LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062616\
Data File : BG022627.D
Acq On : 27 Jun 2016 2:44
Operator : UM/SJ
Sample : H3733-01
Misc :
ALS Vial : 79 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW-14

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-BG062516.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 | 5.240 | 402 | 409 | 416 | rVB2 | 113489 | 186100 | 1.44% | 0.313% |
| 2 | 5.704 | 480 | 488 | 498 | rBV | 1422319 | 2344131 | 18.15% | 3.944% |
| 3 | 7.308 | 754 | 761 | 771 | rVB2 | 989180 | 1698913 | 13.15% | 2.858% |
| 4 | 7.690 | 818 | 826 | 835 | rBV | 2396642 | 4177542 | 32.34% | 7.029% |
| 5 | 8.160 | 899 | 906 | 914 | rVB | 576304 | 979359 | 7.58% | 1.648% |
| 6 | 8.489 | 954 | 962 | 975 | rBV | 2132339 | 3769676 | 29.19% | 6.342% |
| 7 | 9.335 | 1097 | 1106 | 1113 | rBV | 1929604 | 3477986 | 26.93% | 5.852% |
| 8 | 10.986 | 1377 | 1387 | 1396 | rBV | 775637 | 1392564 | 10.78% | 2.343% |
| 9 | 13.419 | 1794 | 1801 | 1809 | rBV | 4784229 | 7599920 | 58.84% | 12.787% |
| 10 | 14.241 | 1936 | 1941 | 1946 | rVB | 103024 | 149388 | 1.16% | 0.251% |
| 11 | 14.799 | 2029 | 2036 | 2042 | rBV2 | 1218326 | 2006907 | 15.54% | 3.377% |
| 12 | 16.039 | 2243 | 2247 | 2253 | rBV4 | 147935 | 221561 | 1.72% | 0.373% |
| 13 | 16.133 | 2258 | 2263 | 2270 | rVB3 | 97414 | 157933 | 1.22% | 0.266% |
| 14 | 16.286 | 2282 | 2289 | 2301 | rBV | 4802928 | 7594161 | 58.80% | 12.777% |
| 15 | 16.415 | 2307 | 2311 | 2316 | rBV | 280556 | 388010 | 3.00% | 0.653% |
| 16 | 17.555 | 2497 | 2505 | 2515 | rVB2 | 1704498 | 2747154 | 21.27% | 4.622% |
| 17 | 18.425 | 2649 | 2653 | 2662 | rBV2 | 287260 | 445801 | 3.45% | 0.750% |
| 18 | 19.694 | 2865 | 2869 | 2878 | rBV | 467008 | 606181 | 4.69% | 1.020% |
| 19 | 20.158 | 2942 | 2948 | 2954 | rBV | 9860192 | 12915993 | 100.00% | 21.731% |
| 20 | 21.850 | 3230 | 3236 | 3242 | rVB2 | 1944538 | 3274147 | 25.35% | 5.509% |
| 21 | 25.217 | 3799 | 3809 | 3824 | rVB | 1094992 | 3303466 | 25.58% | 5.558% |

Sum of corrected areas: 59436893

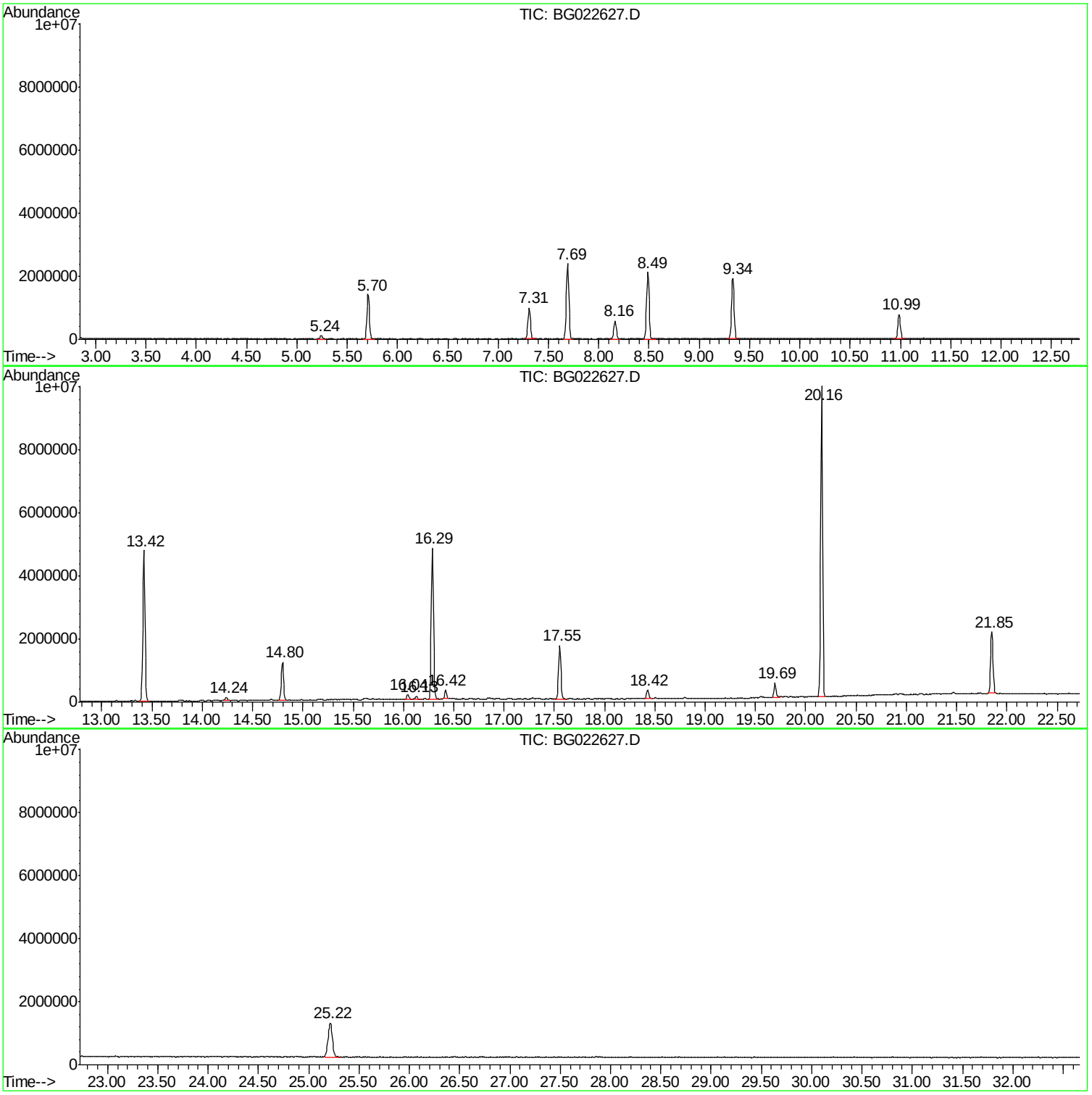
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062616\
Data File : BG022627.D
Acq On : 27 Jun 2016 2:44
Operator : UM/SJ
Sample : H3733-01
Misc :
ALS Vial : 79 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
MW-14

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062616\
Data File : BG022627.D
Acq On : 27 Jun 2016 2:44
Operator : UM/SJ
Sample : H3733-01
Misc :
ALS Vial : 79 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
MW-14

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

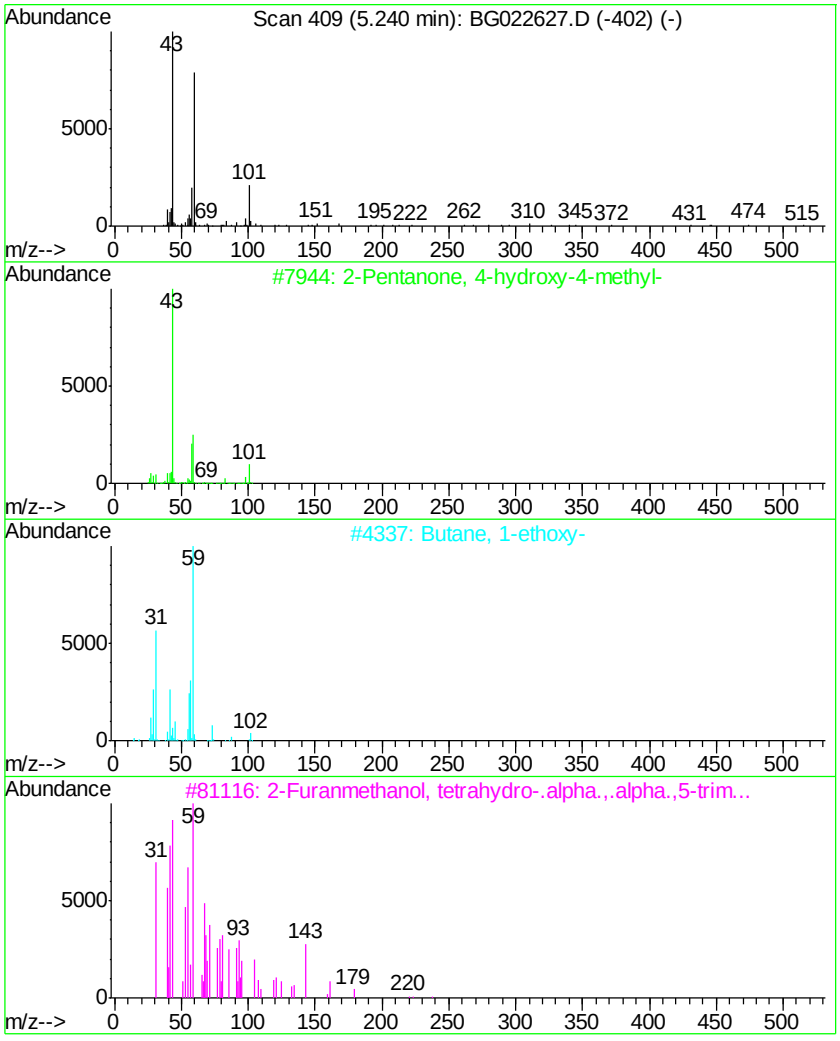
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

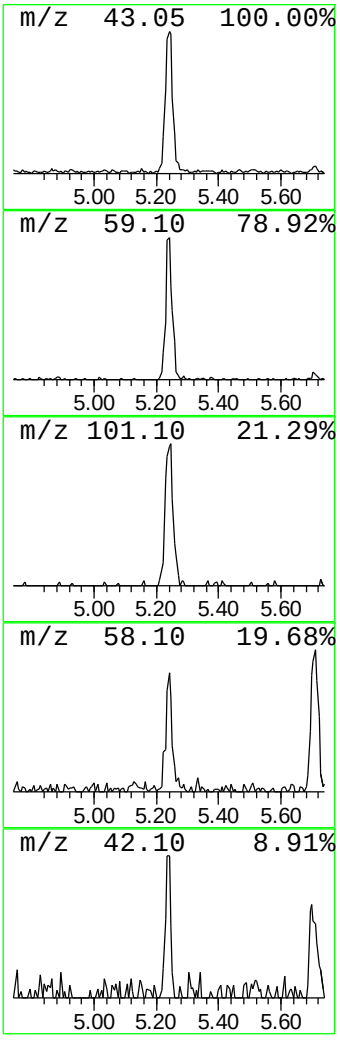
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.24 | 3.80 ng | 186100 | 1,4-Dichlorobenzene-d4 | 8.16 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 42 |
| 2 | Butane, 1-ethoxy- | 102 | C6H14O | 000628-81-9 | 25 |
| 3 | 2-Furanmethanol, tetrahydro-.alp... | 238 | C15H26O2 | 026184-88-3 | 25 |
| 4 | 3-Hydroxy-3-methyl-2-butanone | 102 | C5H10O2 | 000115-22-0 | 25 |
| 5 | Guanidine | 59 | CH5N3 | 000113-00-8 | 9 |



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062616\
Data File : BG022627.D
Acq On : 27 Jun 2016 2:44
Operator : UM/SJ
Sample : H3733-01
Misc :
ALS Vial : 79 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW-14

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

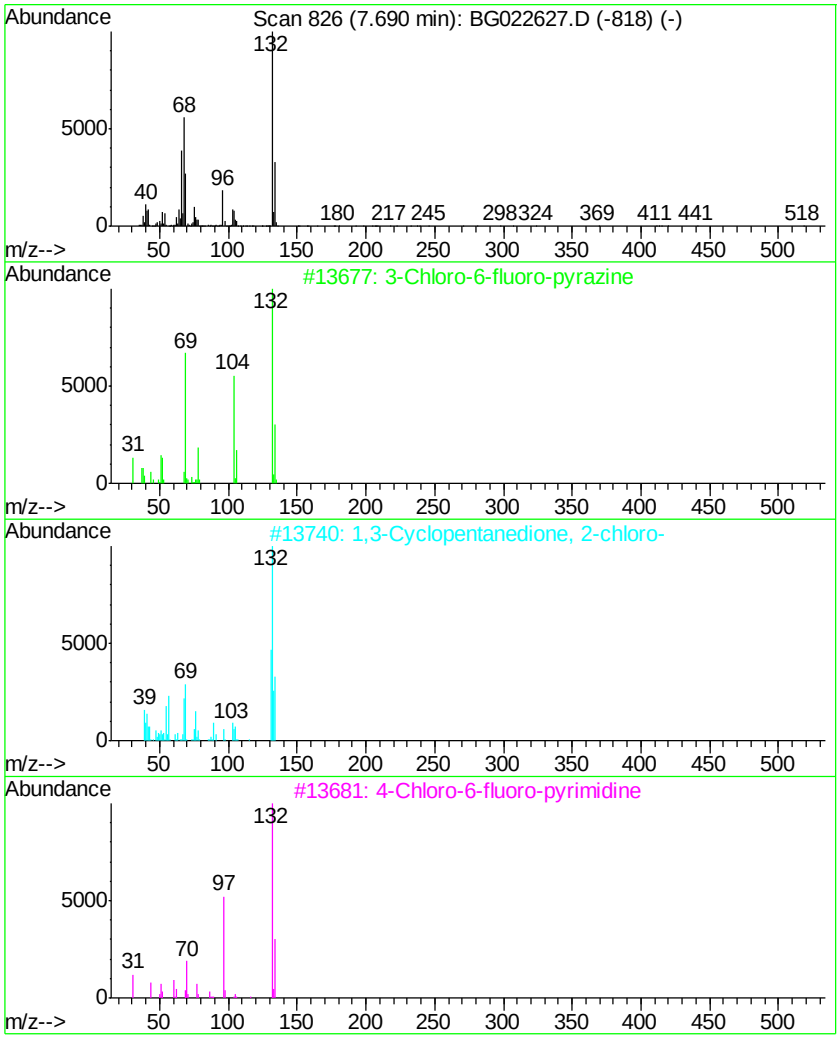
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

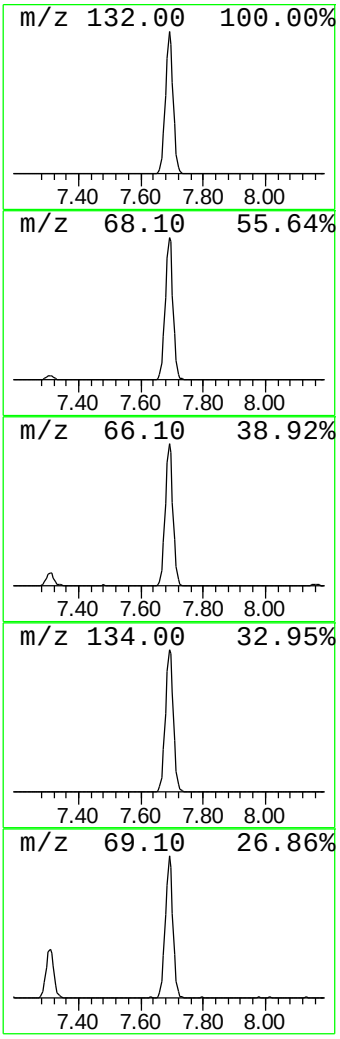
**********

Peak Number 2 unknown7.69 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.69 | 85.31 ng | 4177540 | 1,4-Dichlorobenzene-d4 | 8.16 |

| 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 | 16 |
| 3 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 14 |
| 4 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 14 |
| 5 | 1,2,3-Trifluorobenzene | 132 | C6H3F3 | 001489-53-8 | 9 |



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062616\
Data File : BG022627.D
Acq On : 27 Jun 2016 2:44
Operator : UM/SJ
Sample : H3733-01
Misc :
ALS Vial : 79 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW-14

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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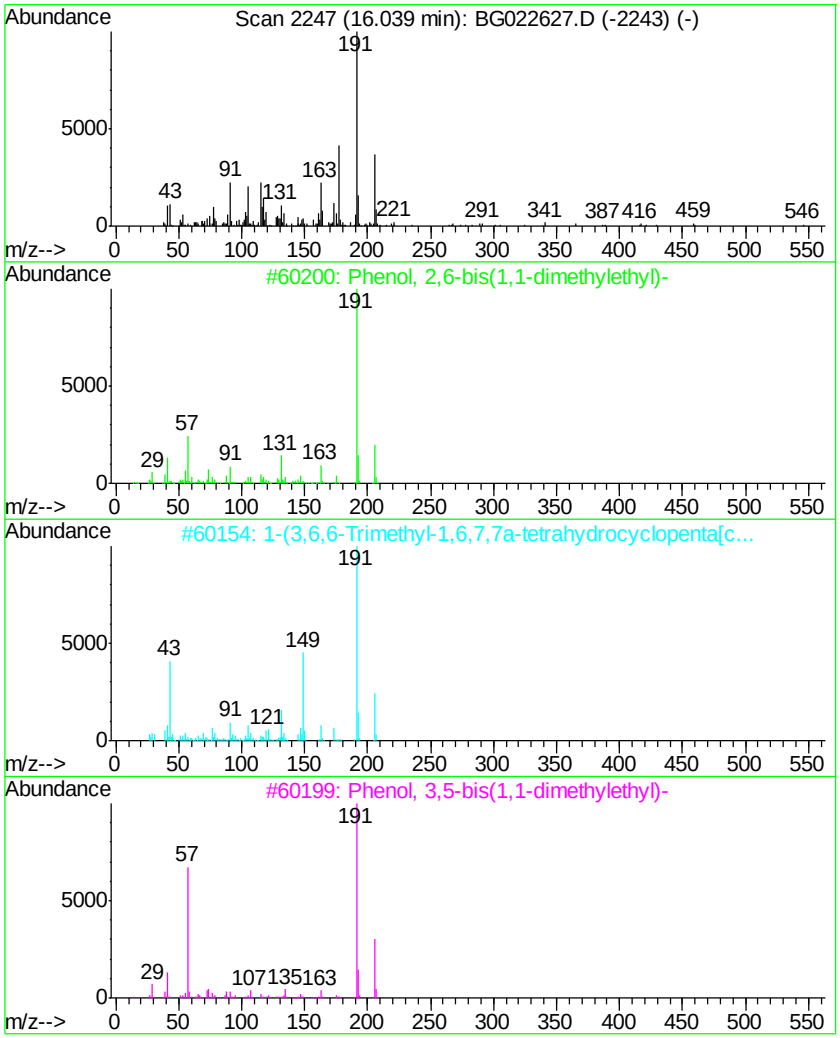
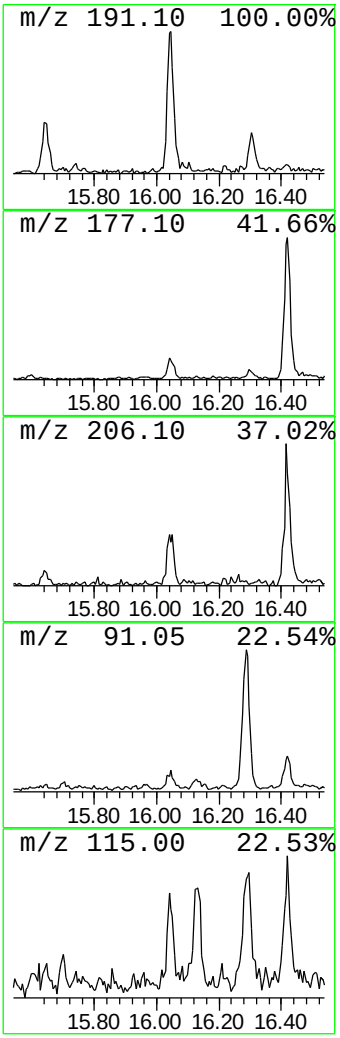
Peak Number 4 unknown16.04 Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.04 | 2.21 ng | 221561 | Acenaphthene-d10 | 14.80 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Phenol, 2,6-bis(1,1-dimethylethyl)- | 206 | C14H22O | 000128-39-2 | 47 |
| 2 | 1-(3,6,6-Trimethyl-1,6,7,7a-tetr... | 206 | C13H18O2 | 1000194-97-2 | 47 |
| 3 | Phenol, 3,5-bis(1,1-dimethylethyl)- | 206 | C14H22O | 001138-52-9 | 46 |
| 4 | Pentanoic acid, 5-hydroxy-, 2,4-... | 306 | C19H30O3 | 166273-38-7 | 43 |
| 5 | 4,5-Dihydrothiazol-4-one, 2-(2-m... | 222 | C10H10N2O2S | 022476-61-5 | 43 |



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062616\
Data File : BG022627.D
Acq On : 27 Jun 2016 2:44
Operator : UM/SJ
Sample : H3733-01
Misc :
ALS Vial : 79 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW-14

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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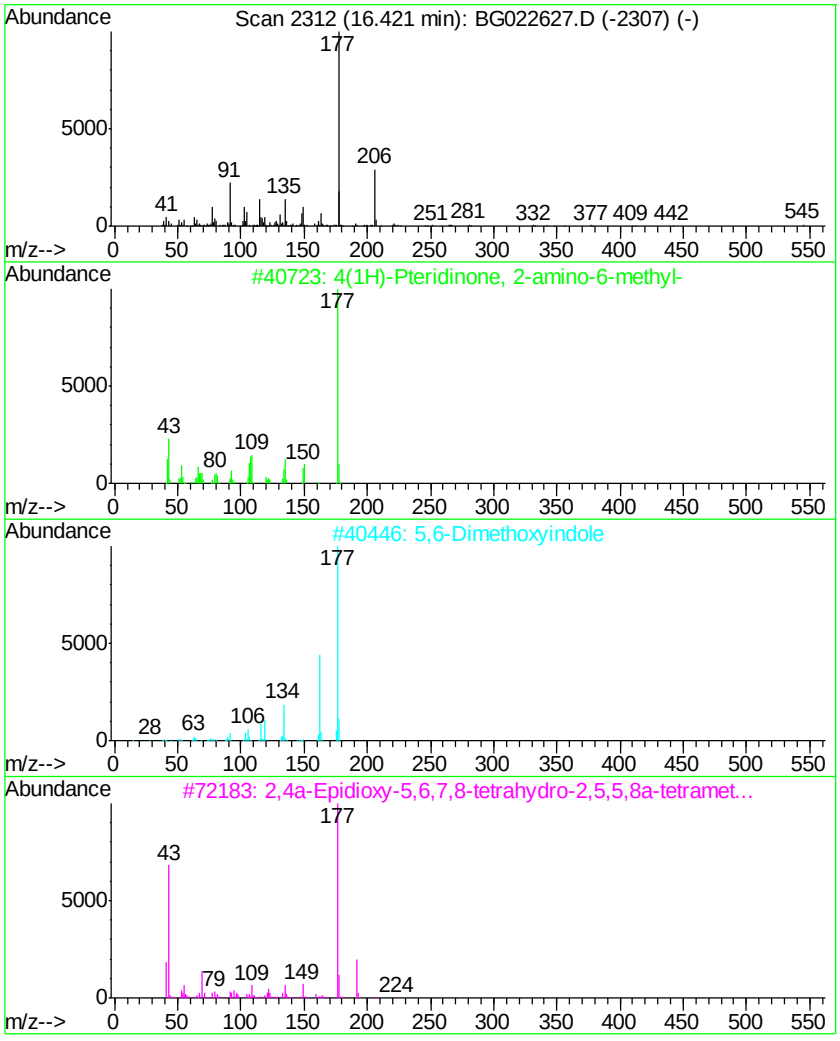
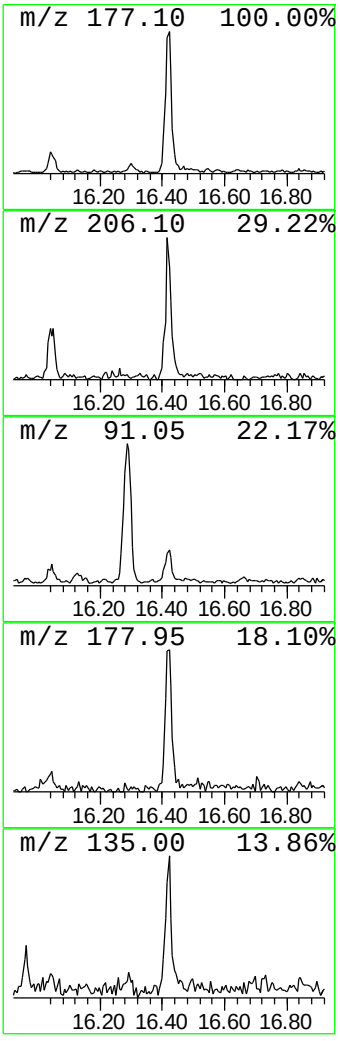
Peak Number 5 unknown16.42 Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.42 | 2.82 ng | 388010 | Phenanthrene-d10 | 17.55 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4(1H)-Pteridinone, 2-amino-6-met... | 177 | C7H7N5O | 000708-75-8 | 47 |
| 2 | 5,6-Dimethoxyindole | 177 | C10H11NO2 | 014430-23-0 | 47 |
| 3 | 2,4a-Epidioxy-5,6,7,8-tetrahydro... | 224 | C13H20O3 | 1000212-29-9 | 43 |
| 4 | 2,6-DI-SEC-BUTYLPHENYL ACETATE | 248 | C16H24O2 | 1000233-09-3 | 39 |
| 5 | Benzene, 1-(1-carboxyethyl)-4-(1... | 206 | C12H14O3 | 1000161-22-9 | 38 |



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062616\
Data File : BG022627.D
Acq On : 27 Jun 2016 2:44
Operator : UM/SJ
Sample : H3733-01
Misc :
ALS Vial : 79 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW-14

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

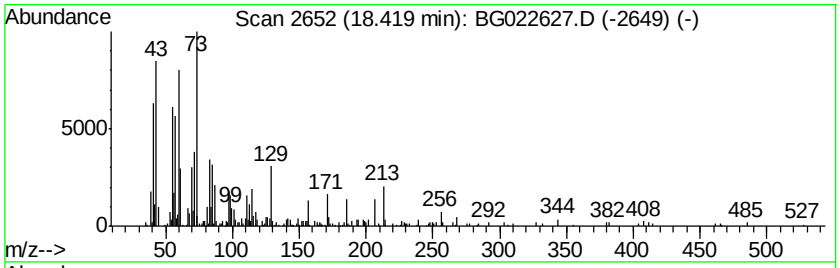
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

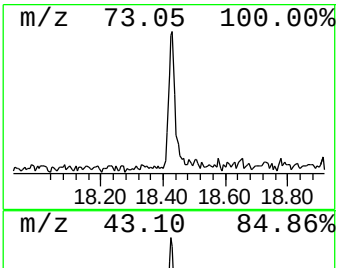
**********

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.42 | 3.25 ng | 445801 | Phenanthrene-d10 | 17.55 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 68 |
| 3 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 60 |
| 4 | Ether, dodecyl isopropyl | 228 | C15H32O | 029379-42-8 | 30 |
| 5 | D-Glucose, 4-O-.alpha.-D-glucopy... | 342 | C12H22O11 | 000069-79-4 | 27 |



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062616\
Data File : BG022627.D
Acq On : 27 Jun 2016 2:44
Operator : UM/SJ
Sample : H3733-01
Misc :
ALS Vial : 79 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW-14

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

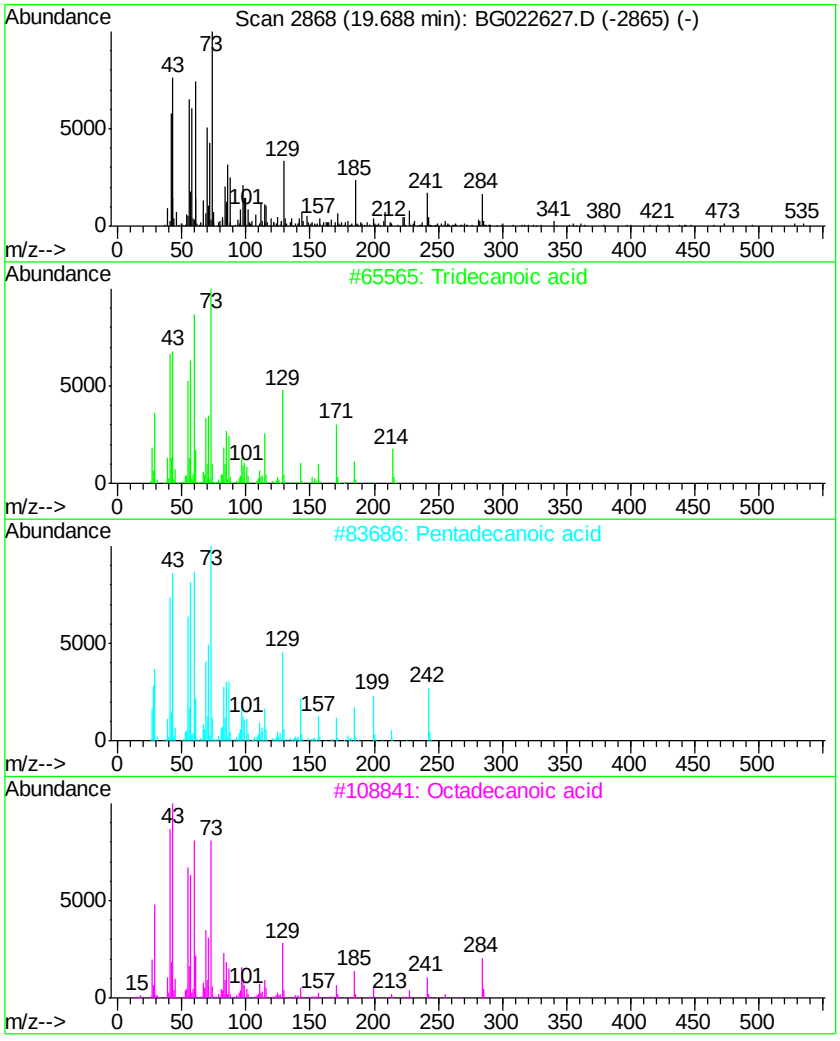
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

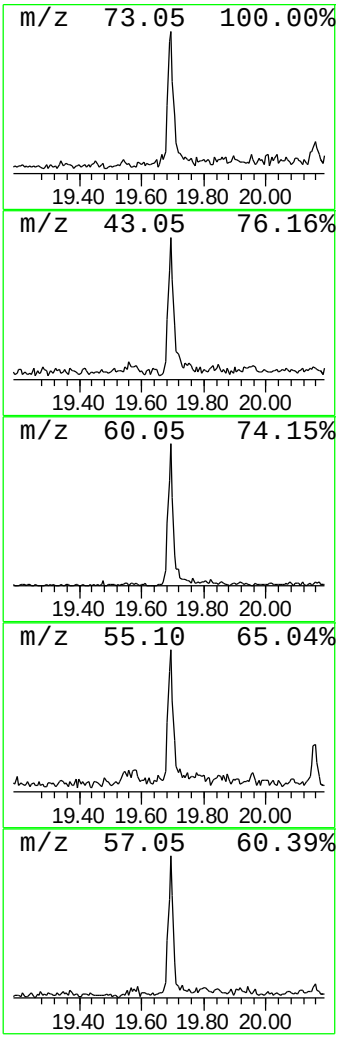
**********

Peak Number 7 Tridecanoic acid Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.69 | 4.41 ng | 606181 | Phenanthrene-d10 | 17.55 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 90 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 89 |
| 3 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 72 |
| 4 | Docosanoic acid | 340 | C22H44O2 | 000112-85-6 | 64 |
| 5 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 64 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG062616\
Data File : BG022627.D
Acq On : 27 Jun 2016 2:44
Operator : UM/SJ
Sample : H3733-01
Misc :
ALS Vial : 79 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW-14

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG062516.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 |
| 2-Pentanone, 4-hy... | 5.24 | 3.8 | ng | 186100 | 1 | 8.16 | 979359 | 20.0 |
| unknown7.69 | 7.69 | 85.3 | ng | 4177540 | 1 | 8.16 | 979359 | 20.0 |
| unknown16.04 | 16.04 | 2.2 | ng | 221561 | 3 | 14.80 | 2006910 | 20.0 |
| unknown16.42 | 16.42 | 2.8 | ng | 388010 | 4 | 17.55 | 2747150 | 20.0 |
| n-Hexadecanoic acid | 18.42 | 3.3 | ng | 445801 | 4 | 17.55 | 2747150 | 20.0 |
| Tridecanoic acid | 19.69 | 4.4 | ng | 606181 | 4 | 17.55 | 2747150 | 20.0 |