LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG080316\
Data File : BG023443.D
Acq On : 4 Aug 2016 2:42
Operator : UM/SJ
Sample : H4287-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-58-18.0-19.0

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-BG080116.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 | 2.997 | 23 | 27 | 35 | rVB | 247359 | 331668 | 3.36% | 0.737% |
| 2 | 5.182 | 393 | 399 | 410 | rBV | 381835 | 586595 | 5.94% | 1.303% |
| 3 | 5.658 | 474 | 480 | 490 | rBV | 1316494 | 2093450 | 21.20% | 4.651% |
| 4 | 7.273 | 747 | 755 | 764 | rBV | 1590035 | 2793224 | 28.29% | 6.205% |
| 5 | 7.649 | 811 | 819 | 826 | rBV | 1364075 | 2440242 | 24.72% | 5.421% |
| 6 | 8.119 | 892 | 899 | 908 | rBV | 371043 | 653145 | 6.62% | 1.451% |
| 7 | 8.442 | 946 | 954 | 962 | rBV | 958467 | 1673332 | 16.95% | 3.717% |
| 8 | 9.294 | 1090 | 1099 | 1108 | rBV | 957239 | 1745113 | 17.68% | 3.877% |
| 9 | 10.951 | 1374 | 1381 | 1390 | rVB | 538015 | 992557 | 10.05% | 2.205% |
| 10 | 13.394 | 1790 | 1797 | 1807 | rBV | 2864691 | 4601430 | 46.61% | 10.222% |
| 11 | 14.223 | 1933 | 1938 | 1944 | rBV | 565847 | 803576 | 8.14% | 1.785% |
| 12 | 14.781 | 2026 | 2033 | 2042 | rBV3 | 1001911 | 1667434 | 16.89% | 3.704% |
| 13 | 16.279 | 2281 | 2288 | 2306 | rBV | 3994838 | 6134896 | 62.14% | 13.629% |
| 14 | 16.472 | 2316 | 2321 | 2331 | rBV2 | 91987 | 176080 | 1.78% | 0.391% |
| 15 | 17.542 | 2497 | 2503 | 2512 | rBV2 | 1549218 | 2395750 | 24.27% | 5.322% |
| 16 | 18.417 | 2646 | 2652 | 2661 | rBV | 344258 | 540175 | 5.47% | 1.200% |
| 17 | 19.680 | 2861 | 2867 | 2873 | rBV2 | 169786 | 246085 | 2.49% | 0.547% |
| 18 | 20.150 | 2941 | 2947 | 2954 | rBV | 7072628 | 9872690 | 100.00% | 21.933% |
| 19 | 21.466 | 3165 | 3171 | 3178 | rBV6 | 126674 | 323966 | 3.28% | 0.720% |
| 20 | 21.853 | 3231 | 3237 | 3248 | rVB | 1486032 | 2594268 | 26.28% | 5.763% |
| 21 | 25.237 | 3802 | 3813 | 3823 | rBV2 | 822676 | 2348006 | 23.78% | 5.216% |

Sum of corrected areas: 45013682

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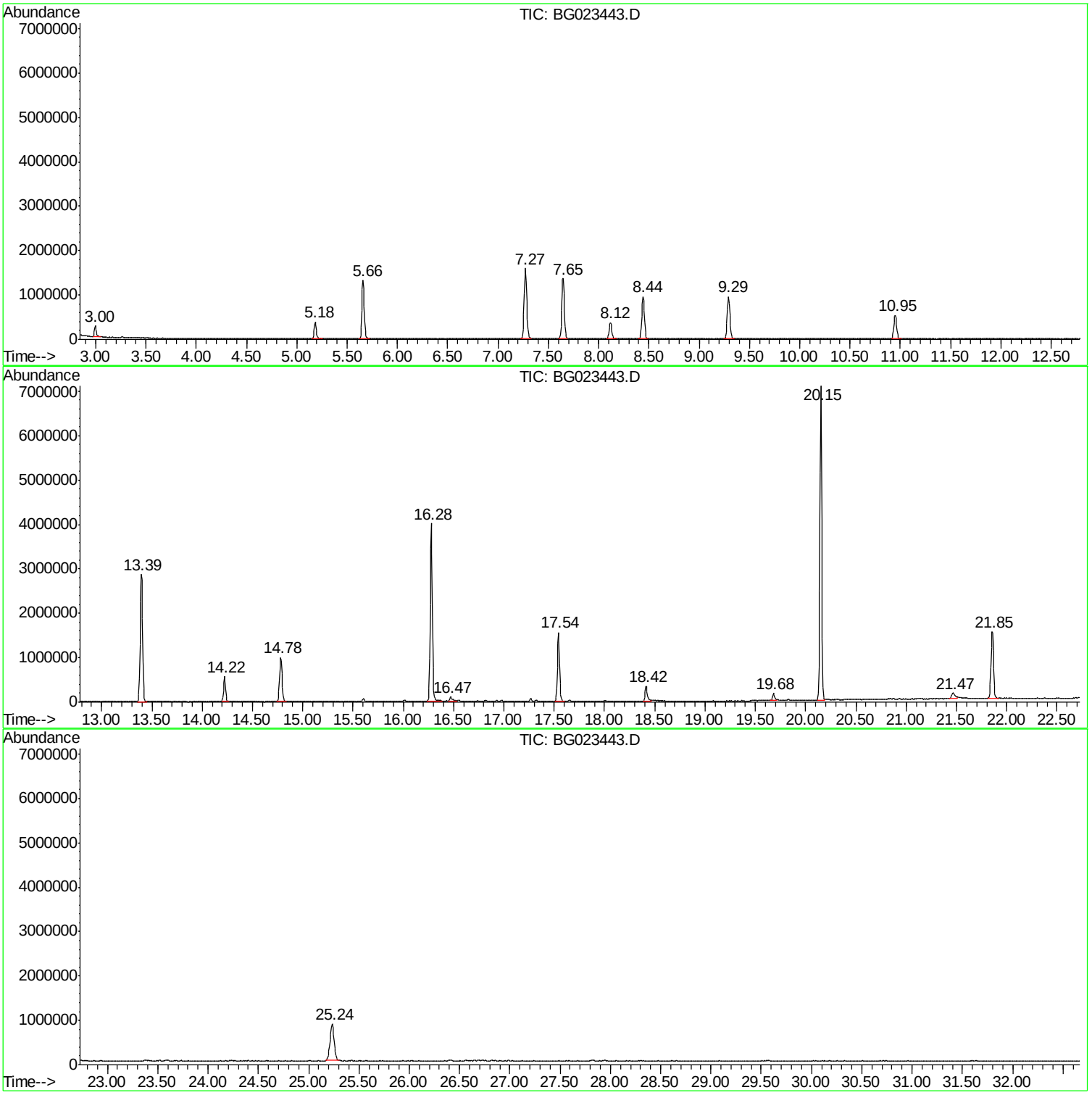
ALS Vial : 16 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
SB-58-18.0-19.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG080316\
Data File : BG023443.D
Acq On : 4 Aug 2016 2:42
Operator : UM/SJ
Sample : H4287-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-58-18.0-19.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

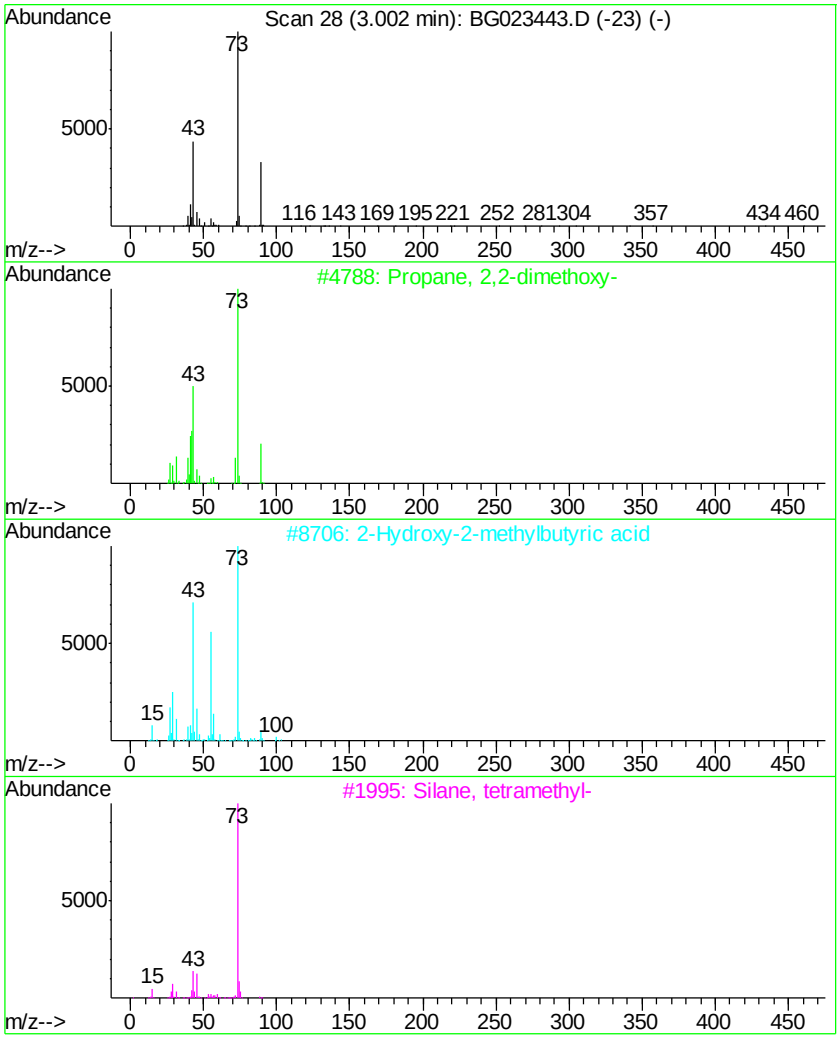
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

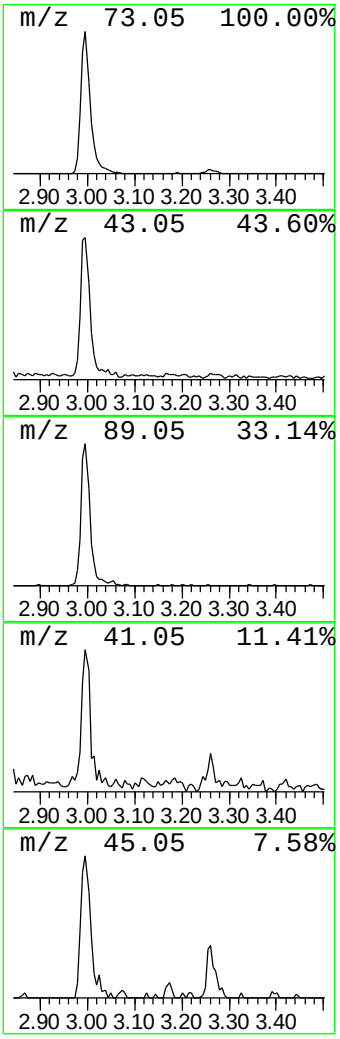
**********

Peak Number 1 unknown3.00 Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.00 | 10.16 ng | 331668 | 1,4-Dichlorobenzene-d4 | 8.11 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Propane, 2,2-dimethoxy- | 104 | C5H12O2 | 000077-76-9 | 42 |
| 2 | 2-Hydroxy-2-methylbutyric acid | 118 | C5H10O3 | 003739-30-8 | 25 |
| 3 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 9 |
| 4 | N-Ethylformamide | 73 | C3H7NO | 000627-45-2 | 9 |
| 5 | 2-Butanone, 3-methoxy-3-methyl- | 116 | C6H12O2 | 036687-98-6 | 9 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG080316\
Data File : BG023443.D
Acq On : 4 Aug 2016 2:42
Operator : UM/SJ
Sample : H4287-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-58-18.0-19.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG080116.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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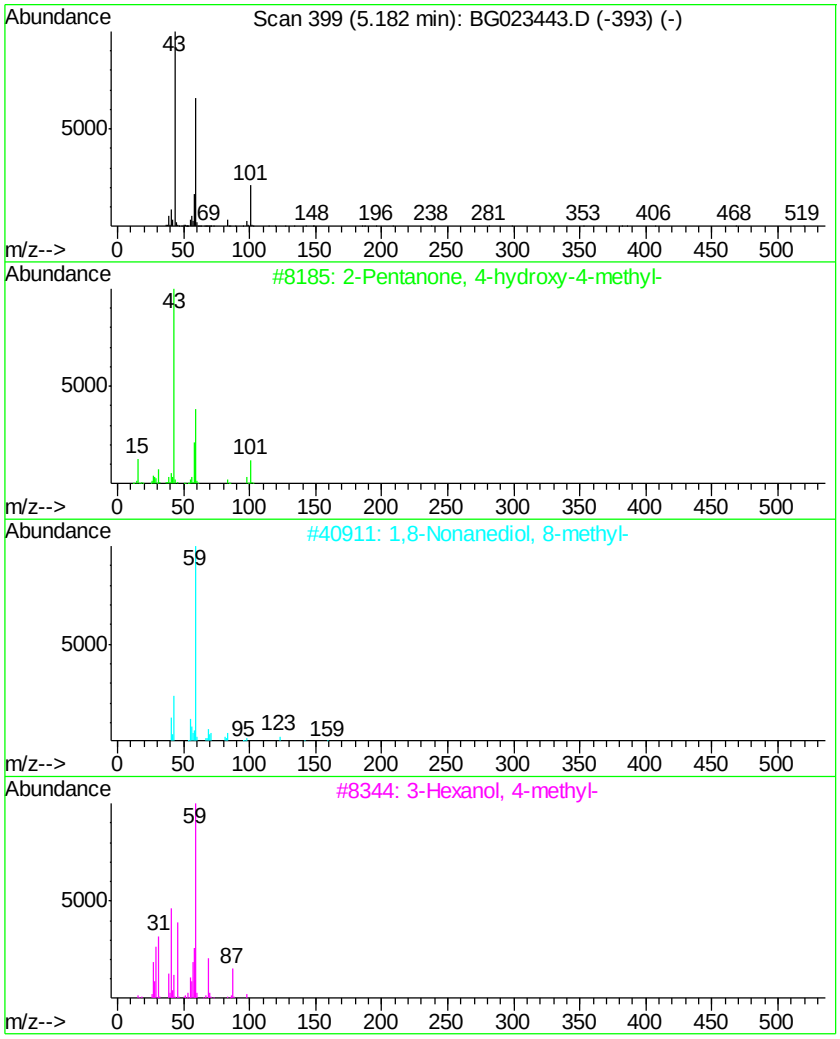
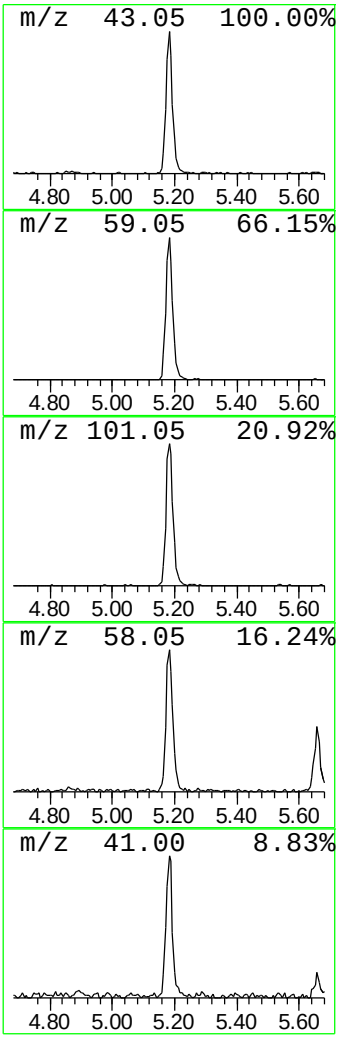
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.18 | 17.96 ng | 586595 | 1,4-Dichlorobenzene-d4 | 8.11 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 56 |
| 2 | 1,8-Nonanediol, 8-methyl- | 174 | C10H22O2 | 054725-73-4 | 37 |
| 3 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 28 |
| 4 | 1,2-Butanediol | 90 | C4H10O2 | 000584-03-2 | 23 |
| 5 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG080316\
Data File : BG023443.D
Acq On : 4 Aug 2016 2:42
Operator : UM/SJ
Sample : H4287-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-58-18.0-19.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

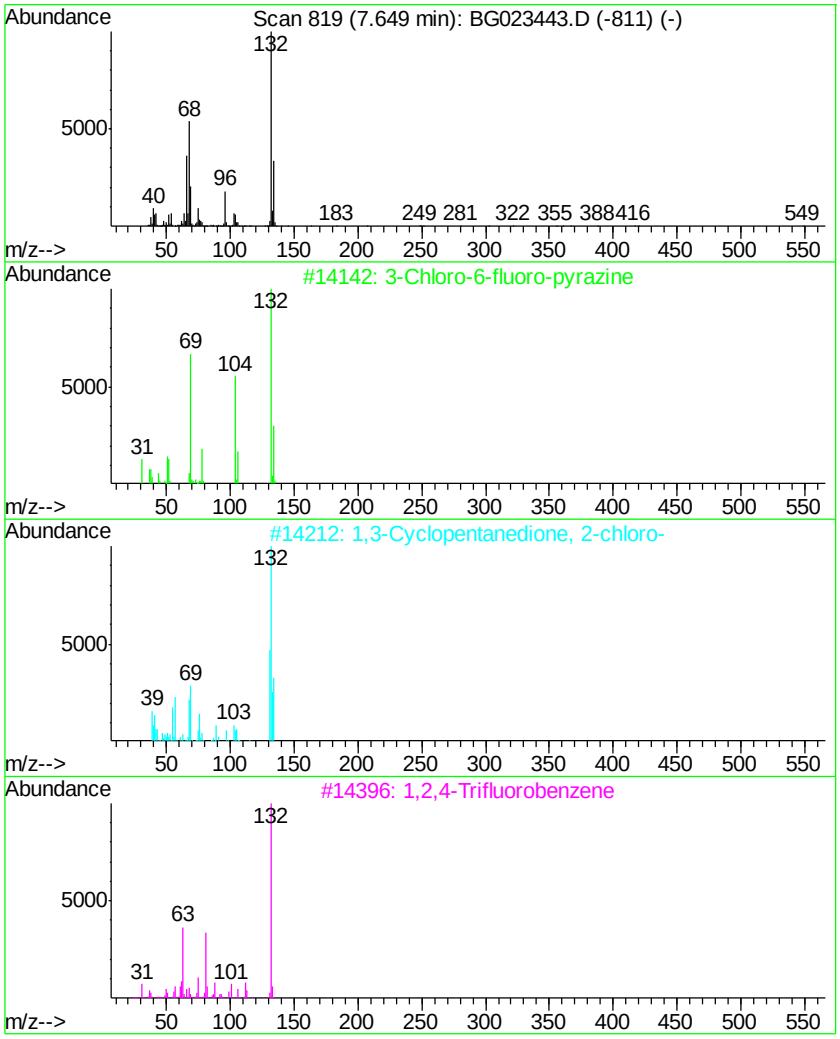
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

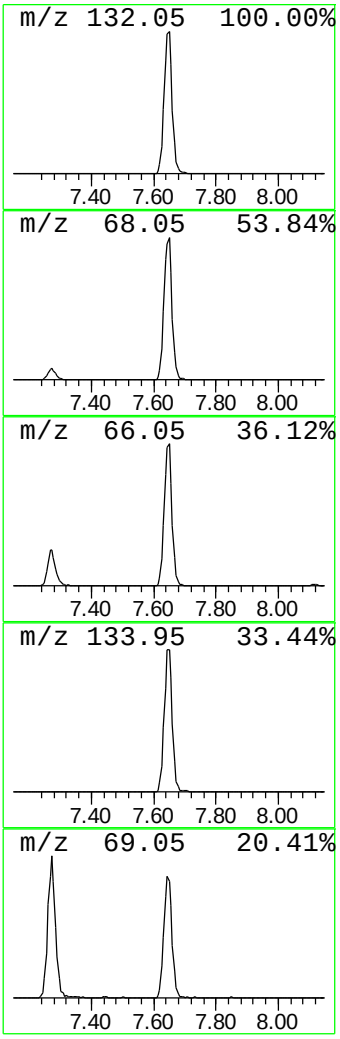
**********

Peak Number 3 unknown7.65 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.65 | 74.72 ng | 2440240 | 1,4-Dichlorobenzene-d4 | 8.11 |

| 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 | 17 |
| 3 | 1,2,4-Trifluorobenzene | 132 | C6H3F3 | 000367-23-7 | 10 |
| 4 | 2-Cyclohexen-1-one | 96 | C6H8O | 000930-68-7 | 10 |
| 5 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG080316\
Data File : BG023443.D
Acq On : 4 Aug 2016 2:42
Operator : UM/SJ
Sample : H4287-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-58-18.0-19.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG080116.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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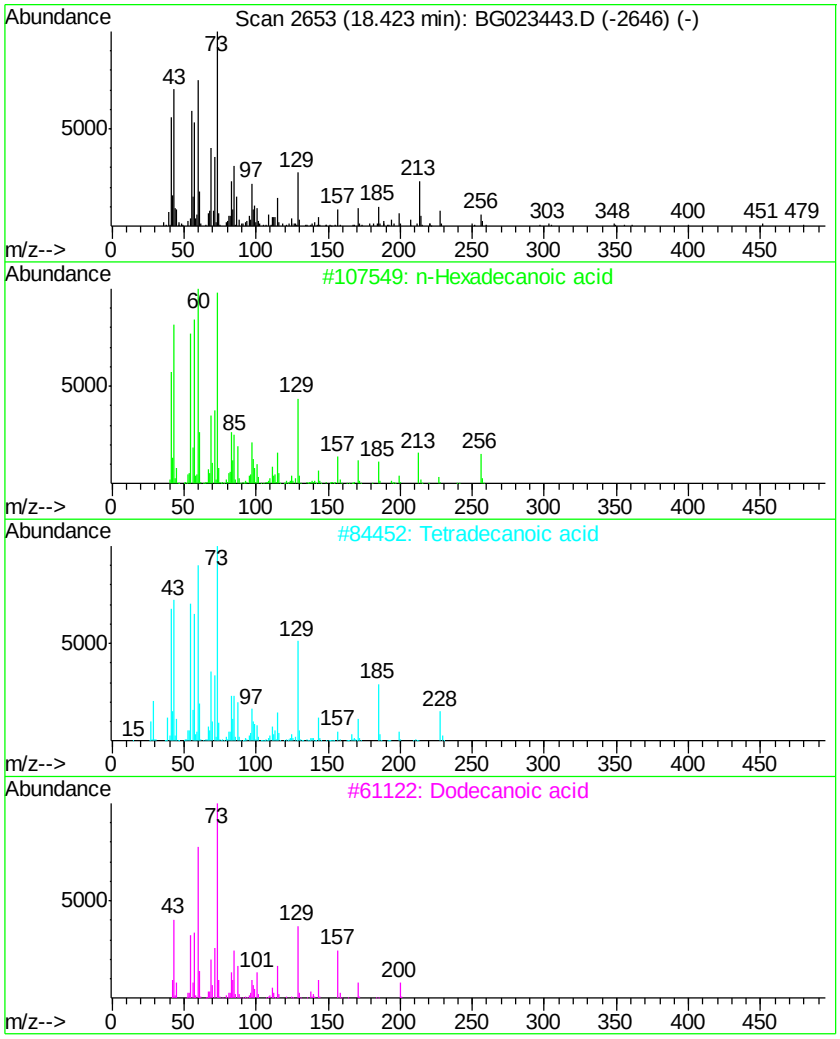
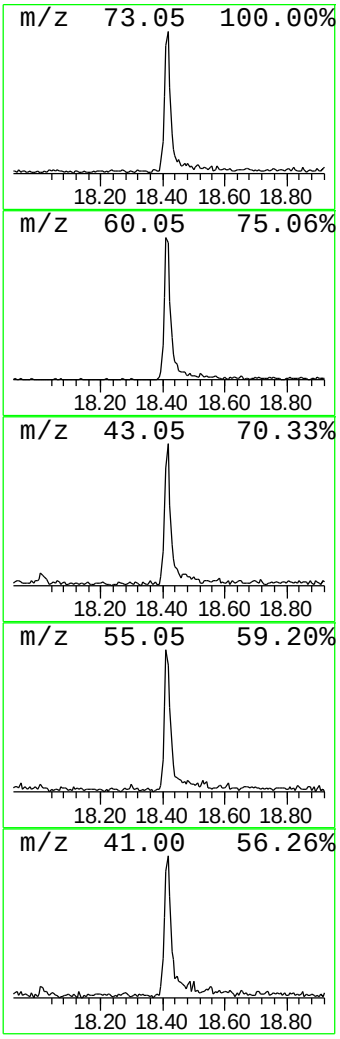
Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.42 | 4.51 ng | 540175 | Phenanthrene-d10 | 17.54 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99 |
| 2 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 72 |
| 3 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 70 |
| 4 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 64 |
| 5 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 62 |



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Data File : BG023443.D
Acq On : 4 Aug 2016 2:42
Operator : UM/SJ
Sample : H4287-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-58-18.0-19.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG080116.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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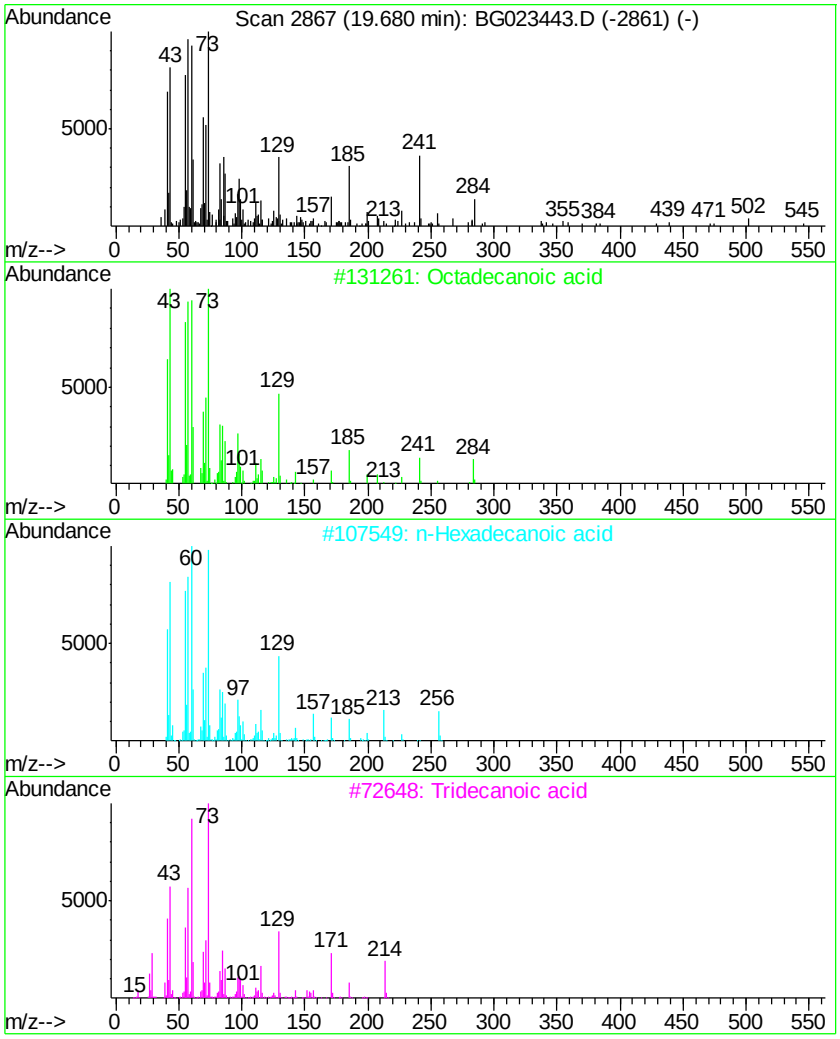
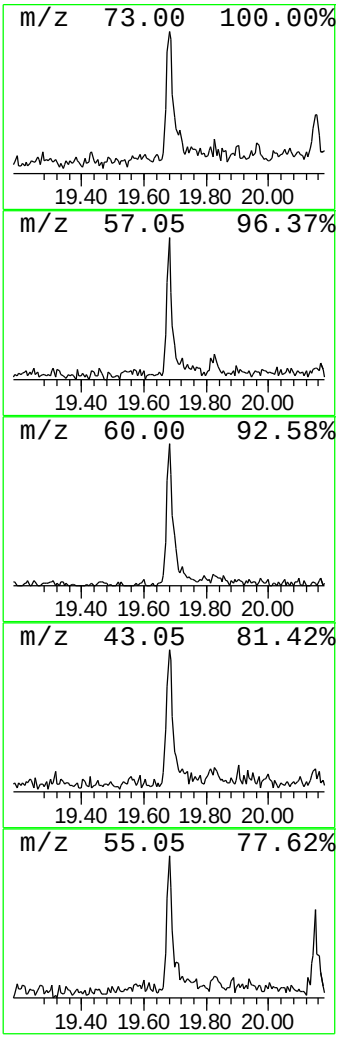
Peak Number 6 Octadecanoic acid Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.68 | 2.05 ng | 246085 | Phenanthrene-d10 | 17.54 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 86 |
| 2 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 58 |
| 3 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 58 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 50 |
| 5 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 47 |



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Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-58-18.0-19.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG080116.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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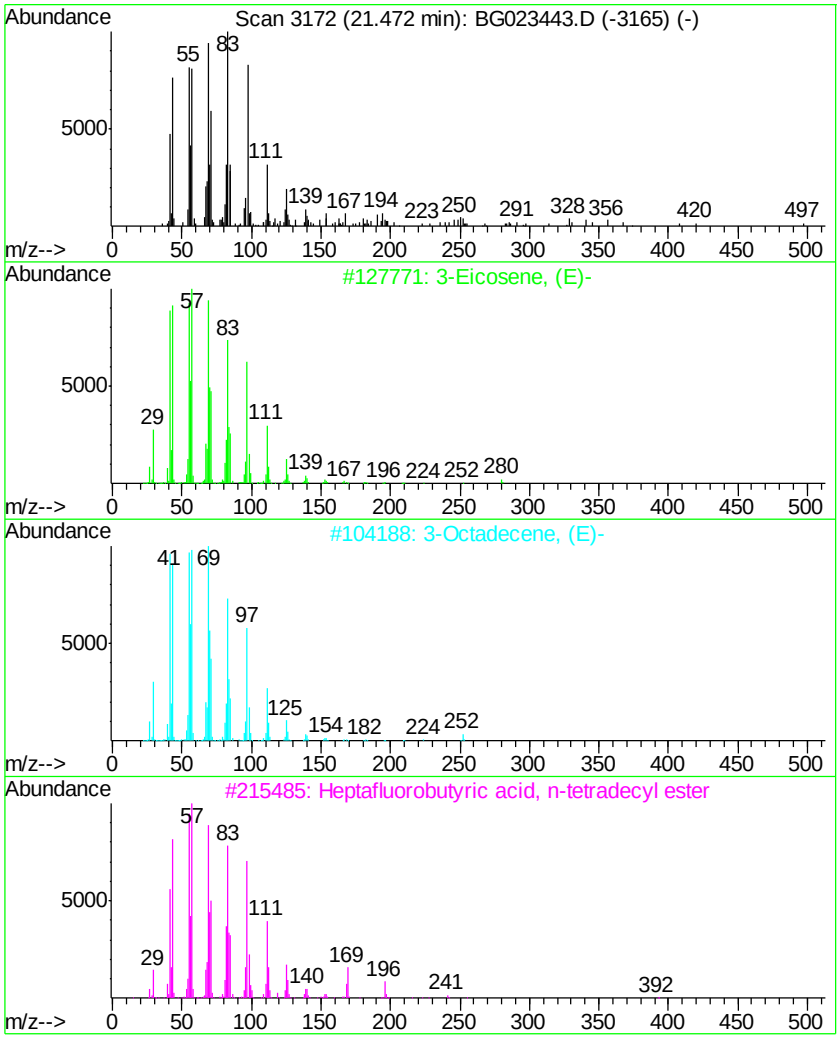
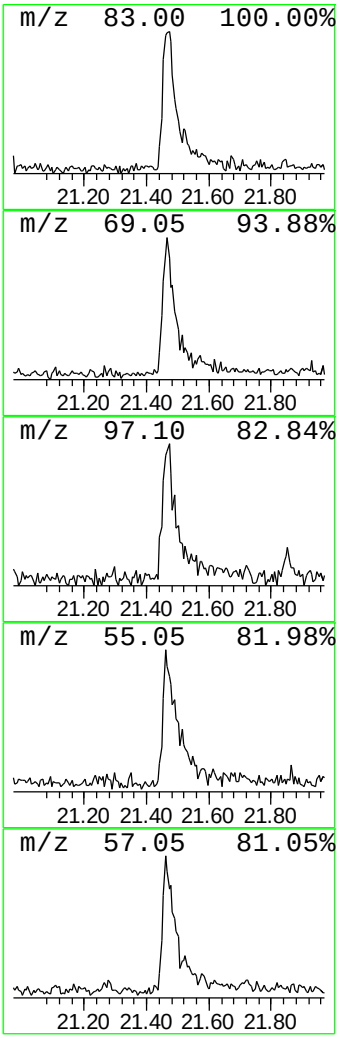
Peak Number 7 3-Eicosene, (E)- Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.47 | 2.50 ng | 323966 | Chrysene-d12 | 21.86 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Eicosene, (E)- | 280 | C20H40 | 074685-33-9 | 98 |
| 2 | 3-Octadecene, (E)- | 252 | C18H36 | 007206-19-1 | 93 |
| 3 | Heptafluorobutyric acid, n-tetra... | 410 | C18H29F7O2 | 007365-36-8 | 93 |
| 4 | Trifluoroacetic acid, pentadecyl... | 324 | C17H31F3O2 | 959010-23-2 | 93 |
| 5 | 9-Octadecene, (E)- | 252 | C18H36 | 007206-25-9 | 93 |



# Tentatively Identified Compound (LSC) summary

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**ClientSampleId :** SB-58-18.0-19.0

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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 |
| unknown3.00 | 3.00 | 10.2 | ng | 331668 | 1 | 8.11 | 653145 | 20.0 |
| 2-Pentanone, 4-hy... | 5.18 | 18.0 | ng | 586595 | 1 | 8.11 | 653145 | 20.0 |
| unknown7.65 | 7.65 | 74.7 | ng | 2440240 | 1 | 8.11 | 653145 | 20.0 |
| n-Hexadecanoic acid | 18.42 | 4.5 | ng | 540175 | 4 | 17.54 | 2395750 | 20.0 |
| Octadecanoic acid | 19.68 | 2.0 | ng | 246085 | 4 | 17.54 | 2395750 | 20.0 |
| 3-Eicosene, (E)- | 21.47 | 2.5 | ng | 323966 | 5 | 21.86 | 2594270 | 20.0 |