LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071915\
Data File : BG017970.D
Acq On : 19 Jul 2015 22:55
Operator : TP/UM
Sample : G2973-02
Misc :
ALS Vial : 46 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TP-2D23

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-BG071715.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 | 2.865 | 25 | 30 | 35 | rBV | 545589 | 675256 | 10.25% | 1.691% |
| 2 | 4.146 | 245 | 248 | 256 | rVB | 61653 | 78077 | 1.19% | 0.196% |
| 3 | 4.739 | 342 | 349 | 359 | rVB | 1122774 | 1615279 | 24.52% | 4.046% |
| 4 | 5.191 | 420 | 426 | 436 | rBV | 1768497 | 2595488 | 39.40% | 6.501% |
| 5 | 5.797 | 524 | 529 | 536 | rVB | 108974 | 160102 | 2.43% | 0.401% |
| 6 | 6.772 | 685 | 695 | 709 | rBV | 1833460 | 2893885 | 43.93% | 7.248% |
| 7 | 7.119 | 747 | 754 | 764 | rBV | 1885643 | 3021217 | 45.87% | 7.567% |
| 8 | 7.583 | 826 | 833 | 842 | rVB | 429845 | 677594 | 10.29% | 1.697% |
| 9 | 7.900 | 880 | 887 | 894 | rBV | 1321522 | 2141654 | 32.51% | 5.364% |
| 10 | 8.740 | 1021 | 1030 | 1038 | rBV | 1077497 | 1798324 | 27.30% | 4.504% |
| 11 | 10.362 | 1299 | 1306 | 1316 | rVB | 612457 | 1035857 | 15.73% | 2.594% |
| 12 | 12.859 | 1724 | 1731 | 1743 | rVB | 2867256 | 4295184 | 65.21% | 10.758% |
| 13 | 13.705 | 1868 | 1875 | 1883 | rBV | 505184 | 690072 | 10.48% | 1.728% |
| 14 | 14.240 | 1960 | 1966 | 1974 | rBV2 | 967797 | 1497241 | 22.73% | 3.750% |
| 15 | 15.738 | 2214 | 2221 | 2238 | rBV | 2512043 | 3574851 | 54.27% | 8.954% |
| 16 | 16.995 | 2428 | 2435 | 2440 | rBV | 1353787 | 1901183 | 28.86% | 4.762% |
| 17 | 17.912 | 2586 | 2591 | 2597 | rBV | 71579 | 108448 | 1.65% | 0.272% |
| 18 | 19.645 | 2879 | 2886 | 2896 | rBV | 5265498 | 6586786 | 100.00% | 16.497% |
| 19 | 20.920 | 3099 | 3103 | 3111 | rBV | 152475 | 225301 | 3.42% | 0.564% |
| 20 | 21.196 | 3144 | 3150 | 3160 | rBV | 1750780 | 2226031 | 33.80% | 5.575% |
| 21 | 23.411 | 3520 | 3527 | 3540 | rVB | 1150708 | 2128219 | 32.31% | 5.330% |

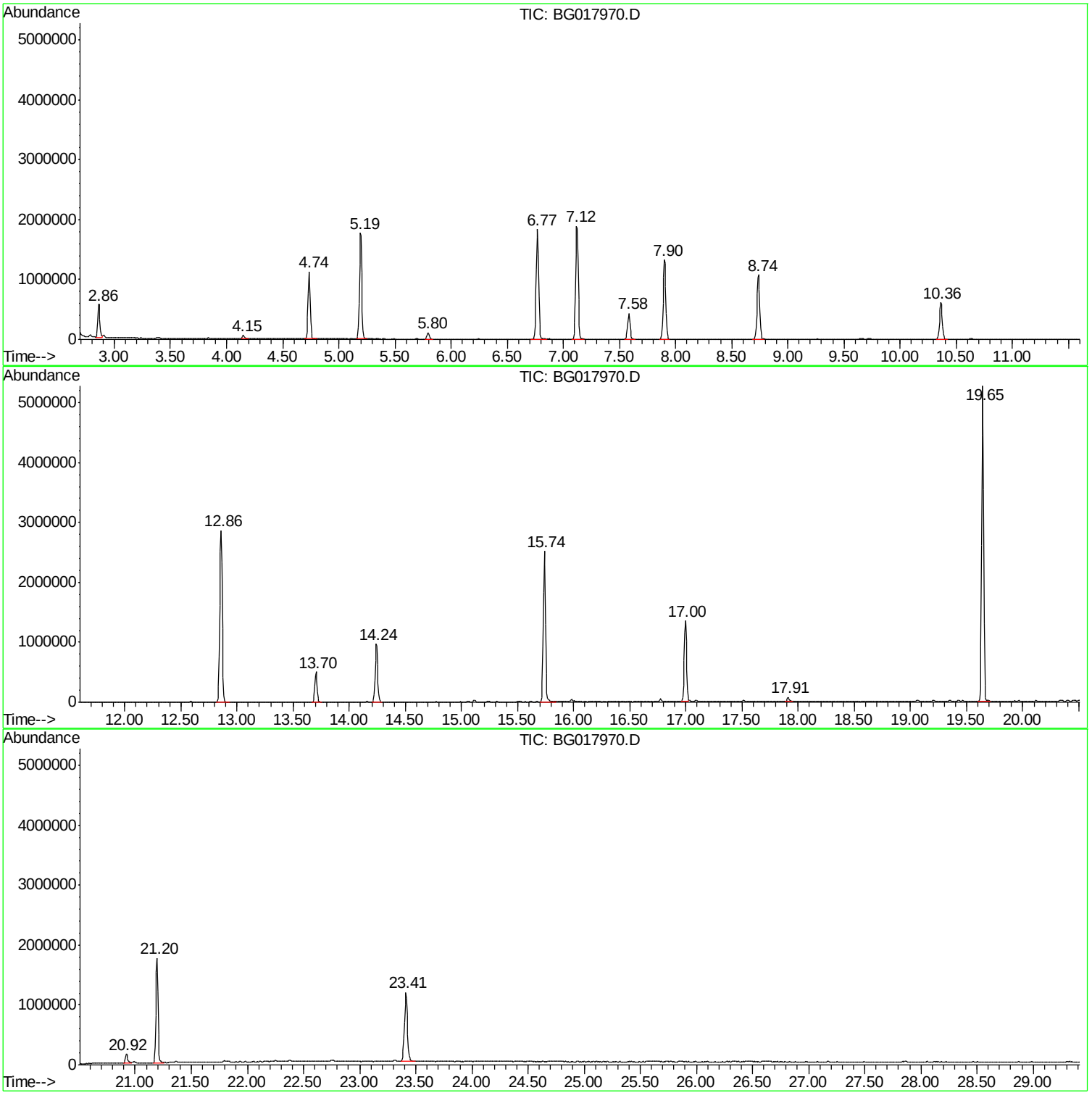
Sum of corrected areas: 39926049

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071915\
Data File : BG017970.D
Acq On : 19 Jul 2015 22:55
Operator : TP/UM
Sample : G2973-02
Misc :
ALS Vial : 46 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TP-2D23

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071915\
Data File : BG017970.D
Acq On : 19 Jul 2015 22:55
Operator : TP/UM
Sample : G2973-02
Misc :
ALS Vial : 46 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TP-2D23

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

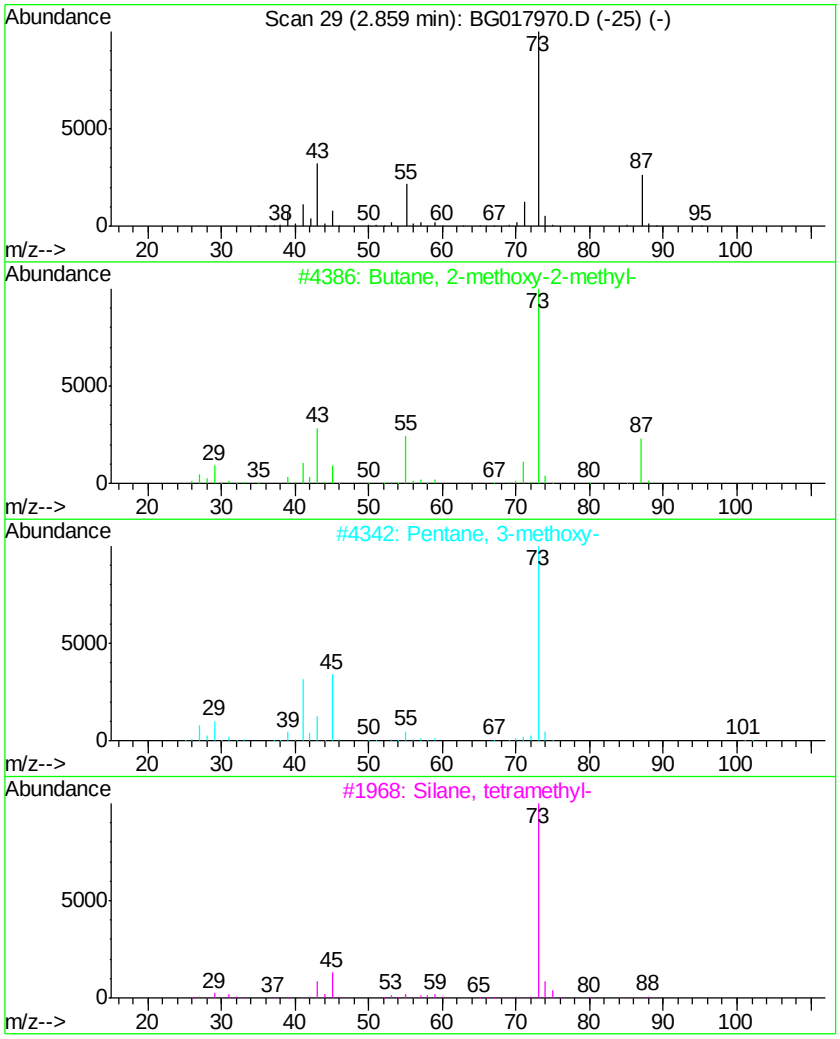
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

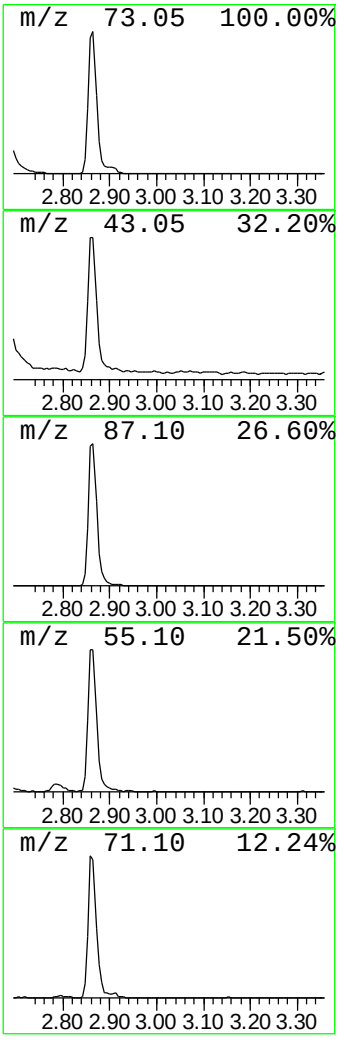
**********

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.86 | 19.93 ng | 675256 | 1,4-Dichlorobenzene-d4 | 7.59 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 90 |
| 2 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 23 |
| 3 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 9 |
| 4 | Acetamide, N-ethyl- | 87 | C4H9NO | 000625-50-3 | 9 |
| 5 | N-Ethylformamide | 73 | C3H7NO | 000627-45-2 | 9 |



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071915\
Data File : BG017970.D
Acq On : 19 Jul 2015 22:55
Operator : TP/UM
Sample : G2973-02
Misc :
ALS Vial : 46 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TP-2D23

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

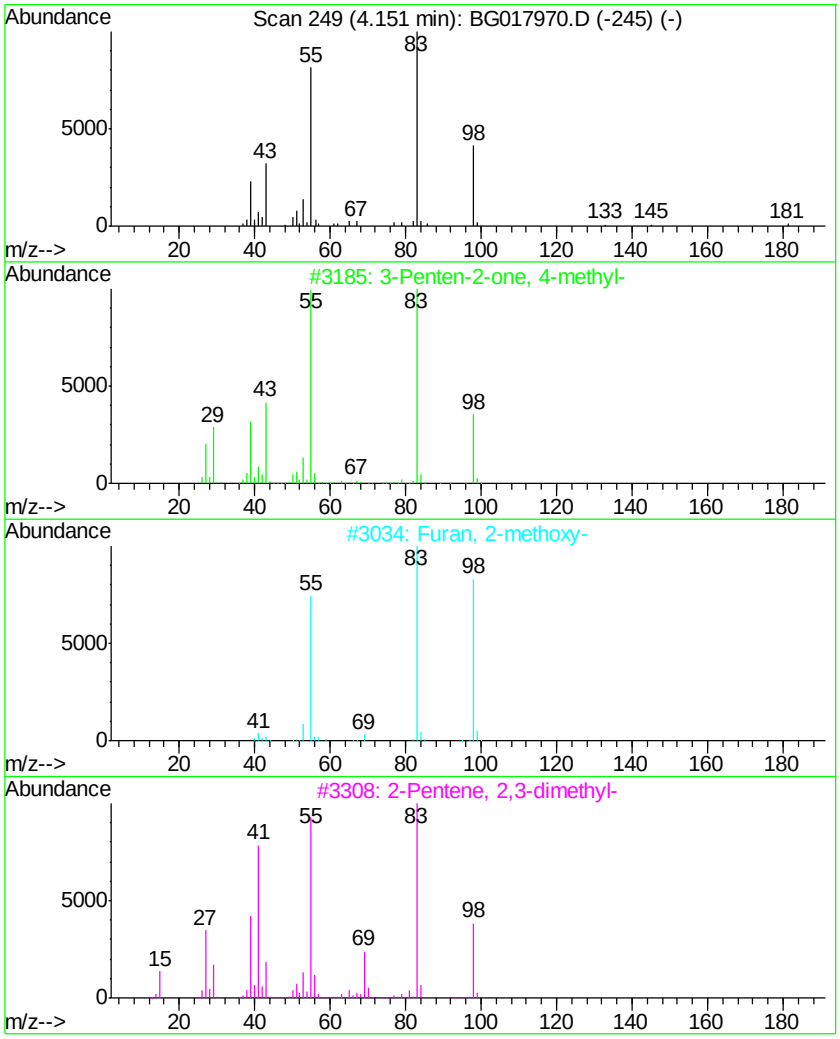
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

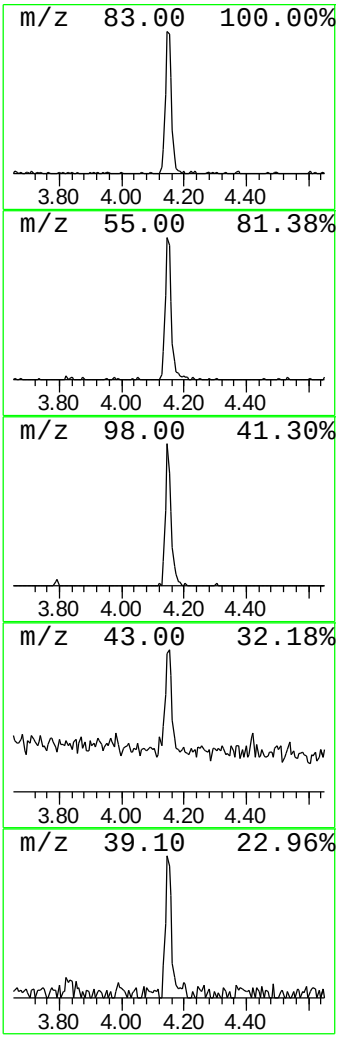
**********

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.15 | 2.30 ng | 78077 | 1,4-Dichlorobenzene-d4 | 7.59 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Penten-2-one, 4-methyl- | 98 | C6H10O | 000141-79-7 | 91 |
| 2 | Furan, 2-methoxy- | 98 | C5H6O2 | 025414-22-6 | 83 |
| 3 | 2-Pentene, 2,3-dimethyl- | 98 | C7H14 | 010574-37-5 | 78 |
| 4 | Cyclohexane, methyl- | 98 | C7H14 | 000108-87-2 | 72 |
| 5 | 1H-Imidazole, 4,5-dihydro-2,4-di... | 98 | C5H10N2 | 000930-61-0 | 64 |



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071915\
Data File : BG017970.D
Acq On : 19 Jul 2015 22:55
Operator : TP/UM
Sample : G2973-02
Misc :
ALS Vial : 46 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TP-2D23

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

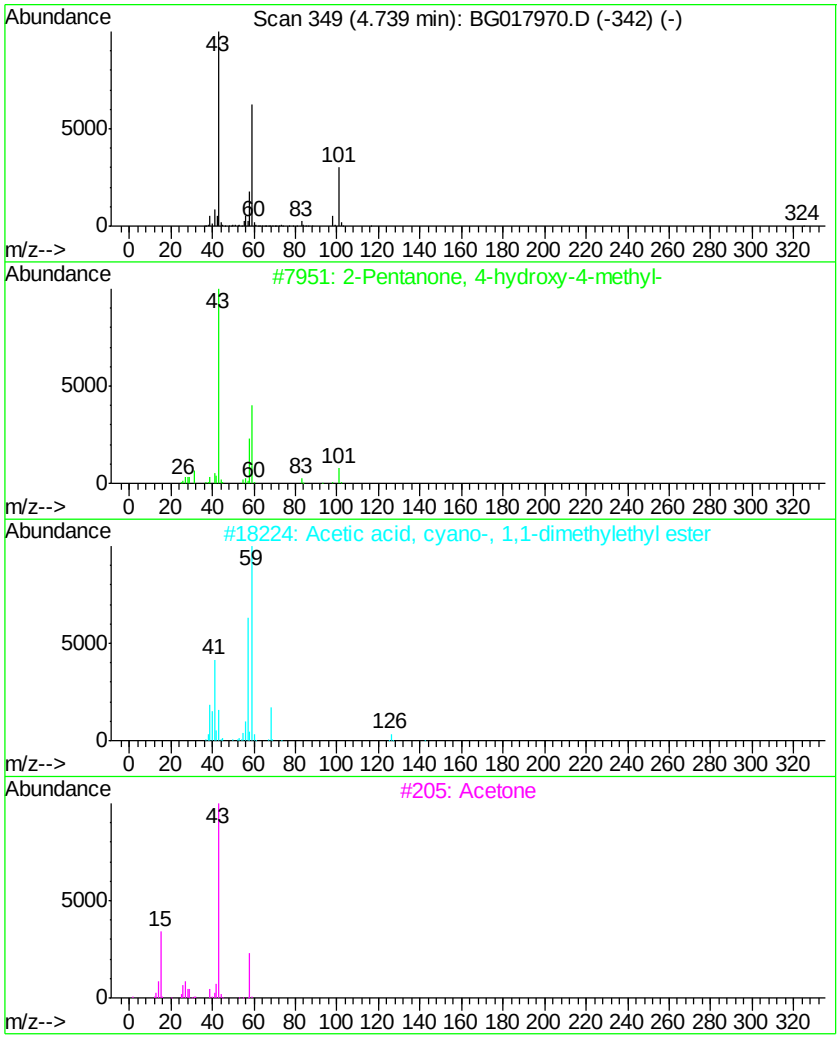
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

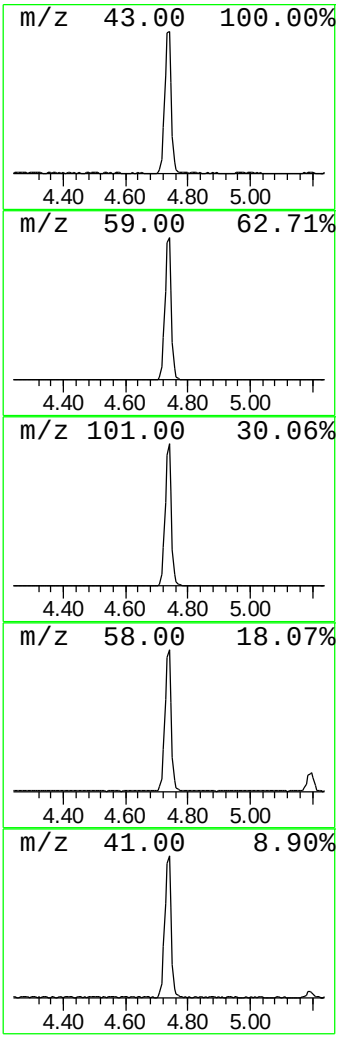
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.74 | 47.68 ng | 1615280 | 1,4-Dichlorobenzene-d4 | 7.59 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 56 |
| 2 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 17 |
| 3 | Acetone | 58 | C3H6O | 000067-64-1 | 10 |
| 4 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |
| 5 | Butane, 1-ethoxy- | 102 | C6H14O | 000628-81-9 | 9 |



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071915\
Data File : BG017970.D
Acq On : 19 Jul 2015 22:55
Operator : TP/UM
Sample : G2973-02
Misc :
ALS Vial : 46 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TP-2D23

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

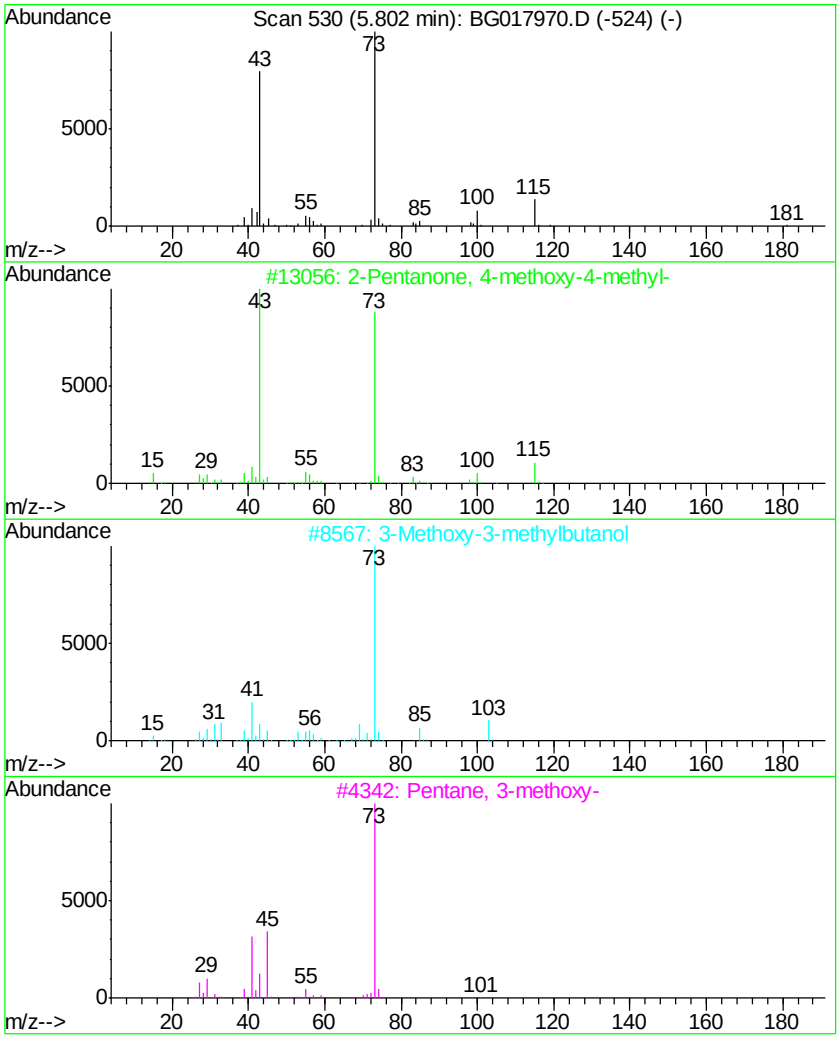
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

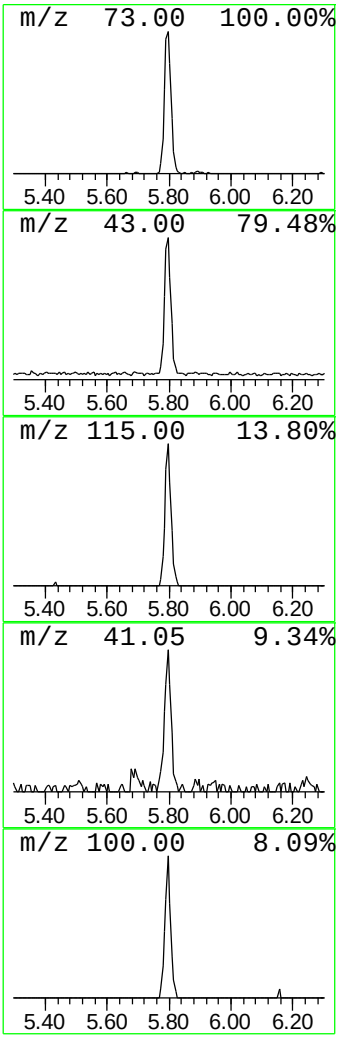
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.80 | 4.73 ng | 160102 | 1,4-Dichlorobenzene-d4 | 7.59 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-methoxy-4-methyl- | 130 | C7H14O2 | 000107-70-0 | 78 |
| 2 | 3-Methoxy-3-methylbutanol | 118 | C6H14O2 | 056539-66-3 | 12 |
| 3 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 10 |
| 4 | N-Ethylformamide | 73 | C3H7NO | 000627-45-2 | 9 |
| 5 | 5H-1,4-Dioxepin, 2,3-dihydro- | 100 | C5H8O2 | 004040-81-7 | 9 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071915\
Data File : BG017970.D
Acq On : 19 Jul 2015 22:55
Operator : TP/UM
Sample : G2973-02
Misc :
ALS Vial : 46 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TP-2D23

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

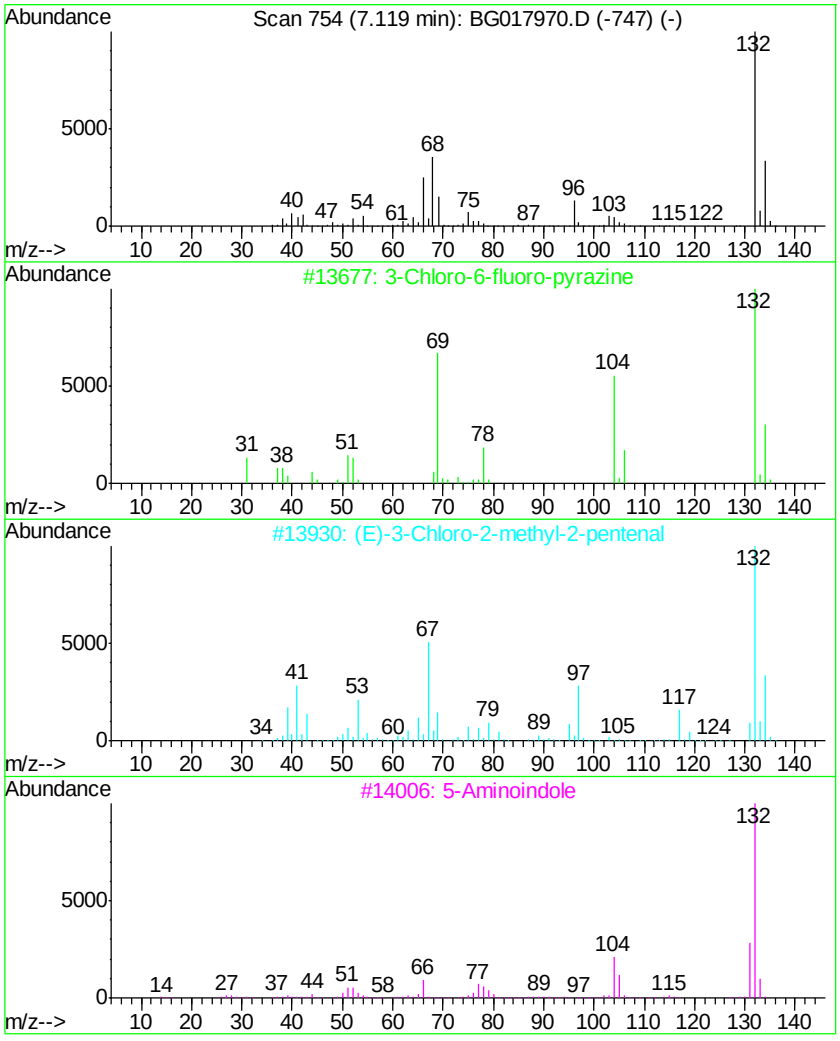
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

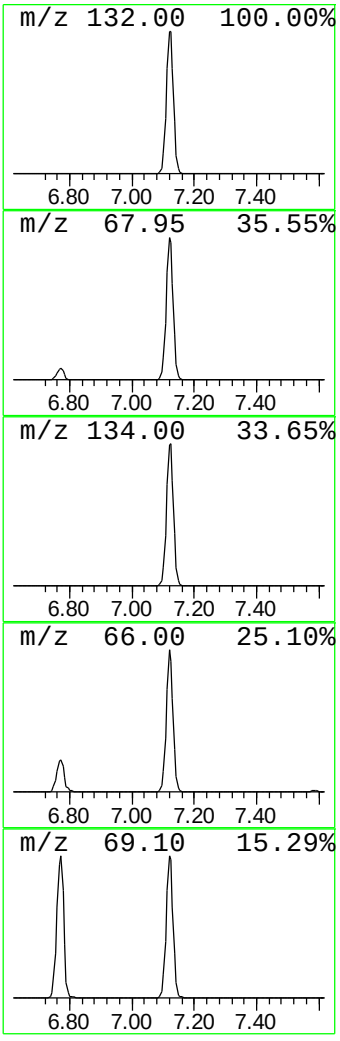
**********

Peak Number 5 unknown7.12 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.12 | 89.17 ng | 3021220 | 1,4-Dichlorobenzene-d4 | 7.59 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 25 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 17 |
| 3 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 10 |
| 4 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |
| 5 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 9 |



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071915\
Data File : BG017970.D
Acq On : 19 Jul 2015 22:55
Operator : TP/UM
Sample : G2973-02
Misc :
ALS Vial : 46 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TP-2D23

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

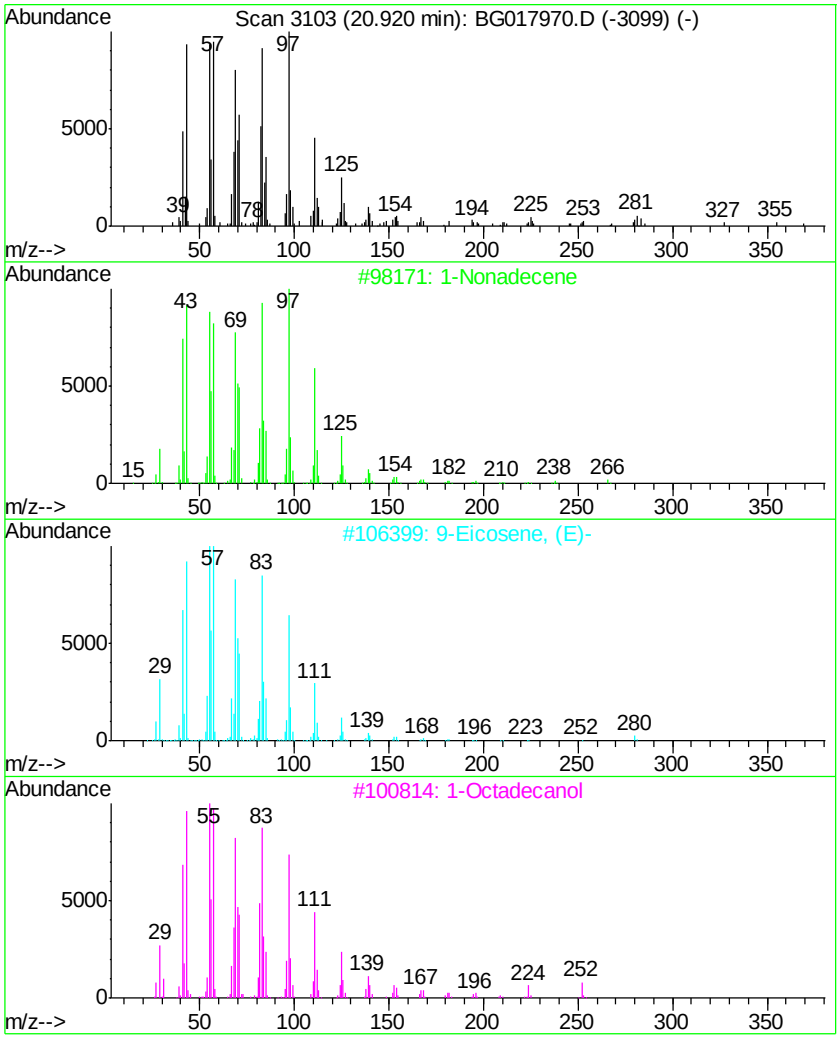
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

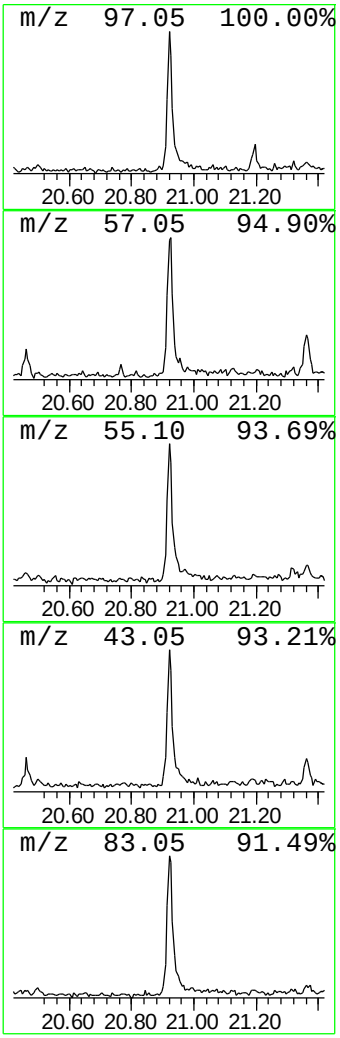
**********

Peak Number 7 1-Nonadecene Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.92 | 2.02 ng | 225301 | Chrysene-d12 | 21.20 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Nonadecene | 266 | C19H38 | 018435-45-5 | 90 |
| 2 | 9-Eicosene, (E)- | 280 | C20H40 | 074685-29-3 | 86 |
| 3 | 1-Octadecanol | 270 | C18H38O | 000112-92-5 | 83 |
| 4 | 1-Hexacosanol | 382 | C26H54O | 000506-52-5 | 81 |
| 5 | Heptafluorobutanoic acid, heptad... | 452 | C21H35F7O2 | 1000282-97-3 | 81 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071915\
Data File : BG017970.D
Acq On : 19 Jul 2015 22:55
Operator : TP/UM
Sample : G2973-02
Misc :
ALS Vial : 46 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** TP-2D23

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.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 |
| Butane, 2-methoxy... | 2.86 | 19.9 | ng | 675256 | 1 | 7.59 | 677594 | 20.0 |
| 3-Penten-2-one, 4... | 4.15 | 2.3 | ng | 78077 | 1 | 7.59 | 677594 | 20.0 |
| 2-Pentanone, 4-hy... | 4.74 | 47.7 | ng | 1615280 | 1 | 7.59 | 677594 | 20.0 |
| 2-Pentanone, 4-me... | 5.80 | 4.7 | ng | 160102 | 1 | 7.59 | 677594 | 20.0 |
| unknown7.12 | 7.12 | 89.2 | ng | 3021220 | 1 | 7.59 | 677594 | 20.0 |
| 1-Nonadecene | 20.92 | 2.0 | ng | 225301 | 5 | 21.20 | 2226030 | 20.0 |