LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG050515\
Data File : BG016887.D
Acq On : 6 May 2015 5:31
Operator : TP/IZ
Sample : G2114-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** GRID-2(12-18)

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-BG050515.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 | 2.788 | 13 | 17 | 35 | rBV | 6451253 | 8681710 | 100.00% | 19.891% |
| 2 | 2.923 | 36 | 40 | 49 | rVV2 | 159048 | 301805 | 3.48% | 0.691% |
| 3 | 3.005 | 49 | 54 | 58 | rVV | 253933 | 313496 | 3.61% | 0.718% |
| 4 | 4.920 | 375 | 380 | 387 | rVB | 195186 | 283504 | 3.27% | 0.650% |
| 5 | 5.385 | 453 | 459 | 470 | rVB | 1847619 | 2660365 | 30.64% | 6.095% |
| 6 | 6.971 | 721 | 729 | 740 | rBV | 1953600 | 3158745 | 36.38% | 7.237% |
| 7 | 7.335 | 783 | 791 | 798 | rBV | 1851191 | 2910621 | 33.53% | 6.669% |
| 8 | 7.799 | 863 | 870 | 877 | rBV | 347206 | 549346 | 6.33% | 1.259% |
| 9 | 8.123 | 915 | 925 | 931 | rBV | 1224114 | 1953912 | 22.51% | 4.477% |
| 10 | 8.963 | 1056 | 1068 | 1078 | rBV | 1108998 | 1882800 | 21.69% | 4.314% |
| 11 | 10.596 | 1336 | 1346 | 1354 | rBV | 492181 | 821361 | 9.46% | 1.882% |
| 12 | 11.912 | 1564 | 1570 | 1577 | rBV2 | 108091 | 162299 | 1.87% | 0.372% |
| 13 | 12.799 | 1716 | 1721 | 1728 | rVB | 80980 | 114643 | 1.32% | 0.263% |
| 14 | 13.064 | 1756 | 1766 | 1773 | rBV | 2641368 | 3875133 | 44.64% | 8.878% |
| 15 | 13.898 | 1901 | 1908 | 1917 | rVB | 215668 | 303516 | 3.50% | 0.695% |
| 16 | 14.439 | 1994 | 2000 | 2007 | rBV2 | 764003 | 1131430 | 13.03% | 2.592% |
| 17 | 15.802 | 2225 | 2232 | 2239 | rVB | 495285 | 656041 | 7.56% | 1.503% |
| 18 | 15.925 | 2245 | 2253 | 2265 | rBV | 2211831 | 3282356 | 37.81% | 7.520% |
| 19 | 17.183 | 2460 | 2467 | 2477 | rBV | 981791 | 1392219 | 16.04% | 3.190% |
| 20 | 18.087 | 2615 | 2621 | 2630 | rBV | 261279 | 426425 | 4.91% | 0.977% |
| 21 | 19.362 | 2834 | 2838 | 2849 | rBV2 | 108265 | 202123 | 2.33% | 0.463% |
| 22 | 19.815 | 2909 | 2915 | 2920 | rBV | 4251862 | 5090382 | 58.63% | 11.663% |
| 23 | 20.502 | 3025 | 3032 | 3038 | rBV3 | 84460 | 174642 | 2.01% | 0.400% |
| 24 | 21.078 | 3126 | 3130 | 3140 | rBV | 353988 | 443495 | 5.11% | 1.016% |
| 25 | 21.360 | 3173 | 3178 | 3186 | rBV | 1209744 | 1473729 | 16.98% | 3.377% |
| 26 | 23.669 | 3563 | 3571 | 3579 | rVB2 | 698319 | 1400315 | 16.13% | 3.208% |

Sum of corrected areas: 43646413

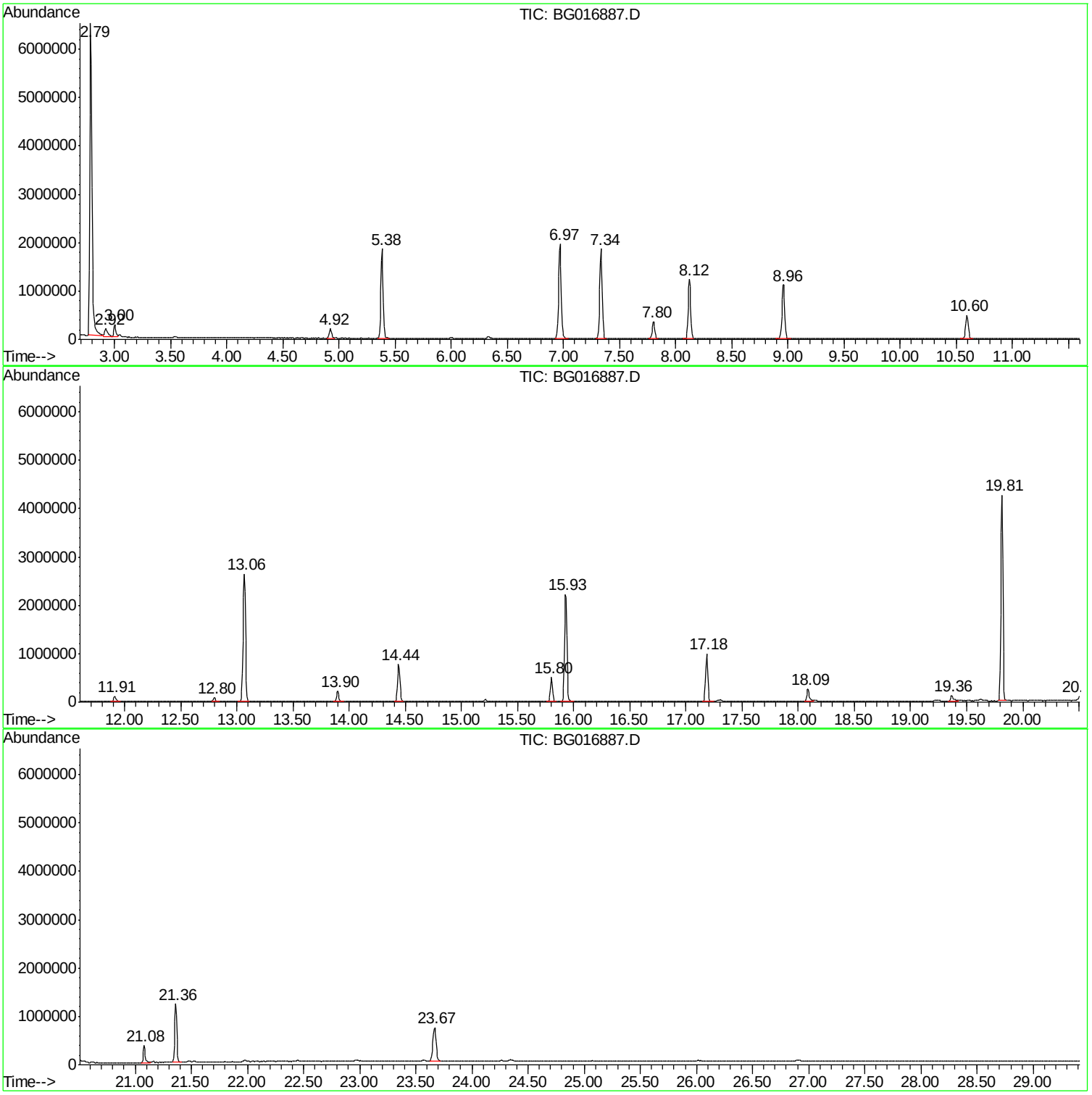
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA G\DATA\BG050515\
Data File : BG016887.D
Acq On : 6 May 2015 5:31
Operator : TP/IZ
Sample : G2114-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** GRID-2(12-18)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA G\DATA\BG050515\
Data File : BG016887.D
Acq On : 6 May 2015 5:31
Operator : TP/IZ
Sample : G2114-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** GRID-2(12-18)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

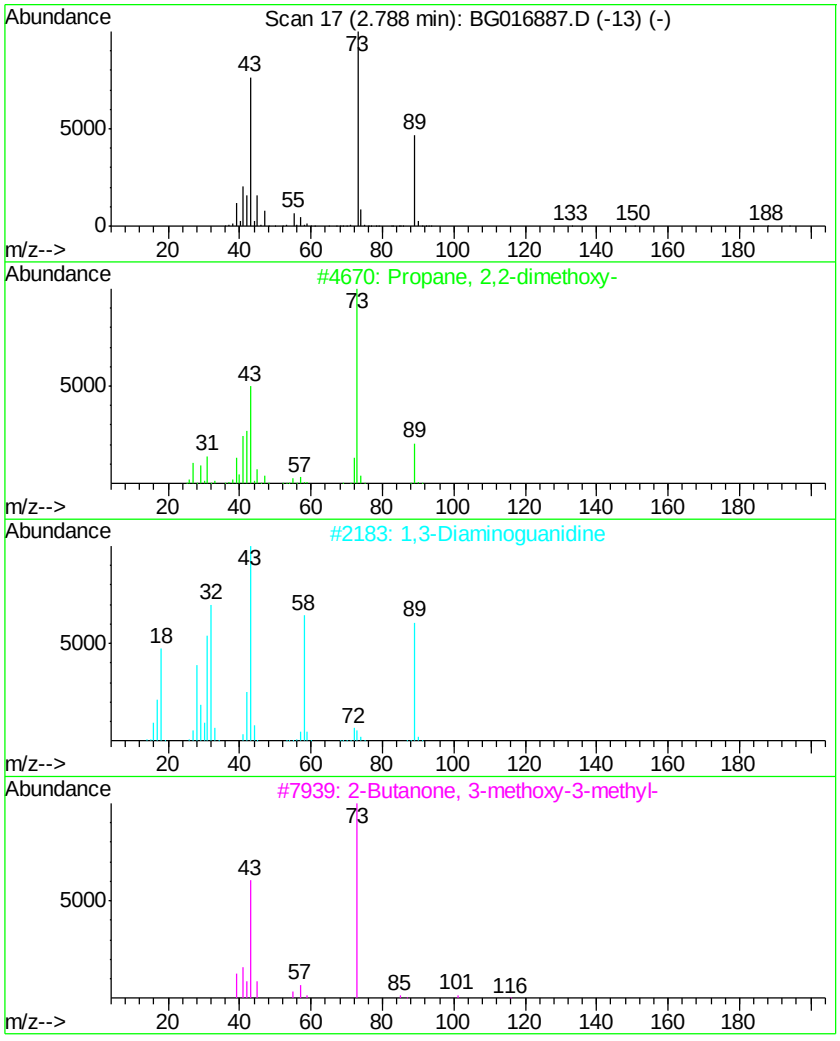
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

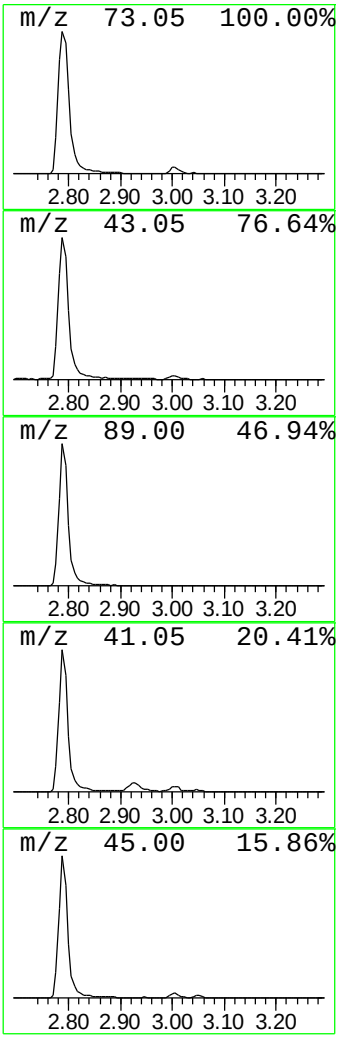
**********

Peak Number 1 unknown2.79 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.79 | 316.07 ng | 8681710 | 1,4-Dichlorobenzene-d4 | 7.81 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Propane, 2,2-dimethoxy- | 104 | C5H12O2 | 000077-76-9 | 42 |
| 2 | 1,3-Diaminoguanidine | 89 | CH7N5 | 004364-78-7 | 33 |
| 3 | 2-Butanone, 3-methoxy-3-methyl- | 116 | C6H12O2 | 036687-98-6 | 32 |
| 4 | Acetamide, N-methyl- | 73 | C3H7NO | 000079-16-3 | 32 |
| 5 | 1-Propanol, 2-methyl- | 74 | C4H10O | 000078-83-1 | 9 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG050515\
Data File : BG016887.D
Acq On : 6 May 2015 5:31
Operator : TP/IZ
Sample : G2114-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** GRID-2(12-18)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

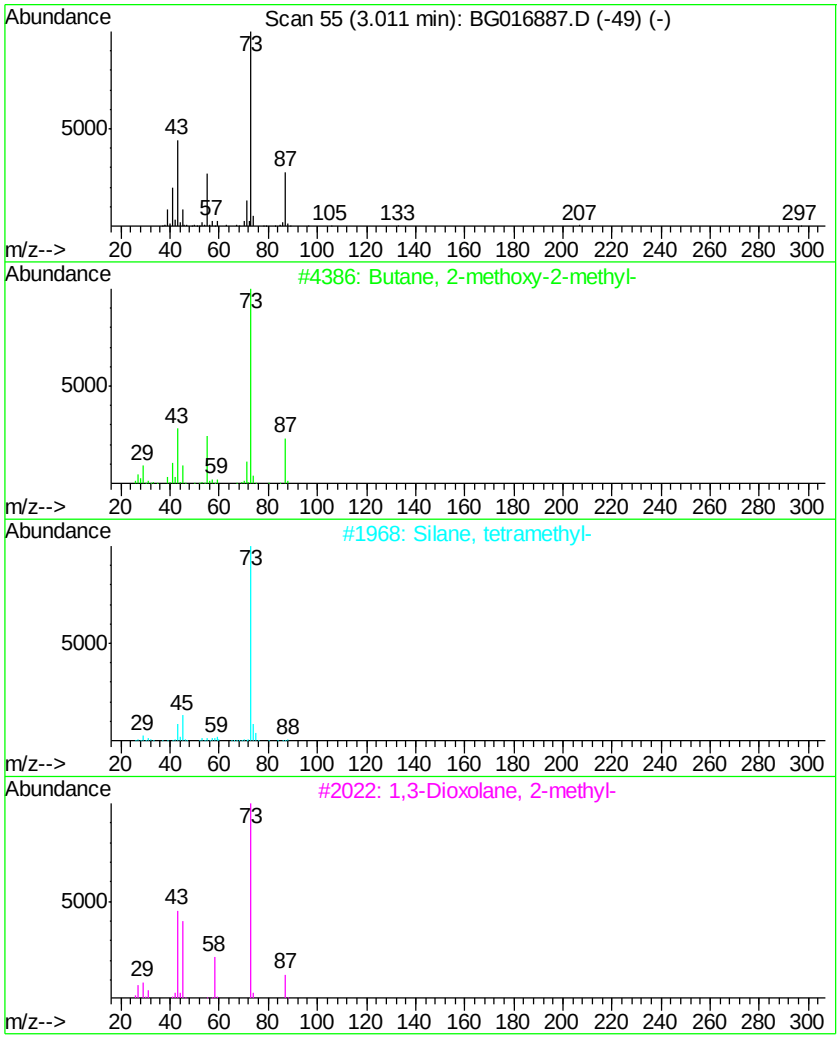
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

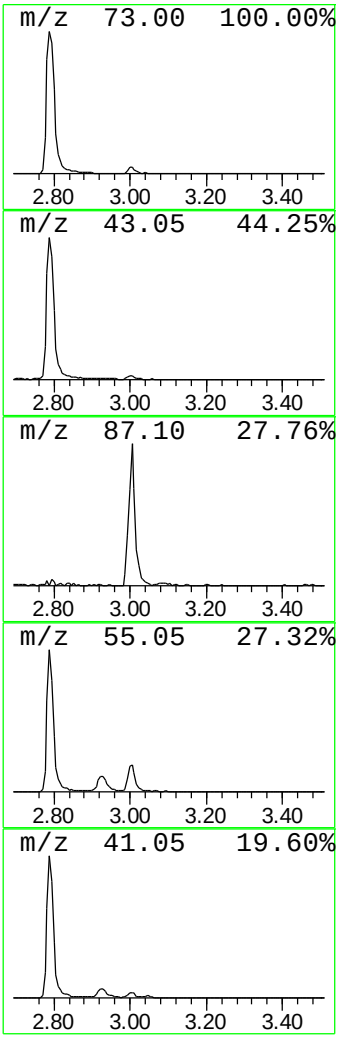
**********

Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.01 | 11.41 ng | 313496 | 1,4-Dichlorobenzene-d4 | 7.81 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 78 |
| 2 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 35 |
| 3 | 1,3-Dioxolane, 2-methyl- | 88 | C4H8O2 | 000497-26-7 | 23 |
| 4 | N-Ethylformamide | 73 | C3H7NO | 000627-45-2 | 9 |
| 5 | Butanoic acid, 2-hydroxy-2-methy... | 132 | C6H12O3 | 032793-34-3 | 9 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG050515\
Data File : BG016887.D
Acq On : 6 May 2015 5:31
Operator : TP/IZ
Sample : G2114-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** GRID-2(12-18)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

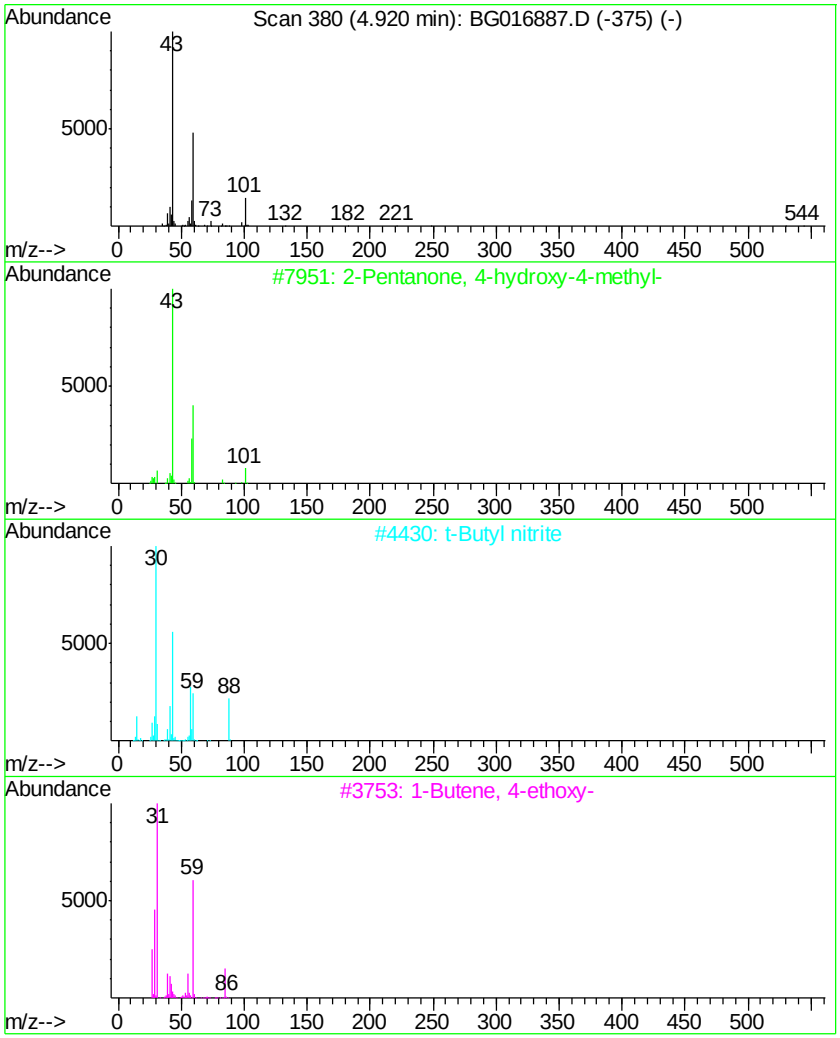
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

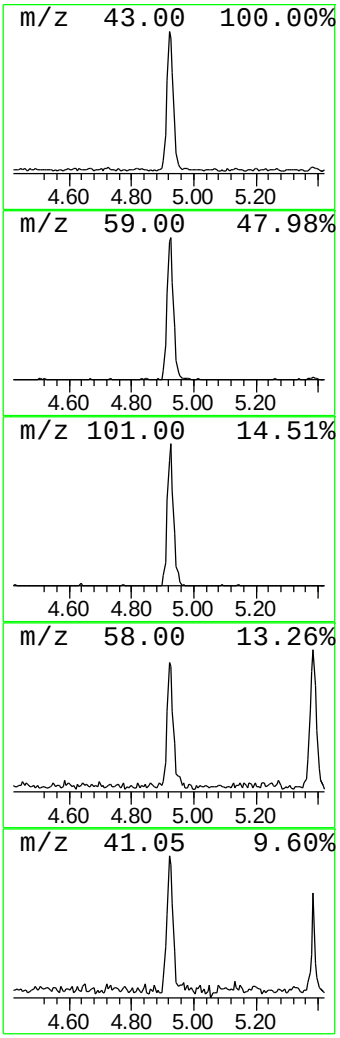
**********

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.92 | 10.32 ng | 283504 | 1,4-Dichlorobenzene-d4 | 7.81 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 50 |
| 2 | t-Butyl nitrite | 103 | C4H9NO2 | 000540-80-7 | 39 |
| 3 | 1-Butene, 4-ethoxy- | 100 | C6H12O | 044611-46-3 | 23 |
| 4 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |
| 5 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 9 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG050515\
Data File : BG016887.D
Acq On : 6 May 2015 5:31
Operator : TP/IZ
Sample : G2114-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** GRID-2(12-18)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

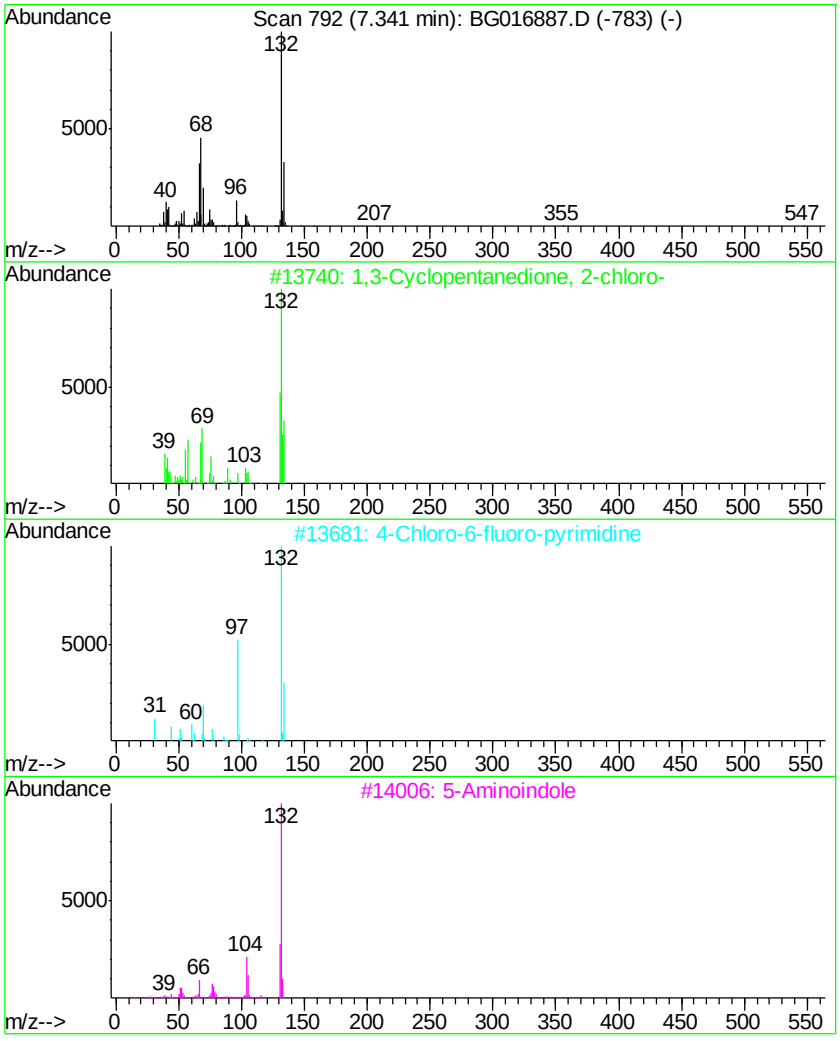
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

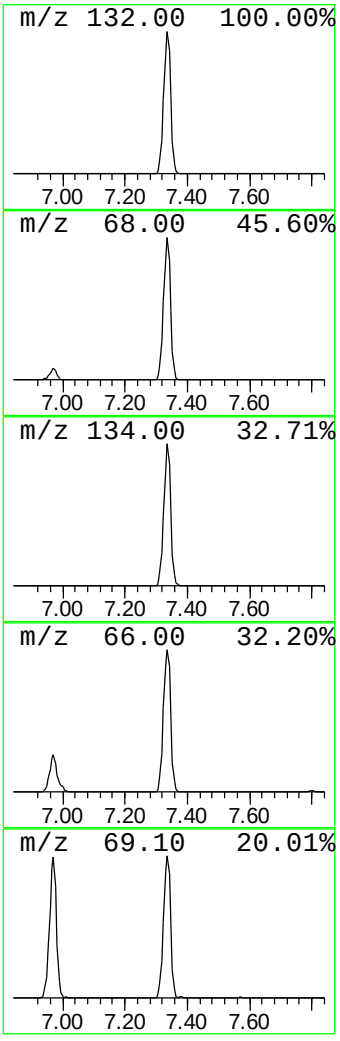
**********

Peak Number 5 unknown7.34 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.34 | 105.97 ng | 2910620 | 1,4-Dichlorobenzene-d4 | 7.81 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,3-Cyclopentanedione, 2-chloro- | 132 | C5H5ClO2 | 014203-19-1 | 35 |
| 2 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 27 |
| 3 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 22 |
| 4 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 12 |
| 5 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG050515\
Data File : BG016887.D
Acq On : 6 May 2015 5:31
Operator : TP/IZ
Sample : G2114-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** GRID-2(12-18)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

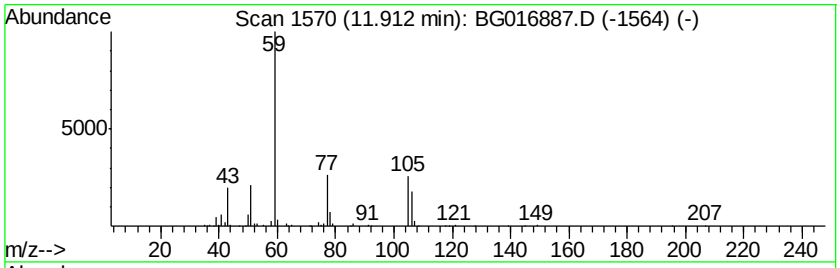
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

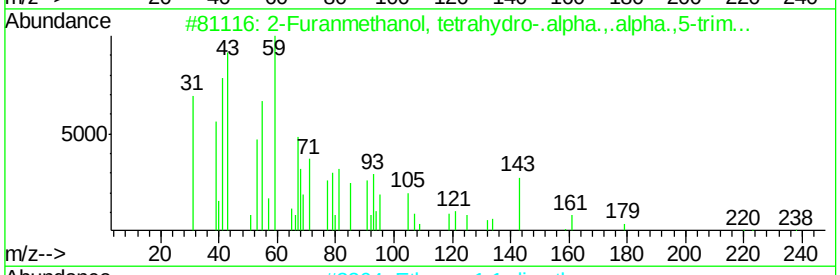
**********

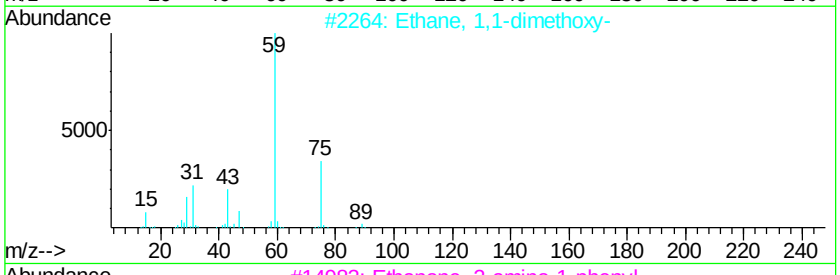
Peak Number 7 unknown11.91 Concentration Rank 10

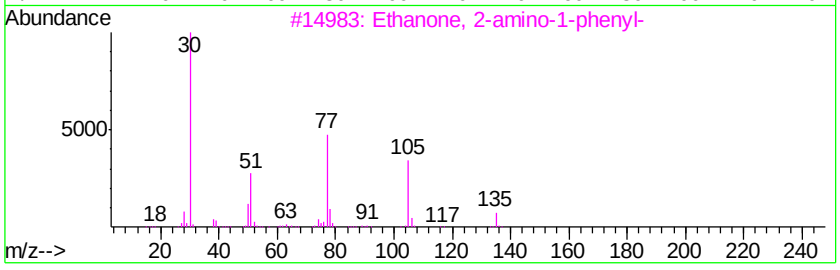
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.91 | 3.95 ng | 162299 | Naphthalene-d8 | 10.60 |

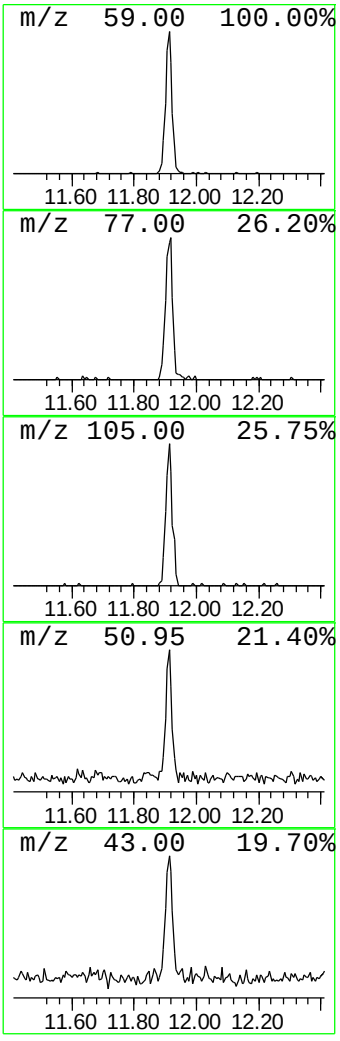
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Furanmethanol, tetrahydro-.alp... | 238 | C15H26O2 | 026184-88-3 | 32 |
| 2 | Ethane, 1,1-dimethoxy- | 90 | C4H10O2 | 000534-15-6 | 23 |
| 3 | Ethanone, 2-amino-1-phenyl- | 135 | C8H9NO | 000613-89-8 | 16 |
| 4 | Guanidine | 59 | CH5N3 | 000113-00-8 | 9 |
| 5 | Propanoic acid, 2-hydroxy-2-methyl- | 104 | C4H8O3 | 000594-61-6 | 9 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG050515\
Data File : BG016887.D
Acq On : 6 May 2015 5:31
Operator : TP/IZ
Sample : G2114-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** GRID-2(12-18)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

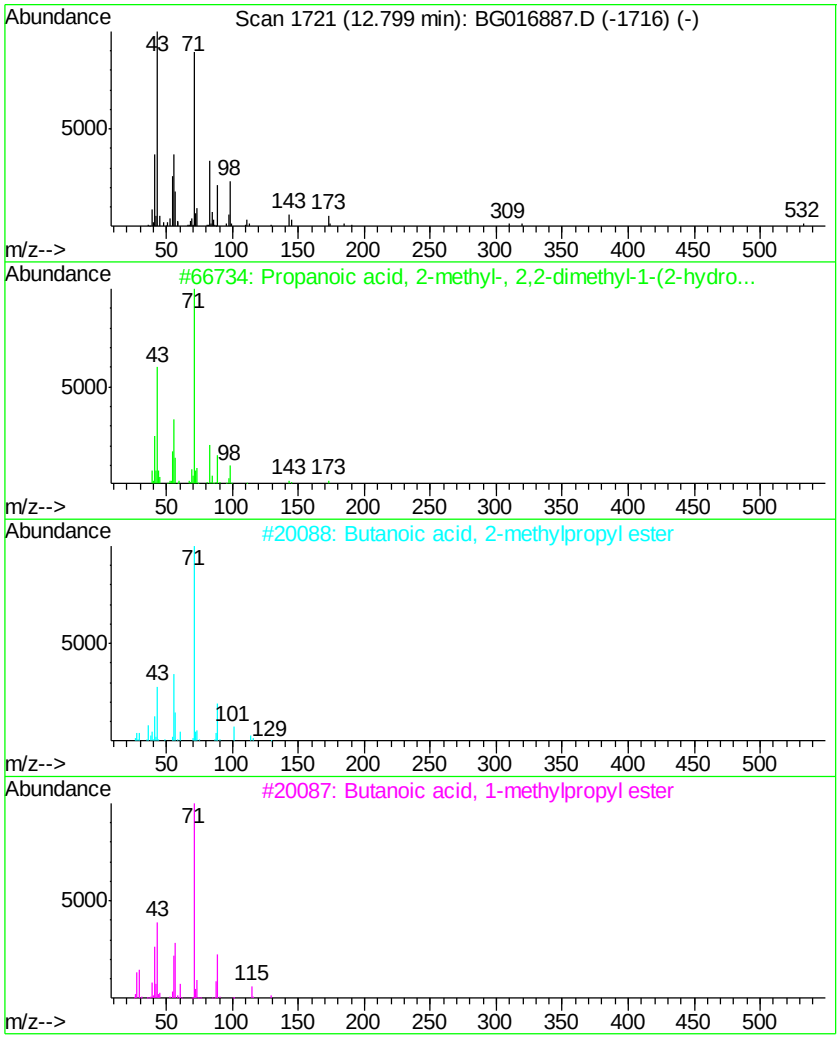
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

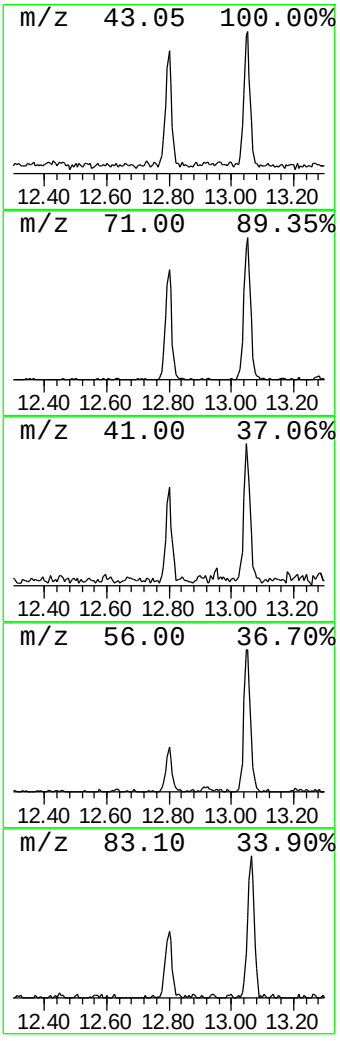
**********

Peak Number 8 Propanoic acid, 2-methyl-, ... Concentration Rank 13

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.80 | 2.03 ng | 114643 | Acenaphthene-d10 | 14.44 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Propanoic acid, 2-methyl-, 2,2-d... | 216 | C12H24O3 | 074367-33-2 | 59 |
| 2 | Butanoic acid, 2-methylpropyl ester | 144 | C8H16O2 | 000539-90-2 | 53 |
| 3 | Butanoic acid, 1-methylpropyl ester | 144 | C8H16O2 | 000819-97-6 | 40 |
| 4 | Propanoic acid, 2-methyl-, 2-met... | 144 | C8H16O2 | 000097-85-8 | 40 |
| 5 | Butyric acid, 3-tridecyl ester | 270 | C17H34O2 | 1000280-56-8 | 38 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG050515\
Data File : BG016887.D
Acq On : 6 May 2015 5:31
Operator : TP/IZ
Sample : G2114-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** GRID-2(12-18)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

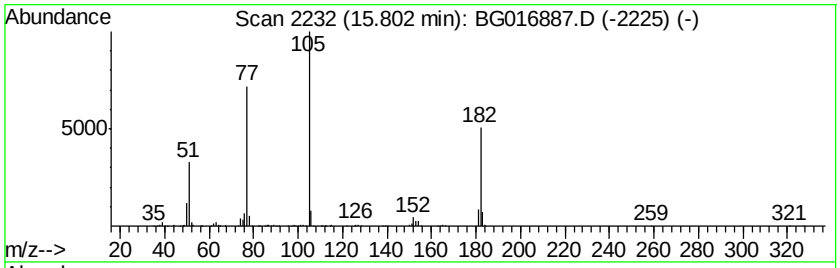
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

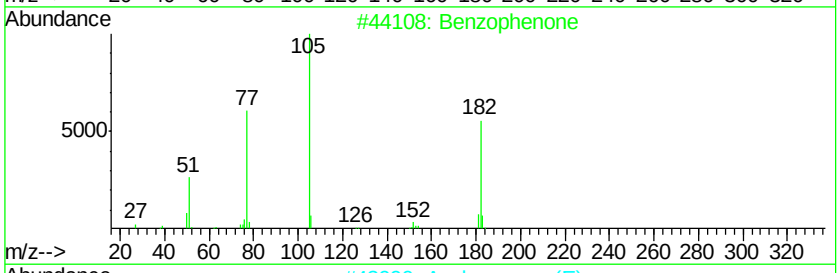
**********

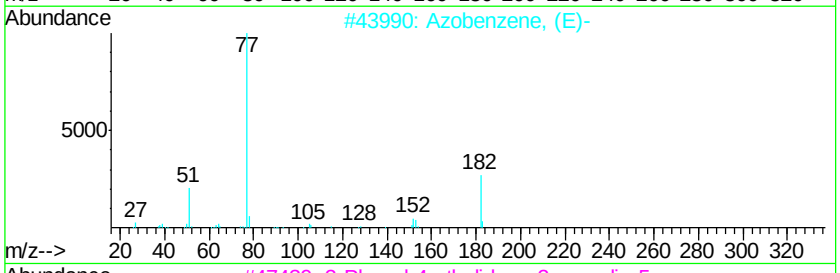
Peak Number 9 Benzophenone Concentration Rank 4

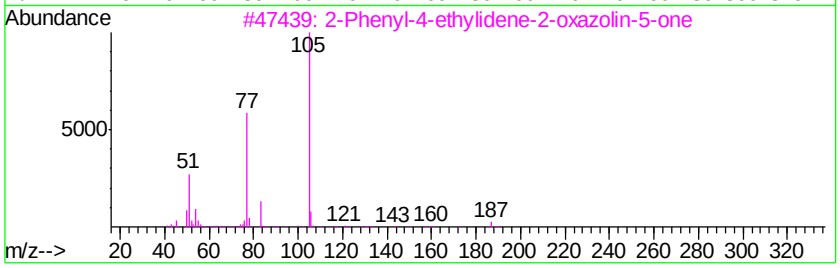
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.80 | 11.60 ng | 656041 | Acenaphthene-d10 | 14.44 |

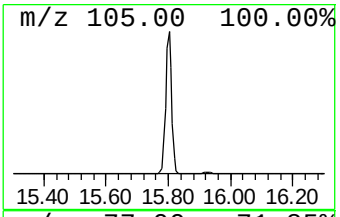
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzophenone | 182 | C13H10O | 000119-61-9 | 96 |
| 2 | Azobenzene, (E)- | 182 | C12H10N2 | 017082-12-1 | 53 |
| 3 | 2-Phenyl-4-ethylidene-2-oxazolin... | 187 | C11H9NO2 | 037791-41-6 | 50 |
| 4 | Benzenepropanenitrile, .beta.-oxo- | 145 | C9H7NO | 000614-16-4 | 50 |
| 5 | Benzenebutanoic acid, .gamma.-oxo- | 178 | C10H10O3 | 002051-95-8 | 50 |

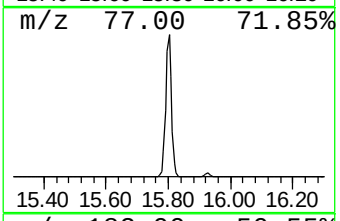


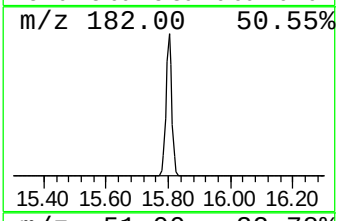



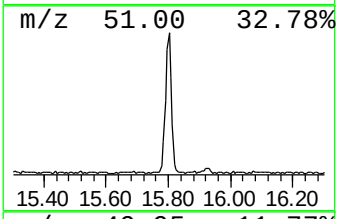



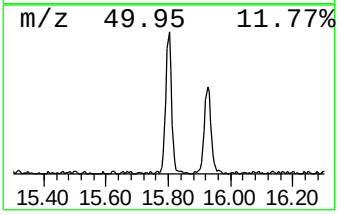



Data Path : Z:\HPCHEM1\BNA G\DATA\BG050515\
Data File : BG016887.D
Acq On : 6 May 2015 5:31
Operator : TP/IZ
Sample : G2114-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** GRID-2(12-18)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

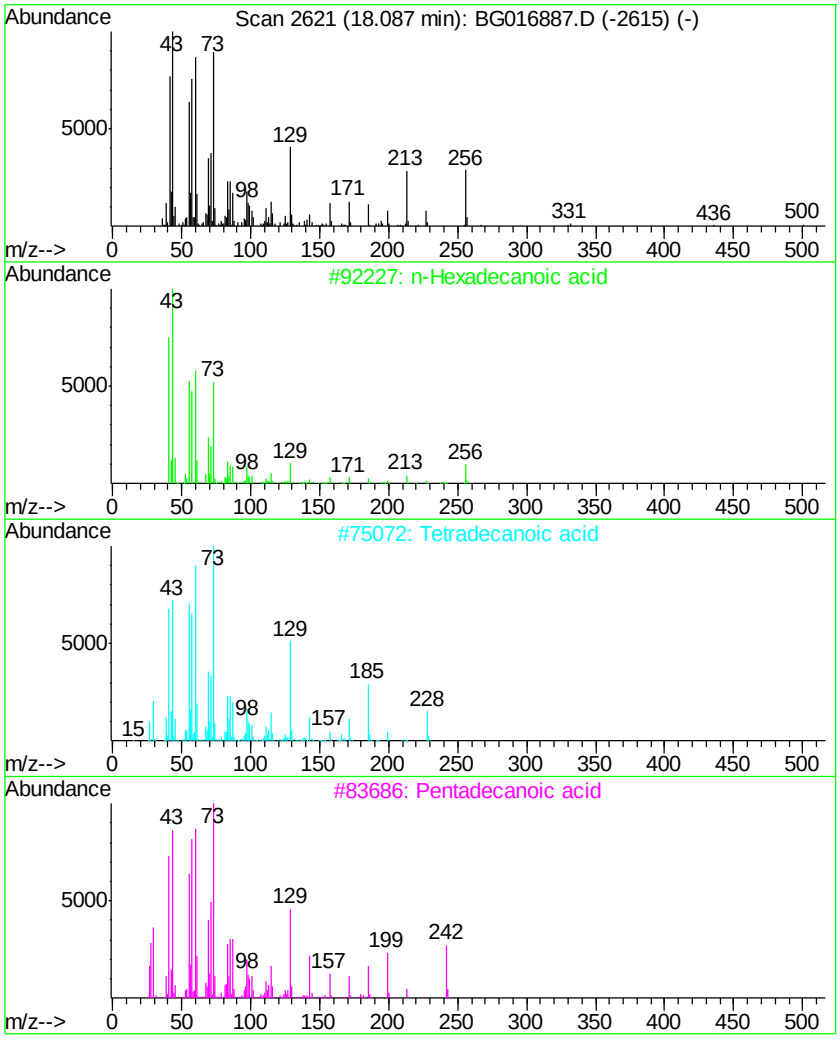
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

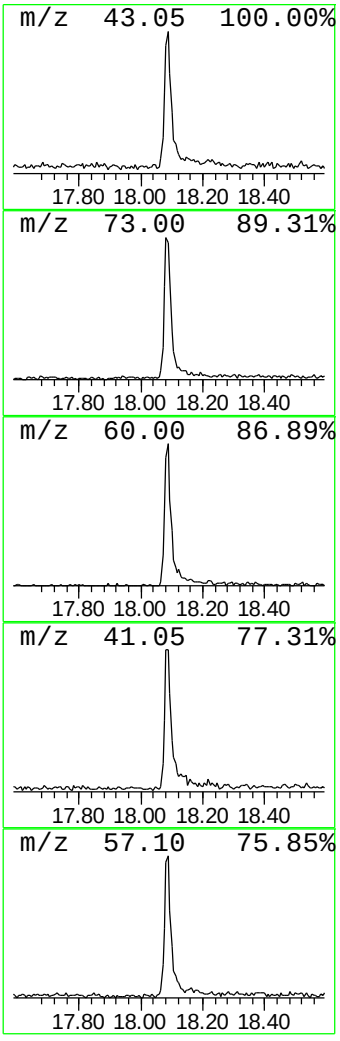
**********

Peak Number 10 n-Hexadecanoic acid Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.09 | 6.13 ng | 426425 | Phenanthrene-d10 | 17.18 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 92 |
| 2 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 86 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 81 |
| 4 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 64 |
| 5 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 55 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG050515\
Data File : BG016887.D
Acq On : 6 May 2015 5:31
Operator : TP/IZ
Sample : G2114-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** GRID-2(12-18)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

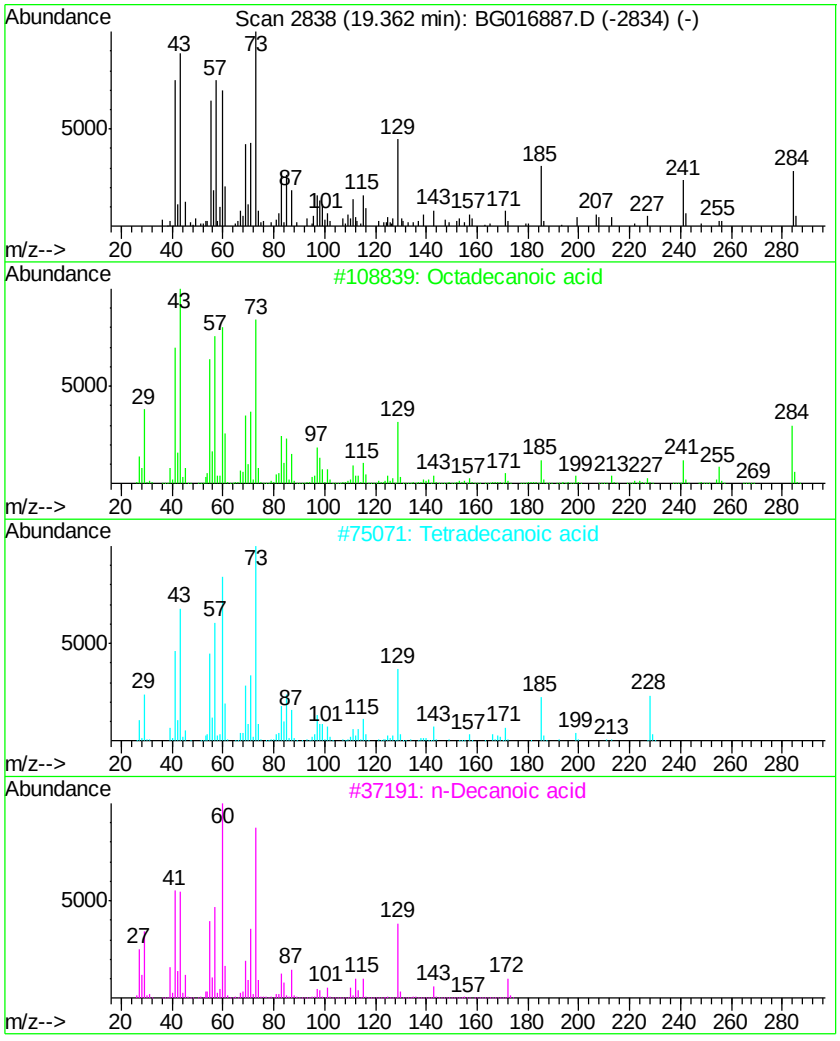
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

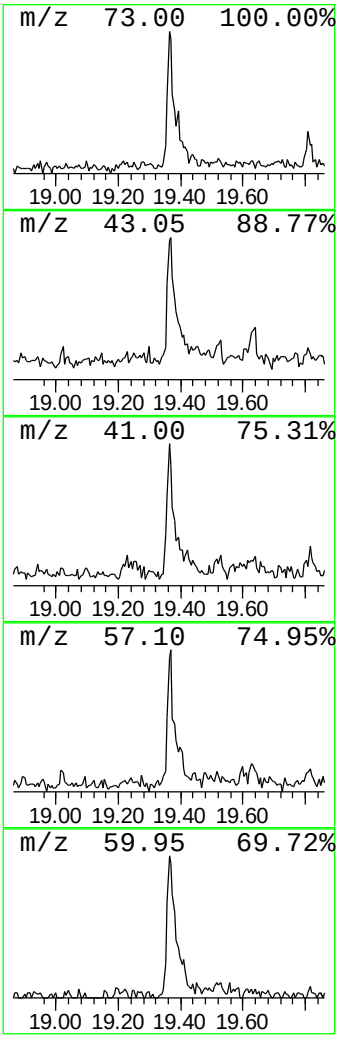
**********

Peak Number 11 Octadecanoic acid Concentration Rank 11

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.36 | 2.74 ng | 202123 | Chrysene-d12 | 21.36 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 94 |
| 2 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 58 |
| 3 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 53 |
| 4 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 47 |
| 5 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 46 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG050515\
Data File : BG016887.D
Acq On : 6 May 2015 5:31
Operator : TP/IZ
Sample : G2114-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** GRID-2(12-18)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

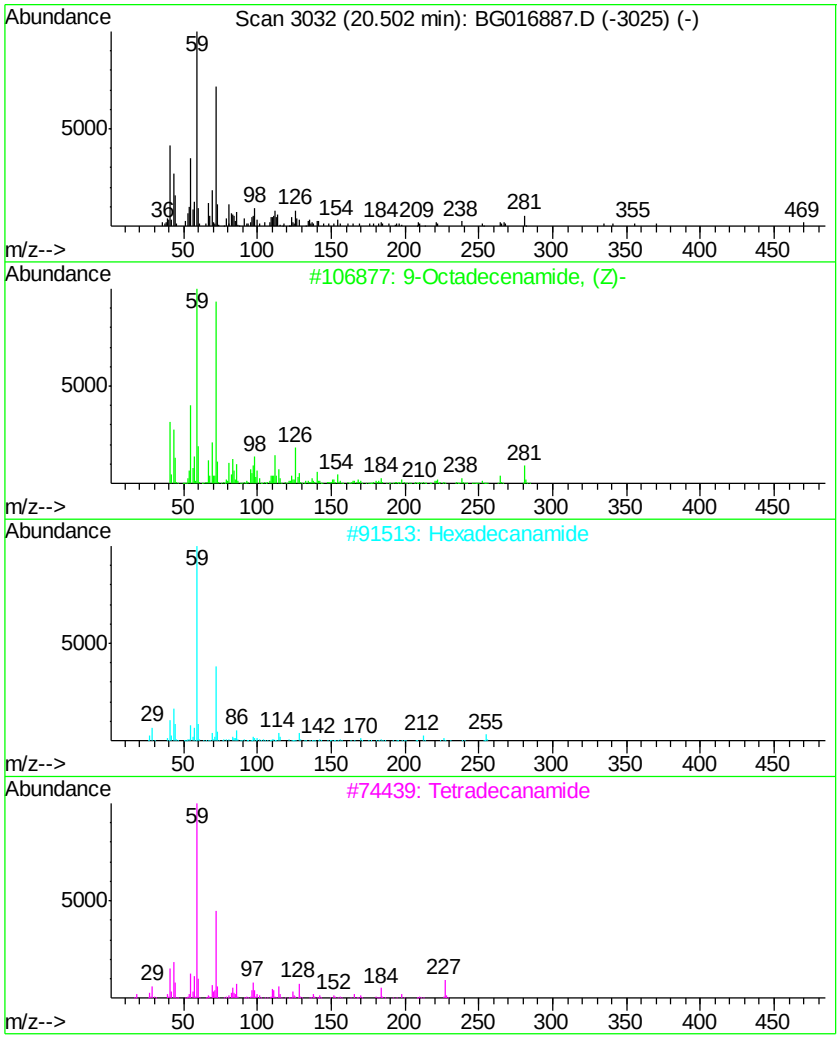
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

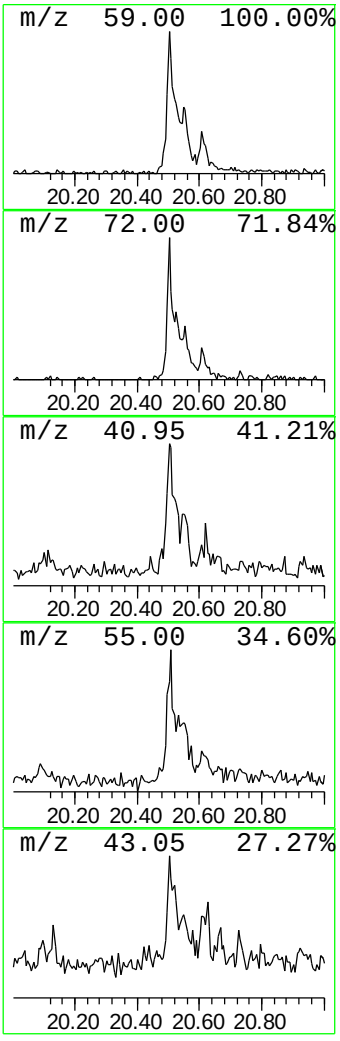
**********

Peak Number 12 9-Octadecenamide, (Z)- Concentration Rank 12

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.50 | 2.37 ng | 174642 | Chrysene-d12 | 21.36 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 9-Octadecenamide, (Z)- | 281 | C18H35NO | 000301-02-0 | 90 |
| 2 | Hexadecanamide | 255 | C16H33NO | 000629-54-9 | 72 |
| 3 | Tetradecanamide | 227 | C14H29NO | 000638-58-4 | 64 |
| 4 | 7-Nonenamide | 155 | C9H17NO | 090949-53-4 | 64 |
| 5 | Dodecanamide | 199 | C12H25NO | 001120-16-7 | 59 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG050515\
Data File : BG016887.D
Acq On : 6 May 2015 5:31
Operator : TP/IZ
Sample : G2114-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** GRID-2(12-18)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

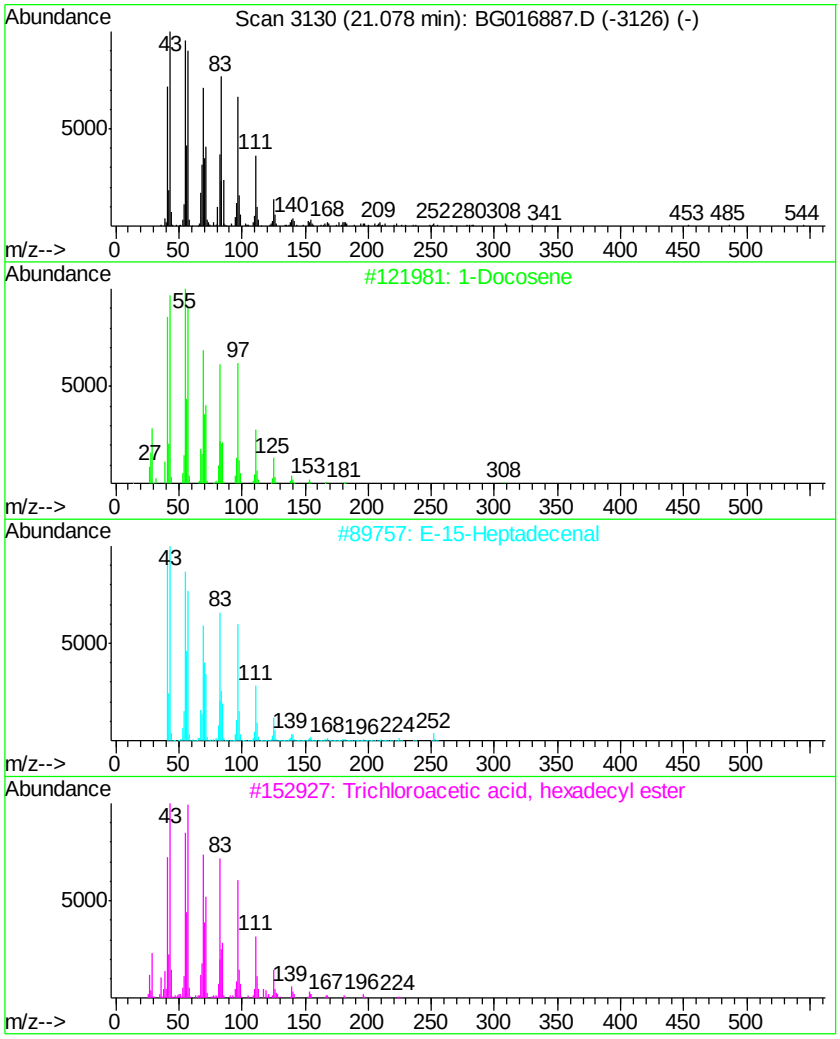
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

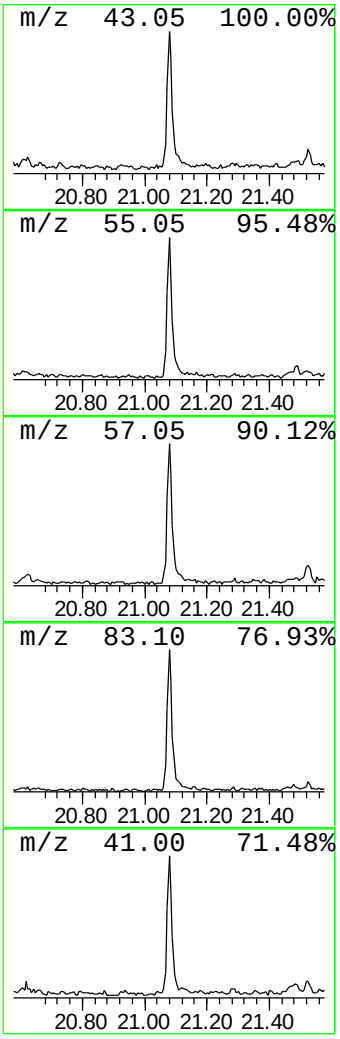
**********

Peak Number 13 1-Docosene Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.08 | 6.02 ng | 443495 | Chrysene-d12 | 21.36 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Docosene | 308 | C22H44 | 001599-67-3 | 98 |
| 2 | E-15-Heptadecenal | 252 | C17H32O | 1000130-97-9 | 98 |
| 3 | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 94 |
| 4 | Trichloroacetic acid, pentadecyl... | 372 | C17H31Cl3O2 | 074339-53-0 | 91 |
| 5 | 1-Eicosanol | 298 | C20H42O | 000629-96-9 | 91 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050515\
Data File : BG016887.D
Acq On : 6 May 2015 5:31
Operator : TP/IZ
Sample : G2114-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** GRID-2(12-18)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| unknown2.79 | 2.79 | 316.1 | ng | 8681710 | 1 | 7.81 | 549346 | 20.0 |
| Butane, 2-methoxy... | 3.01 | 11.4 | ng | 313496 | 1 | 7.81 | 549346 | 20.0 |
| 2-Pentanone, 4-hy... | 4.92 | 10.3 | ng | 283504 | 1 | 7.81 | 549346 | 20.0 |
| unknown7.34 | 7.34 | 106.0 | ng | 2910620 | 1 | 7.81 | 549346 | 20.0 |
| unknown11.91 | 11.91 | 4.0 | ng | 162299 | 2 | 10.60 | 821361 | 20.0 |
| Propanoic acid, 2... | 12.80 | 2.0 | ng | 114643 | 3 | 14.44 | 1131430 | 20.0 |
| Benzophenone | 15.80 | 11.6 | ng | 656041 | 3 | 14.44 | 1131430 | 20.0 |
| n-Hexadecanoic acid | 18.09 | 6.1 | ng | 426425 | 4 | 17.18 | 1392220 | 20.0 |
| Octadecanoic acid | 19.36 | 2.7 | ng | 202123 | 5 | 21.36 | 1473730 | 20.0 |
| 9-Octadecenamide,... | 20.50 | 2.4 | ng | 174642 | 5 | 21.36 | 1473730 | 20.0 |
| 1-Docosene | 21.08 | 6.0 | ng | 443495 | 5 | 21.36 | 1473730 | 20.0 |