LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011320\
Data File : BG044021.D
Acq On : 13 Jan 2020 20:59
Operator : JU
Sample : PB126034BL
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** PB126034BL

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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.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 | 3.129 | 3 | 7 | 32 | rVB | 1693397 | 2994692 | 38.00% | 7.534% |
| 2 | 4.457 | 228 | 233 | 241 | rBV | 64810 | 97864 | 1.24% | 0.246% |
| 3 | 5.050 | 328 | 334 | 344 | rBV | 194174 | 317745 | 4.03% | 0.799% |
| 4 | 5.526 | 407 | 415 | 429 | rBV | 868892 | 1434584 | 18.20% | 3.609% |
| 5 | 7.112 | 674 | 685 | 701 | rBV | 550222 | 970401 | 12.31% | 2.441% |
| 6 | 7.482 | 740 | 748 | 759 | rBV | 1680180 | 2996731 | 38.02% | 7.540% |
| 7 | 7.947 | 819 | 827 | 835 | rBV | 405358 | 702040 | 8.91% | 1.766% |
| 8 | 8.270 | 874 | 882 | 892 | rBV | 1583465 | 2771944 | 35.17% | 6.974% |
| 9 | 9.104 | 1015 | 1024 | 1035 | rBV | 1218501 | 2275458 | 28.87% | 5.725% |
| 10 | 10.749 | 1295 | 1304 | 1314 | rBV | 517225 | 953885 | 12.10% | 2.400% |
| 11 | 13.205 | 1713 | 1722 | 1735 | rBV | 3095607 | 5006615 | 63.52% | 12.596% |
| 12 | 14.580 | 1947 | 1956 | 1965 | rBV | 855744 | 1368228 | 17.36% | 3.442% |
| 13 | 16.067 | 2201 | 2209 | 2224 | rBV | 2670796 | 4262945 | 54.09% | 10.725% |
| 14 | 17.318 | 2415 | 2422 | 2434 | rBV | 1115467 | 1671872 | 21.21% | 4.206% |
| 15 | 19.938 | 2861 | 2868 | 2878 | rBV | 5644724 | 7881653 | 100.00% | 19.830% |
| 16 | 21.566 | 3138 | 3145 | 3156 | rBV | 1107722 | 1895686 | 24.05% | 4.769% |
| 17 | 24.680 | 3665 | 3675 | 3685 | rBV2 | 666474 | 1867490 | 23.69% | 4.698% |
| 18 | 25.561 | 3817 | 3825 | 3834 | rVB5 | 38526 | 112870 | 1.43% | 0.284% |
| 19 | 27.148 | 4089 | 4095 | 4106 | rVB7 | 46996 | 164071 | 2.08% | 0.413% |

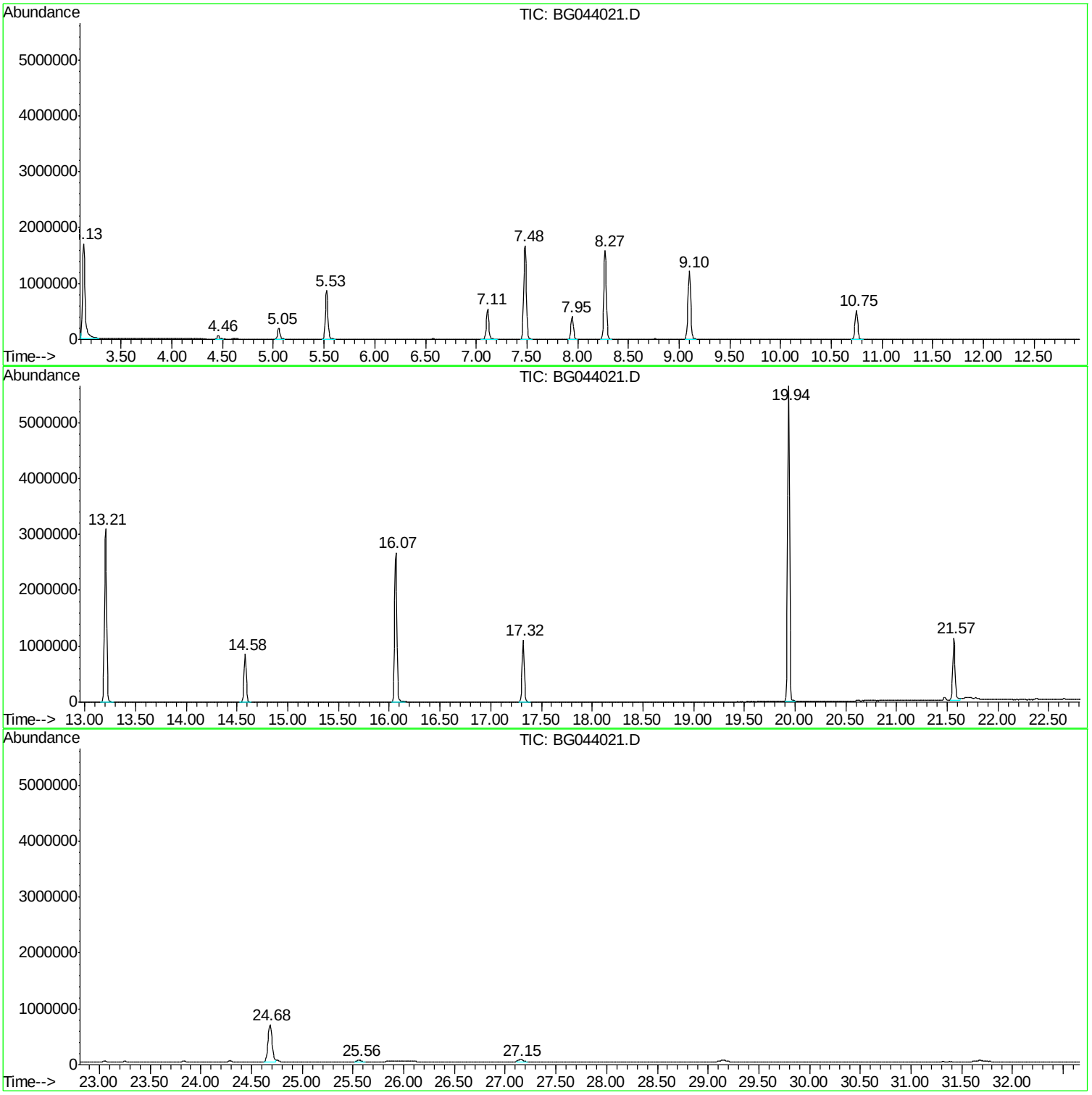
Sum of corrected areas: 39746774

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011320\
Data File : BG044021.D
Acq On : 13 Jan 2020 20:59
Operator : JU
Sample : PB126034BL
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :**
BNA_G
**ClientSampleId :**
PB126034BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011320\
Data File : BG044021.D
Acq On : 13 Jan 2020 20:59
Operator : JU
Sample : PB126034BL
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** PB126034BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

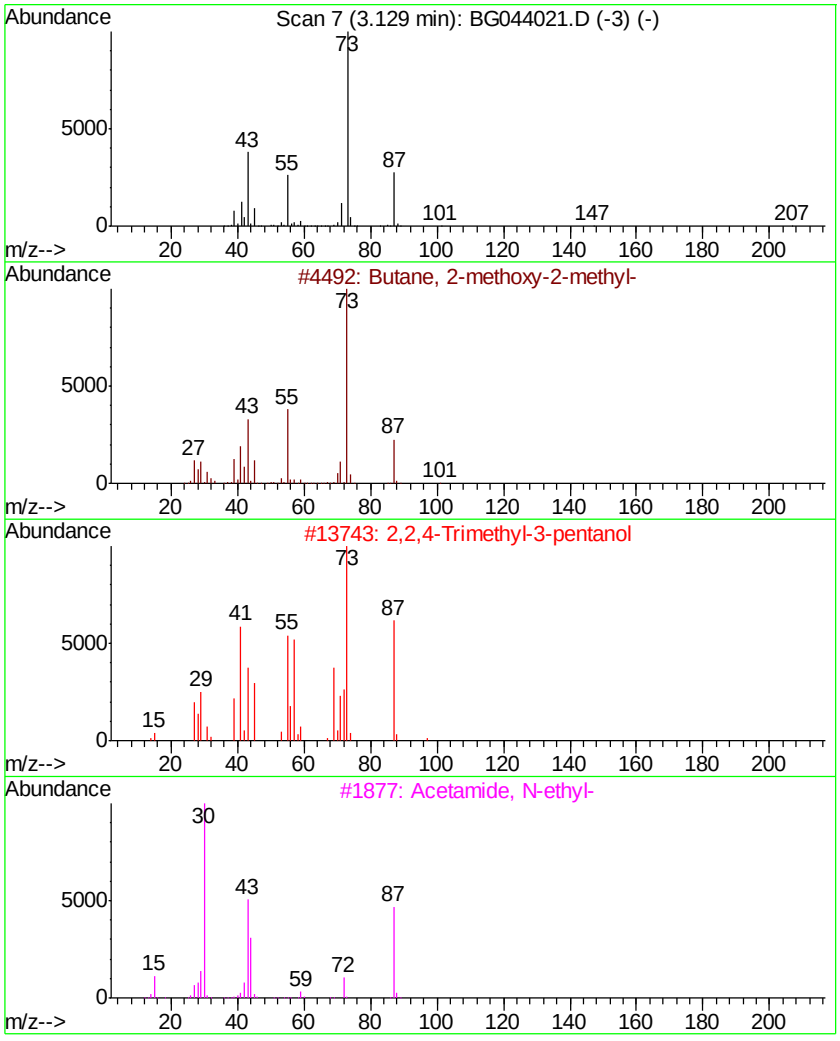
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

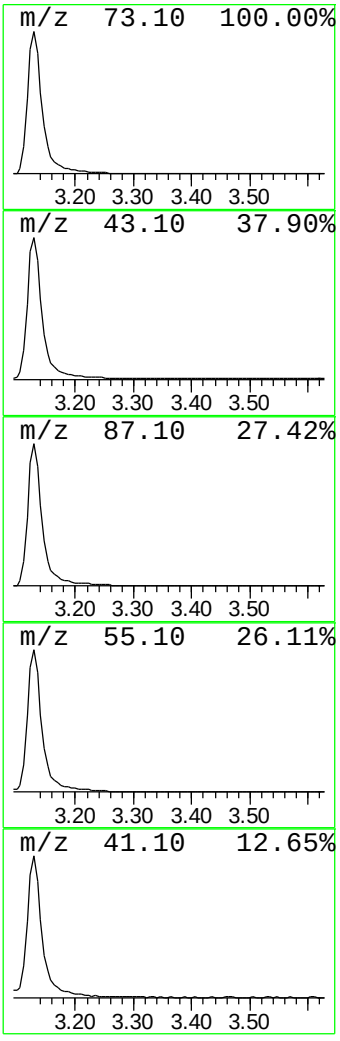
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.13 | 85.31 ng | 2994690 | 1,4-Dichlorobenzene-d4 | 7.95 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 83 |
| 2 | 2,2,4-Trimethyl-3-pentanol | 130 | C8H18O | 005162-48-1 | 40 |
| 3 | Acetamide, N-ethyl- | 87 | C4H9NO | 000625-50-3 | 27 |
| 4 | 1,3-Dioxolane, 2-methyl- | 88 | C4H8O2 | 000497-26-7 | 25 |
| 5 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 17 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011320\
Data File : BG044021.D
Acq On : 13 Jan 2020 20:59
Operator : JU
Sample : PB126034BL
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** PB126034BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

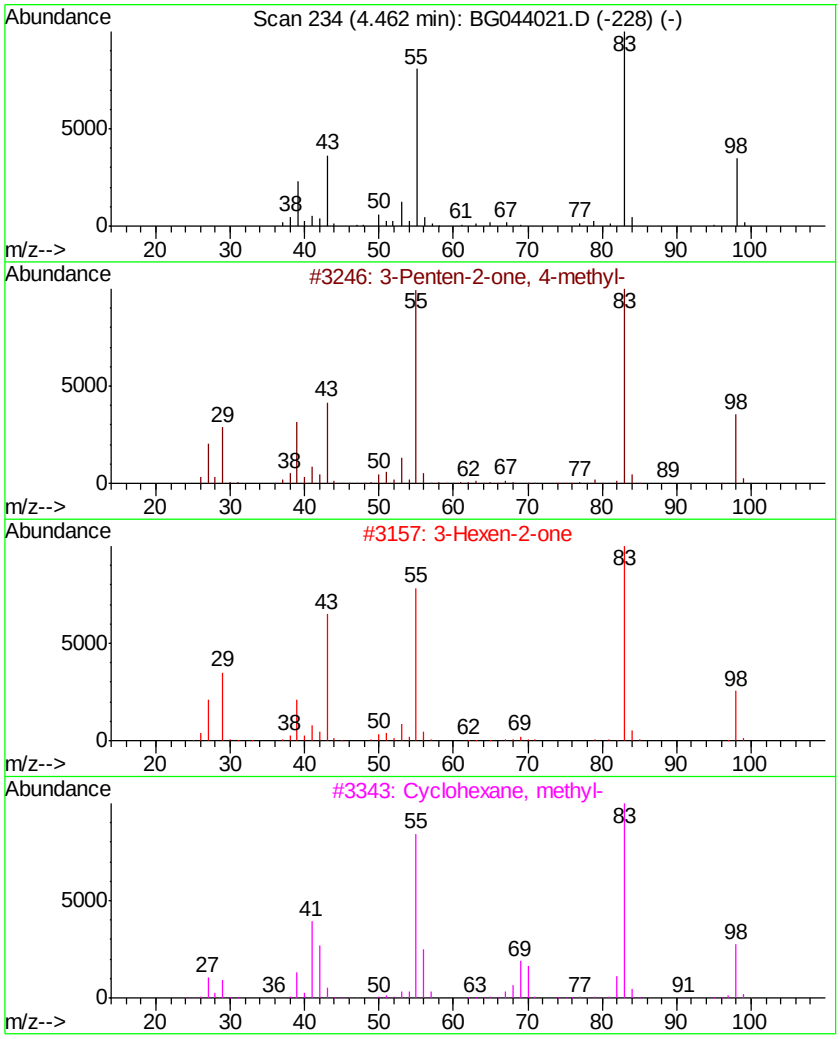
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

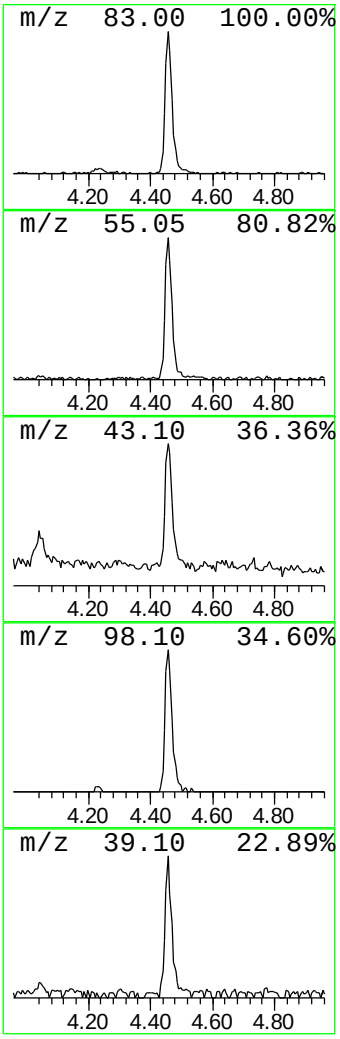
**********

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.46 | 2.79 ng | 97864 | 1,4-Dichlorobenzene-d4 | 7.95 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Penten-2-one, 4-methyl- | 98 | C6H10O | 000141-79-7 | 91 |
| 2 | 3-Hexen-2-one | 98 | C6H10O | 000763-93-9 | 86 |
| 3 | Cyclohexane, methyl- | 98 | C7H14 | 000108-87-2 | 80 |
| 4 | 2,4-Azetidinedione, 3,3-diethyl- | 141 | C7H11NO2 | 042282-85-9 | 78 |
| 5 | 2-Pentene, 3,4-dimethyl-, (E)- | 98 | C7H14 | 004914-92-5 | 72 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011320\
Data File : BG044021.D
Acq On : 13 Jan 2020 20:59
Operator : JU
Sample : PB126034BL
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** PB126034BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

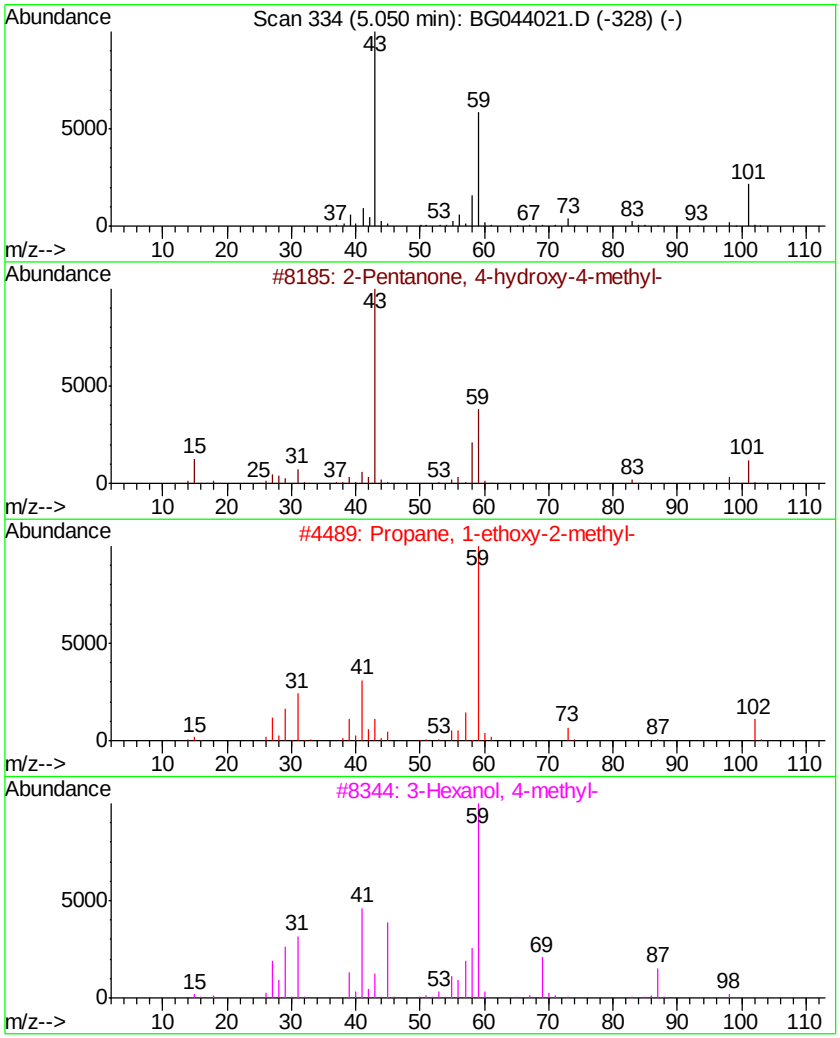
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

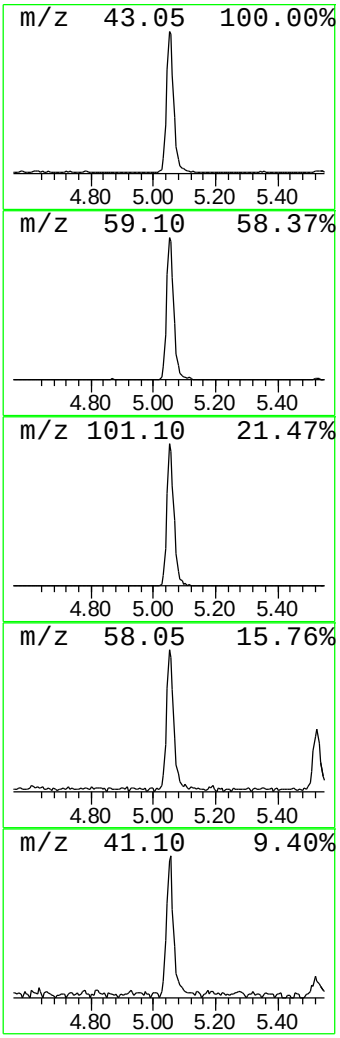
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.05 | 9.05 ng | 317745 | 1,4-Dichlorobenzene-d4 | 7.95 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 50 |
| 2 | Propane, 1-ethoxy-2-methyl- | 102 | C6H14O | 000627-02-1 | 35 |
| 3 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 25 |
| 4 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25 |
| 5 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 25 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011320\
Data File : BG044021.D
Acq On : 13 Jan 2020 20:59
Operator : JU
Sample : PB126034BL
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** PB126034BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

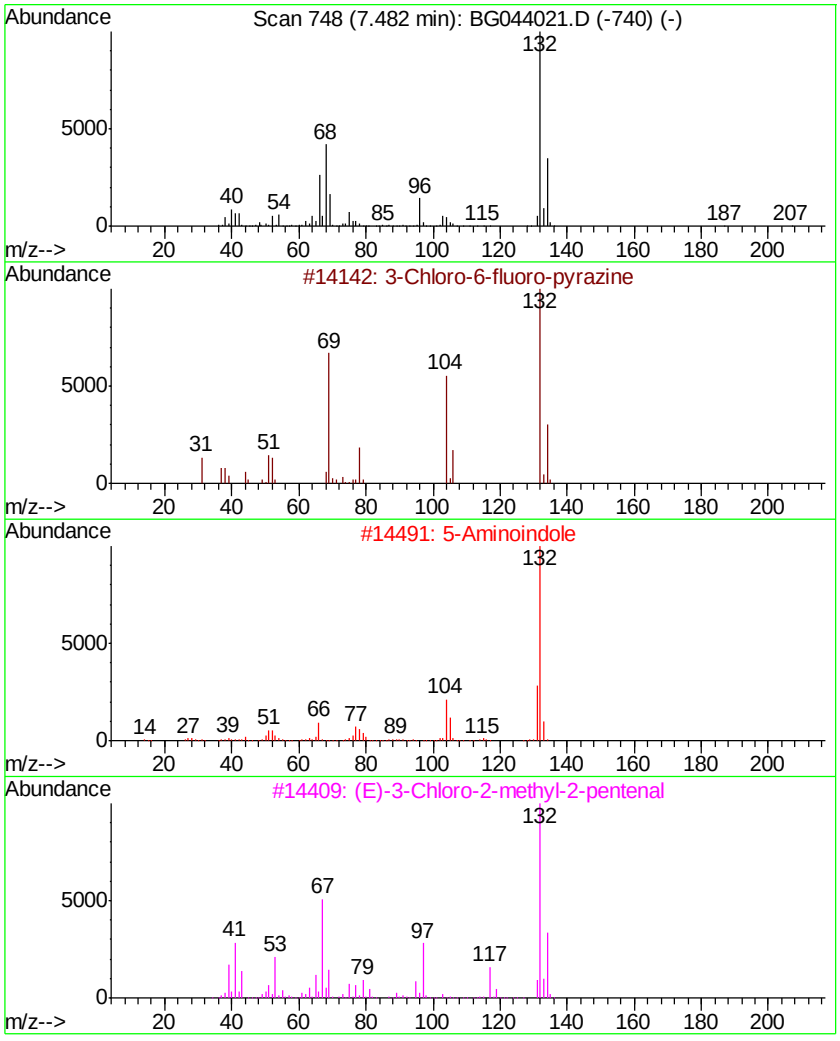
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

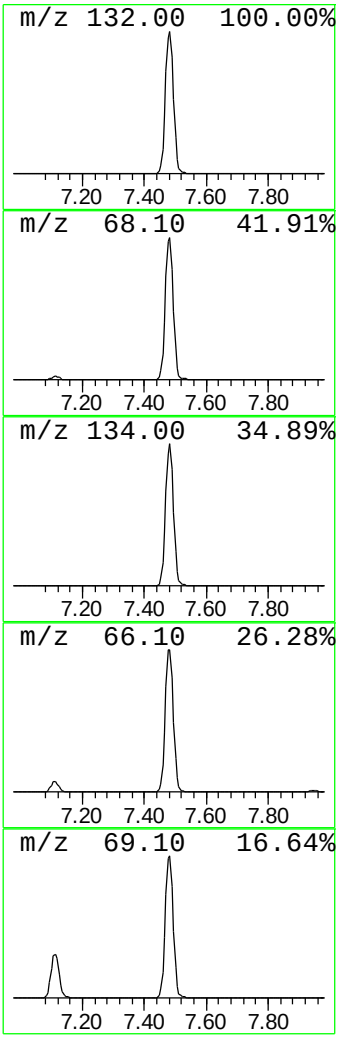
**********

Peak Number 4 unknown7.48 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.48 | 85.37 ng | 2996730 | 1,4-Dichlorobenzene-d4 | 7.95 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 22 |
| 3 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 16 |
| 4 | 1-Isoquinolinemethanol, .alpha.-... | 191 | C12H17NO | 114608-92-3 | 12 |
| 5 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 12 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG011320\
Data File : BG044021.D
Acq On : 13 Jan 2020 20:59
Operator : JU
Sample : PB126034BL
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** PB126034BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| Butane, 2-methoxy... | 3.13 | 85.3 | ng | 2994690 | 1 | 7.95 | 702040 | 20.0 |
| 3-Penten-2-one, 4... | 4.46 | 2.8 | ng | 97864 | 1 | 7.95 | 702040 | 20.0 |
| 2-Pentanone, 4-hy... | 5.05 | 9.1 | ng | 317745 | 1 | 7.95 | 702040 | 20.0 |
| unknown7.48 | 7.48 | 85.4 | ng | 2996730 | 1 | 7.95 | 702040 | 20.0 |