LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071315\
Data File : BF080442.D
Acq On : 13 Jul 2015 22:58
Operator : TP/UM
Sample : G2945-14
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TE-PMW-40

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-BF071015.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 | 2.155 | 4 | 6 | 14 | rBV | 76183 | 118562 | 13.40% | 2.236% |
| 2 | 2.281 | 14 | 17 | 26 | rVB | 303052 | 476101 | 53.79% | 8.979% |
| 3 | 2.693 | 50 | 53 | 55 | rBV | 7734 | 10527 | 1.19% | 0.199% |
| 4 | 5.356 | 283 | 286 | 296 | rBB | 50523 | 70455 | 7.96% | 1.329% |
| 5 | 5.767 | 320 | 322 | 331 | rBB | 208713 | 206929 | 23.38% | 3.903% |
| 6 | 6.156 | 354 | 356 | 359 | rBB | 13239 | 19379 | 2.19% | 0.365% |
| 7 | 6.773 | 409 | 410 | 420 | rBB | 74256 | 116505 | 13.16% | 2.197% |
| 8 | 6.910 | 420 | 422 | 424 | rBV | 533682 | 431165 | 48.71% | 8.132% |
| 9 | 7.127 | 440 | 441 | 444 | rBB | 99169 | 111701 | 12.62% | 2.107% |
| 10 | 7.287 | 453 | 455 | 458 | rBB | 391963 | 389136 | 43.96% | 7.339% |
| 11 | 7.699 | 489 | 491 | 493 | rBV | 403555 | 324979 | 36.72% | 6.129% |
| 12 | 8.419 | 552 | 554 | 557 | rBV | 195975 | 157857 | 17.83% | 2.977% |
| 13 | 9.493 | 645 | 648 | 650 | rBV | 881507 | 704592 | 79.61% | 13.289% |
| 14 | 10.179 | 706 | 708 | 710 | rVB | 222097 | 179156 | 20.24% | 3.379% |
| 15 | 10.968 | 775 | 777 | 780 | rBV | 468921 | 387483 | 43.78% | 7.308% |
| 16 | 11.665 | 836 | 838 | 841 | rBV | 173155 | 187943 | 21.23% | 3.545% |
| 17 | 12.248 | 887 | 889 | 891 | rBB | 17165 | 20238 | 2.29% | 0.382% |
| 18 | 13.288 | 978 | 980 | 982 | rBV | 994836 | 885108 | 100.00% | 16.693% |
| 19 | 14.419 | 1077 | 1079 | 1081 | rBV2 | 10356 | 11607 | 1.31% | 0.219% |
| 20 | 14.465 | 1081 | 1083 | 1086 | rBV | 225151 | 232490 | 26.27% | 4.385% |
| 21 | 16.168 | 1229 | 1232 | 1236 | rBV | 194345 | 260240 | 29.40% | 4.908% |

Sum of corrected areas: 5302153

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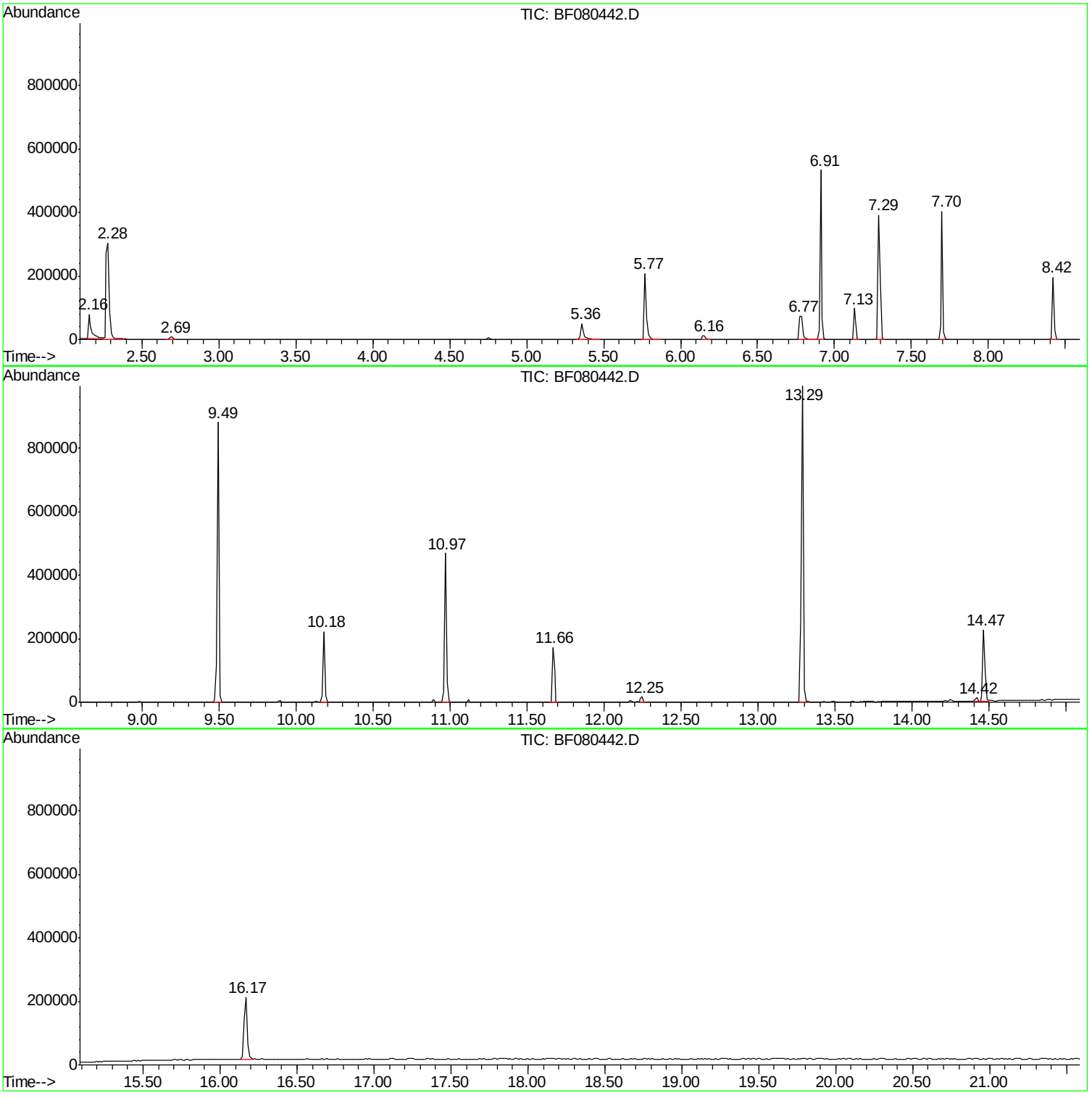
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TE-PMW-40

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071015.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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**Instrument :** BNA_F
**ClientSampleId :** TE-PMW-40

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

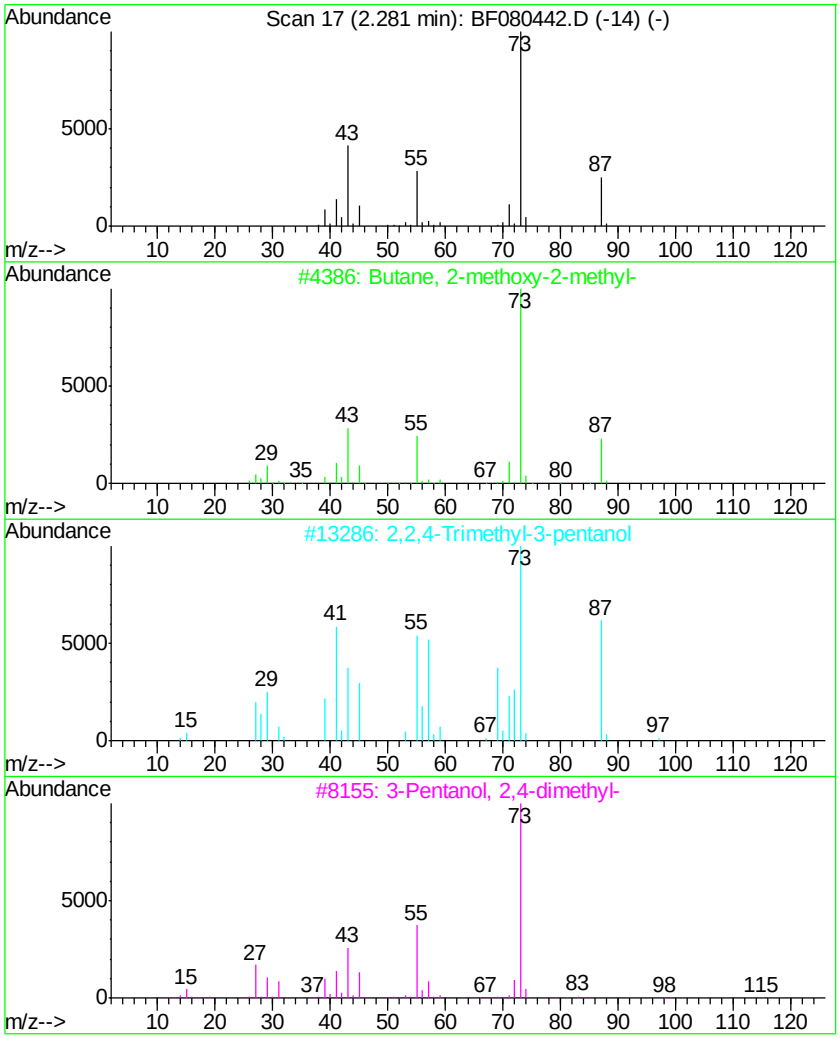
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

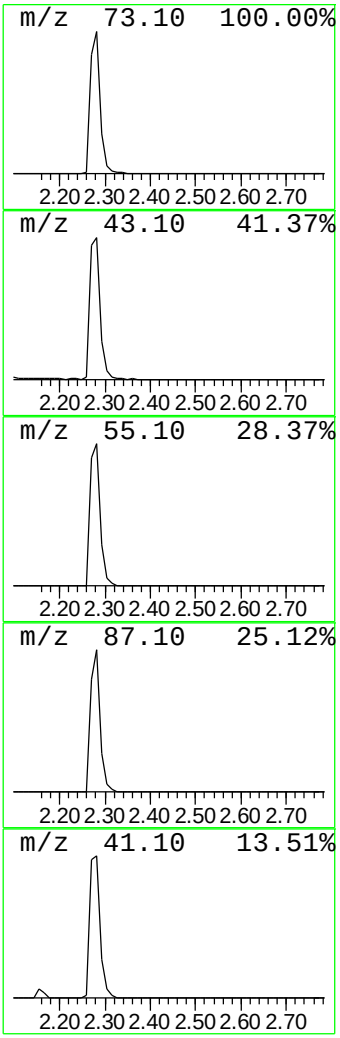
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.28 | 85.25 ng | 476101 | 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 | 2,2,4-Trimethyl-3-pentanol | 130 | C8H18O | 005162-48-1 | 39 |
| 3 | 3-Pentanol, 2,4-dimethyl- | 116 | C7H16O | 000600-36-2 | 37 |
| 4 | 1,3-Dioxolane, 2-methyl- | 88 | C4H8O2 | 000497-26-7 | 25 |
| 5 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 12 |



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Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TE-PMW-40

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071015.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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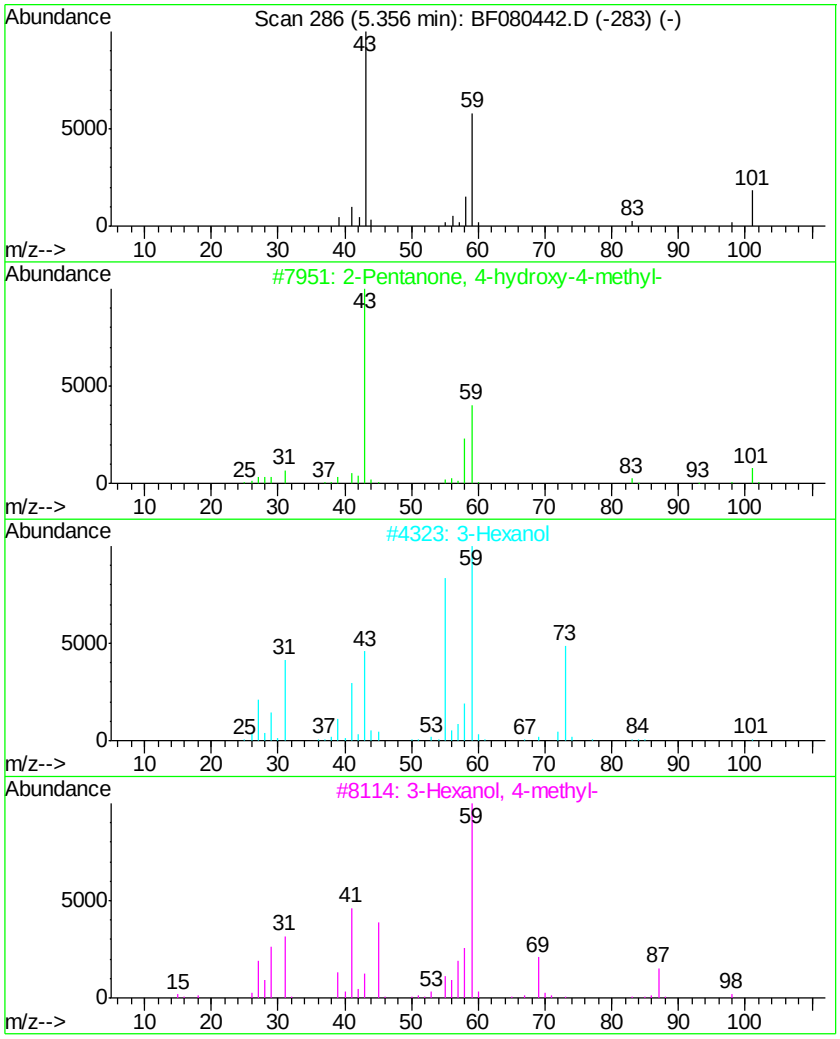
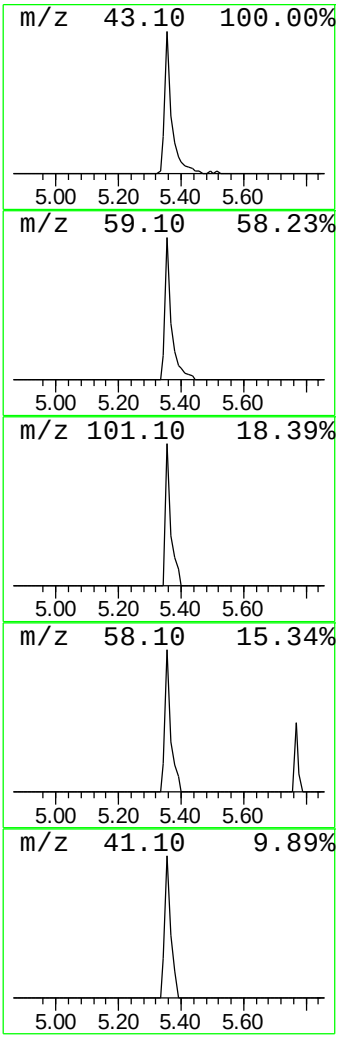
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.36 | 12.61 ng | 70455 | 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 | 50 |
| 2 | 3-Hexanol | 102 | C6H14O | 000623-37-0 | 36 |
| 3 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 33 |
| 4 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |
| 5 | 1-Propen-2-ol, acetate | 100 | C5H8O2 | 000108-22-5 | 9 |



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Data File : BF080442.D
Acq On : 13 Jul 2015 22:58
Operator : TP/UM
Sample : G2945-14
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TE-PMW-40

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071015.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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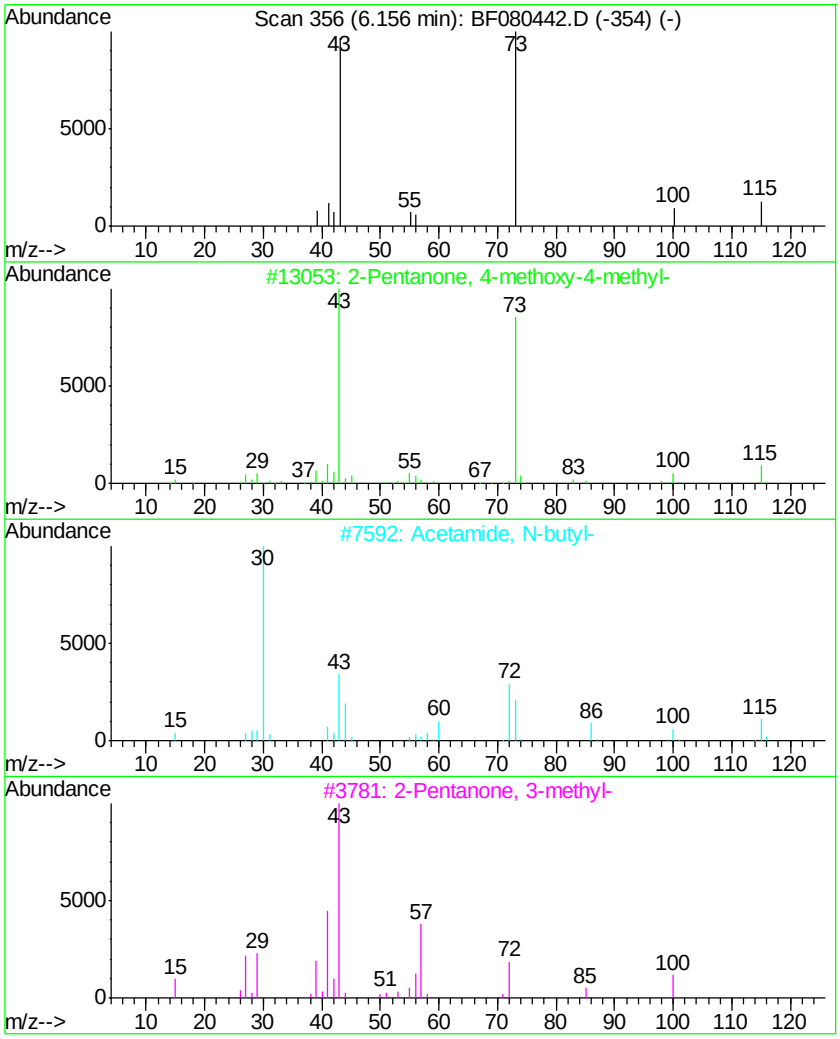
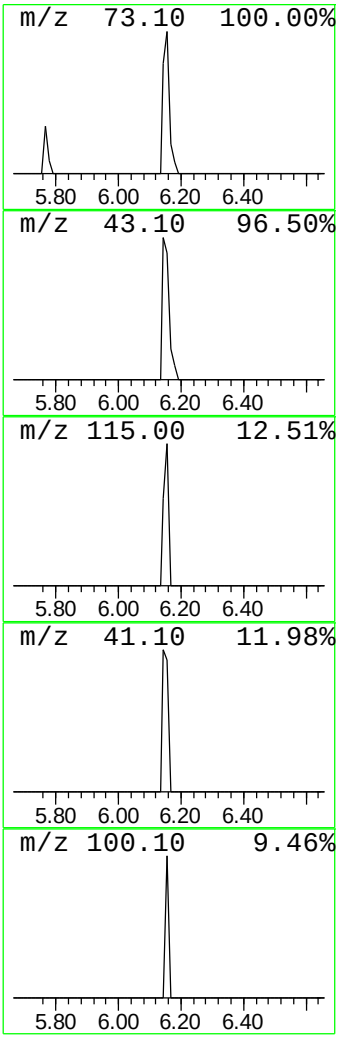
Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.16 | 3.47 ng | 19379 | 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 | 74 |
| 2 | Acetamide, N-butyl- | 115 | C6H13NO | 001119-49-9 | 5 |
| 3 | 2-Pentanone, 3-methyl- | 100 | C6H12O | 000565-61-7 | 5 |
| 4 | 2,3-Pentanedione | 100 | C5H8O2 | 000600-14-6 | 5 |
| 5 | Acetamide, N-(2-methylpropyl)- | 115 | C6H13NO | 001540-94-9 | 4 |



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Operator : TP/UM
Sample : G2945-14
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TE-PMW-40

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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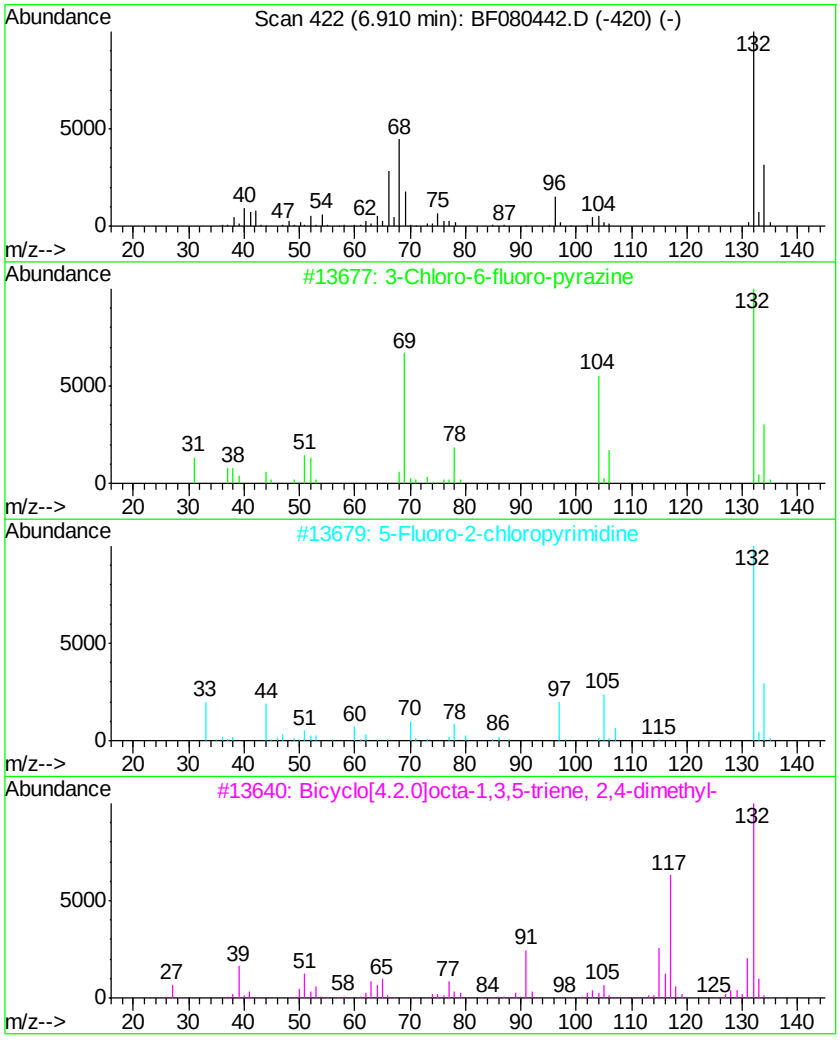
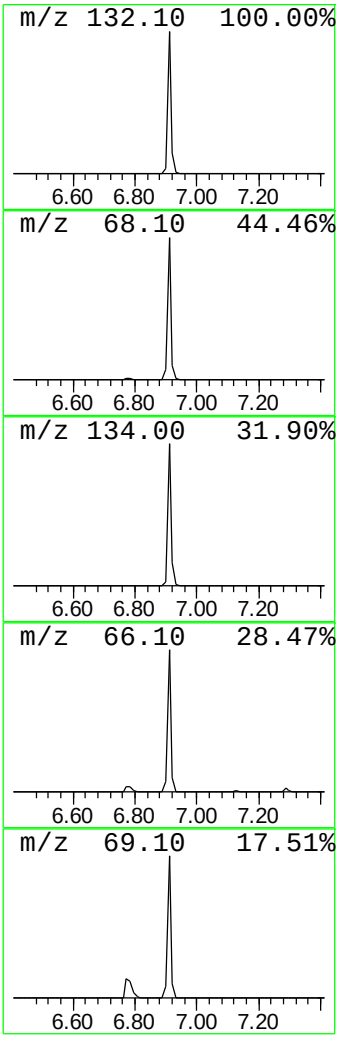
**********

Peak Number 5 unknown6.91 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.91 | 77.20 ng | 431165 | 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 | 27 |
| 2 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 16 |
| 3 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |
| 4 | Benzene, 1-ethenyl-3,5-dimethyl- | 132 | C10H12 | 005379-20-4 | 9 |
| 5 | 1-Methylpyrrolo[1,2-a]pyrazine | 132 | C8H8N2 | 064608-59-9 | 9 |



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Misc :
ALS Vial : 17 Sample Multiplier: 1

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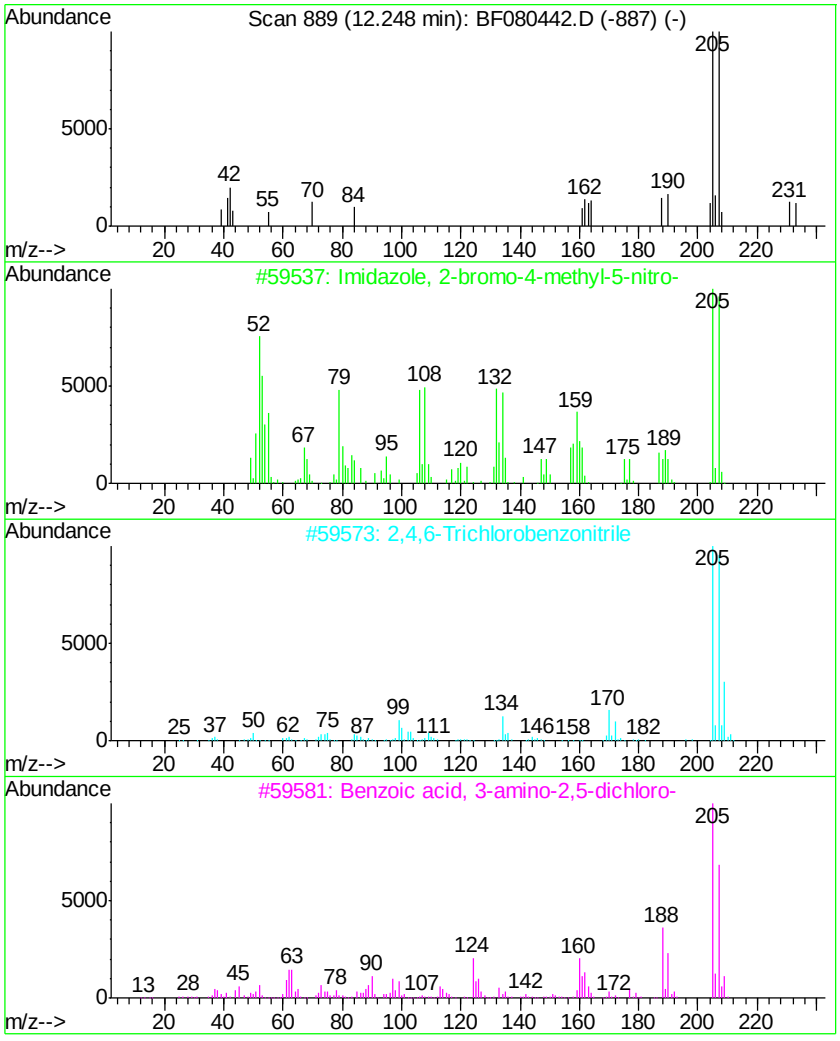
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

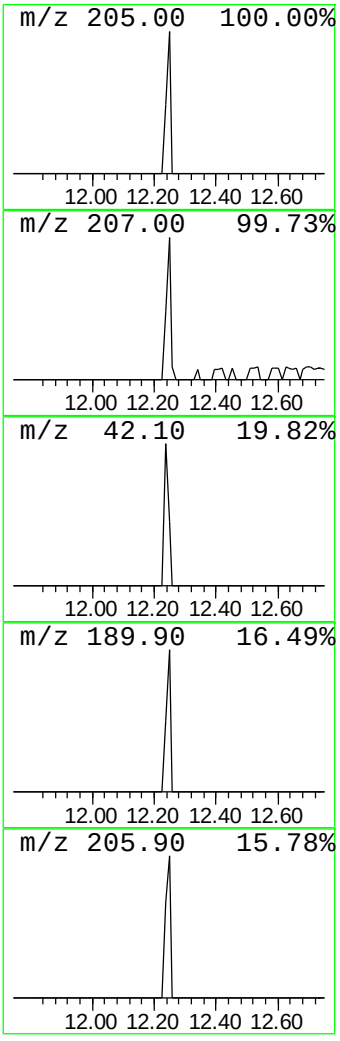
**********

Peak Number 7 Imidazole, 2-bromo-4-methyl... Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.25 | 2.15 ng | 20238 | Phenanthrene-d10 | 11.66 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Imidazole, 2-bromo-4-methyl-5-ni... | 205 | C4H4BrN3O2 | 105983-46-8 | 72 |
| 2 | 2,4,6-Trichlorobenzonitrile | 205 | C7H2Cl3N | 006575-05-9 | 59 |
| 3 | Benzoic acid, 3-amino-2,5-dichloro- | 205 | C7H5Cl2NO2 | 000133-90-4 | 47 |
| 4 | Thiazolo[5,4-d]pyrimidine, 5,7-d... | 205 | C5HCl2N3S | 013479-88-4 | 45 |
| 5 | Thiazolo[5,4-d]pyrimidine, 2,5-d... | 205 | C5HCl2N3S | 013479-89-5 | 45 |



# Tentatively Identified Compound (LSC) summary

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Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| Butane, 2-methoxy... | 2.28 | 85.3 | ng | 476101 | 1 | 7.13 | 111701 | 20.0 |
| 2-Pentanone, 4-hy... | 5.36 | 12.6 | ng | 70455 | 1 | 7.13 | 111701 | 20.0 |
| 2-Pentanone, 4-me... | 6.16 | 3.5 | ng | 19379 | 1 | 7.13 | 111701 | 20.0 |
| unknown6.91 | 6.91 | 77.2 | ng | 431165 | 1 | 7.13 | 111701 | 20.0 |
| Imidazole, 2-brom... | 12.25 | 2.1 | ng | 20238 | 4 | 11.66 | 187943 | 20.0 |