LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110416\
Data File : BG024719.D
Acq On : 5 Nov 2016 19:08
Operator : UM/SJ
Sample : H5527-10
Misc :
ALS Vial : 33 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** GW-107-12.3-26.0

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-BG102516.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 | 3.596 | 123 | 129 | 137 | rBV | 691710 | 1250029 | 12.78% | 2.617% |
| 2 | 5.329 | 418 | 424 | 431 | rVB2 | 181830 | 299548 | 3.06% | 0.627% |
| 3 | 5.799 | 493 | 504 | 513 | rBV | 1099596 | 1861716 | 19.04% | 3.897% |
| 4 | 7.403 | 770 | 777 | 787 | rVB | 732912 | 1316799 | 13.46% | 2.756% |
| 5 | 7.791 | 834 | 843 | 851 | rBV | 1832264 | 3260343 | 33.34% | 6.825% |
| 6 | 8.267 | 916 | 924 | 935 | rBV2 | 388012 | 735023 | 7.52% | 1.539% |
| 7 | 8.590 | 969 | 979 | 992 | rBV | 1639742 | 2923895 | 29.90% | 6.121% |
| 8 | 9.442 | 1114 | 1124 | 1131 | rBV | 1429562 | 2672400 | 27.33% | 5.594% |
| 9 | 11.093 | 1396 | 1405 | 1414 | rVB | 522325 | 980335 | 10.02% | 2.052% |
| 10 | 11.863 | 1527 | 1536 | 1543 | rBV3 | 117349 | 323845 | 3.31% | 0.678% |
| 11 | 13.508 | 1806 | 1816 | 1824 | rVB | 3754098 | 5895093 | 60.28% | 12.340% |
| 12 | 14.319 | 1947 | 1954 | 1960 | rBV | 505065 | 745571 | 7.62% | 1.561% |
| 13 | 14.883 | 2043 | 2050 | 2057 | rVB | 889034 | 1417697 | 14.50% | 2.968% |
| 14 | 15.253 | 2104 | 2113 | 2118 | rBV9 | 54853 | 106306 | 1.09% | 0.223% |
| 15 | 16.363 | 2295 | 2302 | 2313 | rBV | 3776716 | 6013253 | 61.49% | 12.587% |
| 16 | 16.534 | 2327 | 2331 | 2338 | rBV3 | 99422 | 205067 | 2.10% | 0.429% |
| 17 | 17.327 | 2462 | 2466 | 2470 | rBV2 | 76068 | 110207 | 1.13% | 0.231% |
| 18 | 17.621 | 2509 | 2516 | 2523 | rBV | 1165063 | 1951986 | 19.96% | 4.086% |
| 19 | 18.467 | 2656 | 2660 | 2671 | rBV2 | 248415 | 404272 | 4.13% | 0.846% |
| 20 | 19.724 | 2870 | 2874 | 2882 | rBV8 | 107848 | 189353 | 1.94% | 0.396% |
| 21 | 20.206 | 2950 | 2956 | 2962 | rBV | 7119309 | 9779863 | 100.00% | 20.472% |
| 22 | 21.498 | 3171 | 3176 | 3181 | rBV2 | 183103 | 300917 | 3.08% | 0.630% |
| 23 | 21.916 | 3241 | 3247 | 3256 | rVB | 1426649 | 2564204 | 26.22% | 5.368% |
| 24 | 25.347 | 3821 | 3831 | 3844 | rVB3 | 782087 | 2464435 | 25.20% | 5.159% |

Sum of corrected areas: 47772157

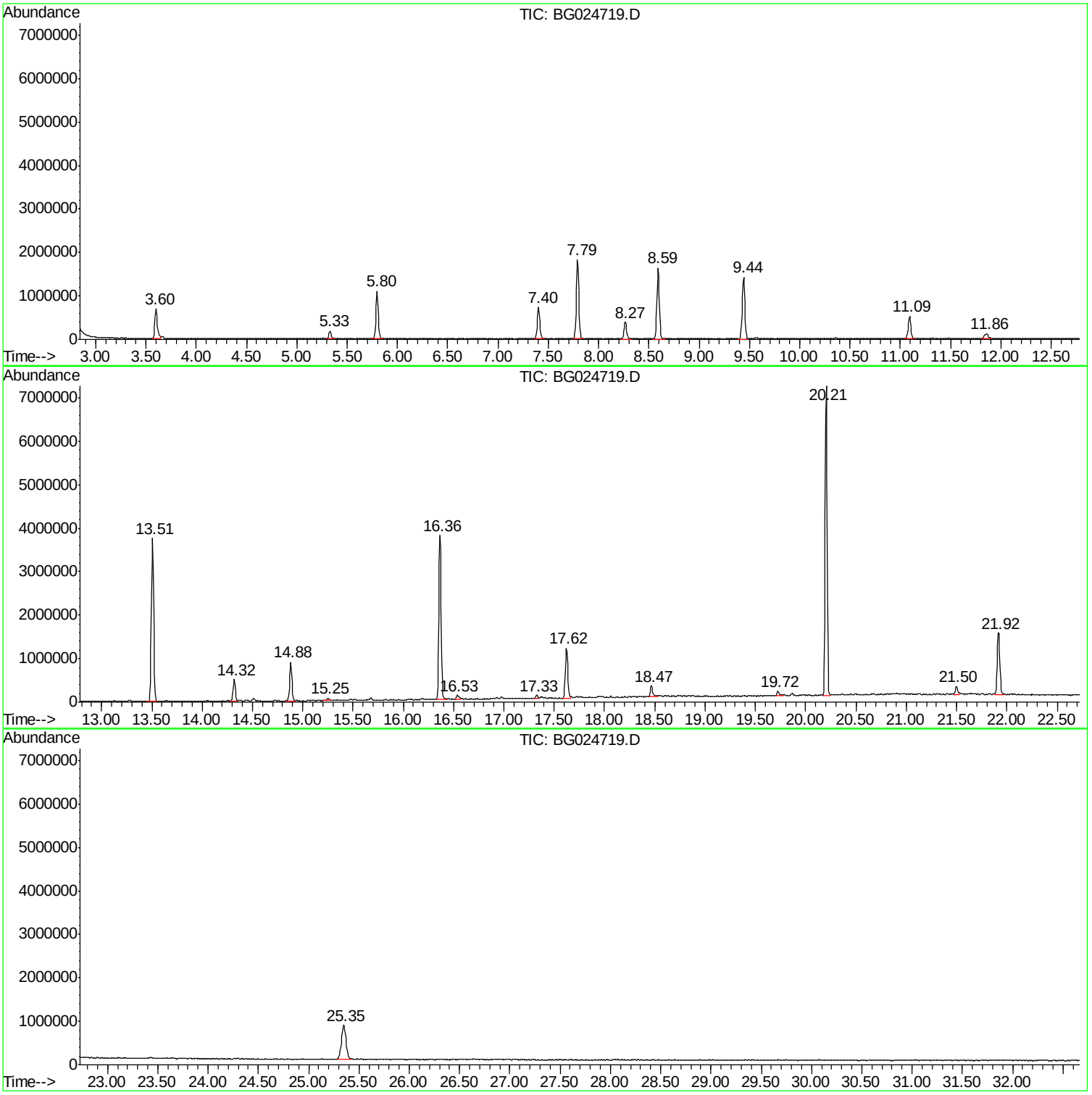
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110416\
Data File : BG024719.D
Acq On : 5 Nov 2016 19:08
Operator : UM/SJ
Sample : H5527-10
Misc :
ALS Vial : 33 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** GW-107-12.3-26.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA G\DATA\BG110416\
Data File : BG024719.D
Acq On : 5 Nov 2016 19:08
Operator : UM/SJ
Sample : H5527-10
Misc :
ALS Vial : 33 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** GW-107-12.3-26.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

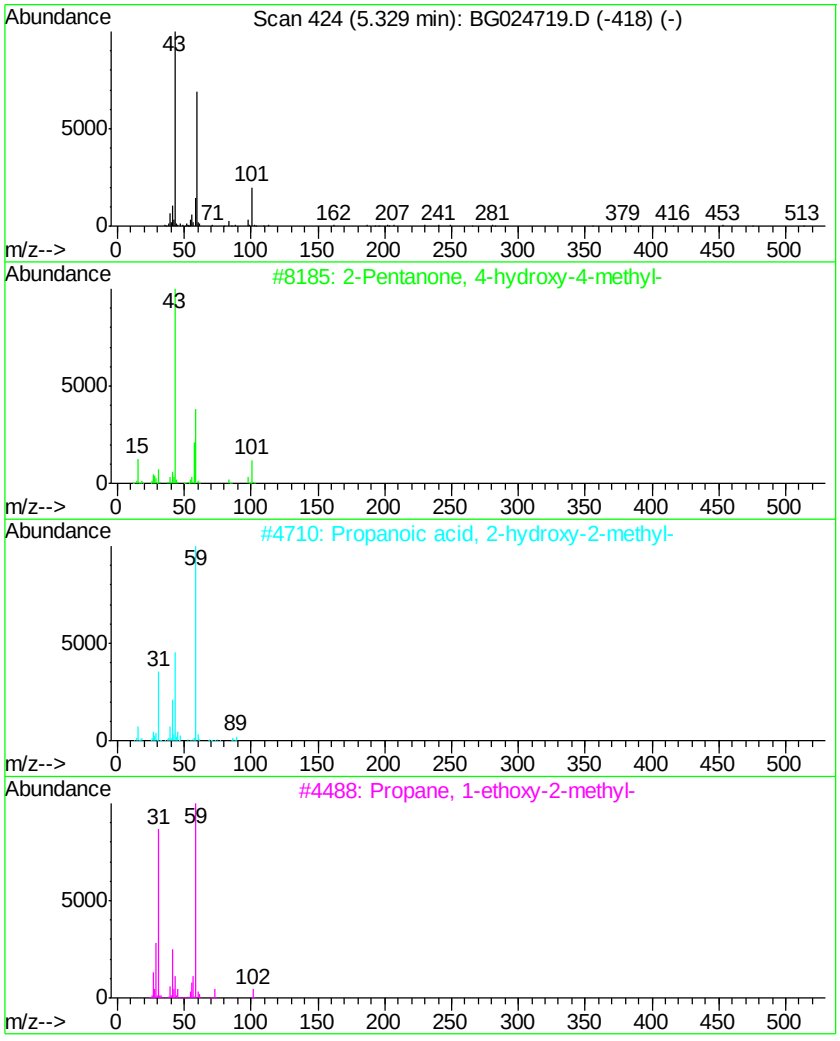
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

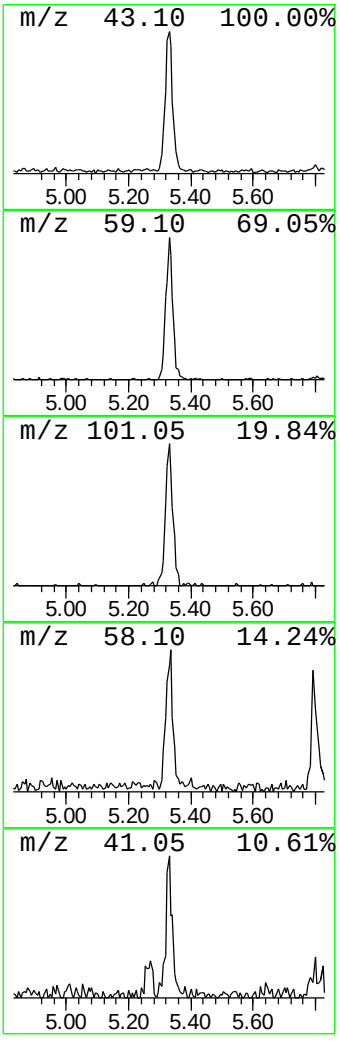
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.33 | 8.15 ng | 299548 | 1,4-Dichlorobenzene-d4 | 8.27 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 38 |
| 2 | Propanoic acid, 2-hydroxy-2-methyl- | 104 | C4H8O3 | 000594-61-6 | 17 |
| 3 | Propane, 1-ethoxy-2-methyl- | 102 | C6H14O | 000627-02-1 | 12 |
| 4 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 12 |
| 5 | 3-Hexanol | 102 | C6H14O | 000623-37-0 | 9 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG110416\
Data File : BG024719.D
Acq On : 5 Nov 2016 19:08
Operator : UM/SJ
Sample : H5527-10
Misc :
ALS Vial : 33 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** GW-107-12.3-26.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

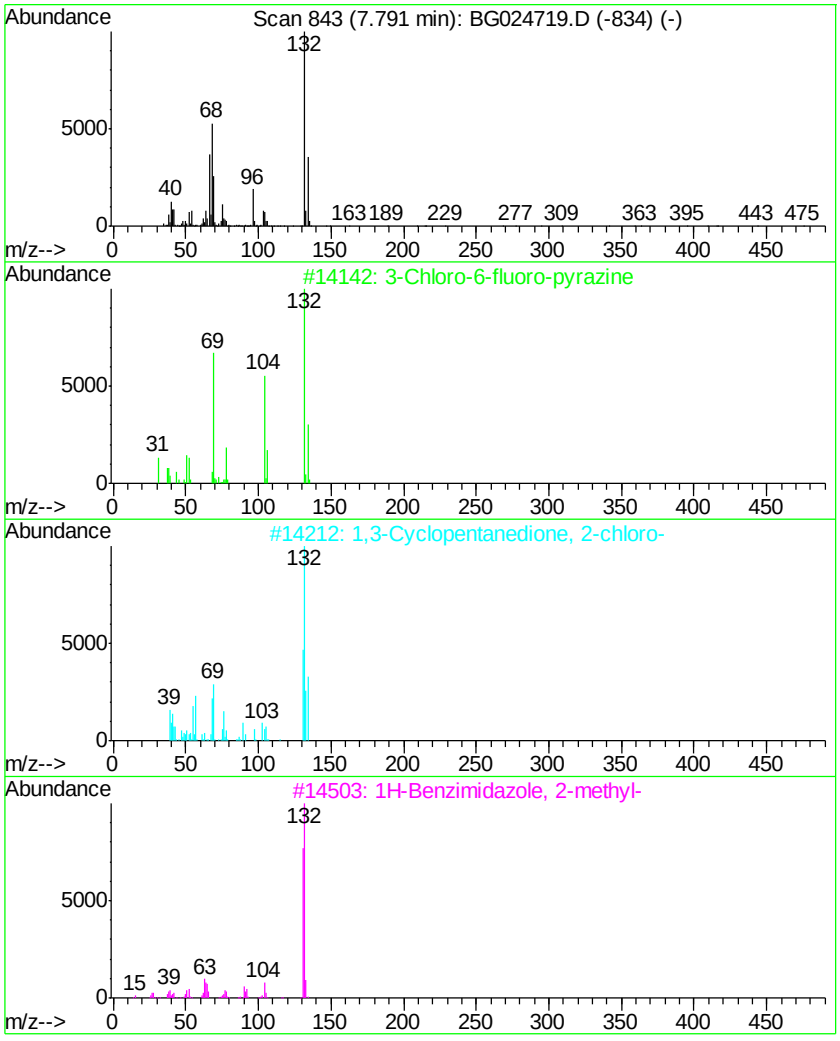
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

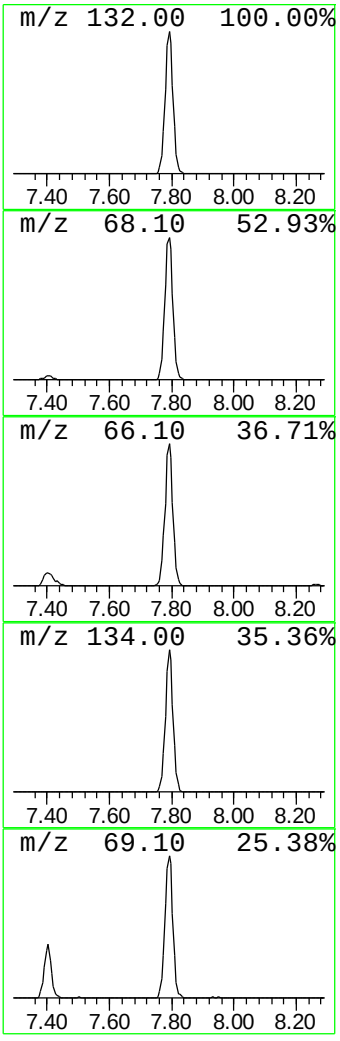
**********

Peak Number 3 unknown7.79 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.79 | 88.71 ng | 3260340 | 1,4-Dichlorobenzene-d4 | 8.27 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 1,3-Cyclopentanedione, 2-chloro- | 132 | C5H5ClO2 | 014203-19-1 | 23 |
| 3 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 22 |
| 4 | Cyclopropanamine, 1-phenyl- | 133 | C9H11N | 1000351-26-2 | 14 |
| 5 | Pyrazolo(2,3-a)pyridine, 7-methyl- | 132 | C8H8N2 | 034760-58-2 | 12 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110416\
Data File : BG024719.D
Acq On : 5 Nov 2016 19:08
Operator : UM/SJ
Sample : H5527-10
Misc :
ALS Vial : 33 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** GW-107-12.3-26.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

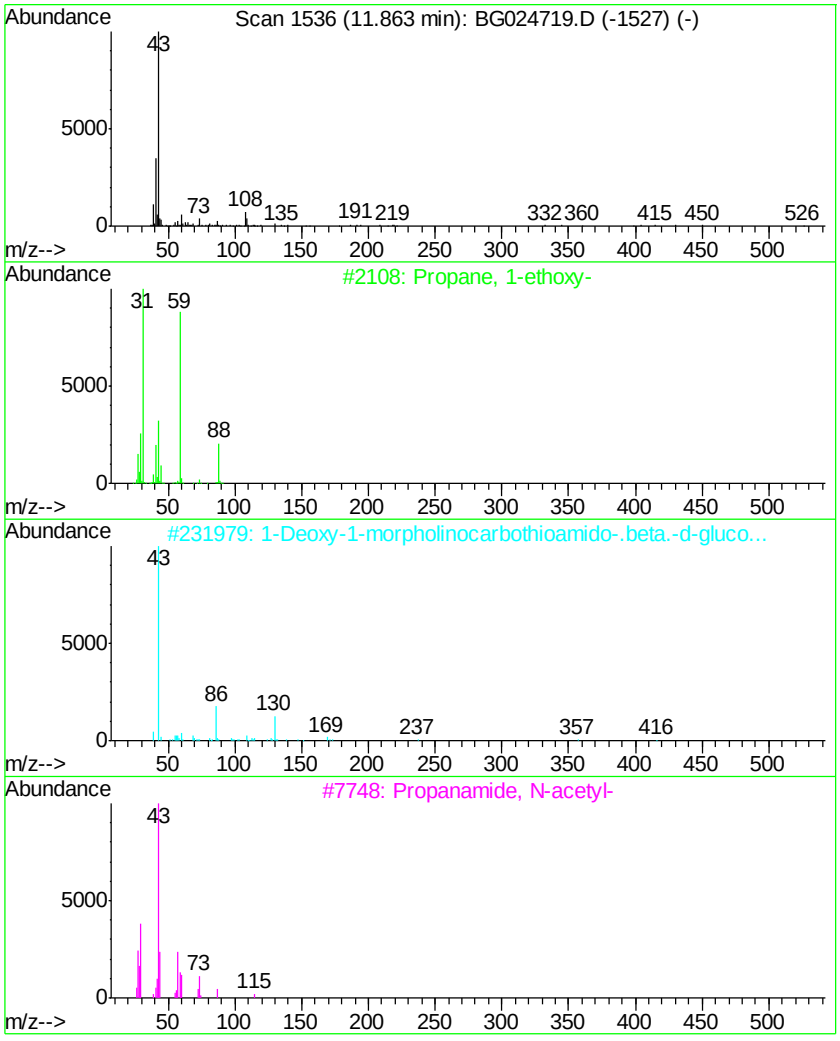
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

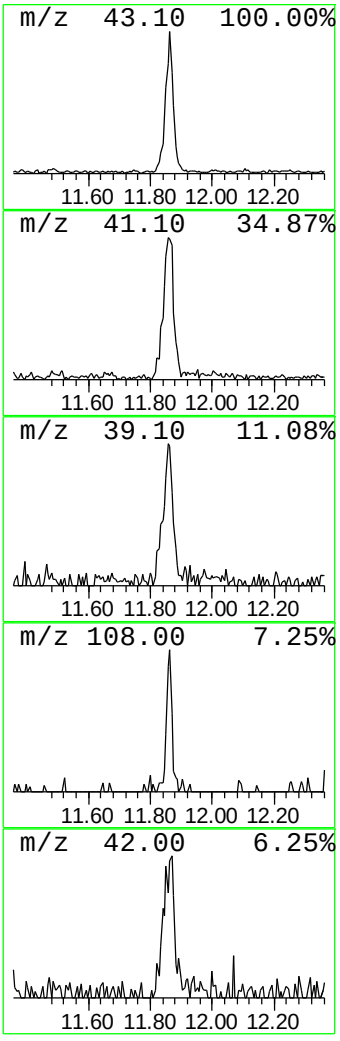
**********

Peak Number 5 unknown11.86 Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.86 | 6.61 ng | 323845 | Naphthalene-d8 | 11.09 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Propane, 1-ethoxy- | 88 | C5H12O | 000628-32-0 | 9 |
| 2 | 1-Deoxy-1-morpholinocarbothioami... | 476 | C19H28N2O10S | 1000223-13-8 | 9 |
| 3 | Propanamide, N-acetyl- | 115 | C5H9NO2 | 019264-34-7 | 7 |
| 4 | N-Acetyl-D-glucosamine | 221 | C8H15NO6 | 007512-17-6 | 7 |
| 5 | Propane, 1,1'-sulfonylbis- | 150 | C6H14O2S | 000598-03-8 | 7 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110416\
Data File : BG024719.D
Acq On : 5 Nov 2016 19:08
Operator : UM/SJ
Sample : H5527-10
Misc :
ALS Vial : 33 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** GW-107-12.3-26.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

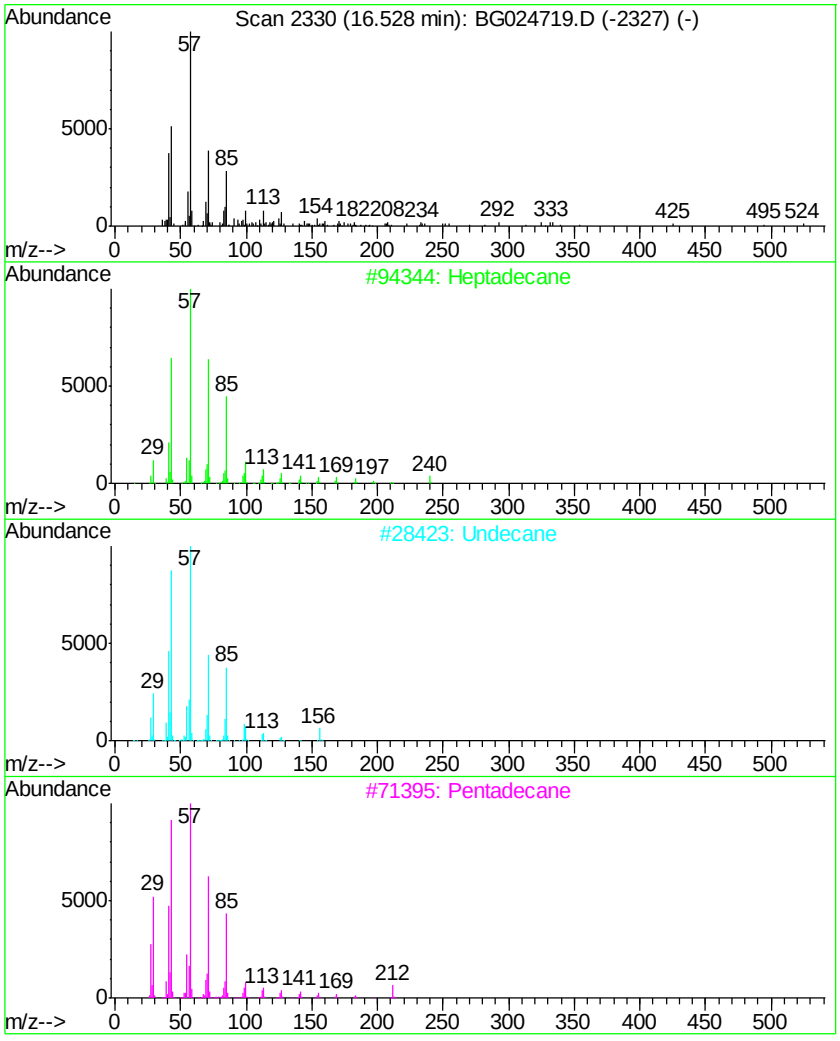
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

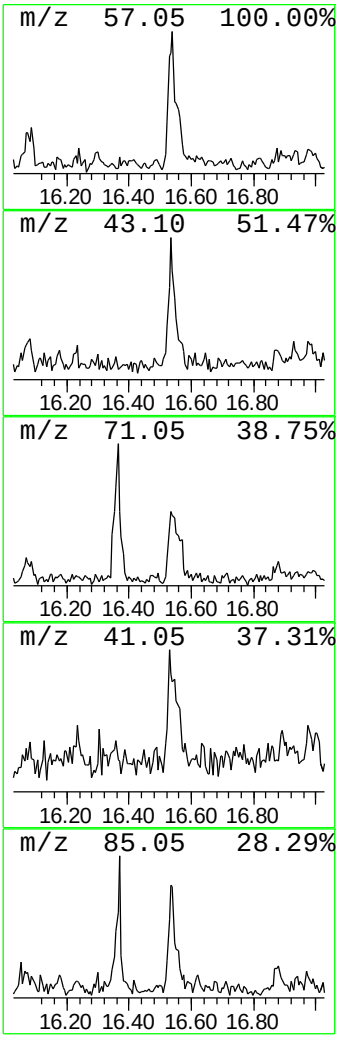
**********

Peak Number 6 Heptadecane Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.53 | 2.10 ng | 205067 | Phenanthrene-d10 | 17.62 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptadecane | 240 | C17H36 | 000629-78-7 | 87 |
| 2 | Undecane | 156 | C11H24 | 001120-21-4 | 87 |
| 3 | Pentadecane | 212 | C15H32 | 000629-62-9 | 78 |
| 4 | Tetradecane | 198 | C14H30 | 000629-59-4 | 78 |
| 5 | 10-Methylnonadecane | 282 | C20H42 | 056862-62-5 | 64 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG110416\
Data File : BG024719.D
Acq On : 5 Nov 2016 19:08
Operator : UM/SJ
Sample : H5527-10
Misc :
ALS Vial : 33 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** GW-107-12.3-26.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

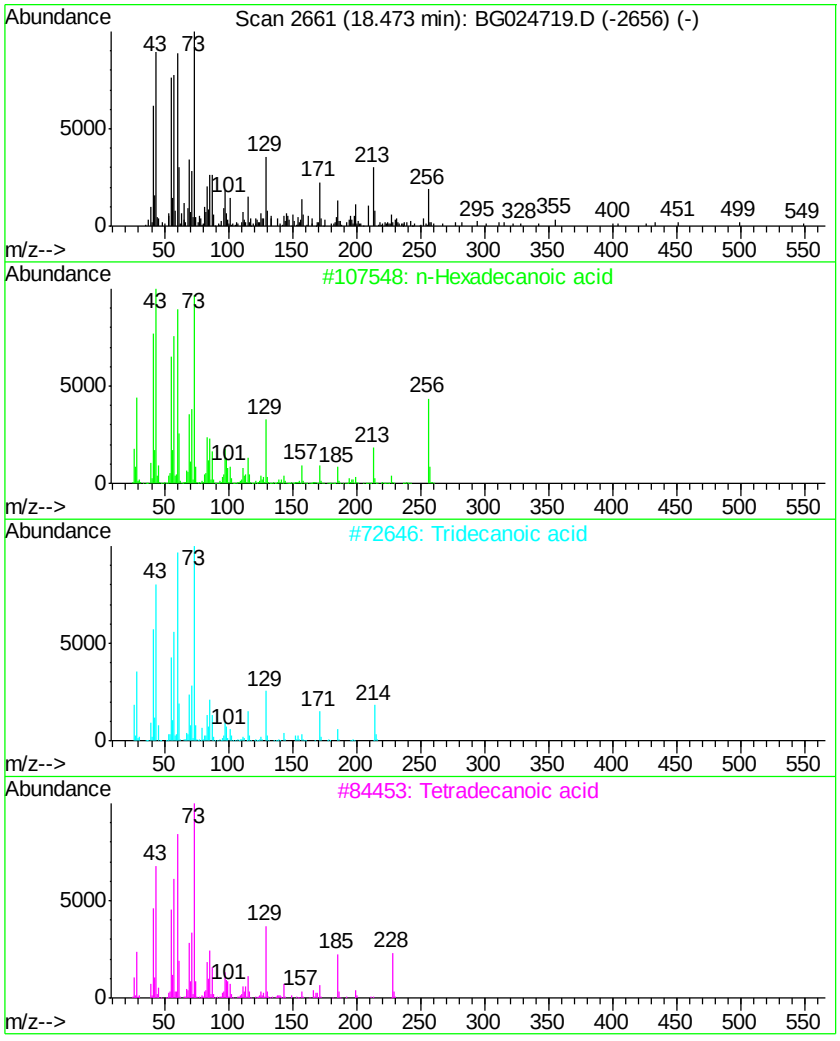
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

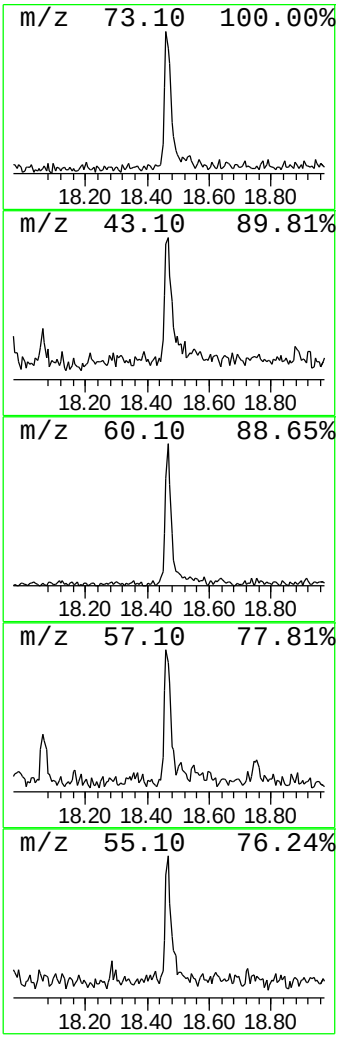
**********

Peak Number 7 n-Hexadecanoic acid Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.47 | 4.14 ng | 404272 | Phenanthrene-d10 | 17.62 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 95 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 64 |
| 3 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 59 |
| 4 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 59 |
| 5 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 55 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG110416\
Data File : BG024719.D
Acq On : 5 Nov 2016 19:08
Operator : UM/SJ
Sample : H5527-10
Misc :
ALS Vial : 33 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** GW-107-12.3-26.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

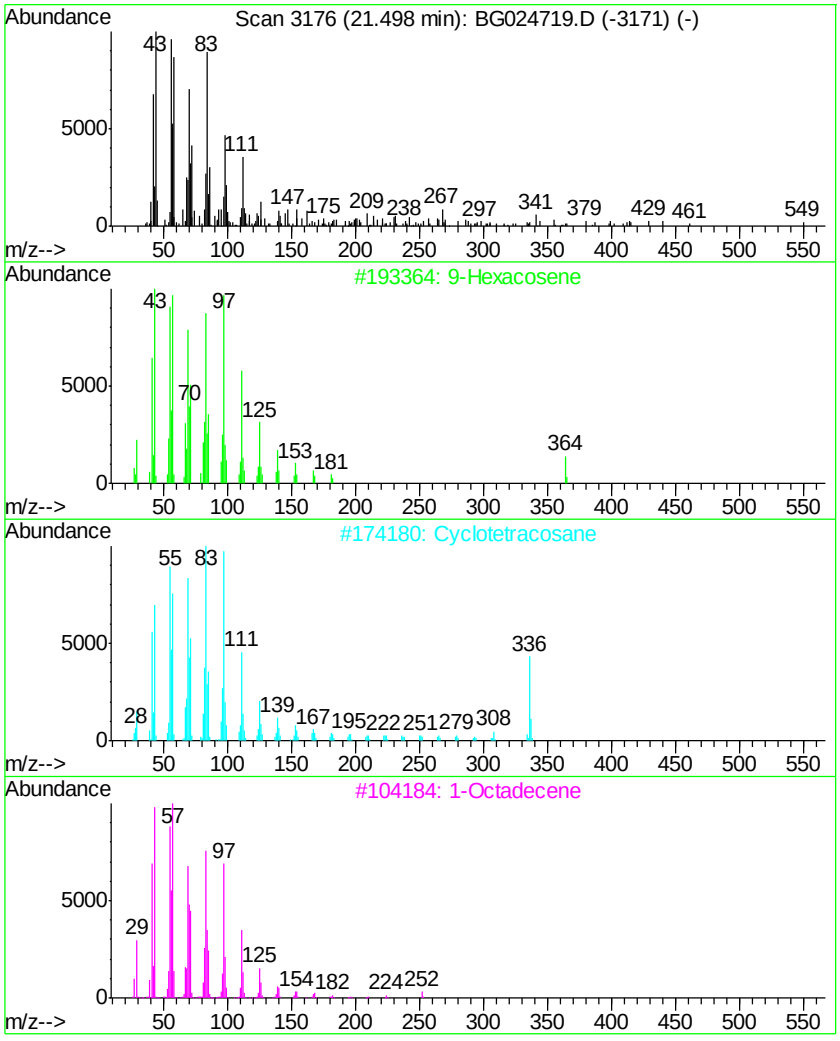
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

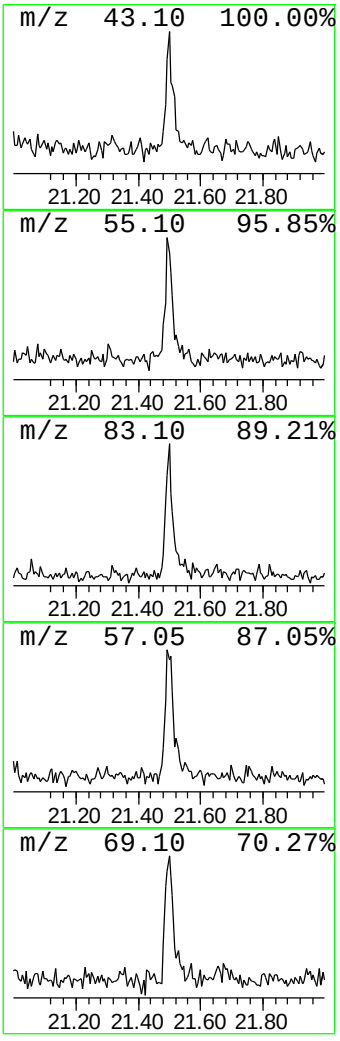
**********

Peak Number 8 9-Hexacosene Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.50 | 2.35 ng | 300917 | Chrysene-d12 | 21.92 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 9-Hexacosene | 364 | C26H52 | 071502-22-2 | 95 |
| 2 | Cyclotetracosane | 336 | C24H48 | 000297-03-0 | 95 |
| 3 | 1-Octadecene | 252 | C18H36 | 000112-88-9 | 93 |
| 4 | Dichloroacetic acid, tridecyl ester | 310 | C15H28Cl2O2 | 1000280-48-3 | 91 |
| 5 | 2-Methyl-2-docosene | 322 | C23H46 | 1000131-16-9 | 91 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110416\
Data File : BG024719.D
Acq On : 5 Nov 2016 19:08
Operator : UM/SJ
Sample : H5527-10
Misc :
ALS Vial : 33 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** GW-107-12.3-26.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.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 |
| 2-Pentanone, 4-hy... | 5.33 | 8.2 | ng | 299548 | 1 | 8.27 | 735023 | 20.0 |
| unknown7.79 | 7.79 | 88.7 | ng | 3260340 | 1 | 8.27 | 735023 | 20.0 |
| unknown11.86 | 11.86 | 6.6 | ng | 323845 | 2 | 11.09 | 980335 | 20.0 |
| Heptadecane | 16.53 | 2.1 | ng | 205067 | 4 | 17.62 | 1951990 | 20.0 |
| n-Hexadecanoic acid | 18.47 | 4.1 | ng | 404272 | 4 | 17.62 | 1951990 | 20.0 |
| 9-Hexacosene | 21.50 | 2.4 | ng | 300917 | 5 | 21.92 | 2564200 | 20.0 |