# LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG052015\
Data File : BG017237.D
Acq On : 21 May 2015 6:38
Operator : TP/IZ
Sample : G2301-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW7

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-BG051315.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 | 2.779 | 11 | 15 | 24 | rBV | 81516 | 138189 | 3.98% | 0.861% |
| 2 | 2.861 | 24 | 29 | 42 | rVB | 388206 | 526726 | 15.18% | 3.280% |
| 3 | 4.800 | 354 | 359 | 364 | rVB | 43183 | 57375 | 1.65% | 0.357% |
| 4 | 5.287 | 436 | 442 | 449 | rBV | 347293 | 500713 | 14.43% | 3.118% |
| 5 | 6.891 | 707 | 715 | 726 | rBV | 229725 | 344696 | 9.93% | 2.147% |
| 6 | 7.232 | 765 | 773 | 781 | rBV | 722883 | 1088374 | 31.36% | 6.778% |
| 7 | 7.691 | 844 | 851 | 860 | rBV | 177585 | 269824 | 7.77% | 1.680% |
| 8 | 8.014 | 899 | 906 | 914 | rVB | 615067 | 958728 | 27.63% | 5.971% |
| 9 | 8.854 | 1041 | 1049 | 1058 | rBV | 576942 | 925439 | 26.67% | 5.764% |
| 10 | 10.487 | 1320 | 1327 | 1334 | rBV | 219220 | 372624 | 10.74% | 2.321% |
| 11 | 12.967 | 1741 | 1749 | 1757 | rBV | 1346407 | 1978332 | 57.01% | 12.321% |
| 12 | 14.353 | 1979 | 1985 | 1991 | rBV2 | 346394 | 523134 | 15.07% | 3.258% |
| 13 | 15.846 | 2232 | 2239 | 2254 | rBV | 1307441 | 1887390 | 54.38% | 11.754% |
| 14 | 16.098 | 2278 | 2282 | 2287 | rVB | 26484 | 37421 | 1.08% | 0.233% |
| 15 | 16.192 | 2293 | 2298 | 2302 | rBV | 35928 | 46756 | 1.35% | 0.291% |
| 16 | 16.245 | 2302 | 2307 | 2314 | rVV4 | 47219 | 84663 | 2.44% | 0.527% |
| 17 | 16.310 | 2314 | 2318 | 2321 | rVV2 | 40822 | 55837 | 1.61% | 0.348% |
| 18 | 16.351 | 2321 | 2325 | 2330 | rVB | 28068 | 39586 | 1.14% | 0.247% |
| 19 | 16.510 | 2347 | 2352 | 2358 | rVB4 | 40600 | 78430 | 2.26% | 0.488% |
| 20 | 16.574 | 2358 | 2363 | 2366 | rBV | 40927 | 55579 | 1.60% | 0.346% |
| 21 | 16.651 | 2373 | 2376 | 2382 | rVB4 | 29884 | 38546 | 1.11% | 0.240% |
| 22 | 17.097 | 2446 | 2452 | 2458 | rBV2 | 509467 | 708619 | 20.42% | 4.413% |
| 23 | 18.002 | 2601 | 2606 | 2614 | rBV2 | 45064 | 66527 | 1.92% | 0.414% |
| 24 | 19.283 | 2821 | 2824 | 2830 | rVB4 | 33872 | 45880 | 1.32% | 0.286% |
| 25 | 19.735 | 2895 | 2901 | 2907 | rBV | 2775397 | 3470438 | 100.00% | 21.613% |
| 26 | 20.998 | 3112 | 3116 | 3124 | rBV4 | 38812 | 69792 | 2.01% | 0.435% |
| 27 | 21.280 | 3159 | 3164 | 3173 | rBV | 689441 | 857027 | 24.70% | 5.337% |
| 28 | 23.548 | 3542 | 3550 | 3557 | rBV2 | 426452 | 830213 | 23.92% | 5.170% |

Sum of corrected areas: 16056858

LSC Report - Integrated Chromatogram

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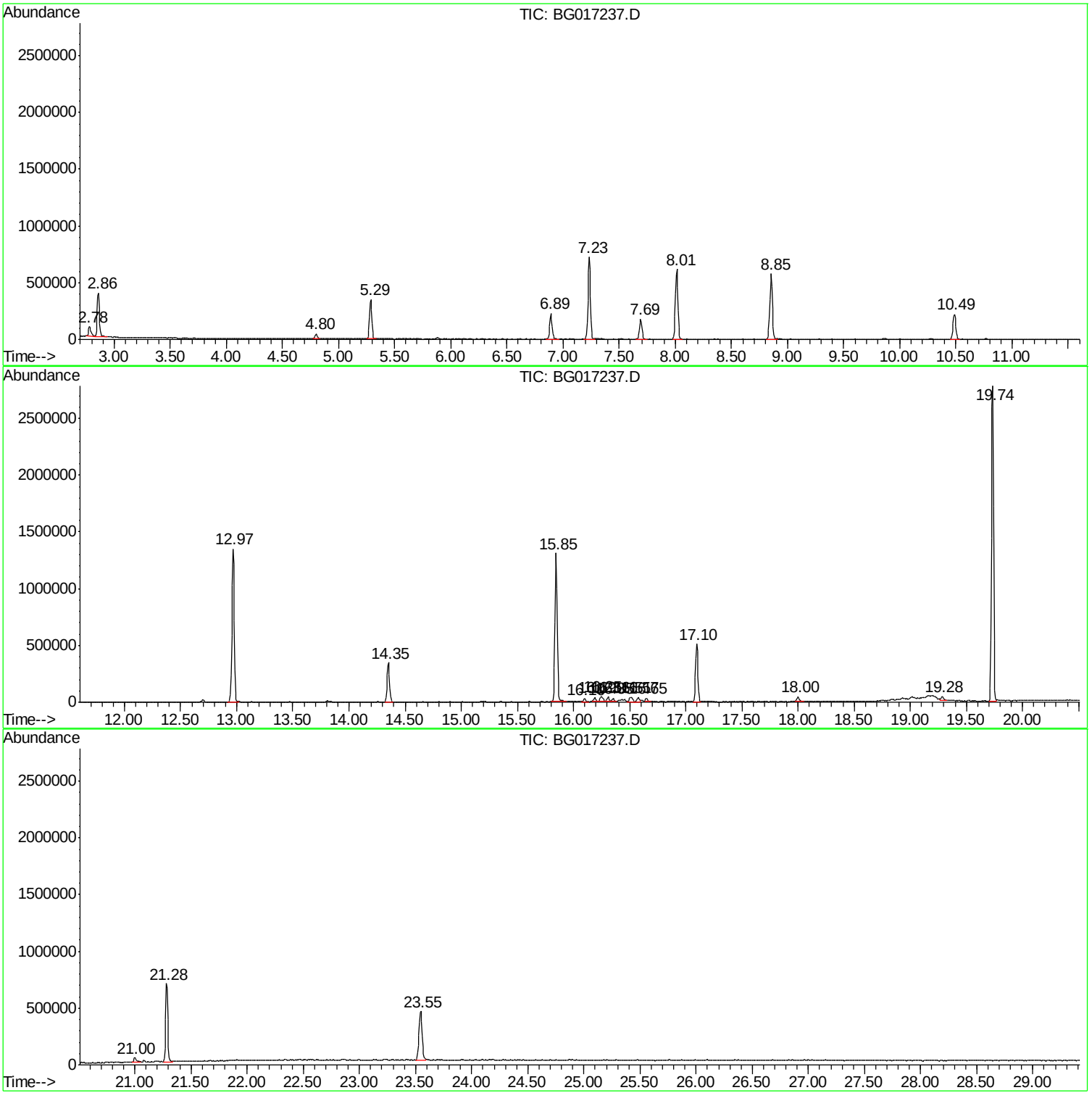
Operator : TP/IZ
Sample : G2301-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW7

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.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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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.M
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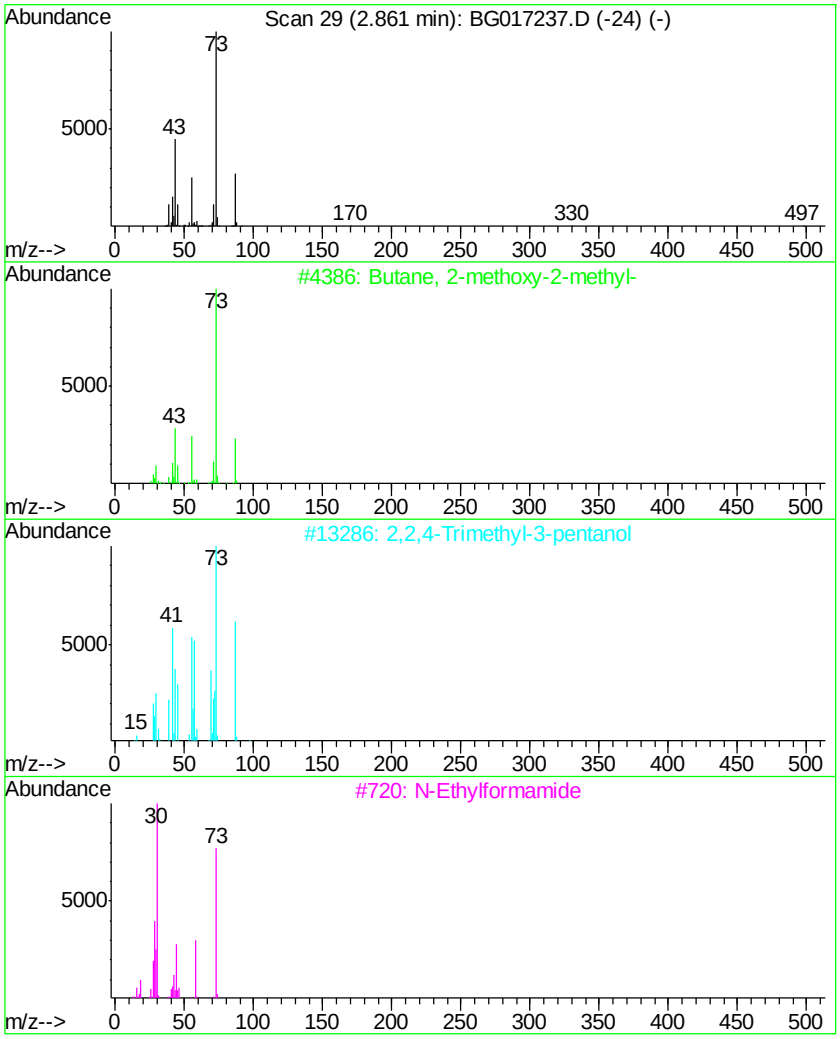
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

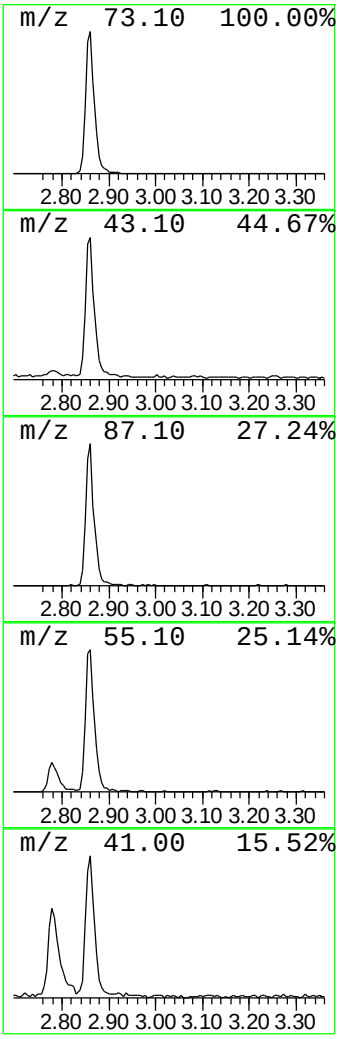
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.86 | 39.04 ng | 526726 | 1,4-Dichlorobenzene-d4 | 7.69 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 72 |
| 2 | 2,2,4-Trimethyl-3-pentanol | 130 | C8H18O | 005162-48-1 | 50 |
| 3 | N-Ethylformamide | 73 | C3H7NO | 000627-45-2 | 9 |
| 4 | Acetamide, N-ethyl- | 87 | C4H9NO | 000625-50-3 | 9 |
| 5 | 2-Methyl-5-hexen-3-ol | 114 | C7H14O | 032815-70-6 | 9 |



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Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW7

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

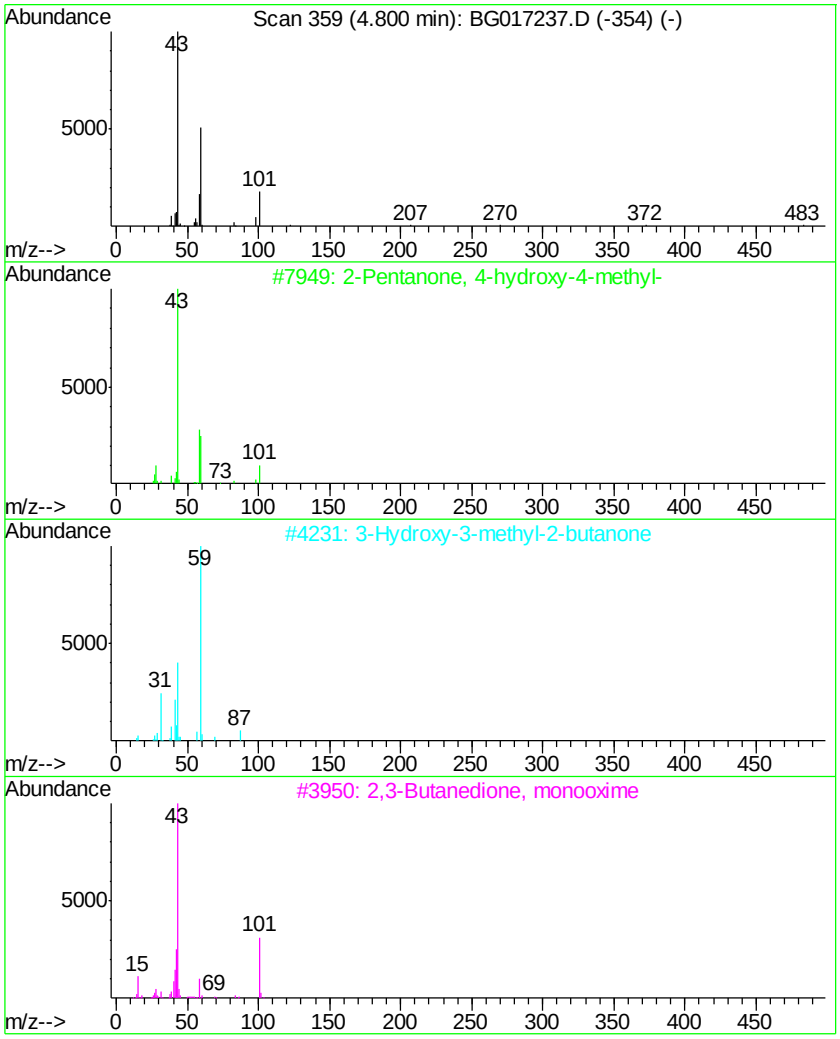
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

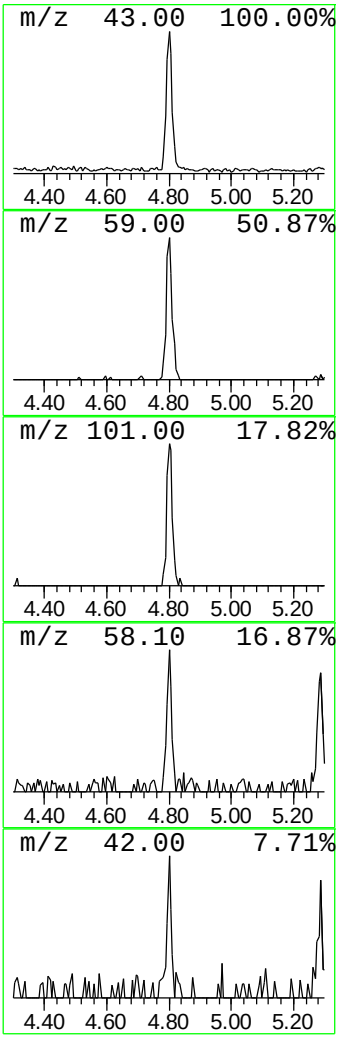
**********

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.80 | 4.25 ng | 57375 | 1,4-Dichlorobenzene-d4 | 7.69 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 43 |
| 2 | 3-Hydroxy-3-methyl-2-butanone | 102 | C5H10O2 | 000115-22-0 | 17 |
| 3 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |
| 4 | Guanidine | 59 | CH5N3 | 000113-00-8 | 9 |
| 5 | Silane, trimethyl- | 74 | C3H10Si | 000993-07-7 | 9 |



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Data File : BG017237.D
Acq On : 21 May 2015 6:38
Operator : TP/IZ
Sample : G2301-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW7

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.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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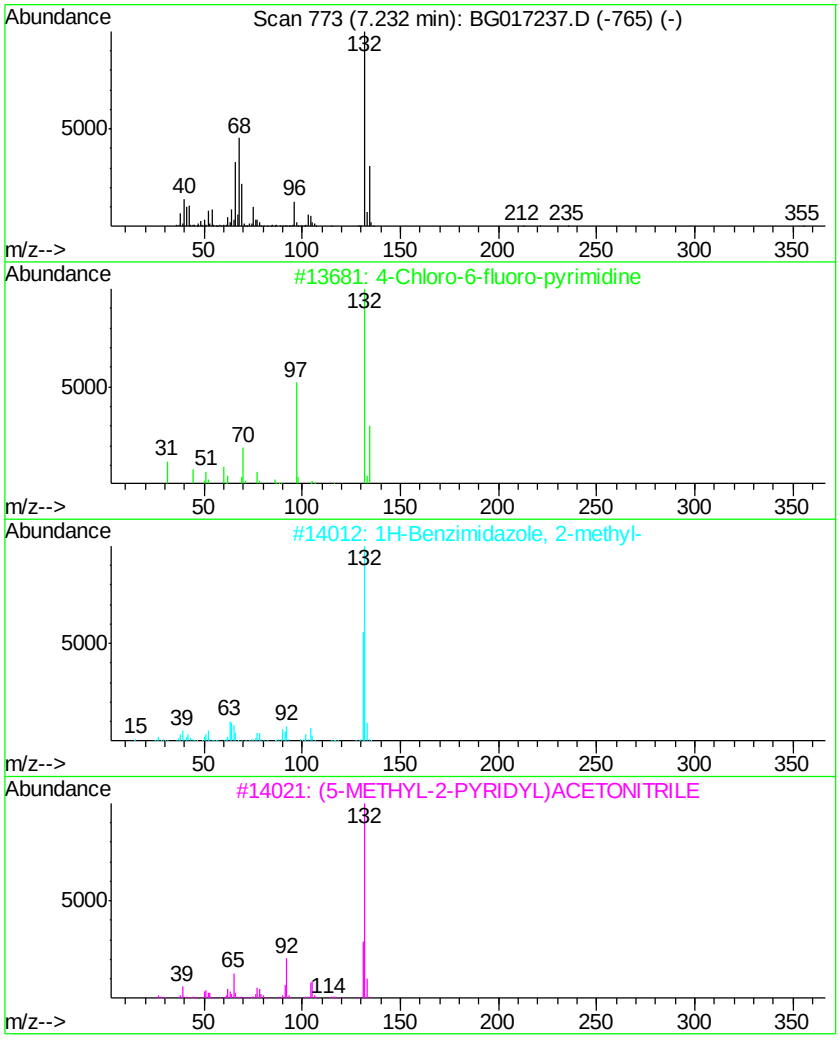
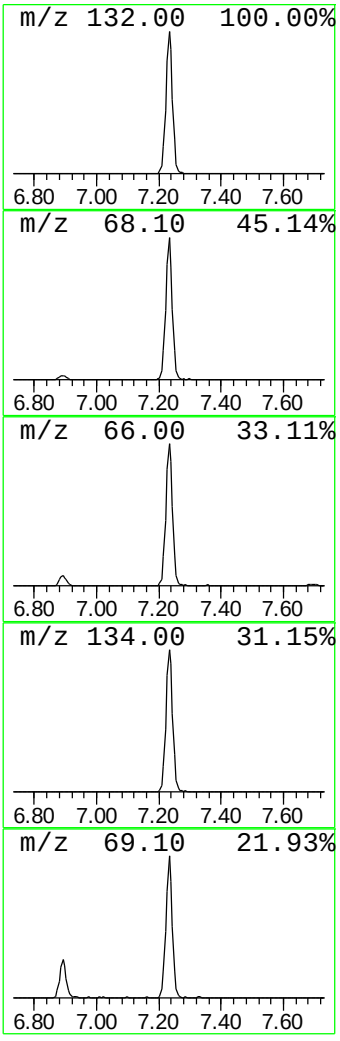
Peak Number 4 unknown7.23 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.23 | 80.67 ng | 1088370 | 1,4-Dichlorobenzene-d4 | 7.69 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 27 |
| 2 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 22 |
| 3 | (5-METHYL-2-PYRIDYL)ACETONITRILE | 132 | C8H8N2 | 1000241-93-9 | 22 |
| 4 | 1,3-Cyclopentanedione, 2-chloro- | 132 | C5H5ClO2 | 014203-19-1 | 13 |
| 5 | Pyrazolo(2,3-a)pyridine, 7-methyl- | 132 | C8H8N2 | 034760-58-2 | 12 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG052015\
Data File : BG017237.D
Acq On : 21 May 2015 6:38
Operator : TP/IZ
Sample : G2301-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW7

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

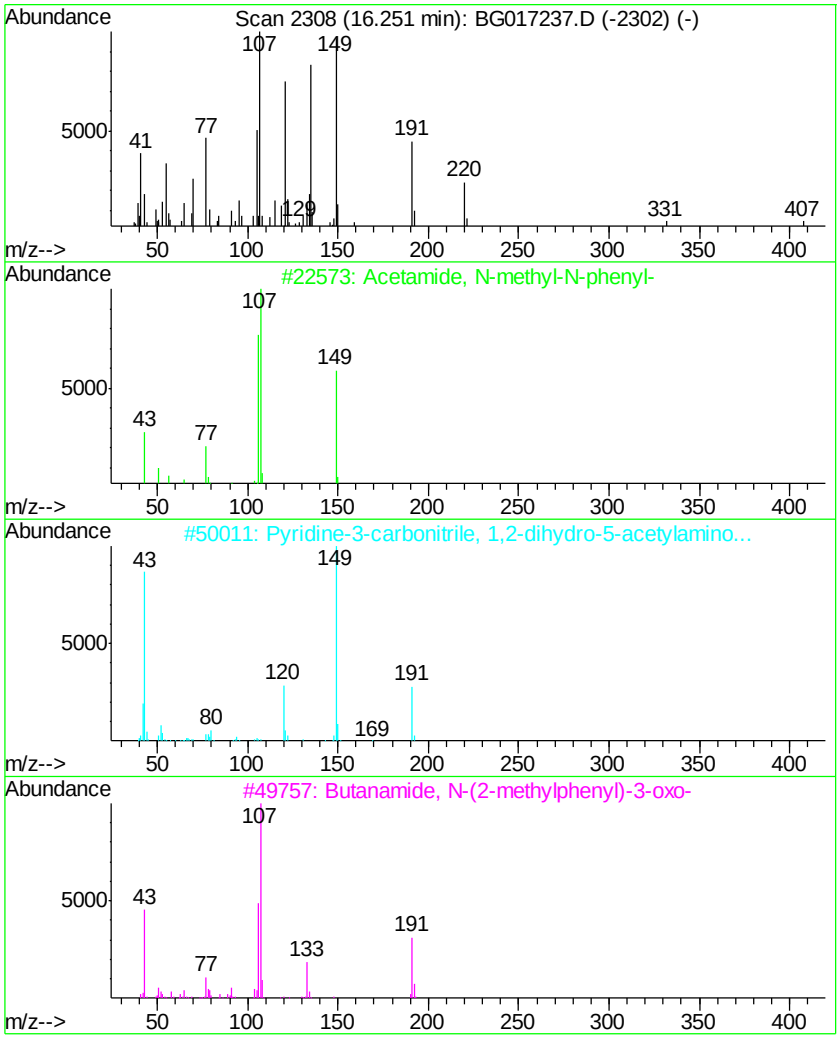
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

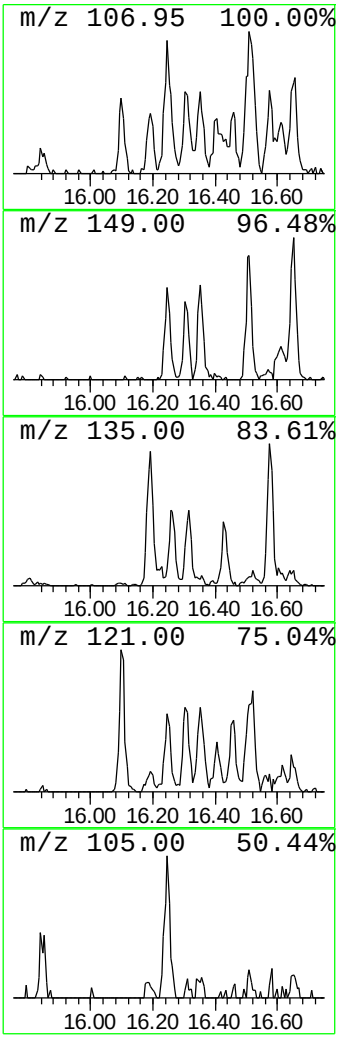
**********

Peak Number 6 Acetamide, N-methyl-N-phenyl- Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.25 | 2.39 ng | 84663 | Phenanthrene-d10 | 17.10 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Acetamide, N-methyl-N-phenyl- | 149 | C9H11NO | 000579-10-2 | 59 |
| 2 | Pyridine-3-carbonitrile, 1,2-dih... | 191 | C9H9N3O2 | 220098-92-0 | 38 |
| 3 | Butanamide, N-(2-methylphenyl)-3... | 191 | C11H13NO2 | 000093-68-5 | 35 |
| 4 | Phenol, 4-(2-methylpropyl)- | 150 | C10H14O | 004167-74-2 | 30 |
| 5 | 4-Methyl-2-tert-octylphenol | 220 | C15H24O | 004979-46-8 | 30 |



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Acq On : 21 May 2015 6:38
Operator : TP/IZ
Sample : G2301-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** MW7

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

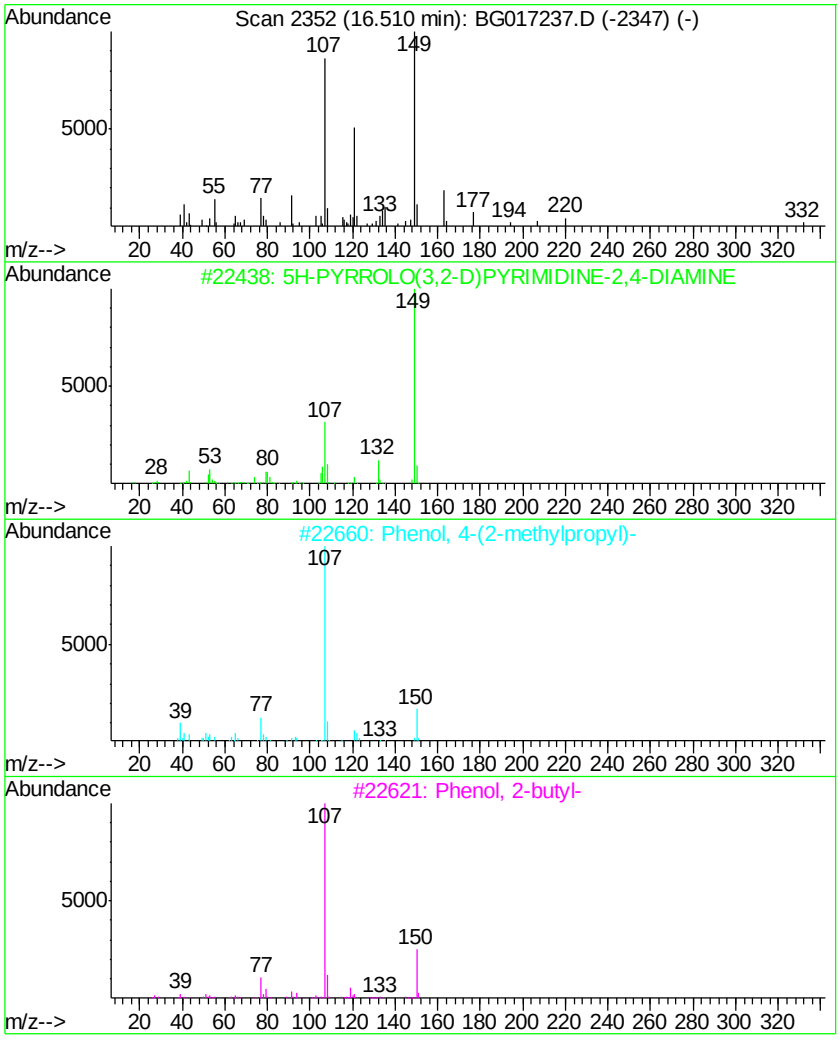
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

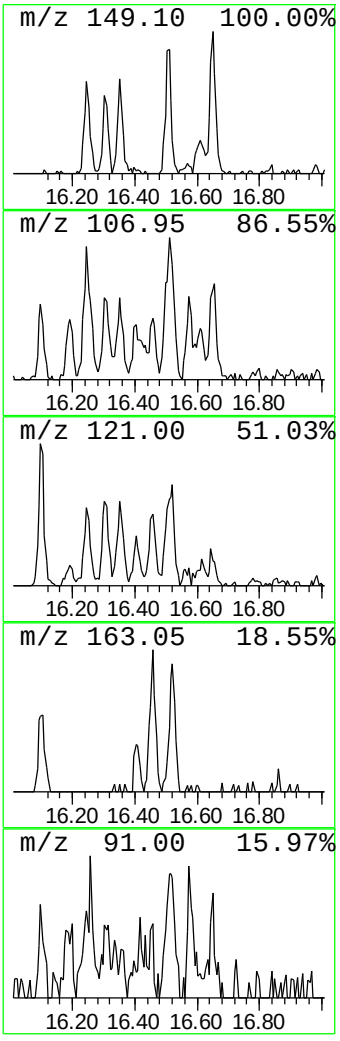
**********

Peak Number 7 5H-PYRROLO(3,2-D)PYRIMIDINE... Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.51 | 2.21 ng | 78430 | Phenanthrene-d10 | 17.10 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 5H-PYRROLO(3,2-D)PYRIMIDINE-2,4-... | 149 | C6H7N5 | 1000244-21-4 | 59 |
| 2 | Phenol, 4-(2-methylpropyl)- | 150 | C10H14O | 004167-74-2 | 43 |
| 3 | Phenol, 2-butyl- | 150 | C10H14O | 003180-09-4 | 35 |
| 4 | 2H-Indol-2-one, 1,3-dihydro-5-hy... | 149 | C8H7NO2 | 003416-18-0 | 35 |
| 5 | 2-Butanone, 4-(4-hydroxyphenyl)- | 164 | C10H12O2 | 005471-51-2 | 35 |



Tentatively Identified Compound (LSC) summary

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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 |
| Butane, 2-methoxy... | 2.86 | 39.0 | ng | 526726 | 1 | 7.69 | 269824 | 20.0 |
| 2-Pentanone, 4-hy... | 4.80 | 4.3 | ng | 57375 | 1 | 7.69 | 269824 | 20.0 |
| unknown7.23 | 7.23 | 80.7 | ng | 1088370 | 1 | 7.69 | 269824 | 20.0 |
| Acetamide, N-meth... | 16.25 | 2.4 | ng | 84663 | 4 | 17.10 | 708619 | 20.0 |
| 5H-PYRROLO(3,2-D)... | 16.51 | 2.2 | ng | 78430 | 4 | 17.10 | 708619 | 20.0 |