LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071415\
Data File : BF080490.D
Acq On : 15 Jul 2015 13:59
Operator : TP/UM
Sample : G2973-14
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TP-9S

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_F\METHODS\8270-BF071415.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 | 2.156 | 4 | 6 | 14 | rBV | 93990 | 181064 | 28.29% | 2.664% |
| 2 | 2.281 | 14 | 17 | 26 | rVB | 120020 | 187896 | 29.36% | 2.765% |
| 3 | 2.430 | 29 | 30 | 37 | rVB | 6919 | 11076 | 1.73% | 0.163% |
| 4 | 4.739 | 230 | 232 | 240 | rBV | 7245 | 13933 | 2.18% | 0.205% |
| 5 | 5.333 | 281 | 284 | 298 | rBV | 323911 | 397346 | 62.08% | 5.847% |
| 6 | 5.756 | 319 | 321 | 334 | rVB | 573632 | 548386 | 85.68% | 8.070% |
| 7 | 6.133 | 352 | 354 | 360 | rBB | 34431 | 36989 | 5.78% | 0.544% |
| 8 | 6.762 | 407 | 409 | 419 | rBV | 627977 | 602081 | 94.07% | 8.860% |
| 9 | 6.899 | 419 | 421 | 423 | rBV | 764159 | 616152 | 96.27% | 9.067% |
| 10 | 7.127 | 439 | 441 | 443 | rBB | 134328 | 177894 | 27.79% | 2.618% |
| 11 | 7.276 | 453 | 454 | 457 | rBV | 343864 | 394593 | 61.65% | 5.807% |
| 12 | 7.688 | 488 | 490 | 492 | rBV | 456794 | 368430 | 57.56% | 5.422% |
| 13 | 8.408 | 551 | 553 | 556 | rBV | 305646 | 253722 | 39.64% | 3.734% |
| 14 | 9.482 | 645 | 647 | 649 | rVB | 824102 | 640035 | 100.00% | 9.419% |
| 15 | 9.882 | 680 | 682 | 684 | rBV | 130487 | 112820 | 17.63% | 1.660% |
| 16 | 10.168 | 705 | 707 | 710 | rBB | 304011 | 274900 | 42.95% | 4.045% |
| 17 | 10.568 | 739 | 742 | 744 | rBB | 7722 | 8119 | 1.27% | 0.119% |
| 18 | 10.956 | 774 | 776 | 779 | rBV2 | 353751 | 366996 | 57.34% | 5.401% |
| 19 | 11.048 | 782 | 784 | 786 | rBB | 6032 | 10558 | 1.65% | 0.155% |
| 20 | 11.494 | 821 | 823 | 824 | rBV | 8690 | 8380 | 1.31% | 0.123% |
| 21 | 11.665 | 836 | 838 | 840 | rBV | 350505 | 293980 | 45.93% | 4.326% |
| 22 | 13.334 | 981 | 984 | 986 | rBV | 498424 | 602458 | 94.13% | 8.866% |
| 23 | 14.408 | 1076 | 1078 | 1083 | rVB3 | 4406 | 9444 | 1.48% | 0.139% |
| 24 | 14.591 | 1091 | 1094 | 1097 | rBV | 311578 | 322327 | 50.36% | 4.743% |
| 25 | 15.174 | 1142 | 1145 | 1148 | rVB | 13167 | 14826 | 2.32% | 0.218% |
| 26 | 15.768 | 1192 | 1197 | 1200 | rBV2 | 6064 | 12643 | 1.98% | 0.186% |
| 27 | 15.986 | 1214 | 1216 | 1220 | rBV | 16974 | 18869 | 2.95% | 0.278% |
| 28 | 16.408 | 1250 | 1253 | 1256 | rBV | 240363 | 309526 | 48.36% | 4.555% |

Sum of corrected areas: 6795443

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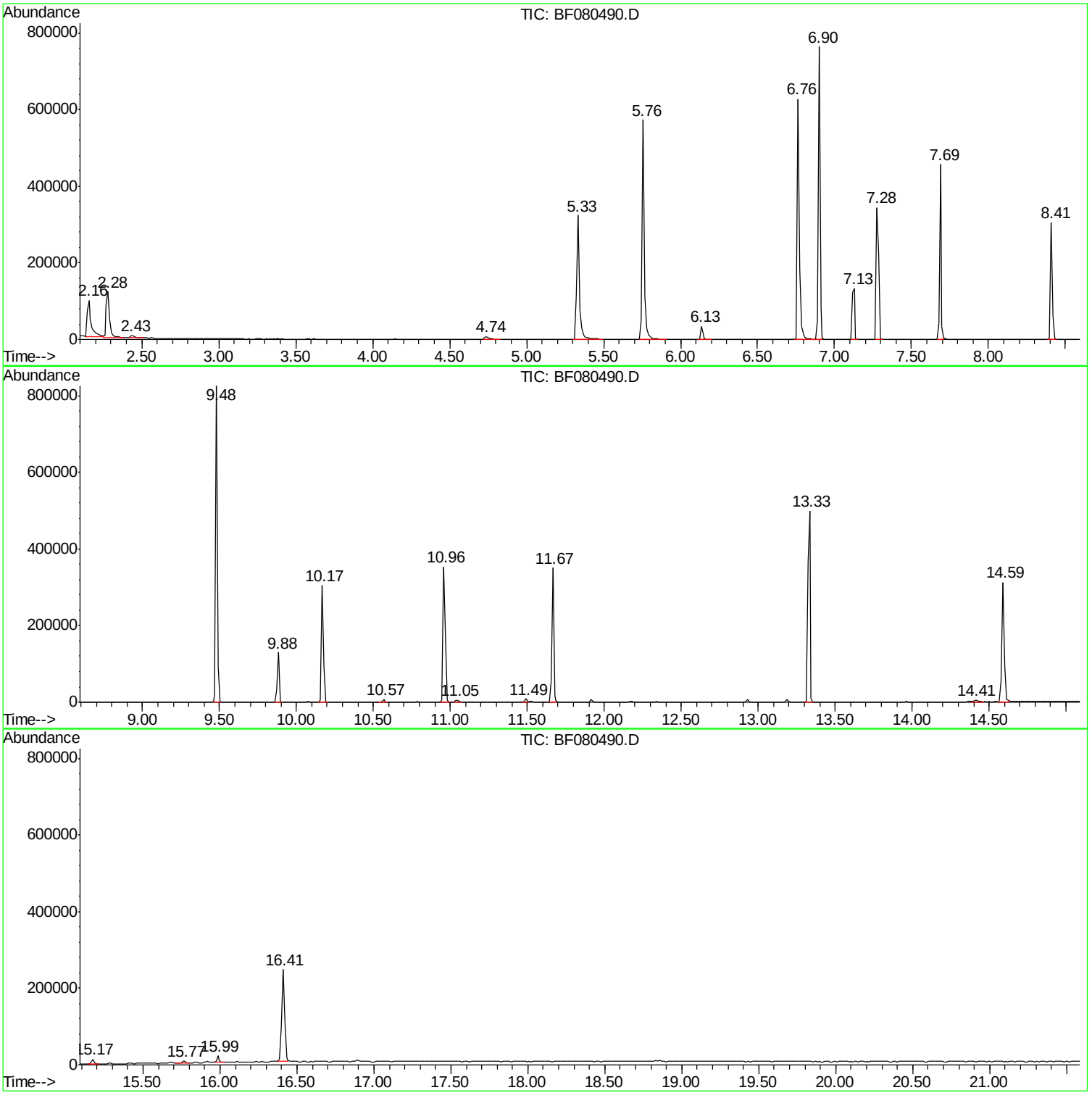
ALS Vial : 23 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TP-9S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071415.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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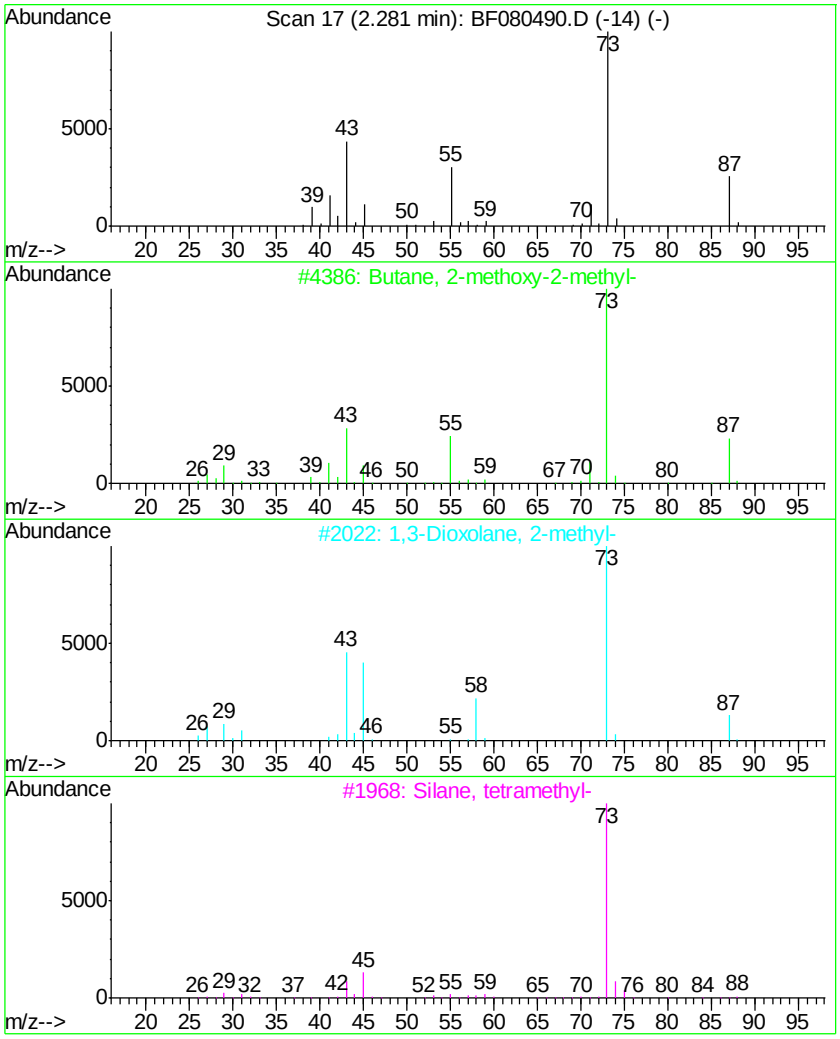
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

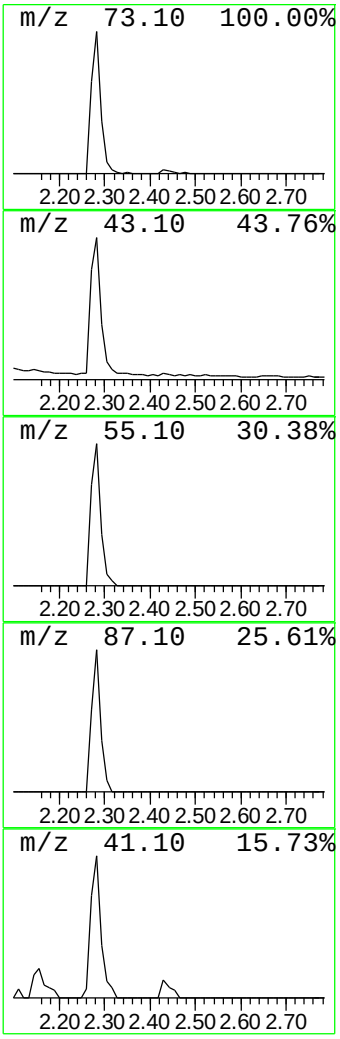
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.28 | 21.12 ng | 187896 | 1,4-Dichlorobenzene-d4 | 7.13 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 83 |
| 2 | 1,3-Dioxolane, 2-methyl- | 88 | C4H8O2 | 000497-26-7 | 37 |
| 3 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 17 |
| 4 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 12 |
| 5 | N-Ethylformamide | 73 | C3H7NO | 000627-45-2 | 9 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071415\
Data File : BF080490.D
Acq On : 15 Jul 2015 13:59
Operator : TP/UM
Sample : G2973-14
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TP-9S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

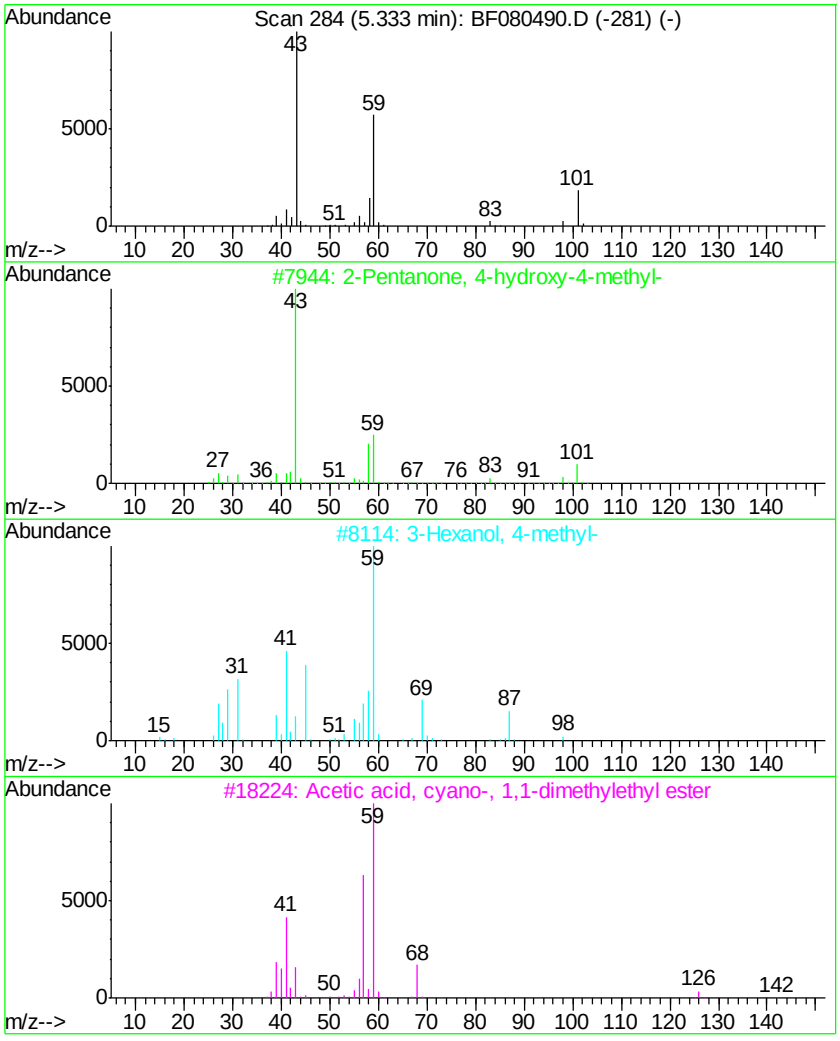
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

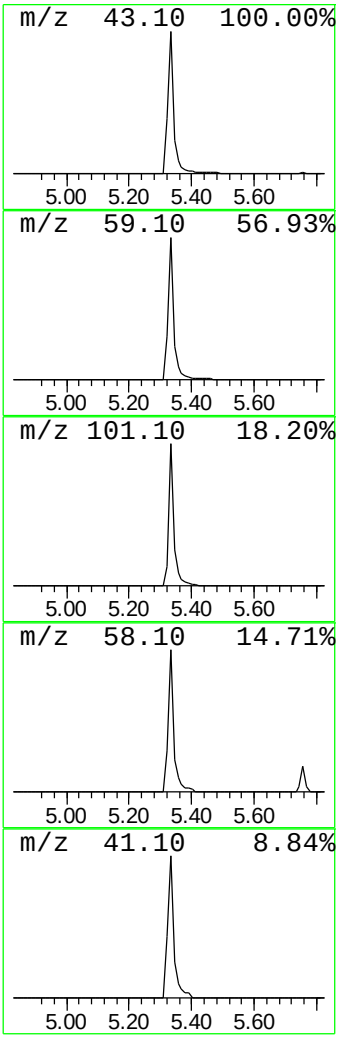
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.33 | 44.67 ng | 397346 | 1,4-Dichlorobenzene-d4 | 7.13 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 59 |
| 2 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 33 |
| 3 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23 |
| 4 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 16 |
| 5 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |



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Operator : TP/UM
Sample : G2973-14
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TP-9S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

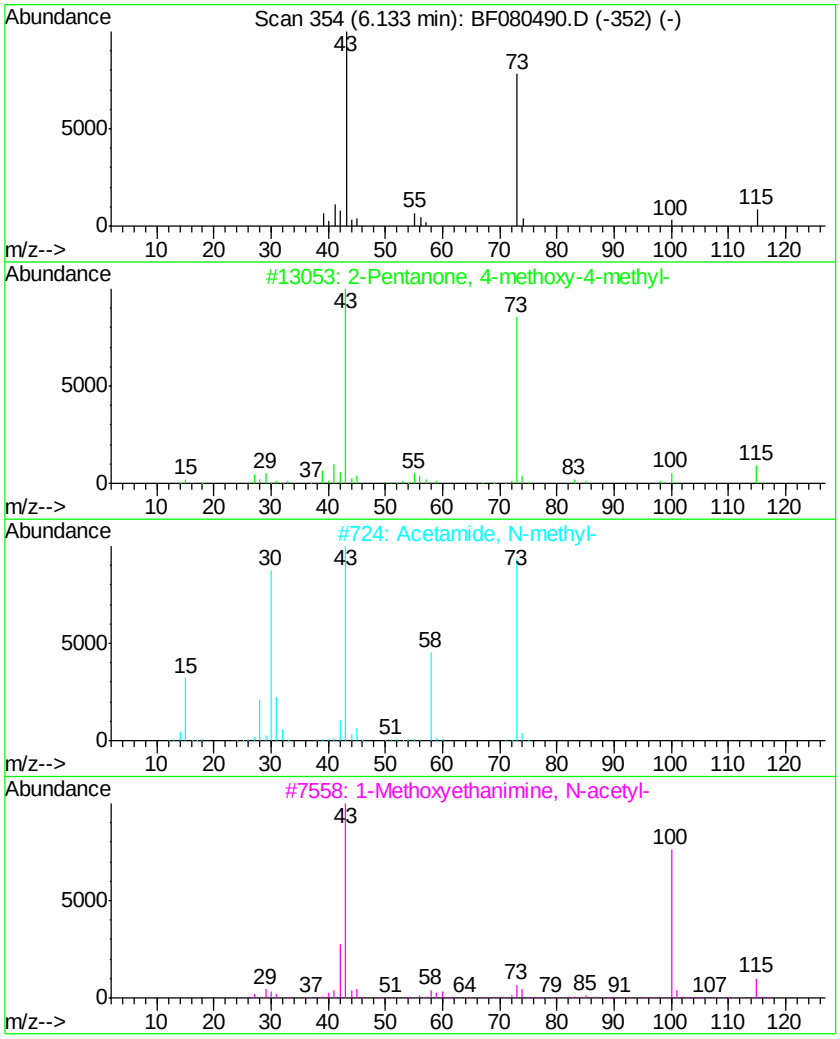
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

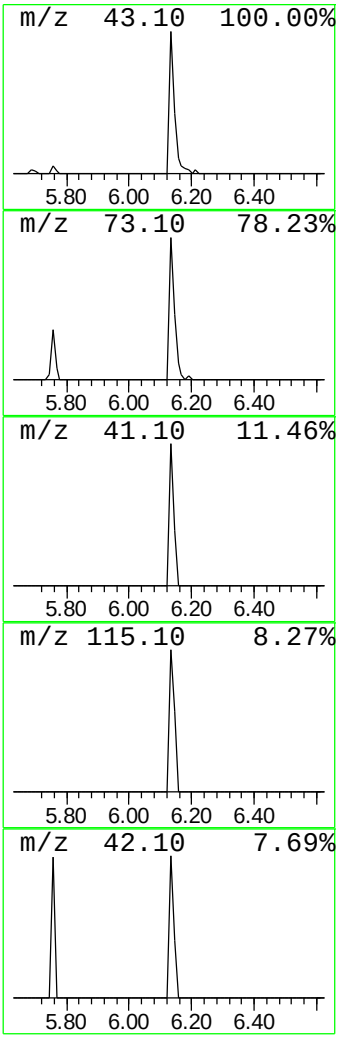
**********

Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.13 | 4.16 ng | 36989 | 1,4-Dichlorobenzene-d4 | 7.13 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-methoxy-4-methyl- | 130 | C7H14O2 | 000107-70-0 | 83 |
| 2 | Acetamide, N-methyl- | 73 | C3H7NO | 000079-16-3 | 9 |
| 3 | 1-Methoxyethanimine, N-acetyl- | 115 | C5H9NO2 | 099028-43-0 | 9 |
| 4 | Propane, 2-methoxy-2-methyl- | 88 | C5H12O | 001634-04-4 | 9 |
| 5 | 5-Aminovaleric acid | 117 | C5H11NO2 | 000660-88-8 | 9 |



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Sample : G2973-14
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TP-9S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

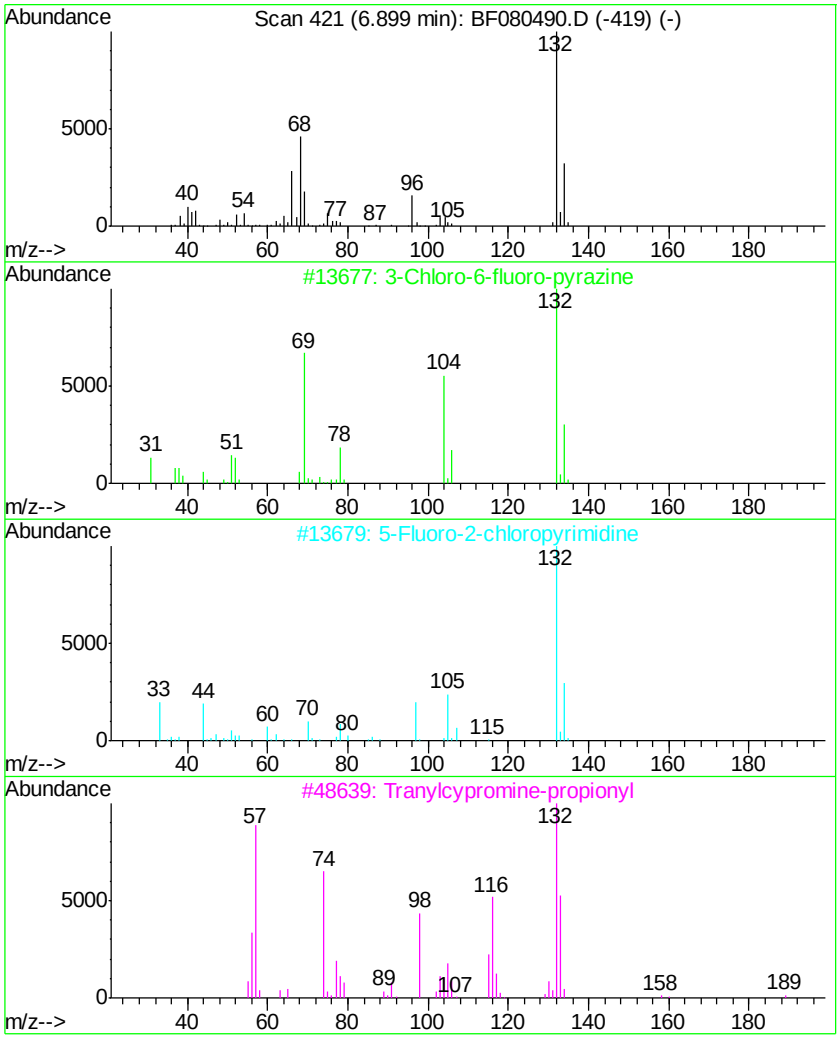
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

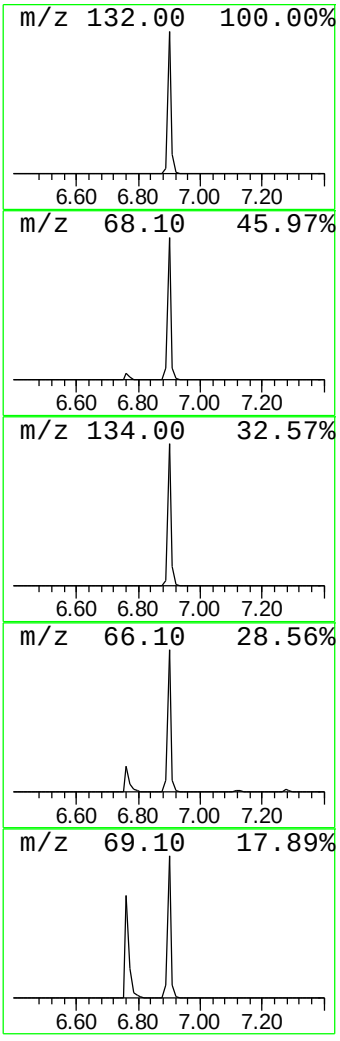
**********

Peak Number 5 unknown6.90 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.90 | 69.27 ng | 616152 | 1,4-Dichlorobenzene-d4 | 7.13 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 35 |
| 2 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 12 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 4 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |
| 5 | 4-Chloro-2-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-00-5 | 9 |



Tentatively Identified Compound (LSC) summary

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ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TP-9S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071415.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... | 2.28 | 21.1 | ng | 187896 | 1 | 7.13 | 177894 | 20.0 |
| 2-Pentanone, 4-hy... | 5.33 | 44.7 | ng | 397346 | 1 | 7.13 | 177894 | 20.0 |
| 2-Pentanone, 4-me... | 6.13 | 4.2 | ng | 36989 | 1 | 7.13 | 177894 | 20.0 |
| unknown6.90 | 6.90 | 69.3 | ng | 616152 | 1 | 7.13 | 177894 | 20.0 |