LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG091916\
Data File : BG024033.D
Acq On : 20 Sep 2016 00:38
Operator : UM/SJ
Sample : H4821-23
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** YORK-SW1-3

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-BG083116.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 | 5.123 | 385 | 389 | 397 | rVB2 | 67598 | 102407 | 1.90% | 0.436% |
| 2 | 5.605 | 465 | 471 | 481 | rBV | 446328 | 767056 | 14.22% | 3.264% |
| 3 | 7.226 | 742 | 747 | 761 | rBV2 | 288573 | 568575 | 10.54% | 2.419% |
| 4 | 7.585 | 801 | 808 | 821 | rBV | 866204 | 1550872 | 28.76% | 6.598% |
| 5 | 8.055 | 880 | 888 | 895 | rBV2 | 177661 | 320487 | 5.94% | 1.364% |
| 6 | 8.378 | 937 | 943 | 954 | rVB | 761063 | 1315657 | 24.39% | 5.598% |
| 7 | 9.235 | 1082 | 1089 | 1103 | rBV | 728846 | 1351290 | 25.06% | 5.749% |
| 8 | 9.623 | 1149 | 1155 | 1166 | rVB3 | 25155 | 64941 | 1.20% | 0.276% |
| 9 | 10.886 | 1363 | 1370 | 1381 | rBV | 246770 | 472018 | 8.75% | 2.008% |
| 10 | 13.342 | 1780 | 1788 | 1798 | rBV | 2073149 | 3287331 | 60.95% | 13.987% |
| 11 | 13.600 | 1824 | 1832 | 1838 | rBV2 | 34344 | 62557 | 1.16% | 0.266% |
| 12 | 14.176 | 1924 | 1930 | 1938 | rBV2 | 258160 | 403103 | 7.47% | 1.715% |
| 13 | 14.728 | 2017 | 2024 | 2031 | rBV | 500097 | 776722 | 14.40% | 3.305% |
| 14 | 16.232 | 2273 | 2280 | 2291 | rBV | 2045933 | 3323157 | 61.62% | 14.139% |
| 15 | 17.495 | 2488 | 2495 | 2504 | rBV2 | 673000 | 1064774 | 19.74% | 4.530% |
| 16 | 18.364 | 2639 | 2643 | 2648 | rBV2 | 112705 | 160773 | 2.98% | 0.684% |
| 17 | 19.633 | 2854 | 2859 | 2869 | rBV2 | 122906 | 201022 | 3.73% | 0.855% |
| 18 | 20.103 | 2932 | 2939 | 2949 | rBV | 4167639 | 5393206 | 100.00% | 22.946% |
| 19 | 21.801 | 3222 | 3228 | 3237 | rBV | 690246 | 1166890 | 21.64% | 4.965% |
| 20 | 22.300 | 3310 | 3313 | 3322 | rVB8 | 41611 | 79373 | 1.47% | 0.338% |
| 21 | 25.149 | 3788 | 3798 | 3810 | rVB | 355210 | 1071227 | 19.86% | 4.558% |

Sum of corrected areas: 23503438

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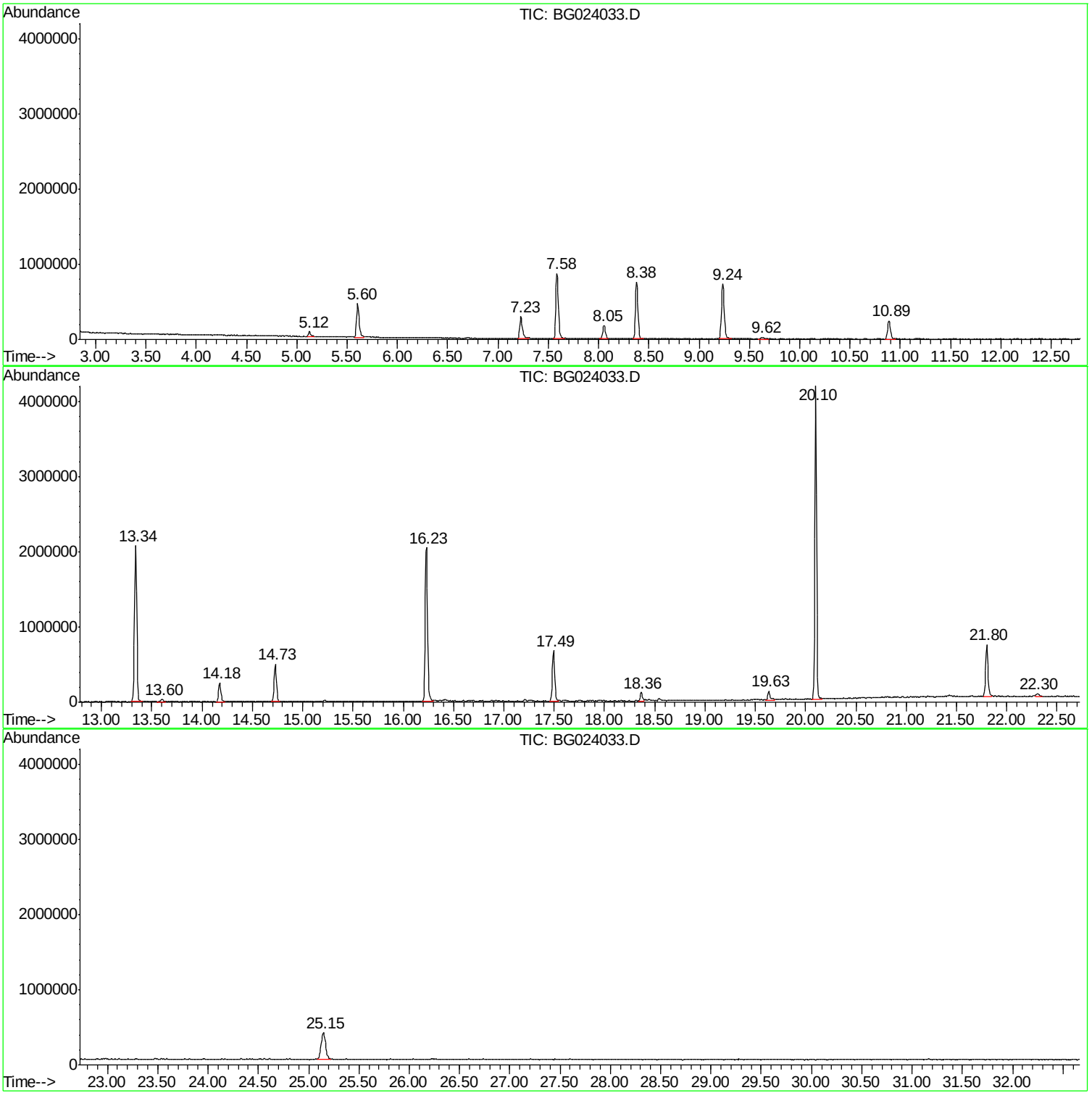
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
YORK-SW1-3

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG083116.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\BG091916\
Data File : BG024033.D
Acq On : 20 Sep 2016 00:38
Operator : UM/SJ
Sample : H4821-23
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** YORK-SW1-3

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG083116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

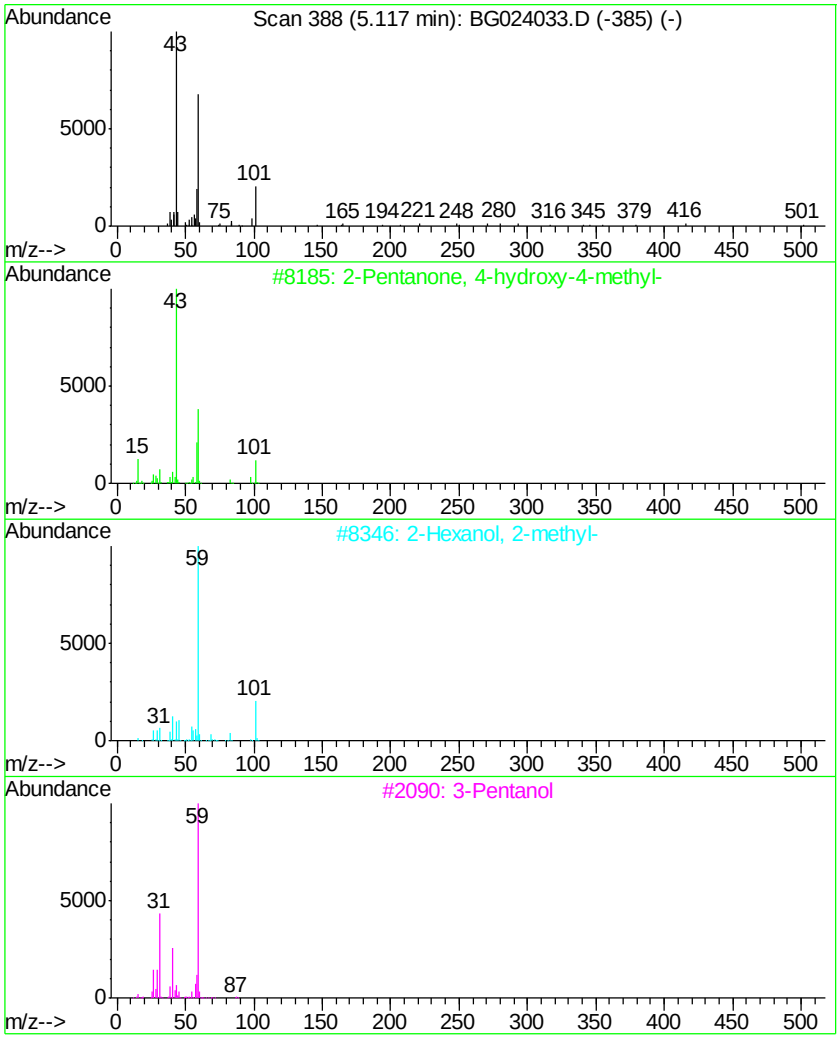
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

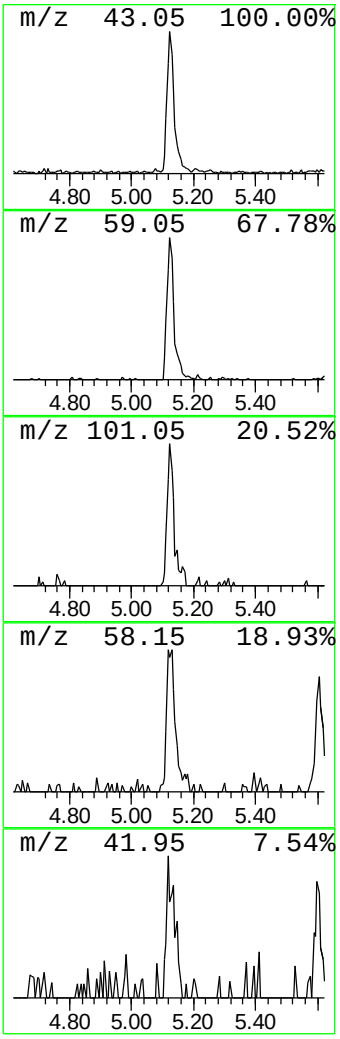
**********

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.12 | 6.39 ng | 102407 | 1,4-Dichlorobenzene-d4 | 8.05 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 45 |
| 2 | 2-Hexanol, 2-methyl- | 116 | C7H16O | 000625-23-0 | 38 |
| 3 | 3-Pentanol | 88 | C5H12O | 000584-02-1 | 23 |
| 4 | 2-Pentanol, 3-chloro-2-methyl- | 136 | C6H13ClO | 074685-49-7 | 17 |
| 5 | Silane, trimethyl- | 74 | C3H10Si | 000993-07-7 | 17 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG091916\
Data File : BG024033.D
Acq On : 20 Sep 2016 00:38
Operator : UM/SJ
Sample : H4821-23
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** YORK-SW1-3

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG083116.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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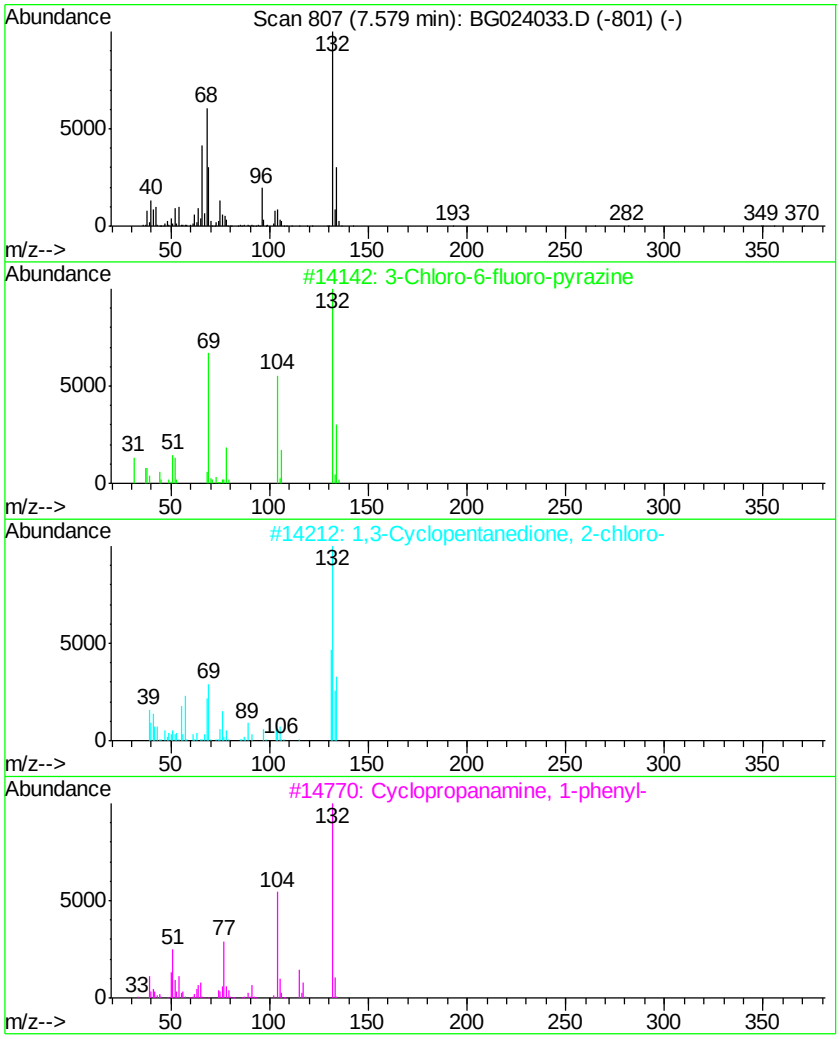
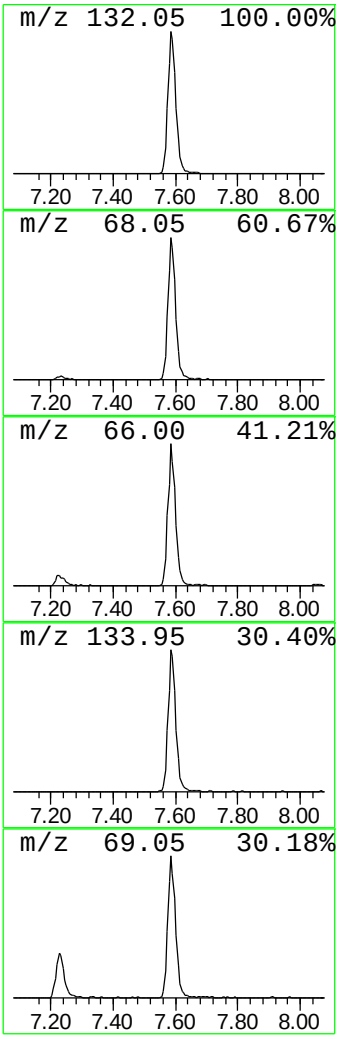
Peak Number 2 unknown7.58 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.58 | 96.78 ng | 1550870 | 1,4-Dichlorobenzene-d4 | 8.05 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 18 |
| 2 | 1,3-Cyclopentanedione, 2-chloro- | 132 | C5H5ClO2 | 014203-19-1 | 12 |
| 3 | Cyclopropanamine, 1-phenyl- | 133 | C9H11N | 1000351-26-2 | 10 |
| 4 | 3H-1,2-Dithiol-3-one, 5-methyl- | 132 | C4H4OS2 | 003620-08-4 | 10 |
| 5 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 9 |



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Data File : BG024033.D
Acq On : 20 Sep 2016 00:38
Operator : UM/SJ
Sample : H4821-23
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** YORK-SW1-3

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG083116.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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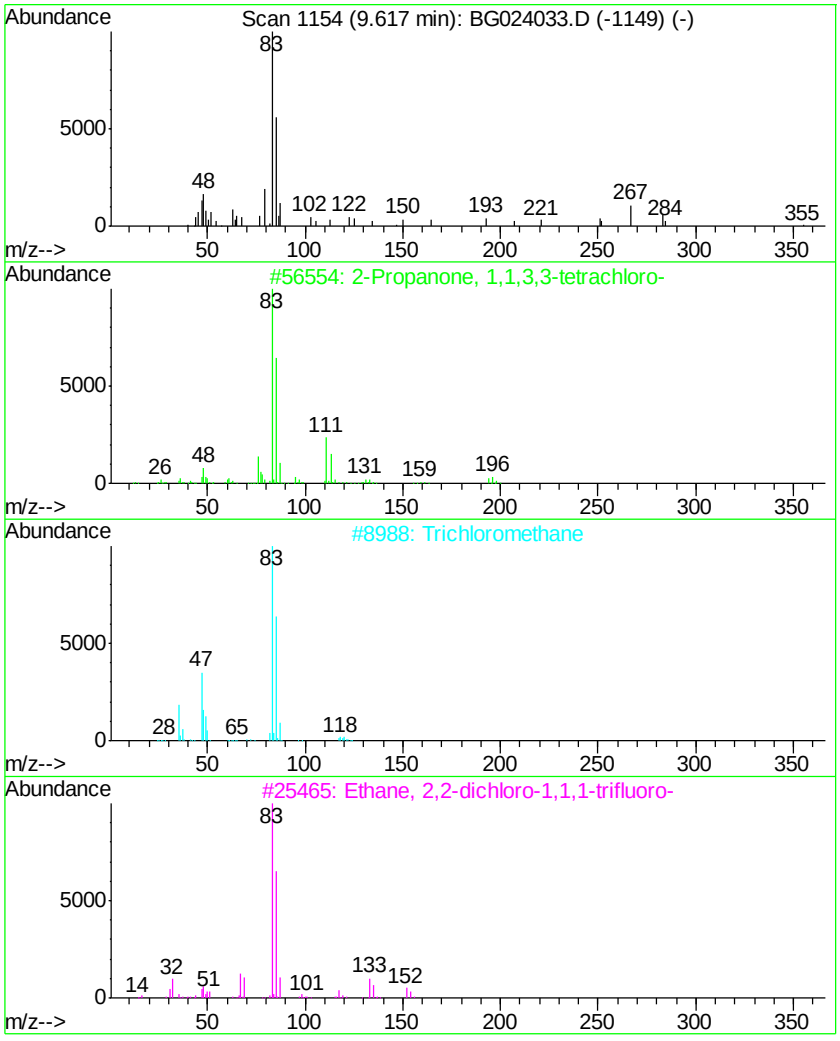
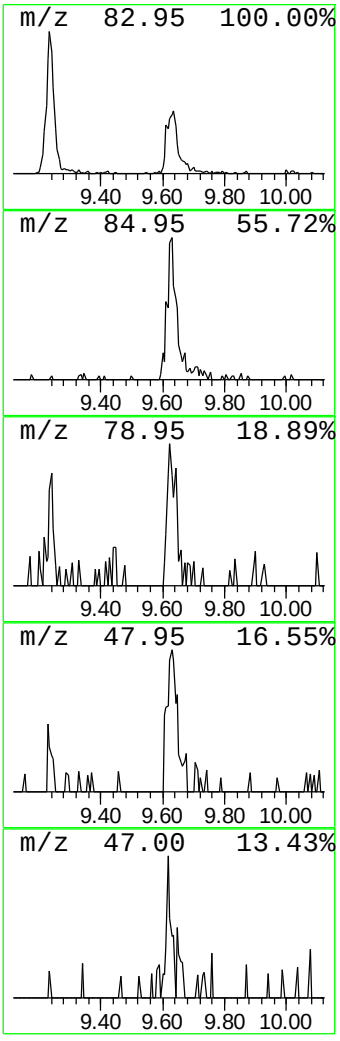
Peak Number 4 2-Propanone, 1,1,3,3-tetrac... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.62 | 2.75 ng | 64941 | Naphthalene-d8 | 10.89 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Propanone, 1,1,3,3-tetrachloro- | 194 | C3H2Cl4O | 000632-21-3 | 64 |
| 2 | Trichloromethane | 118 | CHCl3 | 000067-66-3 | 56 |
| 3 | Ethane, 2,2-dichloro-1,1,1-trifl... | 152 | C2HCl2F3 | 000306-83-2 | 50 |
| 4 | Ethane, 1,2,2-trichloro-1,1-difl... | 168 | C2HCl3F2 | 000354-21-2 | 50 |
| 5 | Methane, dichloronitro- | 129 | CHCl2NO2 | 007119-89-3 | 42 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG091916\
Data File : BG024033.D
Acq On : 20 Sep 2016 00:38
Operator : UM/SJ
Sample : H4821-23
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** YORK-SW1-3

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG083116.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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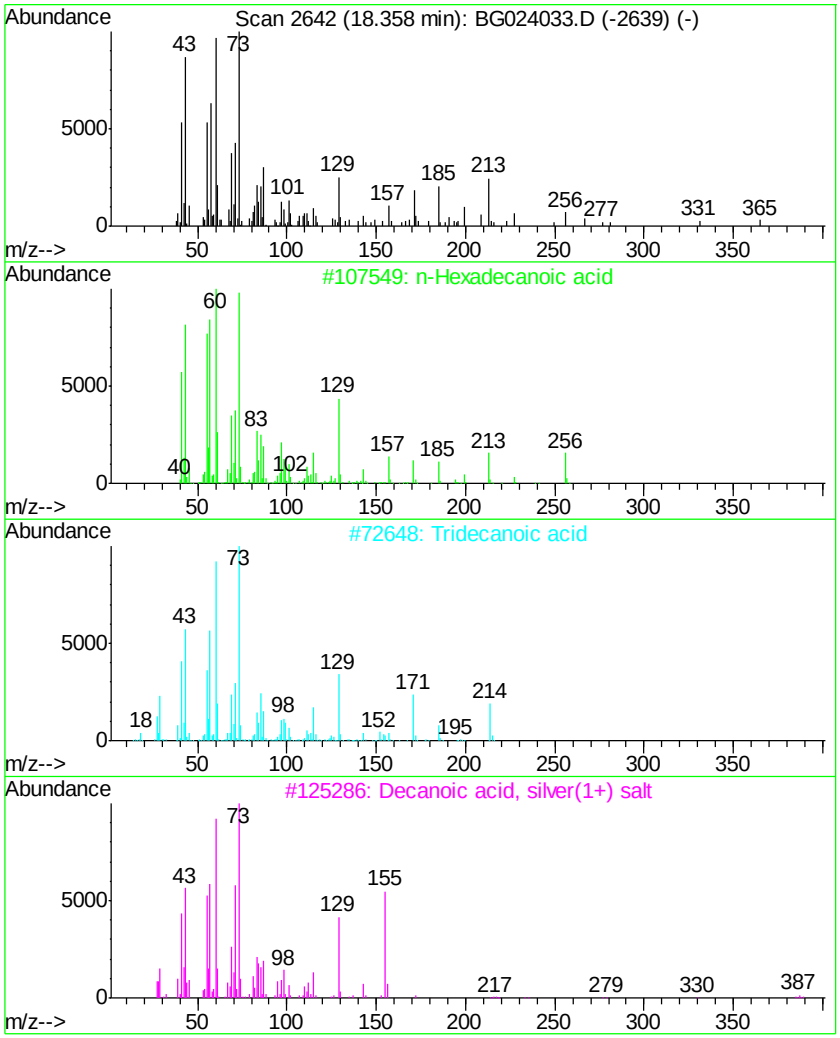
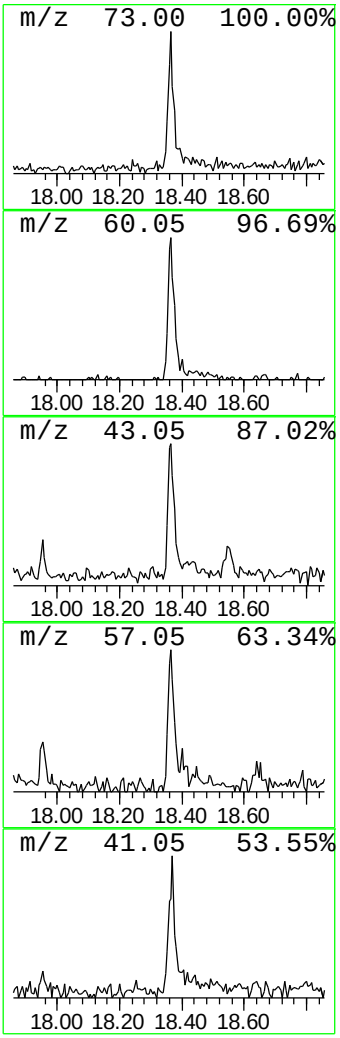
Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.36 | 3.02 ng | 160773 | Phenanthrene-d10 | 17.49 |

| 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 | 53 |
| 3 | Decanoic acid, silver(1+) salt | 278 | C10H19AgO2 | 013126-67-5 | 47 |
| 4 | D-Galactose | 180 | C6H12O6 | 000059-23-4 | 47 |
| 5 | Undecanoic acid | 186 | C11H22O2 | 000112-37-8 | 43 |



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Sample : H4821-23
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** YORK-SW1-3

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG083116.M
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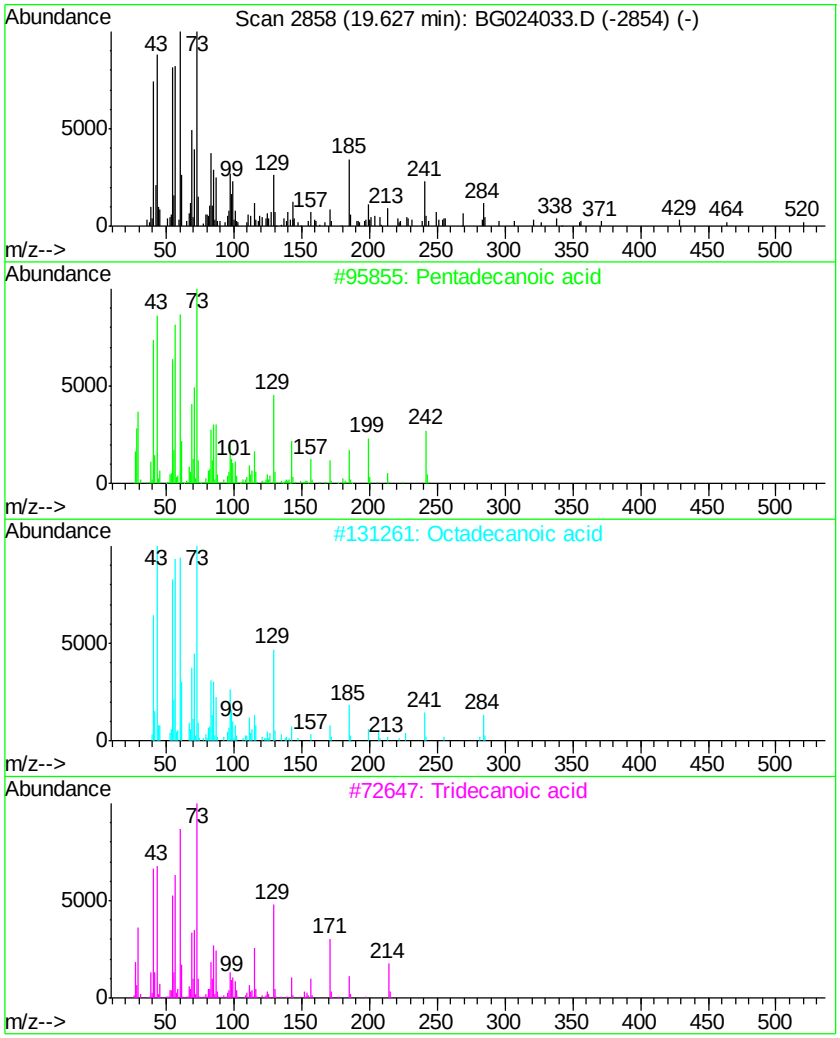
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

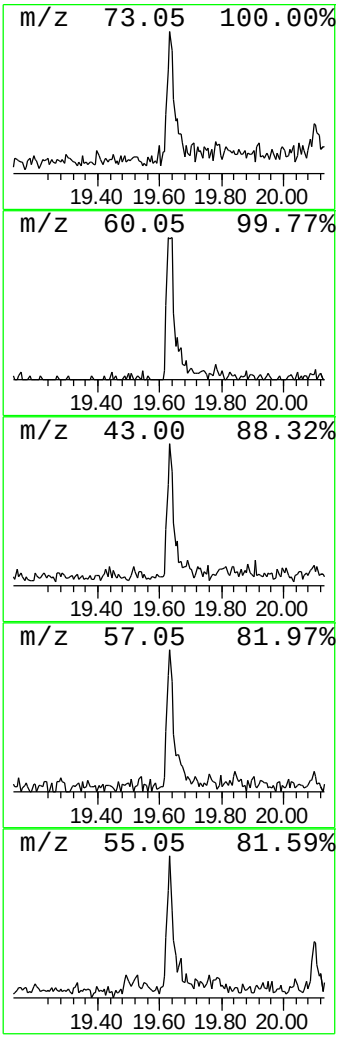
**********

Peak Number 6 Pentadecanoic acid Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.63 | 3.78 ng | 201022 | Phenanthrene-d10 | 17.49 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 70 |
| 2 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 64 |
| 3 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 38 |
| 4 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 38 |
| 5 | Undecanoic acid | 186 | C11H22O2 | 000112-37-8 | 30 |



Tentatively Identified Compound (LSC) summary

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**Instrument :** BNA_G
**ClientSampleId :** YORK-SW1-3

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG083116.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... | 5.12 | 6.4 | ng | 102407 | 1 | 8.05 | 320487 | 20.0 |
| unknown7.58 | 7.58 | 96.8 | ng | 1550870 | 1 | 8.05 | 320487 | 20.0 |
| 2-Propanone, 1,1,... | 9.62 | 2.8 | ng | 64941 | 2 | 10.89 | 472018 | 20.0 |
| n-Hexadecanoic acid | 18.36 | 3.0 | ng | 160773 | 4 | 17.49 | 1064770 | 20.0 |
| Pentadecanoic acid | 19.63 | 3.8 | ng | 201022 | 4 | 17.49 | 1064770 | 20.0 |