LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG092116\
Data File : BG024055.D
Acq On : 21 Sep 2016 15:09
Operator : UM/SJ
Sample : H4820-21
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** YORK-SB3-02

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 | 2.923 | 9 | 14 | 27 | rVB | 2073408 | 3030920 | 74.64% | 11.797% |
| 2 | 5.114 | 382 | 387 | 394 | rBV | 255104 | 393885 | 9.70% | 1.533% |
| 3 | 5.602 | 464 | 470 | 481 | rBV | 722136 | 1176705 | 28.98% | 4.580% |
| 4 | 7.223 | 739 | 746 | 761 | rVB | 1001411 | 1773971 | 43.69% | 6.905% |
| 5 | 7.582 | 799 | 807 | 816 | rBV | 907054 | 1601277 | 39.43% | 6.233% |
| 6 | 8.052 | 880 | 887 | 895 | rBV | 249529 | 442517 | 10.90% | 1.722% |
| 7 | 8.375 | 934 | 942 | 951 | rBV | 760760 | 1317763 | 32.45% | 5.129% |
| 8 | 9.232 | 1080 | 1088 | 1098 | rBV | 708995 | 1298257 | 31.97% | 5.053% |
| 9 | 10.883 | 1361 | 1369 | 1377 | rBV | 341120 | 644896 | 15.88% | 2.510% |
| 10 | 13.339 | 1777 | 1787 | 1796 | rBV | 1954743 | 3071077 | 75.63% | 11.954% |
| 11 | 14.173 | 1923 | 1929 | 1935 | rBV | 346886 | 540696 | 13.31% | 2.105% |
| 12 | 14.725 | 2016 | 2023 | 2031 | rBV | 606758 | 960766 | 23.66% | 3.740% |
| 13 | 16.229 | 2273 | 2279 | 2294 | rBV | 827107 | 1366233 | 33.64% | 5.318% |
| 14 | 16.411 | 2307 | 2310 | 2319 | rVB6 | 25951 | 50449 | 1.24% | 0.196% |
| 15 | 17.210 | 2442 | 2446 | 2450 | rBV4 | 30998 | 46621 | 1.15% | 0.181% |
| 16 | 17.492 | 2488 | 2494 | 2499 | rBV | 690995 | 1099369 | 27.07% | 4.279% |
| 17 | 17.533 | 2499 | 2501 | 2506 | rVB2 | 58506 | 69074 | 1.70% | 0.269% |
| 18 | 19.272 | 2795 | 2797 | 2804 | rVB7 | 36952 | 50616 | 1.25% | 0.197% |
| 19 | 19.548 | 2841 | 2844 | 2850 | rVB2 | 109053 | 141464 | 3.48% | 0.551% |
| 20 | 19.912 | 2903 | 2906 | 2911 | rVB2 | 99780 | 128986 | 3.18% | 0.502% |
| 21 | 20.100 | 2933 | 2938 | 2944 | rBV | 3307539 | 4060813 | 100.00% | 15.806% |
| 22 | 21.398 | 3156 | 3159 | 3168 | rVB8 | 115475 | 251518 | 6.19% | 0.979% |
| 23 | 21.798 | 3221 | 3227 | 3233 | rBV | 699187 | 1155785 | 28.46% | 4.499% |
| 24 | 25.140 | 3789 | 3796 | 3805 | rVB2 | 364455 | 1018068 | 25.07% | 3.963% |

Sum of corrected areas: 25691726

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA G\DATA\BG092116\
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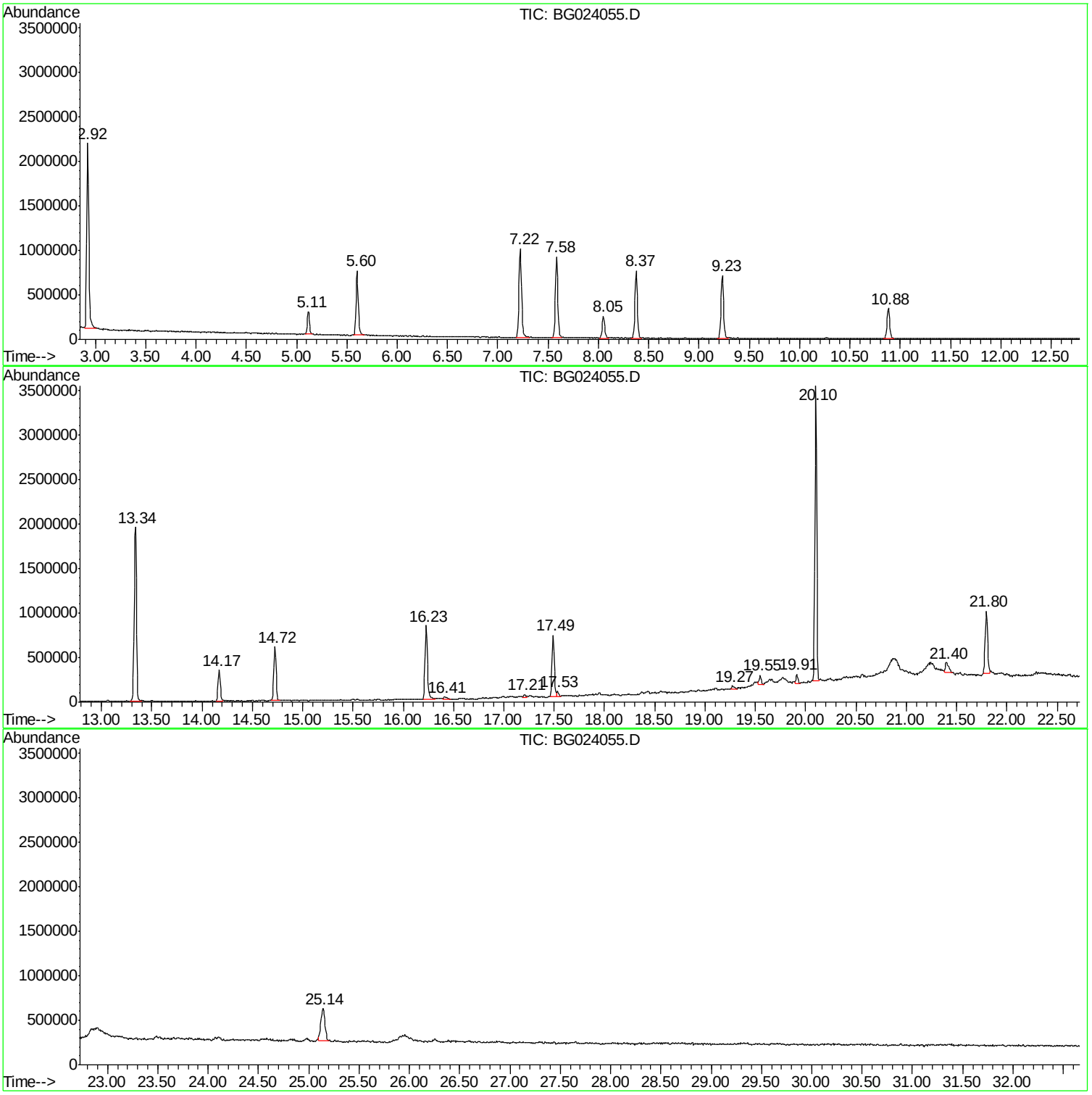
Operator : UM/SJ
Sample : H4820-21
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** YORK-SB3-02

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\BG092116\
Data File : BG024055.D
Acq On : 21 Sep 2016 15:09
Operator : UM/SJ
Sample : H4820-21
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** YORK-SB3-02

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

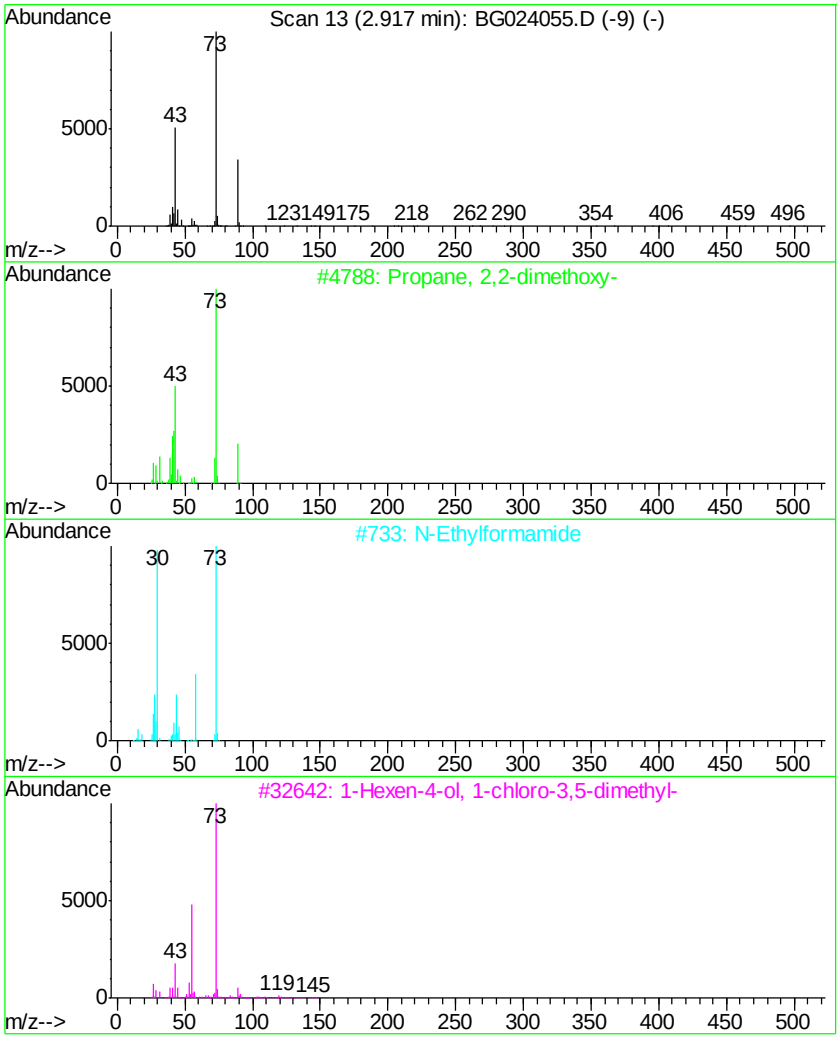
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

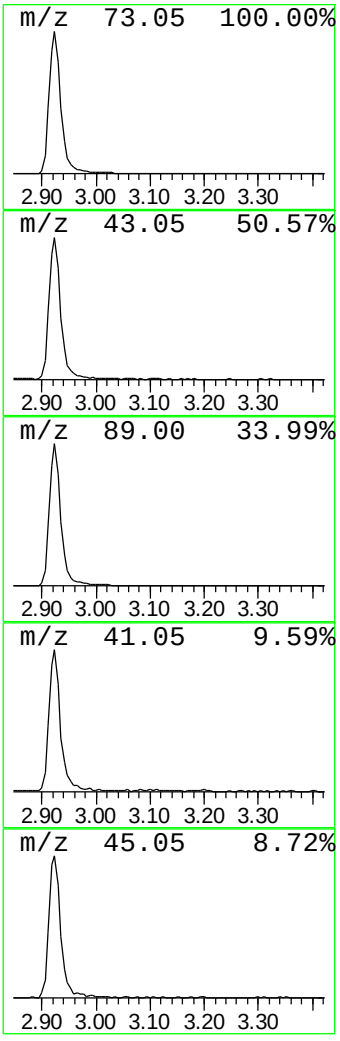
**********

Peak Number 1 unknown2.92 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.92 | 136.99 ng | 3030920 | 1,4-Dichlorobenzene-d4 | 8.05 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Propane, 2,2-dimethoxy- | 104 | C5H12O2 | 000077-76-9 | 38 |
| 2 | N-Ethylformamide | 73 | C3H7NO | 000627-45-2 | 9 |
| 3 | 1-Hexen-4-ol, 1-chloro-3,5-dimet... | 162 | C8H15ClO | 100244-09-5 | 9 |
| 4 | 2-Hydroxy-2-methylbutyric acid | 118 | C5H10O3 | 003739-30-8 | 9 |
| 5 | Propane, 2-methoxy-2-methyl- | 88 | C5H12O | 001634-04-4 | 9 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG092116\
Data File : BG024055.D
Acq On : 21 Sep 2016 15:09
Operator : UM/SJ
Sample : H4820-21
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** YORK-SB3-02

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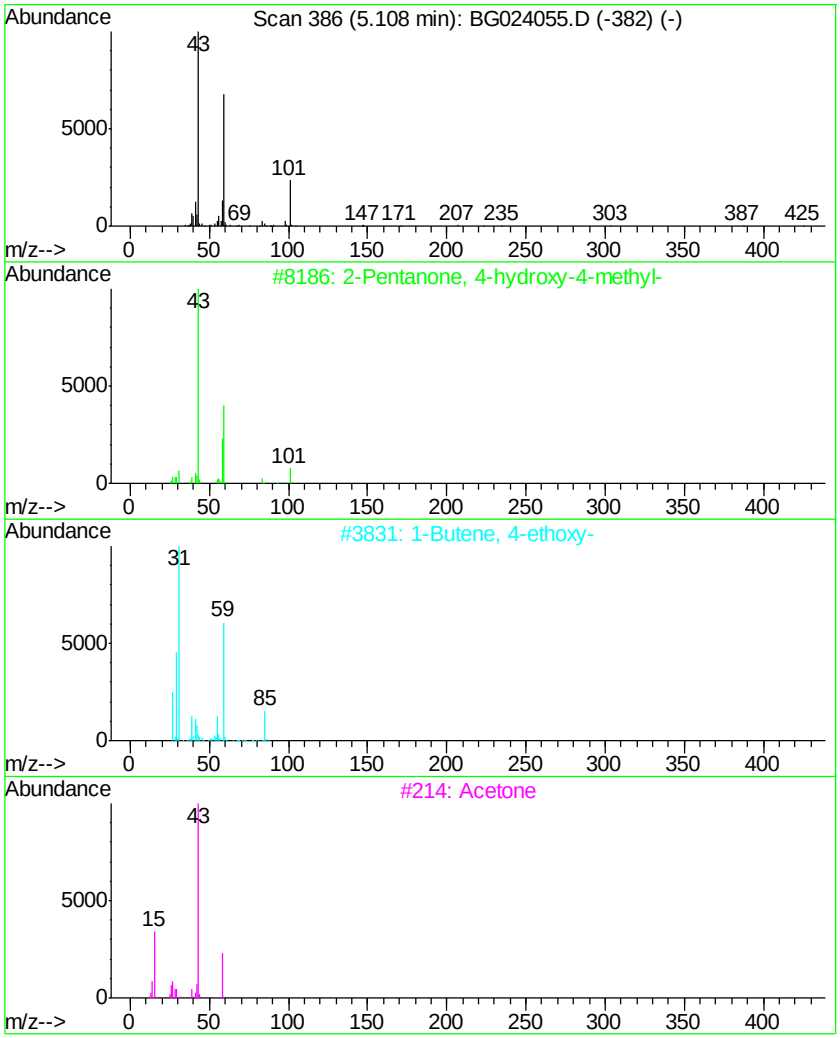
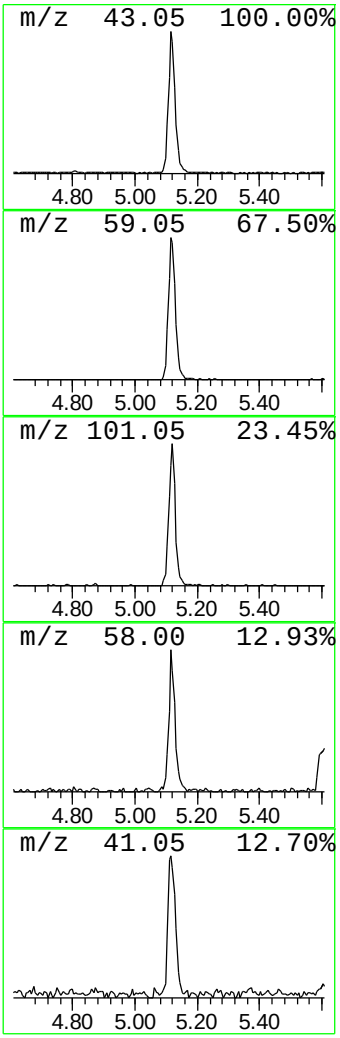
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.11 | 17.80 ng | 393885 | 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 | 56 |
| 2 | 1-Butene, 4-ethoxy- | 100 | C6H12O | 044611-46-3 | 17 |
| 3 | Acetone | 58 | C3H6O | 000067-64-1 | 9 |
| 4 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |
| 5 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG092116\
Data File : BG024055.D
Acq On : 21 Sep 2016 15:09
Operator : UM/SJ
Sample : H4820-21
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** YORK-SB3-02

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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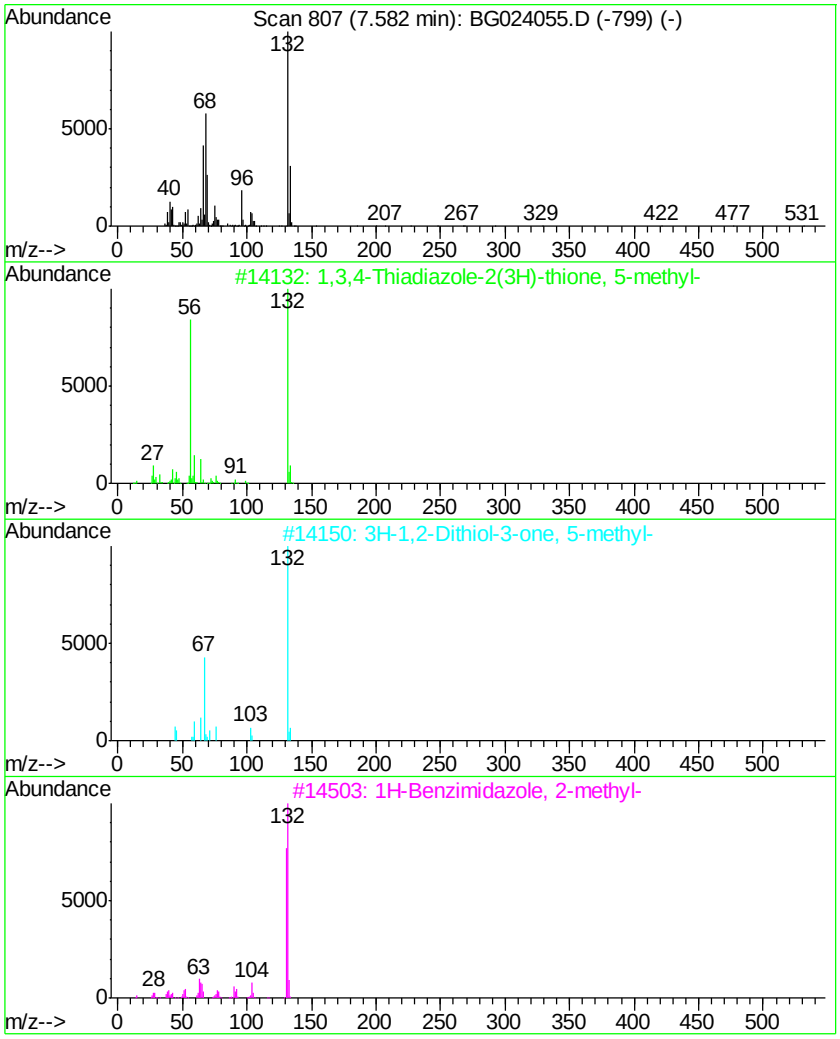
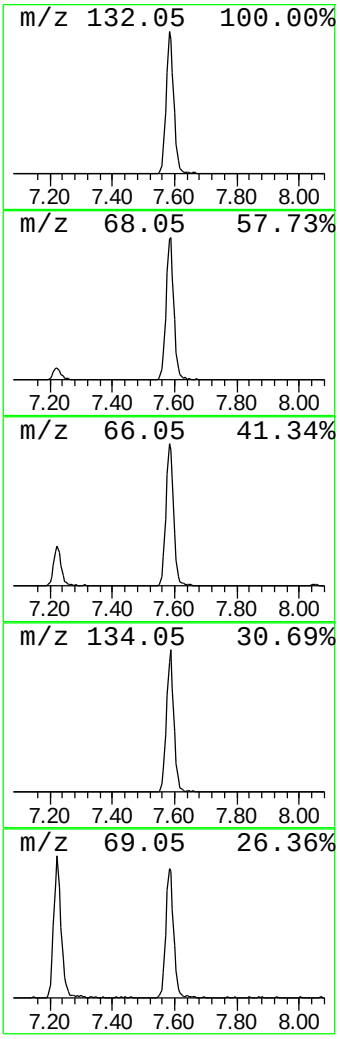
Peak Number 3 unknown7.58 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.58 | 72.37 ng | 1601280 | 1,4-Dichlorobenzene-d4 | 8.05 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,3,4-Thiadiazole-2(3H)-thione, ... | 132 | C3H4N2S2 | 029490-19-5 | 14 |
| 2 | 3H-1,2-Dithiol-3-one, 5-methyl- | 132 | C4H4OS2 | 003620-08-4 | 14 |
| 3 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 14 |
| 4 | 1,3-Cyclopentanedione, 2-chloro- | 132 | C5H5ClO2 | 014203-19-1 | 12 |
| 5 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 10 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG092116\
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Acq On : 21 Sep 2016 15:09
Operator : UM/SJ
Sample : H4820-21
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** YORK-SB3-02

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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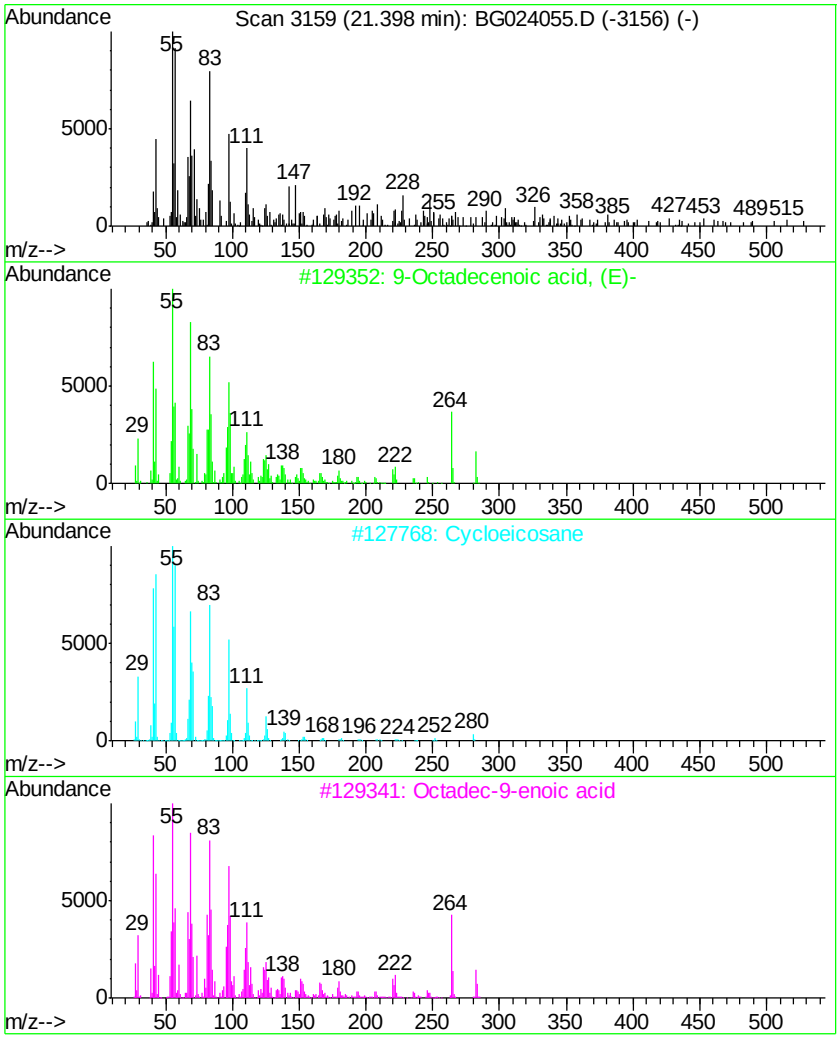
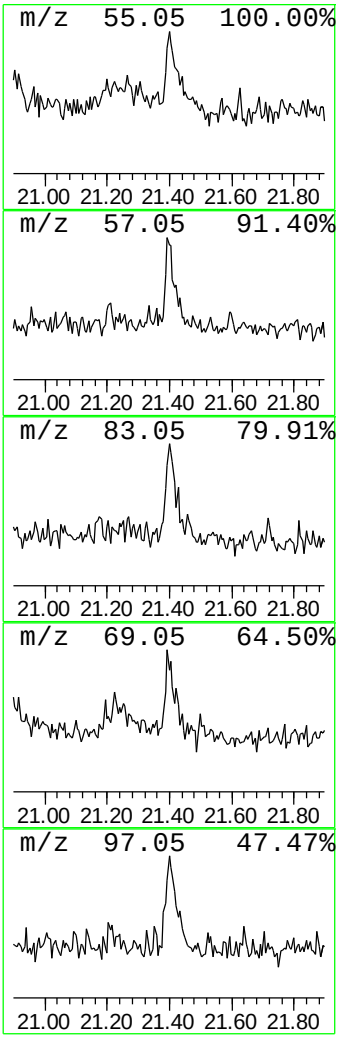
Peak Number 5 9-Octadecenoic acid, (E)- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.40 | 4.35 ng | 251518 | Chrysene-d12 | 21.80 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 9-Octadecenoic acid, (E)- | 282 | C18H34O2 | 000112-79-8 | 66 |
| 2 | Cycloeicosane | 280 | C20H40 | 000296-56-0 | 62 |
| 3 | Octadec-9-enoic acid | 282 | C18H34O2 | 1000190-13-7 | 60 |
| 4 | 3-Chloropropionic acid, heptadec... | 346 | C20H39ClO2 | 1000283-05-1 | 58 |
| 5 | Oleic Acid | 282 | C18H34O2 | 000112-80-1 | 58 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG092116\
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Acq On : 21 Sep 2016 15:09
Operator : UM/SJ
Sample : H4820-21
Misc :
ALS Vial : 3 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** YORK-SB3-02

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 |
| unknown2.92 | 2.92 | 137.0 | ng | 3030920 | 1 | 8.05 | 442517 | 20.0 |
| 2-Pentanone, 4-hy... | 5.11 | 17.8 | ng | 393885 | 1 | 8.05 | 442517 | 20.0 |
| unknown7.58 | 7.58 | 72.4 | ng | 1601280 | 1 | 8.05 | 442517 | 20.0 |
| 9-Octadecenoic ac... | 21.40 | 4.3 | ng | 251518 | 5 | 21.80 | 1155790 | 20.0 |