LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG071316\
Data File : BG023089.D
Acq On : 14 Jul 2016 5:13
Operator : UM/SJ
Sample : H4005-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 071116-P41-E-D-M

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-BG070816.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 | 4.615 | 296 | 302 | 315 | rBV | 1703979 | 2542406 | 25.06% | 5.310% |
| 2 | 5.226 | 398 | 406 | 413 | rBV | 1394390 | 2220332 | 21.89% | 4.637% |
| 3 | 5.697 | 479 | 486 | 497 | rVB | 633153 | 1040428 | 10.26% | 2.173% |
| 4 | 6.308 | 584 | 590 | 598 | rVB | 332479 | 522609 | 5.15% | 1.091% |
| 5 | 7.306 | 753 | 760 | 769 | rBV | 484472 | 830366 | 8.19% | 1.734% |
| 6 | 7.682 | 816 | 824 | 832 | rBV | 1160981 | 2085456 | 20.56% | 4.356% |
| 7 | 8.152 | 895 | 904 | 911 | rVB2 | 432287 | 751109 | 7.40% | 1.569% |
| 8 | 8.476 | 951 | 959 | 968 | rBV | 1437874 | 2587422 | 25.51% | 5.404% |
| 9 | 9.328 | 1096 | 1104 | 1115 | rBV | 1510918 | 2698603 | 26.60% | 5.636% |
| 10 | 10.984 | 1376 | 1386 | 1393 | rBV | 651076 | 1193010 | 11.76% | 2.492% |
| 11 | 13.423 | 1791 | 1801 | 1810 | rBV | 4328305 | 6631843 | 65.38% | 13.851% |
| 12 | 14.245 | 1935 | 1941 | 1948 | rBV | 88156 | 156337 | 1.54% | 0.327% |
| 13 | 14.804 | 2029 | 2036 | 2044 | rBV2 | 1247816 | 2033113 | 20.04% | 4.246% |
| 14 | 16.296 | 2284 | 2290 | 2299 | rBV | 2510099 | 4012949 | 39.56% | 8.381% |
| 15 | 17.559 | 2498 | 2505 | 2511 | rBV2 | 1664692 | 2562643 | 25.26% | 5.352% |
| 16 | 18.423 | 2647 | 2652 | 2657 | rBV3 | 98222 | 138407 | 1.36% | 0.289% |
| 17 | 19.686 | 2863 | 2867 | 2873 | rBV6 | 63895 | 110805 | 1.09% | 0.231% |
| 18 | 20.162 | 2941 | 2948 | 2957 | rBV | 7122701 | 10143914 | 100.00% | 21.186% |
| 19 | 21.860 | 3230 | 3237 | 3245 | rBV2 | 1623089 | 2939817 | 28.98% | 6.140% |
| 20 | 25.244 | 3802 | 3813 | 3826 | rBV2 | 882700 | 2679062 | 26.41% | 5.595% |

Sum of corrected areas: 47880631

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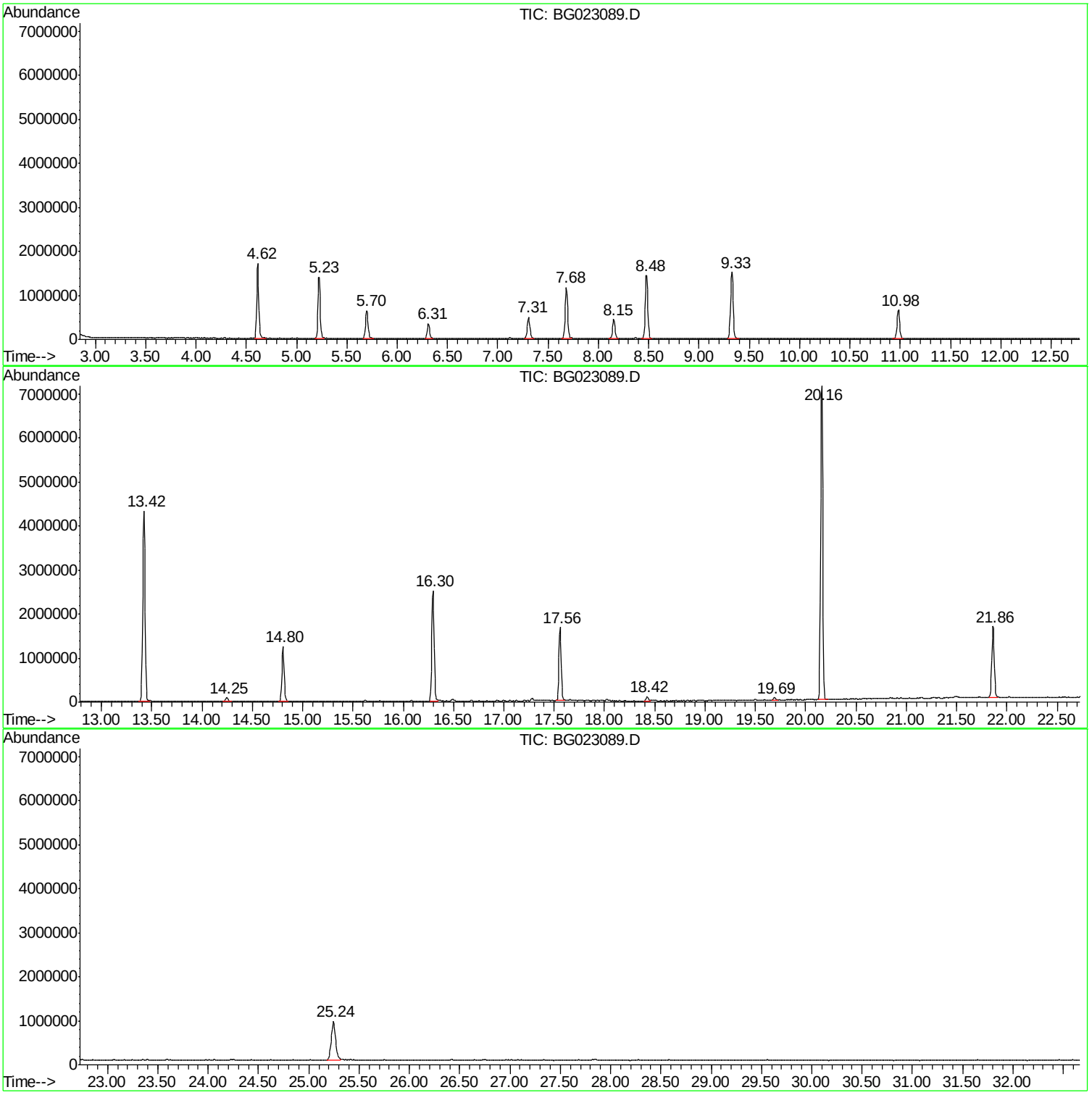
Data File : BG023089.D
Acq On : 14 Jul 2016 5:13
Operator : UM/SJ
Sample : H4005-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
071116-P41-E-D-M

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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\BG071316\
Data File : BG023089.D
Acq On : 14 Jul 2016 5:13
Operator : UM/SJ
Sample : H4005-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 071116-P41-E-D-M

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

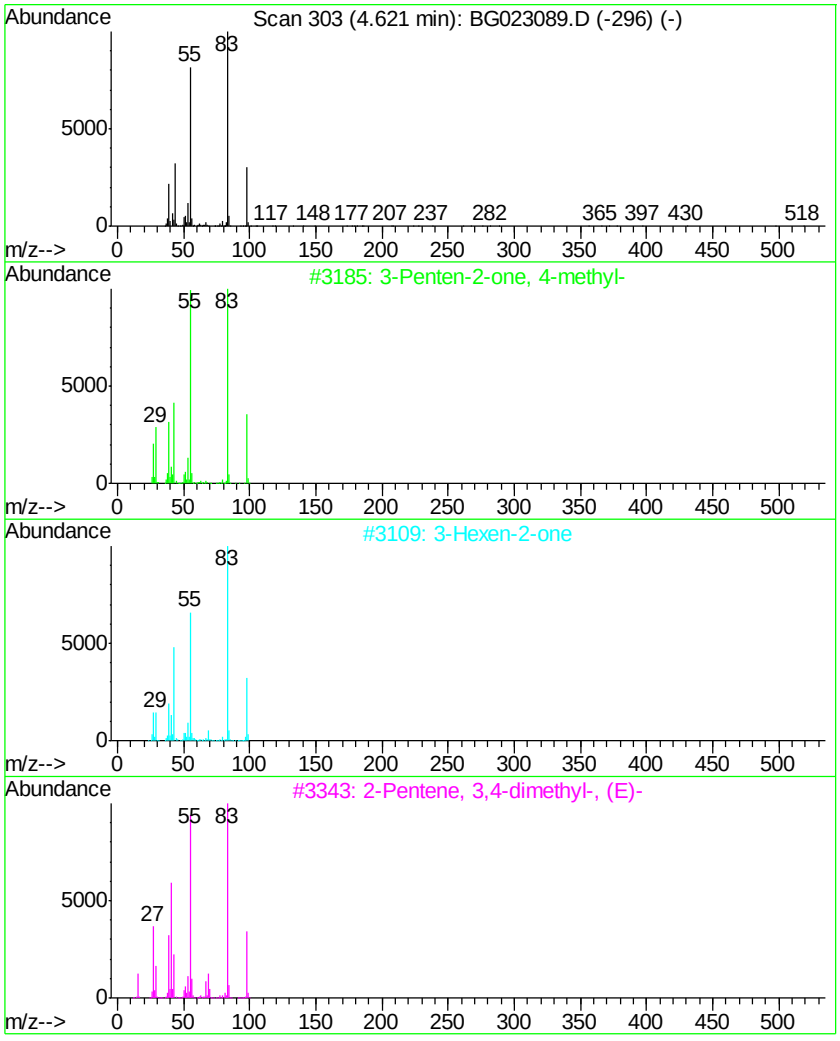
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

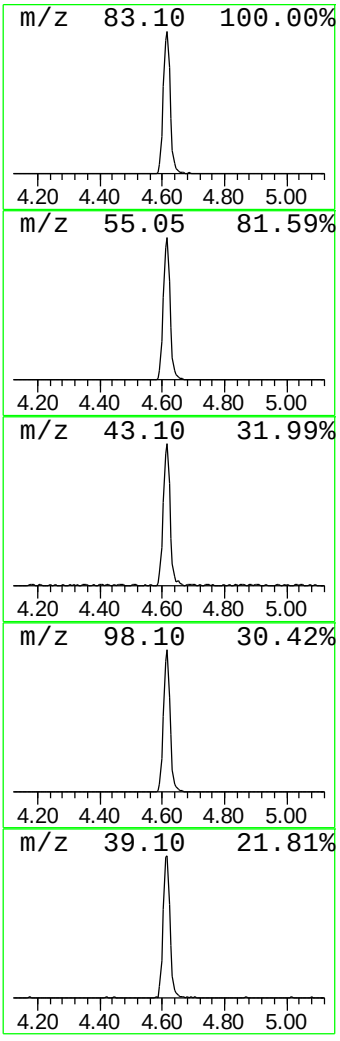
**********

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.62 | 67.70 ng | 2542410 | 1,4-Dichlorobenzene-d4 | 8.15 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Penten-2-one, 4-methyl- | 98 | C6H10O | 000141-79-7 | 94 |
| 2 | 3-Hexen-2-one | 98 | C6H10O | 000763-93-9 | 91 |
| 3 | 2-Pentene, 3,4-dimethyl-, (E)- | 98 | C7H14 | 004914-92-5 | 90 |
| 4 | 2-Pentene, 3,4-dimethyl-, (Z)- | 98 | C7H14 | 004914-91-4 | 86 |
| 5 | 2-Pentene, 2,4-dimethyl- | 98 | C7H14 | 000625-65-0 | 80 |



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG071316\
Data File : BG023089.D
Acq On : 14 Jul 2016 5:13
Operator : UM/SJ
Sample : H4005-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 071116-P41-E-D-M

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

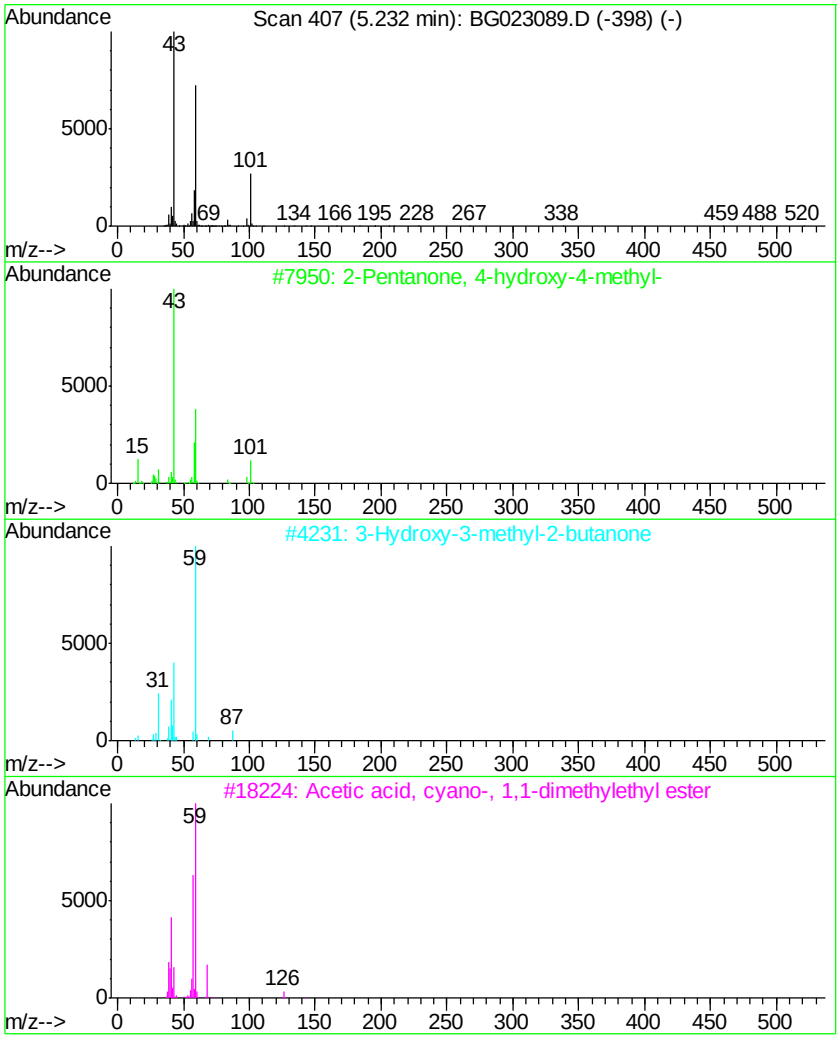
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

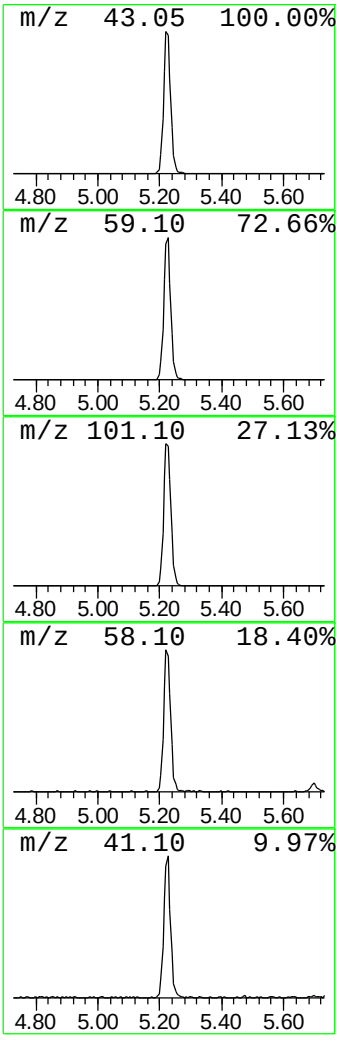
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.23 | 59.12 ng | 2220330 | 1,4-Dichlorobenzene-d4 | 8.15 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 42 |
| 2 | 3-Hydroxy-3-methyl-2-butanone | 102 | C5H10O2 | 000115-22-0 | 38 |
| 3 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 37 |
| 4 | 2-Hexanol, 2-methyl- | 116 | C7H16O | 000625-23-0 | 36 |
| 5 | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O | 017348-59-3 | 33 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG071316\
Data File : BG023089.D
Acq On : 14 Jul 2016 5:13
Operator : UM/SJ
Sample : H4005-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 071116-P41-E-D-M

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

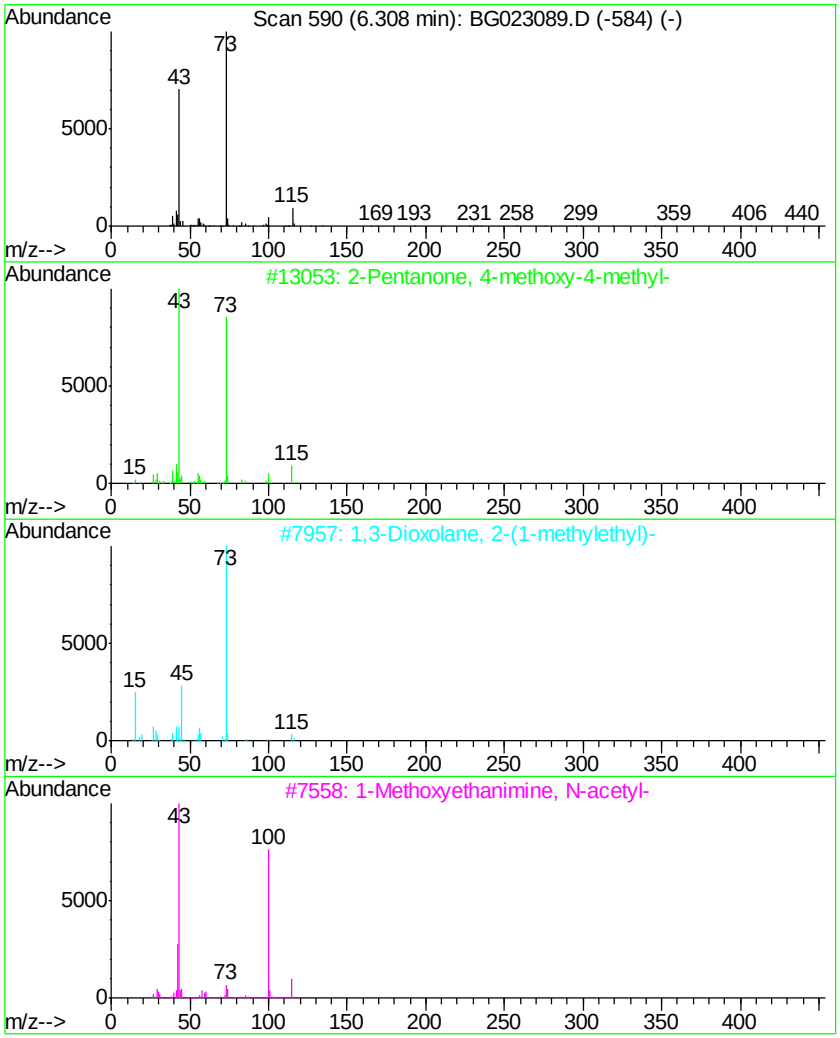
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

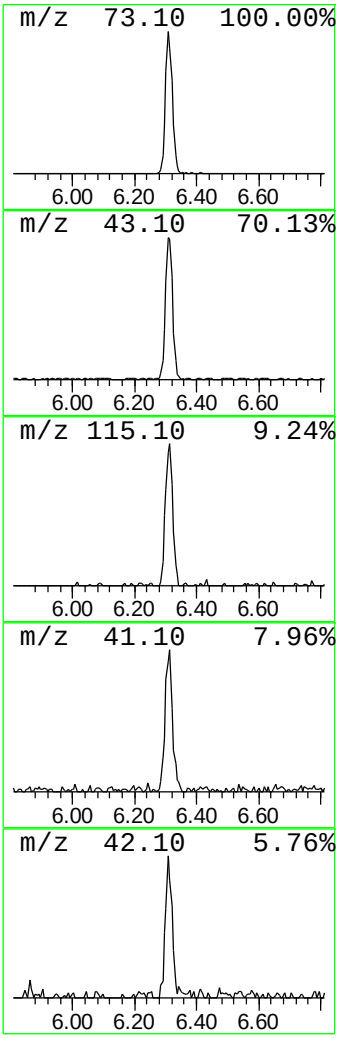
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.31 | 13.92 ng | 522609 | 1,4-Dichlorobenzene-d4 | 8.15 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-methoxy-4-methyl- | 130 | C7H14O2 | 000107-70-0 | 53 |
| 2 | 1,3-Dioxolane, 2-(1-methylethyl)- | 116 | C6H12O2 | 000822-83-3 | 9 |
| 3 | 1-Methoxyethanimine, N-acetyl- | 115 | C5H9NO2 | 099028-43-0 | 9 |
| 4 | 1,3-Dioxolane, 2-propyl- | 116 | C6H12O2 | 003390-13-4 | 9 |
| 5 | 2-Pentanone, 3-methyl- | 100 | C6H12O | 000565-61-7 | 9 |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG071316\
Data File : BG023089.D
Acq On : 14 Jul 2016 5:13
Operator : UM/SJ
Sample : H4005-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 071116-P41-E-D-M

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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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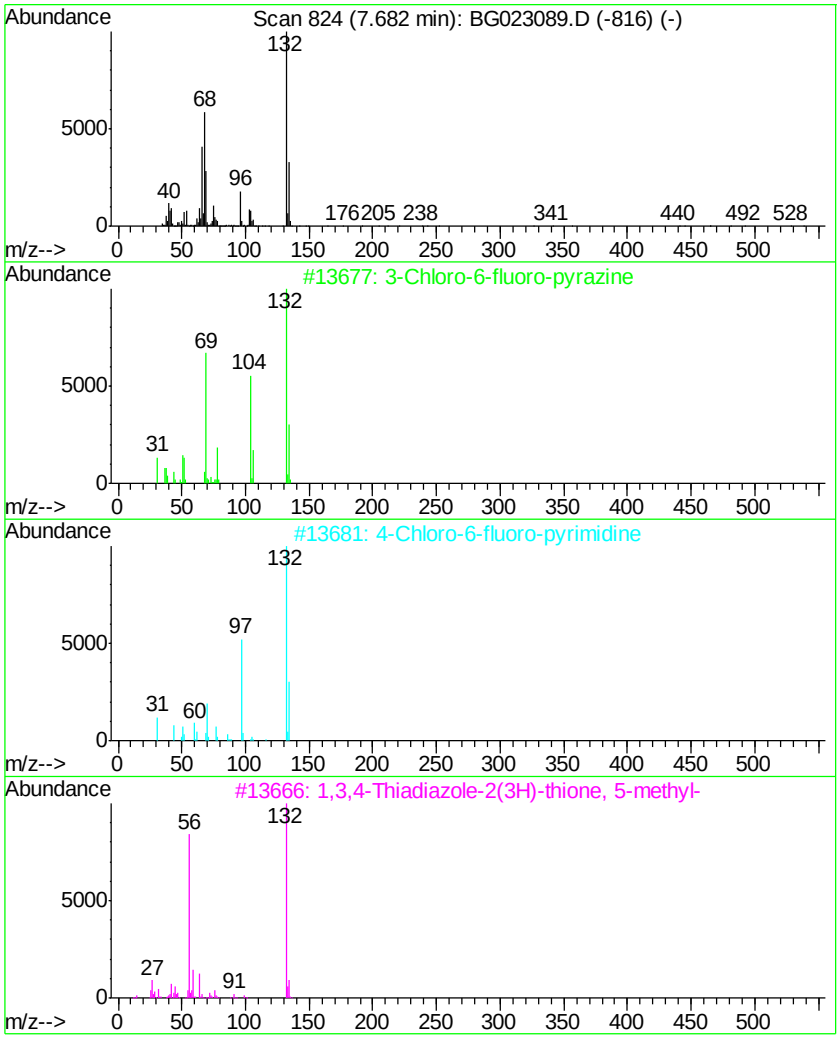
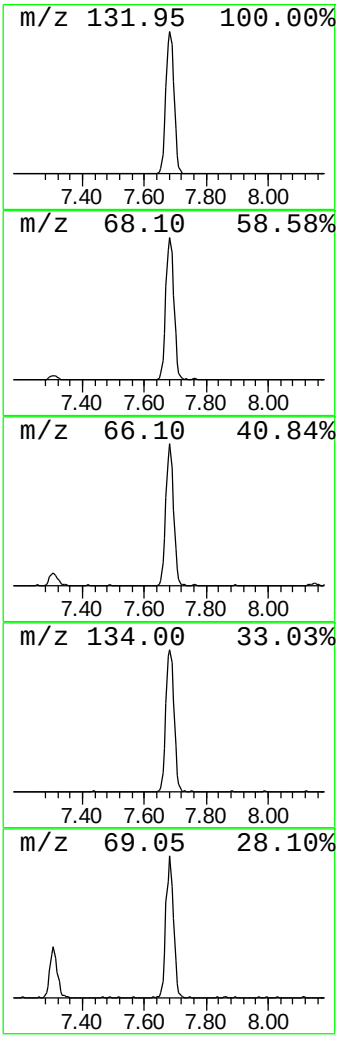
Peak Number 4 unknown7.68 Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.68 | 55.53 ng | 2085460 | 1,4-Dichlorobenzene-d4 | 8.15 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 14 |
| 2 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 14 |
| 3 | 1,3,4-Thiadiazole-2(3H)-thione, ... | 132 | C3H4N2S2 | 029490-19-5 | 14 |
| 4 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 5 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 10 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071316\
Data File : BG023089.D
Acq On : 14 Jul 2016 5:13
Operator : UM/SJ
Sample : H4005-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** 071116-P41-E-D-M

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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 |
| 3-Penten-2-one, 4... | 4.62 | 67.7 | ng | 2542410 | 1 | 8.15 | 751109 | 20.0 |
| 2-Pentanone, 4-hy... | 5.23 | 59.1 | ng | 2220330 | 1 | 8.15 | 751109 | 20.0 |
| 2-Pentanone, 4-me... | 6.31 | 13.9 | ng | 522609 | 1 | 8.15 | 751109 | 20.0 |
| unknown7.68 | 7.68 | 55.5 | ng | 2085460 | 1 | 8.15 | 751109 | 20.0 |