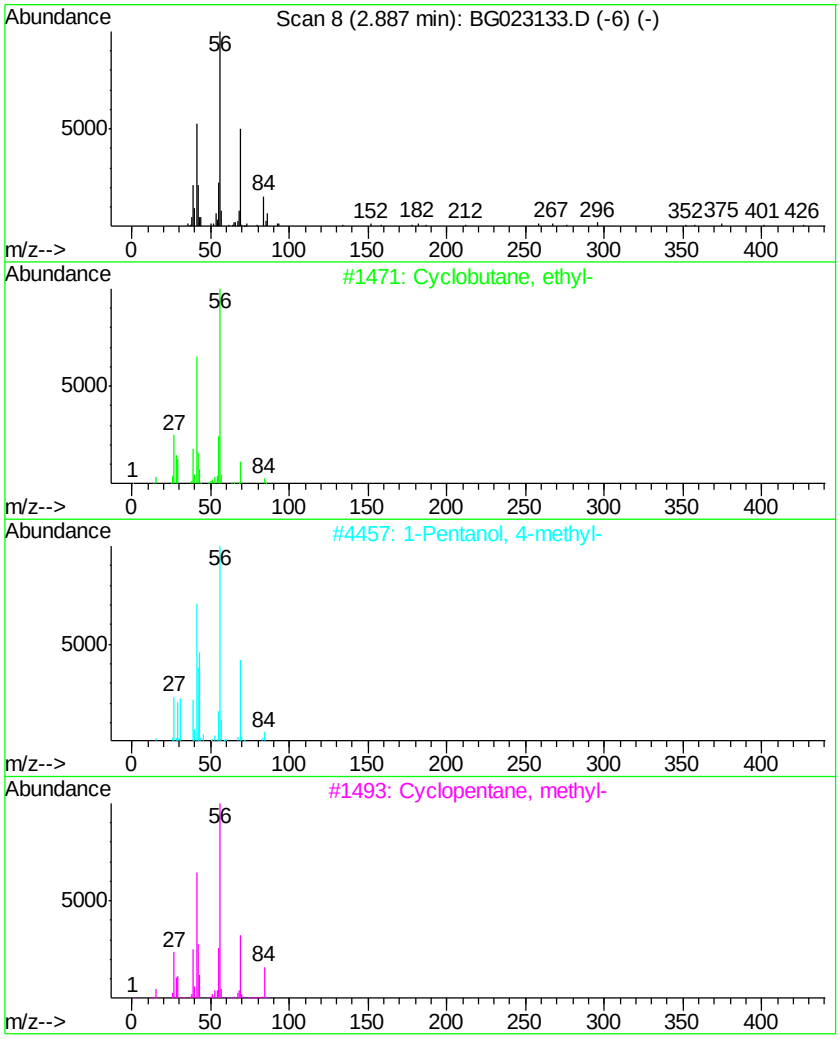
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

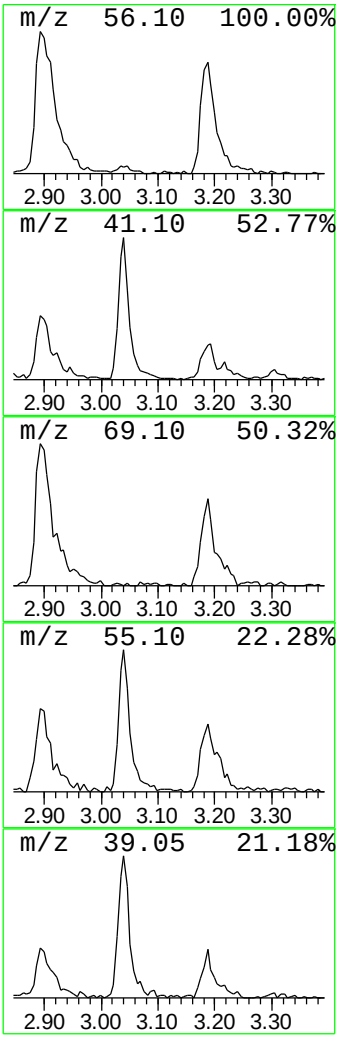
**********

Peak Number 1 Cyclobutane, ethyl- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.89 | 7.68 ng | 246747 | 1,4-Dichlorobenzene-d4 | 8.15 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclobutane, ethyl- | 84 | C6H12 | 004806-61-5 | 59 |
| 2 | 1-Pentanol, 4-methyl- | 102 | C6H14O | 000626-89-1 | 50 |
| 3 | Cyclopentane, methyl- | 84 | C6H12 | 000096-37-7 | 50 |
| 4 | 1-Hexene, 2,5-dimethyl- | 112 | C8H16 | 006975-92-4 | 42 |
| 5 | Cyclobutane | 56 | C4H8 | 000287-23-0 | 40 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071516\
Data File : BG023133.D
Acq On : 16 Jul 2016 5:36
Operator : UM/SJ
Sample : H4016-14
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** C5-16

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

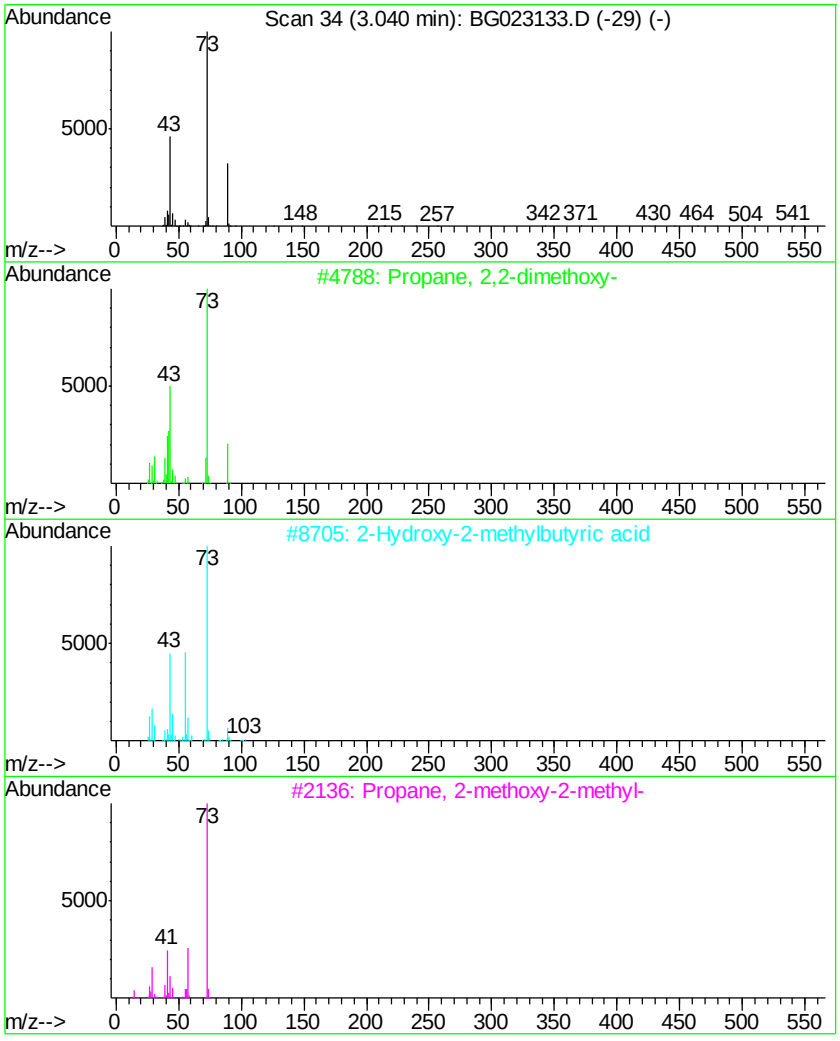
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

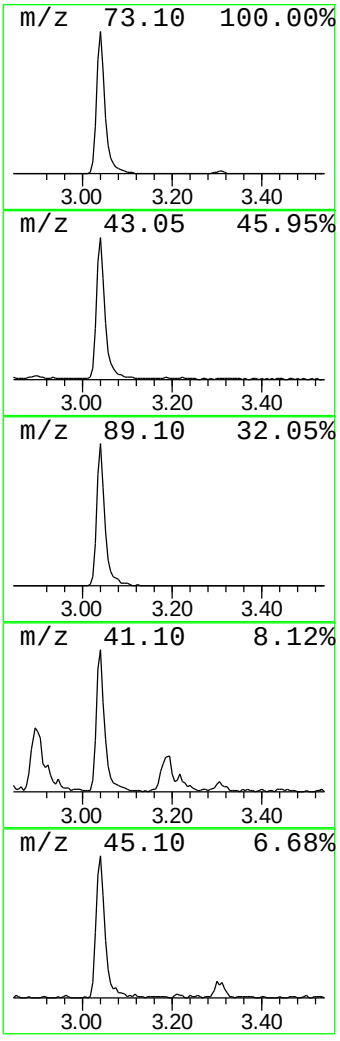
**********

Peak Number 2 Propane, 2,2-dimethoxy- Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.04 | 50.93 ng | 1635710 | 1,4-Dichlorobenzene-d4 | 8.15 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Propane, 2,2-dimethoxy- | 104 | C5H12O2 | 000077-76-9 | 50 |
| 2 | 2-Hydroxy-2-methylbutyric acid | 118 | C5H10O3 | 003739-30-8 | 9 |
| 3 | Propane, 2-methoxy-2-methyl- | 88 | C5H12O | 001634-04-4 | 9 |
| 4 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 9 |
| 5 | N-Ethylformamide | 73 | C3H7NO | 000627-45-2 | 5 |



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071516\
Data File : BG023133.D
Acq On : 16 Jul 2016 5:36
Operator : UM/SJ
Sample : H4016-14
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** C5-16

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

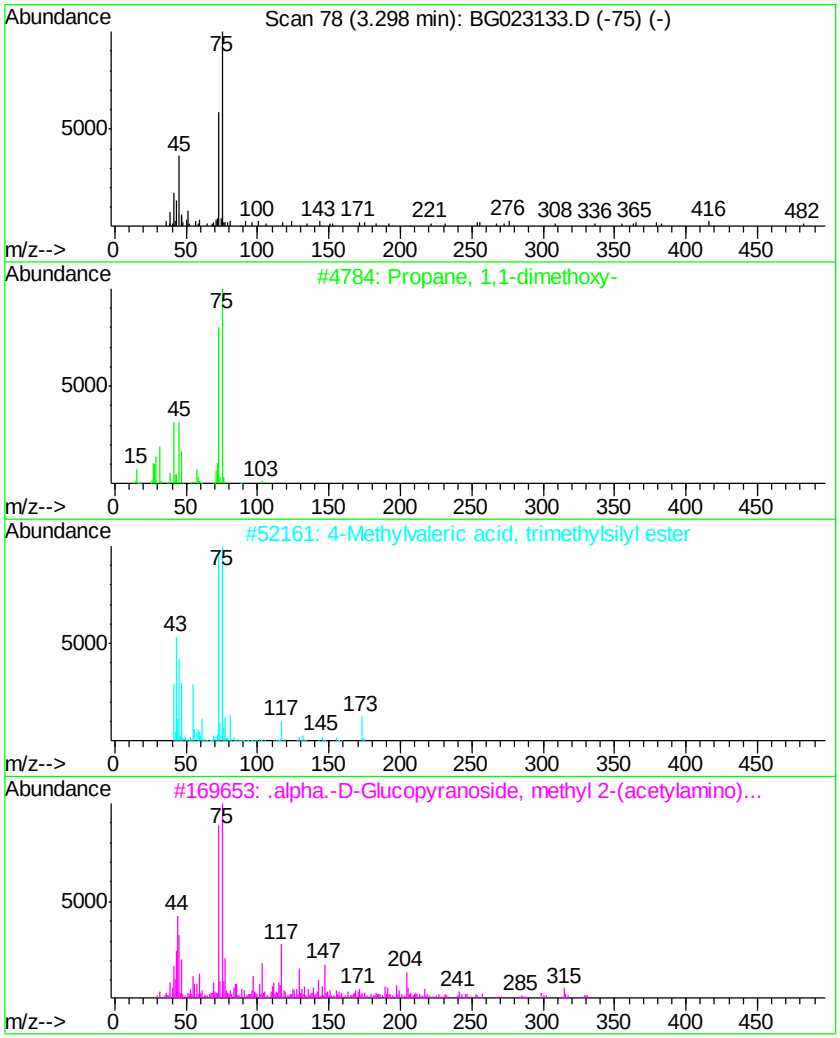
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

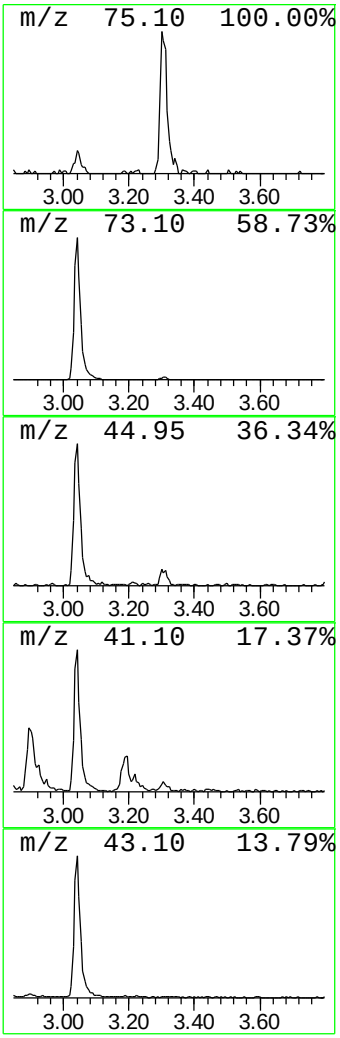
**********

Peak Number 4 Propane, 1,1-dimethoxy- Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.30 | 2.21 ng | 71060 | 1,4-Dichlorobenzene-d4 | 8.15 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Propane, 1,1-dimethoxy- | 104 | C5H12O2 | 004744-10-9 | 72 |
| 2 | 4-Methylvaleric acid, trimethyls... | 188 | C9H20O2Si | 959048-10-3 | 56 |
| 3 | .alpha.-D-Glucopyranoside, methy... | 331 | C13H26BNO6Si | 054477-01-9 | 45 |
| 4 | .beta.-Alanine, trimethylsilyl e... | 161 | C6H15NO2Si | 005269-40-9 | 45 |
| 5 | Pentonic acid, 2-deoxy-3,5-bis-O... | 276 | C11H24O4Si2 | 074742-34-0 | 40 |



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071516\
Data File : BG023133.D
Acq On : 16 Jul 2016 5:36
Operator : UM/SJ
Sample : H4016-14
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** C5-16

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

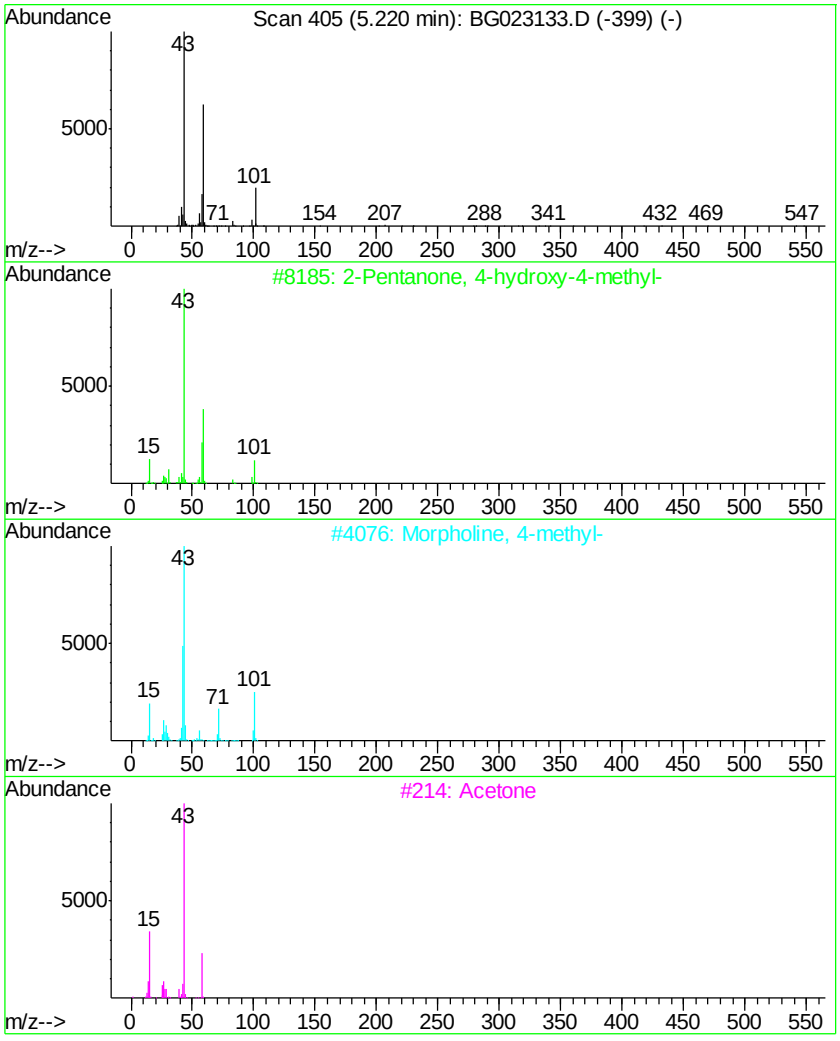
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

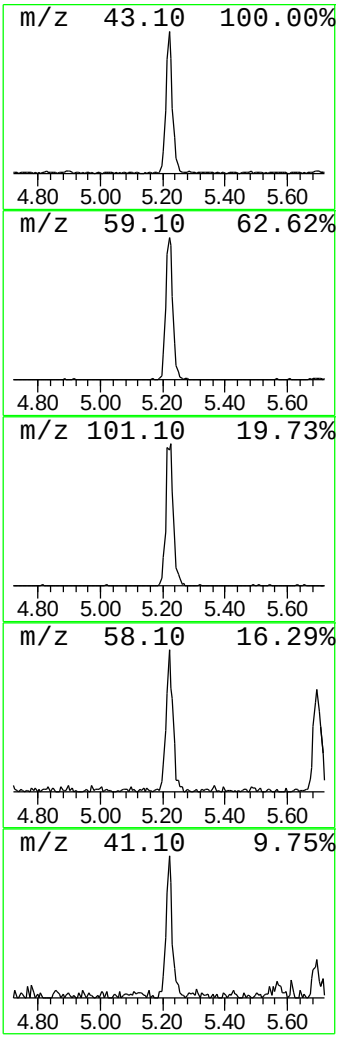
**********

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.22 | 12.57 ng | 403617 | 1,4-Dichlorobenzene-d4 | 8.15 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 50 |
| 2 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |
| 3 | Acetone | 58 | C3H6O | 000067-64-1 | 9 |
| 4 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |
| 5 | Butane, 1-ethoxy- | 102 | C6H14O | 000628-81-9 | 9 |



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Data File : BG023133.D
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Operator : UM/SJ
Sample : H4016-14
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** C5-16

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

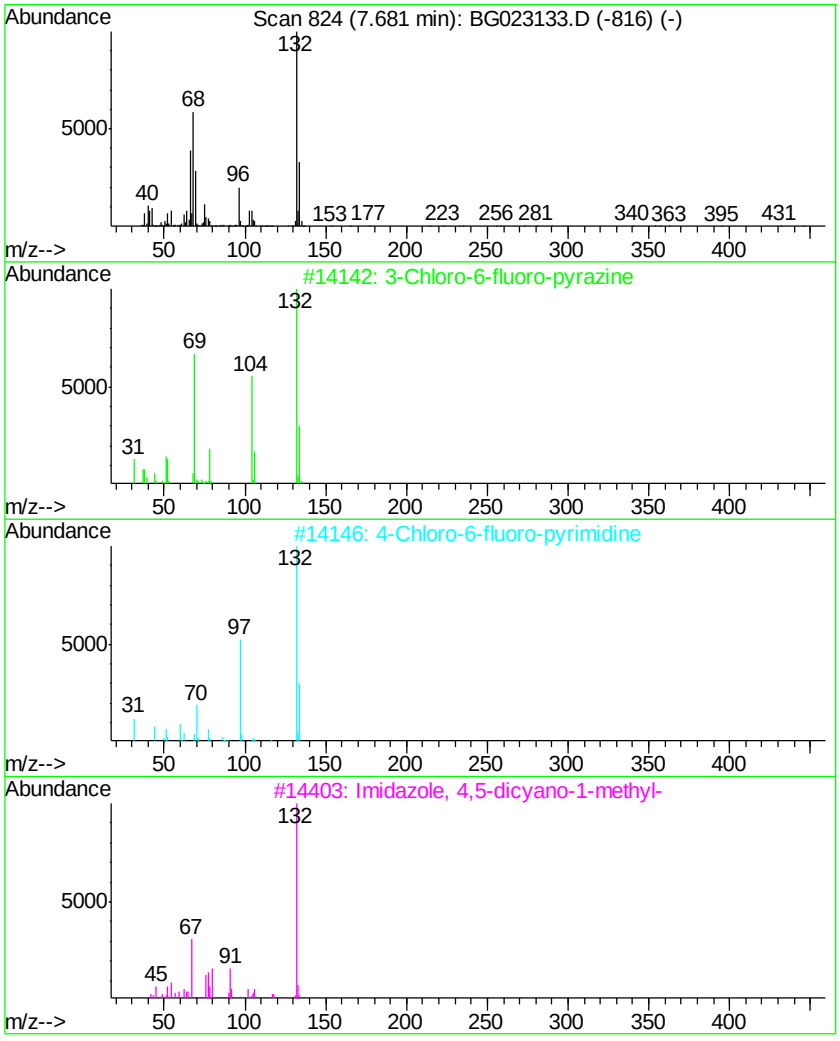
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

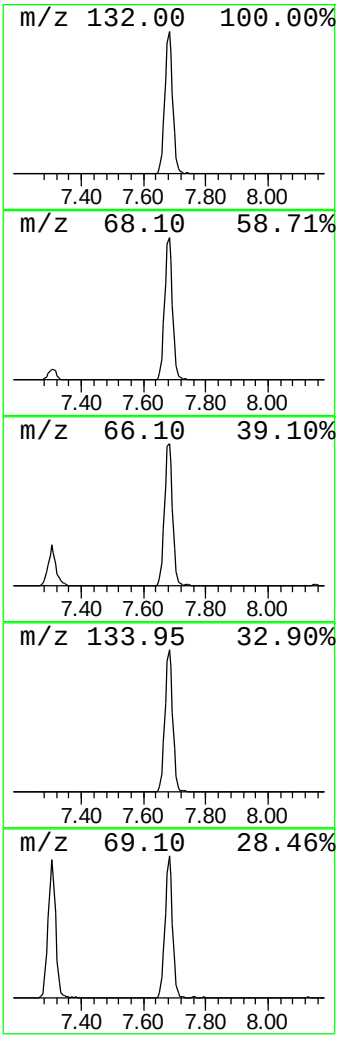
**********

Peak Number 6 unknown7.68 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.68 | 106.52 ng | 3420940 | 1,4-Dichlorobenzene-d4 | 8.15 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 14 |
| 2 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 14 |
| 3 | Imidazole, 4,5-dicyano-1-methyl- | 132 | C6H4N4 | 019485-35-9 | 11 |
| 4 | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2 | 022291-85-6 | 10 |
| 5 | (5-Methyl-2-pyridyl)acetonitrile | 132 | C8H8N2 | 1000241-93-9 | 10 |



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Acq On : 16 Jul 2016 5:36
Operator : UM/SJ
Sample : H4016-14
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** C5-16

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

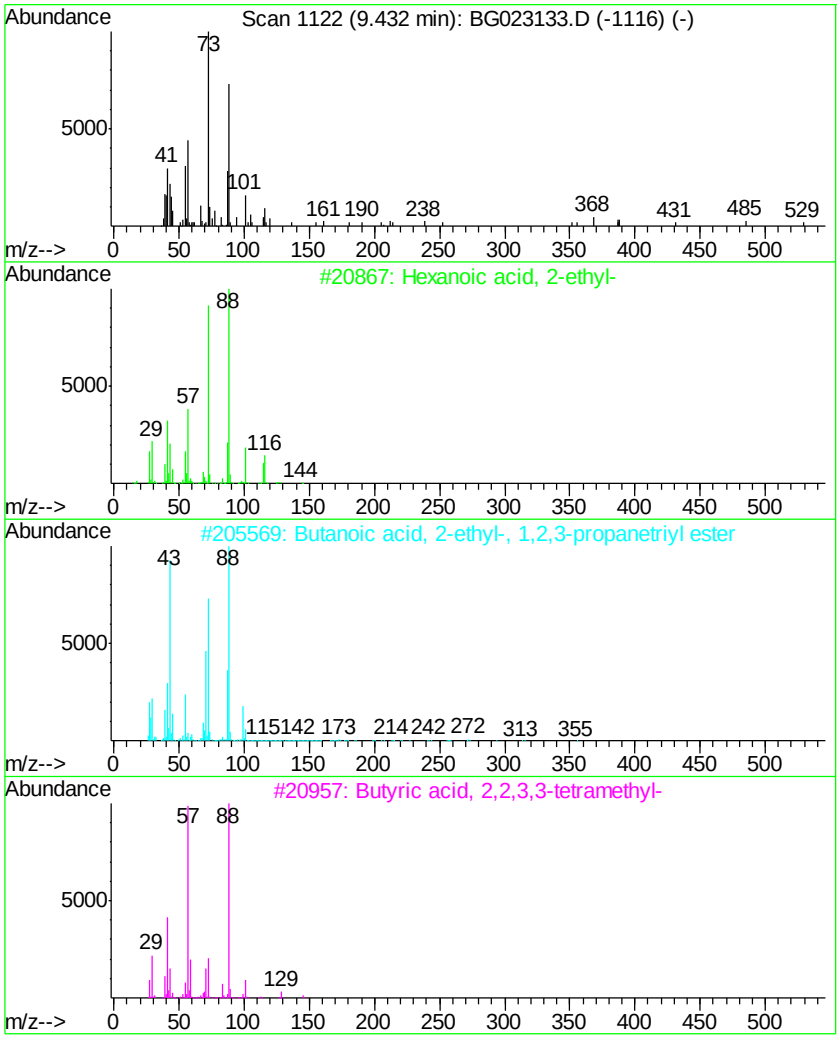
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

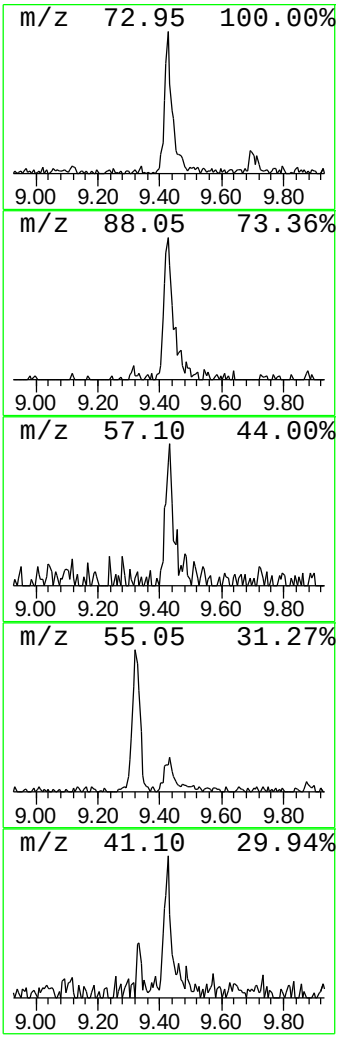
**********

Peak Number 8 Hexanoic acid, 2-ethyl- Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.43 | 2.82 ng | 90464 | 1,4-Dichlorobenzene-d4 | 8.15 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexanoic acid, 2-ethyl- | 144 | C8H16O2 | 000149-57-5 | 59 |
| 2 | Butanoic acid, 2-ethyl-, 1,2,3-p... | 386 | C21H38O6 | 056554-54-2 | 36 |
| 3 | Butyric acid, 2,2,3,3-tetramethyl- | 144 | C8H16O2 | 030407-41-1 | 28 |
| 4 | Nonanoic acid, 5-methyl-, ethyl ... | 200 | C12H24O2 | 116530-40-6 | 25 |
| 5 | Methyl-4-deoxy-2,3-di-O-methyl.b... | 218 | C9H14O6 | 1000312-09-9 | 25 |



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Operator : UM/SJ
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**Instrument :** BNA_G
**ClientSampleId :** C5-16

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

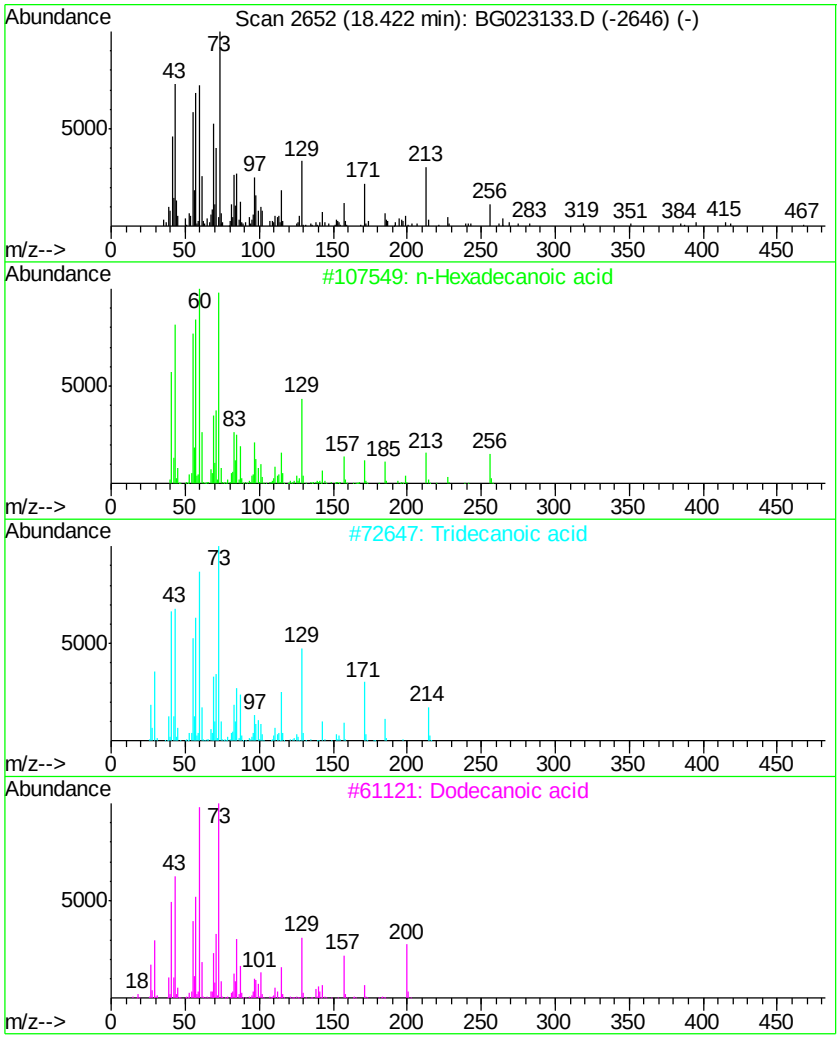
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

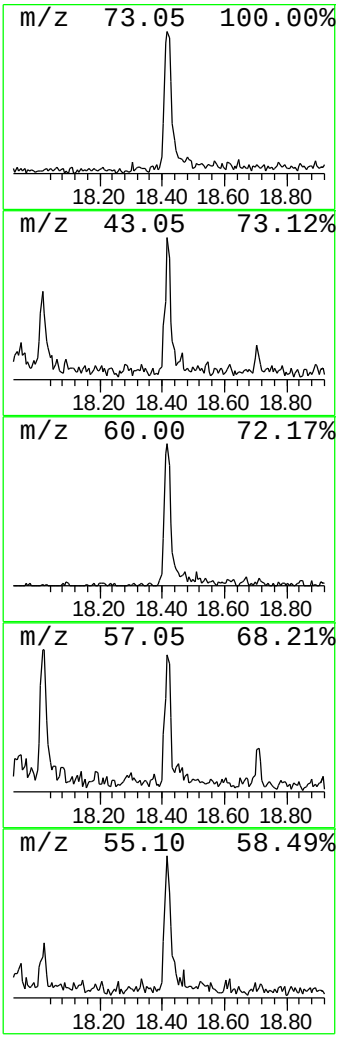
**********

Peak Number 9 n-Hexadecanoic acid Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.42 | 2.90 ng | 298710 | Phenanthrene-d10 | 17.55 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 96 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 83 |
| 3 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 68 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 64 |
| 5 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 58 |



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Operator : UM/SJ
Sample : H4016-14
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** C5-16

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

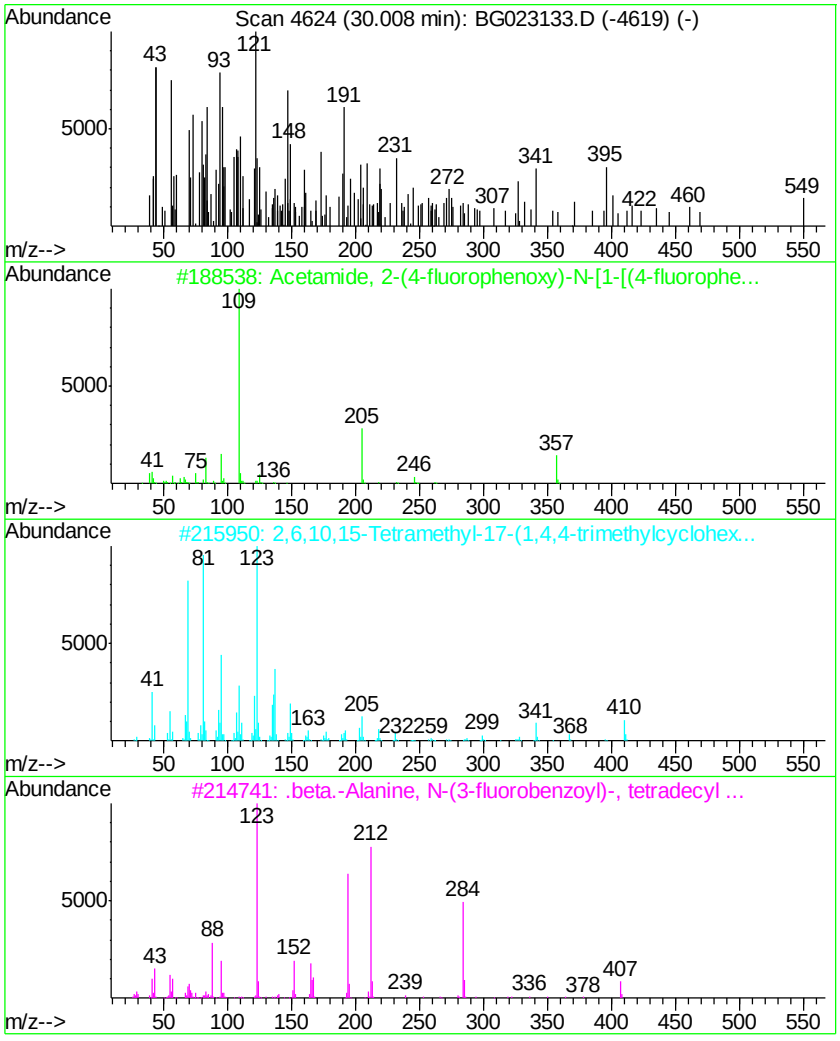
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

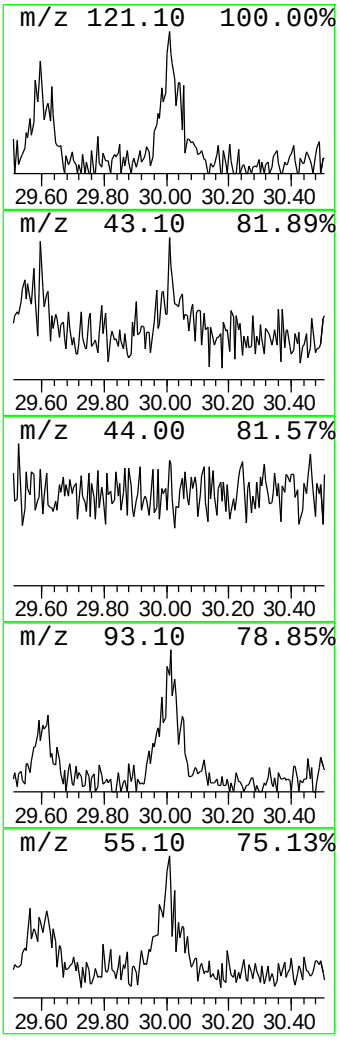
**********

Peak Number 10 unknown30.01 Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 30.01 | 2.71 ng | 291544 | Perylene-d12 | 25.24 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Acetamide, 2-(4-fluorophenoxy)-N... | 357 | C19H17F2N3O2 | 1000319-54-7 | 22 |
| 2 | 2,6,10,15-Tetramethyl-17-(1,4,4-... | 410 | C30H50 | 1000195-23-2 | 14 |
| 3 | .beta.-Alanine, N-(3-fluorobenzo... | 407 | C24H38FNO3 | 1000321-94-2 | 12 |
| 4 | 2-(4-Fluoro-benzylsulfanyl)-N-(2... | 395 | C23H22FNO2S | 339239-45-1 | 10 |
| 5 | Cyclopropanecarboxamide, 2,2-dim... | 329 | C20H27NO3 | 1000320-22-3 | 10 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071516\
Data File : BG023133.D
Acq On : 16 Jul 2016 5:36
Operator : UM/SJ
Sample : H4016-14
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** C5-16

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| Cyclobutane, ethyl- | 2.89 | 7.7 | ng | 246747 | 1 | 8.15 | 642321 | 20.0 |
| Propane, 2,2-dime... | 3.04 | 50.9 | ng | 1635710 | 1 | 8.15 | 642321 | 20.0 |
| Propane, 1,1-dime... | 3.30 | 2.2 | ng | 71060 | 1 | 8.15 | 642321 | 20.0 |
| 2-Pentanone, 4-hy... | 5.22 | 12.6 | ng | 403617 | 1 | 8.15 | 642321 | 20.0 |
| unknown7.68 | 7.68 | 106.5 | ng | 3420940 | 1 | 8.15 | 642321 | 20.0 |
| Hexanoic acid, 2-... | 9.43 | 2.8 | ng | 90464 | 1 | 8.15 | 642321 | 20.0 |
| n-Hexadecanoic acid | 18.42 | 2.9 | ng | 298710 | 4 | 17.55 | 2062530 | 20.0 |
| unknown30.01 | 30.01 | 2.7 | ng | 291544 | 6 | 25.24 | 2155250 | 20.0 |