LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011316\
Data File : BF084471.D
Acq On : 14 Jan 2016 5:57
Operator : SJ/UM
Sample : H1113-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-4

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-BF123115.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 | 4.350 | 196 | 198 | 202 | rBV | 66748 | 84075 | 1.02% | 0.139% |
| 2 | 5.001 | 253 | 255 | 262 | rVB | 1002362 | 1331021 | 16.16% | 2.205% |
| 3 | 5.436 | 290 | 293 | 295 | rBV | 4445469 | 4028947 | 48.90% | 6.673% |
| 4 | 5.836 | 326 | 328 | 330 | rBV | 154028 | 134493 | 1.63% | 0.223% |
| 5 | 6.464 | 381 | 383 | 386 | rBV | 2639066 | 2412780 | 29.29% | 3.996% |
| 6 | 6.602 | 392 | 395 | 397 | rBV | 6631937 | 6377038 | 77.41% | 10.562% |
| 7 | 6.830 | 413 | 415 | 417 | rBV | 1980124 | 1626423 | 19.74% | 2.694% |
| 8 | 6.990 | 426 | 429 | 431 | rBV | 5993487 | 5801462 | 70.42% | 9.609% |
| 9 | 7.402 | 461 | 465 | 467 | rBV | 4615553 | 5489097 | 66.63% | 9.092% |
| 10 | 7.859 | 502 | 505 | 507 | rBV | 82759 | 90622 | 1.10% | 0.150% |
| 11 | 8.122 | 525 | 528 | 530 | rBV | 1559412 | 2104096 | 25.54% | 3.485% |
| 12 | 8.933 | 596 | 599 | 601 | rBV | 107115 | 157292 | 1.91% | 0.261% |
| 13 | 9.196 | 619 | 622 | 624 | rBV | 8152730 | 7940731 | 96.39% | 13.152% |
| 14 | 9.459 | 642 | 645 | 648 | rBV | 98072 | 135725 | 1.65% | 0.225% |
| 15 | 9.528 | 648 | 651 | 652 | rBV | 189624 | 180286 | 2.19% | 0.299% |
| 16 | 9.550 | 652 | 653 | 655 | rVB2 | 76834 | 91752 | 1.11% | 0.152% |
| 17 | 9.642 | 660 | 661 | 664 | rVB | 70886 | 100276 | 1.22% | 0.166% |
| 18 | 9.802 | 673 | 675 | 678 | rBV | 75735 | 83349 | 1.01% | 0.138% |
| 19 | 9.870 | 678 | 681 | 683 | rBV | 2696359 | 2401111 | 29.15% | 3.977% |
| 20 | 10.305 | 713 | 719 | 721 | rBV3 | 119599 | 153668 | 1.87% | 0.255% |
| 21 | 10.659 | 747 | 750 | 753 | rBV | 4860391 | 5216472 | 63.32% | 8.640% |
| 22 | 10.773 | 759 | 760 | 765 | rVB | 64113 | 101537 | 1.23% | 0.168% |
| 23 | 11.356 | 808 | 811 | 813 | rBV | 2122448 | 2372972 | 28.80% | 3.930% |
| 24 | 12.945 | 947 | 950 | 952 | rBV | 7916037 | 8238478 | 100.00% | 13.646% |
| 25 | 13.985 | 1039 | 1041 | 1044 | rBV | 2288934 | 2177353 | 26.43% | 3.606% |
| 26 | 15.402 | 1162 | 1165 | 1168 | rBV | 1213386 | 1543864 | 18.74% | 2.557% |

Sum of corrected areas: 60374920

LSC Report - Integrated Chromatogram

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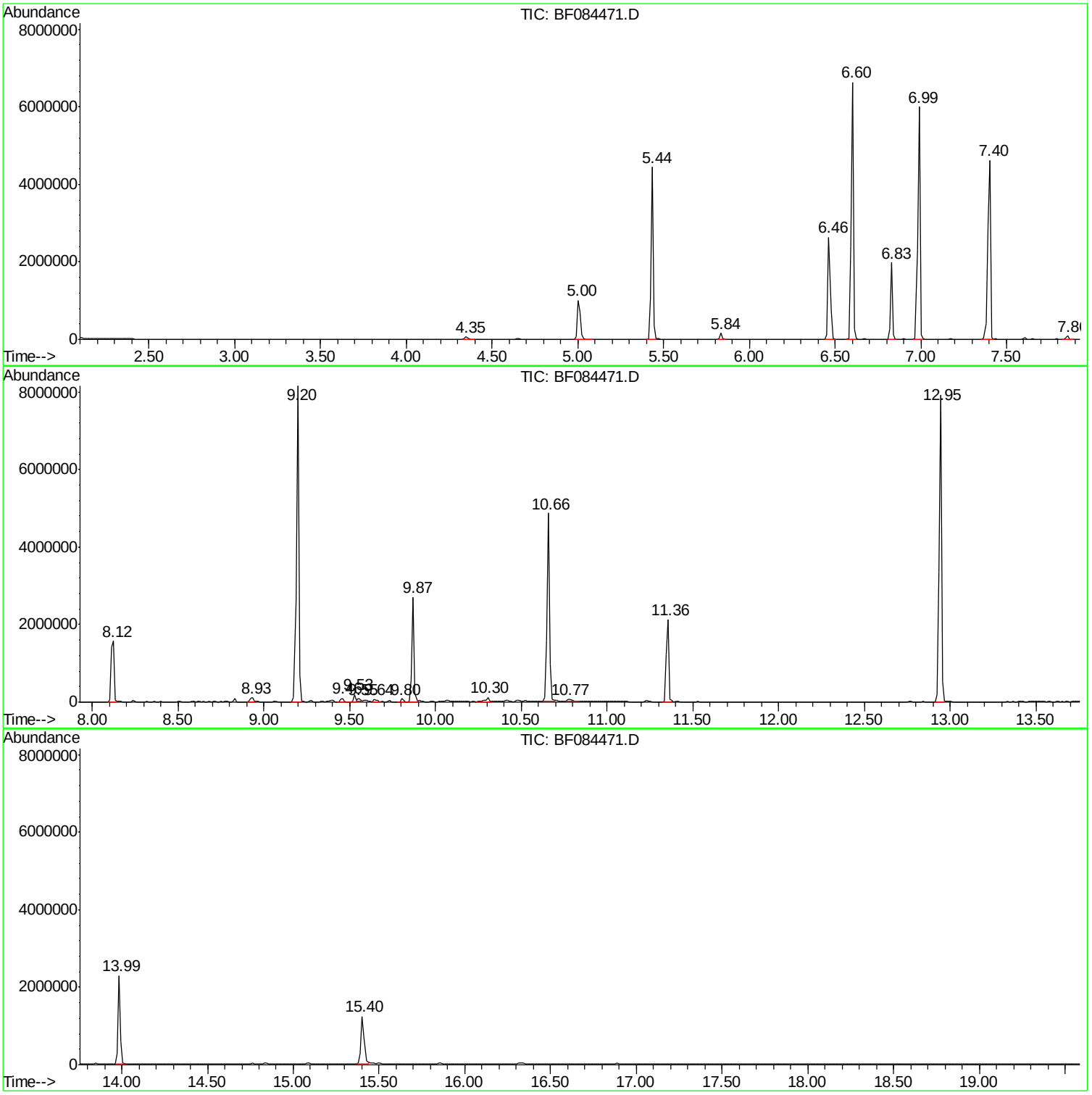
**Instrument :** BNA_F
**ClientSampleId :** MW-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.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
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.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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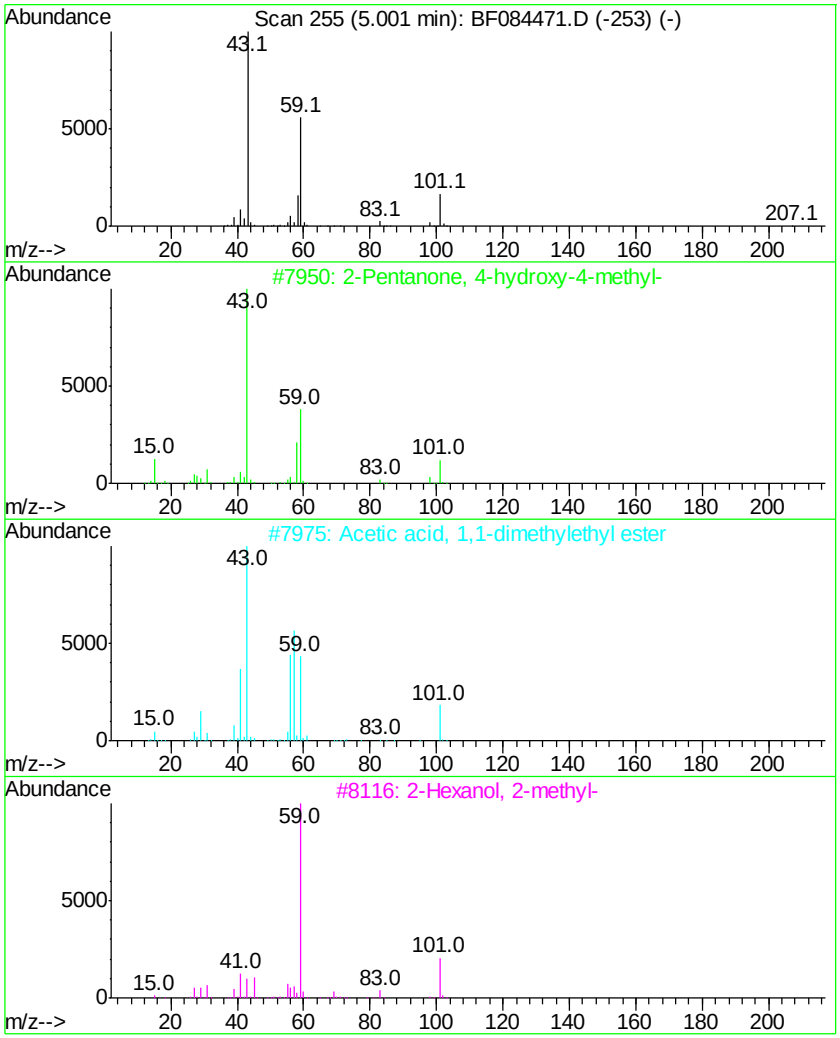
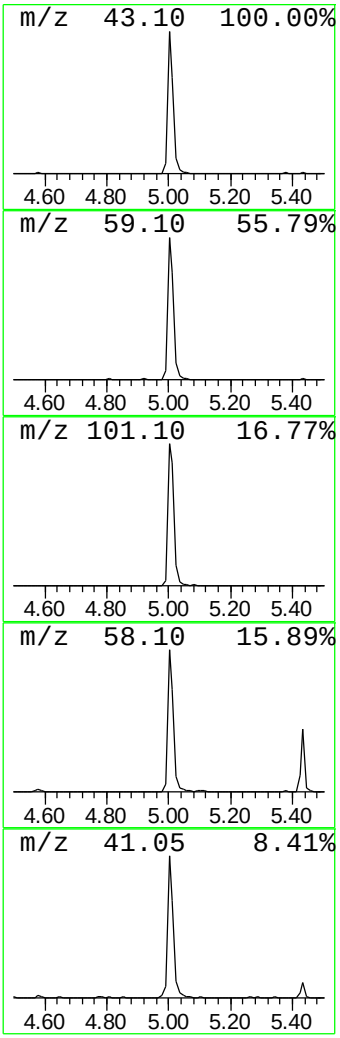
Peak Number 1 unknown5.00 Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.00 | 16.37 ng | 1331020 | 1,4-Dichlorobenzene-d4 | 6.83 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 45 |
| 2 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 39 |
| 3 | 2-Hexanol, 2-methyl- | 116 | C7H16O | 000625-23-0 | 33 |
| 4 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 33 |
| 5 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25 |



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011316\
Data File : BF084471.D
Acq On : 14 Jan 2016 5:57
Operator : SJ/UM
Sample : H1113-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.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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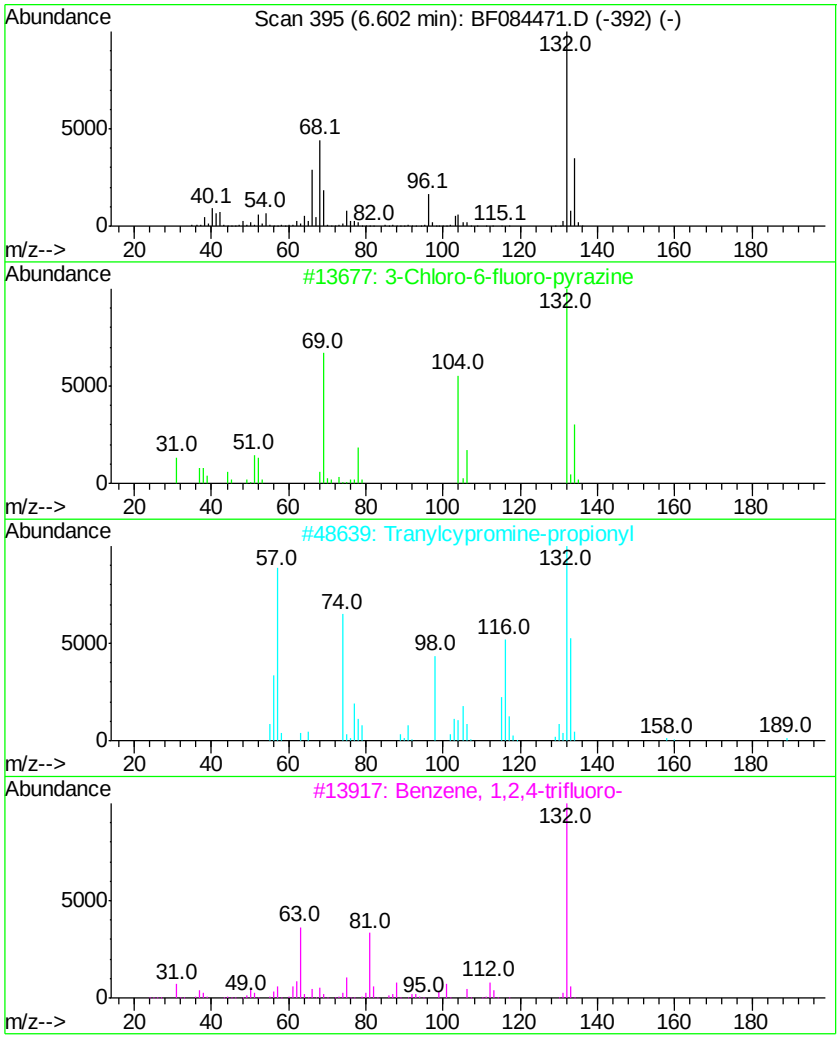
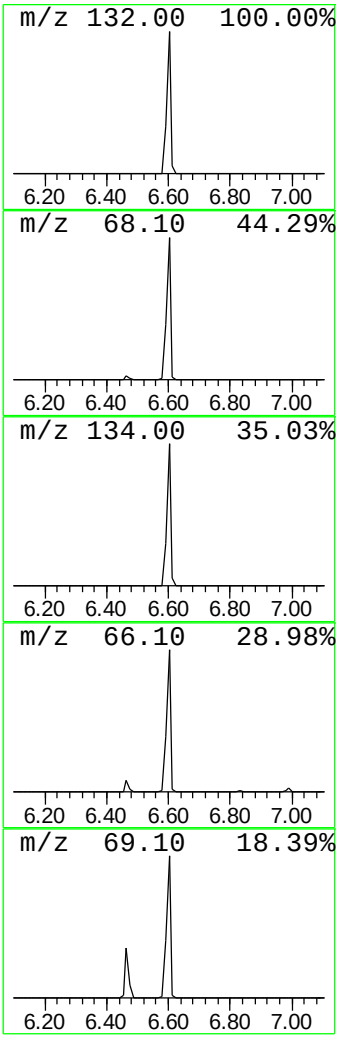
Peak Number 2 unknown6.60 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.60 | 78.42 ng | 6377040 | 1,4-Dichlorobenzene-d4 | 6.83 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 3 | Benzene, 1,2,4-trifluoro- | 132 | C6H3F3 | 000367-23-7 | 9 |
| 4 | Benzene, 1,3,5-trifluoro- | 132 | C6H3F3 | 000372-38-3 | 9 |
| 5 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |



Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| unknown5.00 | 5.00 | 16.4 | ng | 1331020 | 1 | 6.83 | 1626420 | 20.0 |
| unknown6.60 | 6.60 | 78.4 | ng | 6377040 | 1 | 6.83 | 1626420 | 20.0 |