LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062918\
Data File : BF106995.D
Acq On : 30 Jun 2018 1:32
Operator : JU/SJ
Sample : J3718-04
Misc :
ALS Vial : 33 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** W-27

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_F\METHODS\8270-BF061918.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 | 5.184 | 481 | 484 | 493 | rBV | 76968 | 85337 | 4.21% | 0.627% |
| 2 | 5.590 | 550 | 553 | 565 | rBV | 839771 | 818361 | 40.35% | 6.009% |
| 3 | 6.066 | 629 | 634 | 642 | rBV | 16154 | 24622 | 1.21% | 0.181% |
| 4 | 6.595 | 720 | 724 | 735 | rBV | 561132 | 541854 | 26.71% | 3.979% |
| 5 | 6.731 | 743 | 747 | 750 | rBV | 1562252 | 1405316 | 69.29% | 10.319% |
| 6 | 6.948 | 781 | 784 | 790 | rBV | 451858 | 401072 | 19.77% | 2.945% |
| 7 | 7.107 | 807 | 811 | 815 | rBV | 1563070 | 1431359 | 70.57% | 10.510% |
| 8 | 7.519 | 876 | 881 | 884 | rBV | 1157107 | 1136347 | 56.03% | 8.344% |
| 9 | 8.236 | 999 | 1003 | 1017 | rBV | 498230 | 480509 | 23.69% | 3.528% |
| 10 | 9.307 | 1181 | 1185 | 1188 | rBV | 2151132 | 2028282 | 100.00% | 14.893% |
| 11 | 9.648 | 1240 | 1243 | 1248 | rBV | 20833 | 24178 | 1.19% | 0.178% |
| 12 | 9.701 | 1248 | 1252 | 1257 | rVB | 39948 | 40869 | 2.01% | 0.300% |
| 13 | 9.989 | 1298 | 1301 | 1311 | rVB | 512970 | 501087 | 24.70% | 3.679% |
| 14 | 10.401 | 1368 | 1371 | 1373 | rVB | 33018 | 26904 | 1.33% | 0.198% |
| 15 | 10.789 | 1433 | 1437 | 1440 | rBV | 1224230 | 1118702 | 55.16% | 8.215% |
| 16 | 10.901 | 1454 | 1456 | 1462 | rVB | 31656 | 32926 | 1.62% | 0.242% |
| 17 | 10.983 | 1467 | 1470 | 1474 | rVB2 | 20808 | 23369 | 1.15% | 0.172% |
| 18 | 11.019 | 1474 | 1476 | 1479 | rBV2 | 24403 | 21958 | 1.08% | 0.161% |
| 19 | 11.130 | 1493 | 1495 | 1499 | rVB2 | 25000 | 24722 | 1.22% | 0.182% |
| 20 | 11.172 | 1499 | 1502 | 1504 | rBV | 26722 | 20996 | 1.04% | 0.154% |
| 21 | 11.371 | 1530 | 1536 | 1542 | rVB3 | 20297 | 26064 | 1.29% | 0.191% |
| 22 | 11.483 | 1552 | 1555 | 1559 | rBV | 493828 | 450568 | 22.21% | 3.308% |
| 23 | 12.219 | 1677 | 1680 | 1685 | rVB3 | 21808 | 27603 | 1.36% | 0.203% |
| 24 | 12.954 | 1801 | 1805 | 1814 | rVB2 | 18893 | 24635 | 1.21% | 0.181% |
| 25 | 13.071 | 1820 | 1825 | 1828 | rBV | 2048950 | 1919107 | 94.62% | 14.092% |
| 26 | 13.613 | 1913 | 1917 | 1920 | rBV | 39588 | 36219 | 1.79% | 0.266% |
| 27 | 13.948 | 1971 | 1974 | 1978 | rBV | 45297 | 48576 | 2.39% | 0.357% |
| 28 | 14.136 | 2002 | 2006 | 2010 | rBV | 557461 | 508186 | 25.05% | 3.732% |
| 29 | 15.671 | 2262 | 2267 | 2274 | rVB | 283776 | 388865 | 19.17% | 2.855% |

Sum of corrected areas: 13618593

LSC Report - Integrated Chromatogram

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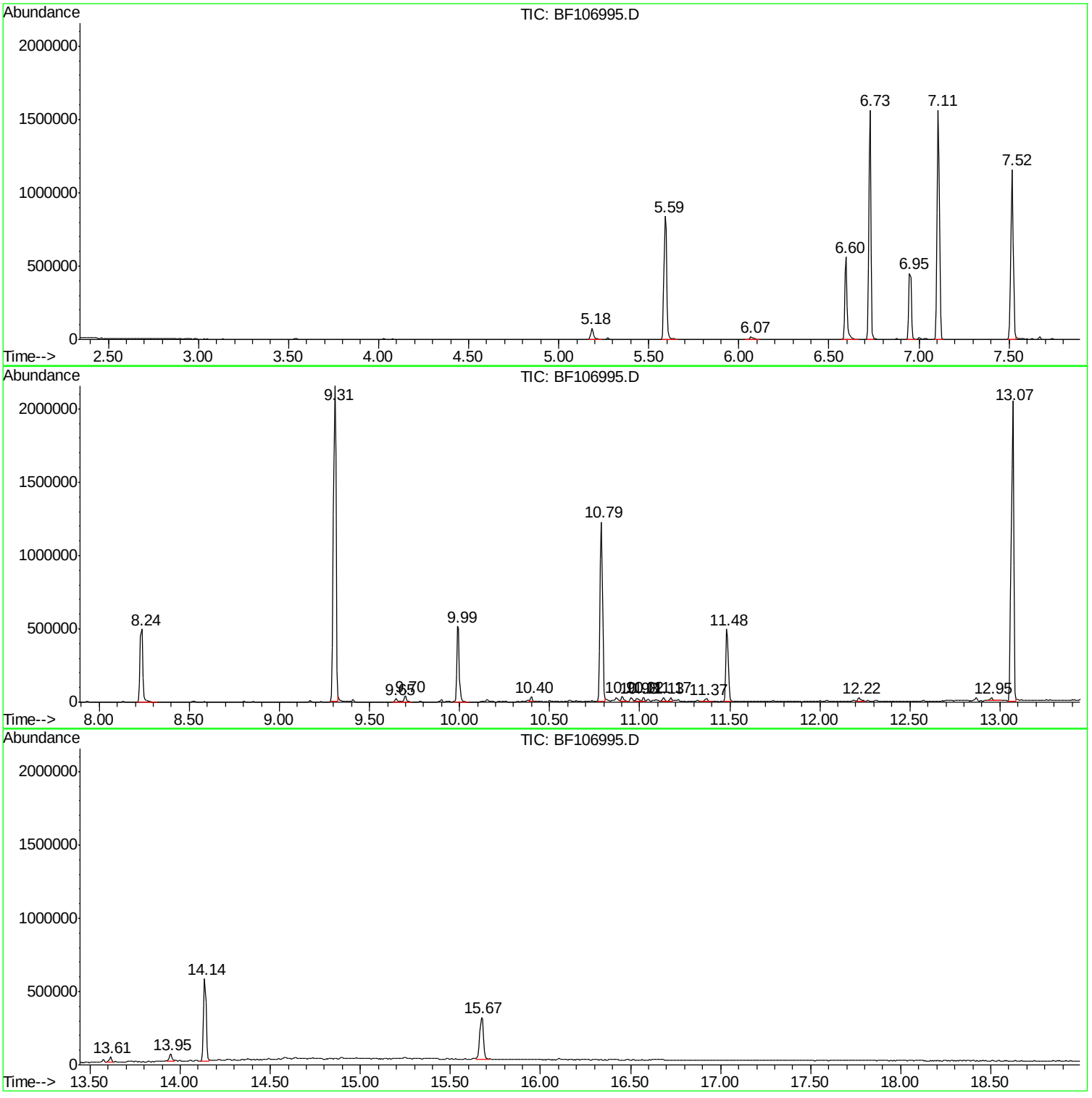
**Instrument :** BNA_F
**ClientSampleId :** W-27

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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

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Data File : BF106995.D
Acq On : 30 Jun 2018 1:32
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Misc :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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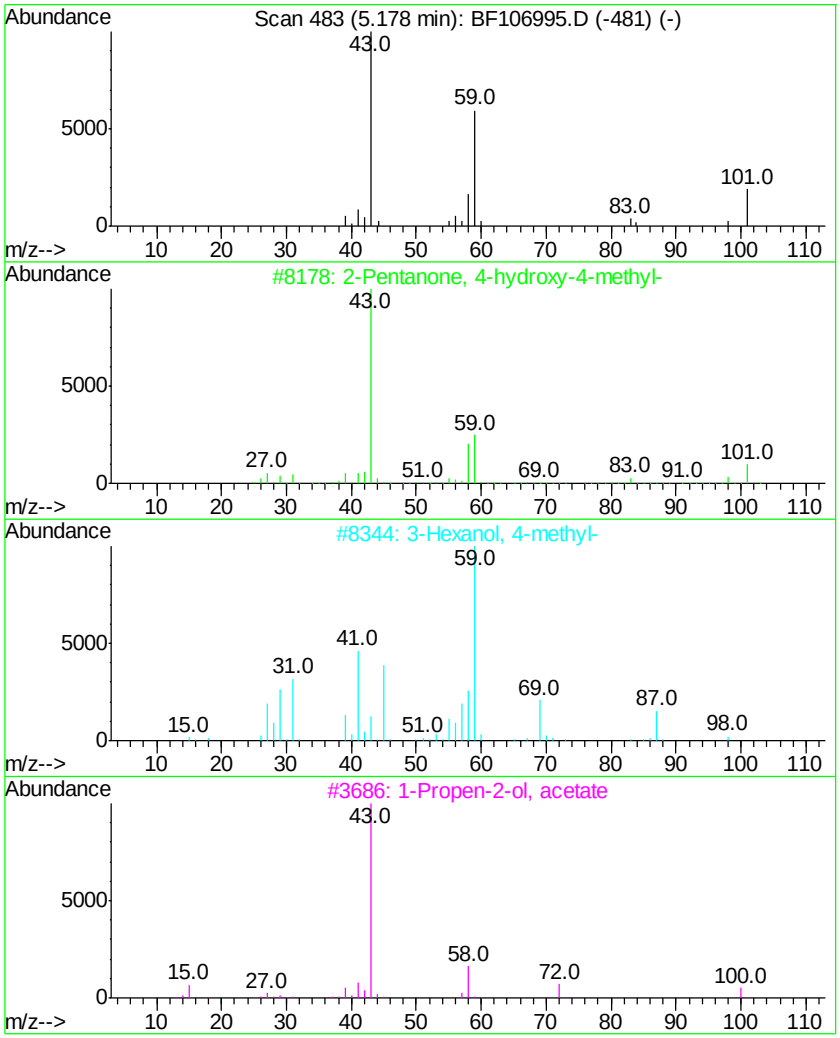
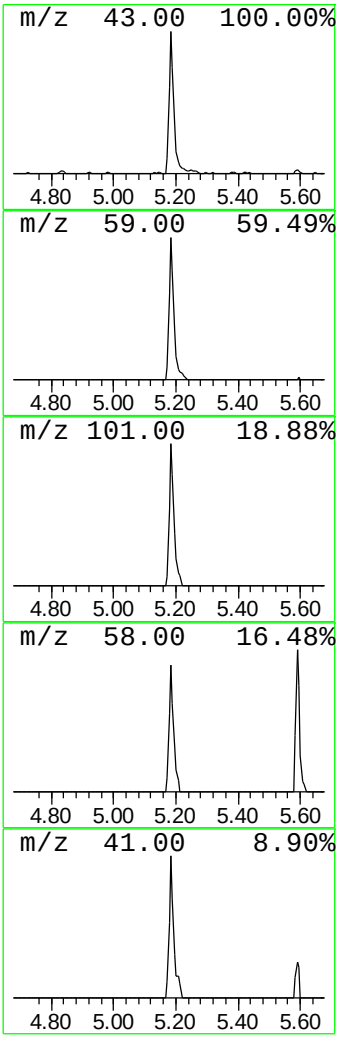
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.18 | 4.26 ng | 85337 | 1,4-Dichlorobenzene-d4 | 6.95 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 64 |
| 2 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 28 |
| 3 | 1-Propen-2-ol, acetate | 100 | C5H8O2 | 000108-22-5 | 9 |
| 4 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 9 |
| 5 | 3-Heptanol | 116 | C7H16O | 000589-82-2 | 9 |



Library Search Compound Report

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Misc :
ALS Vial : 33 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** W-27

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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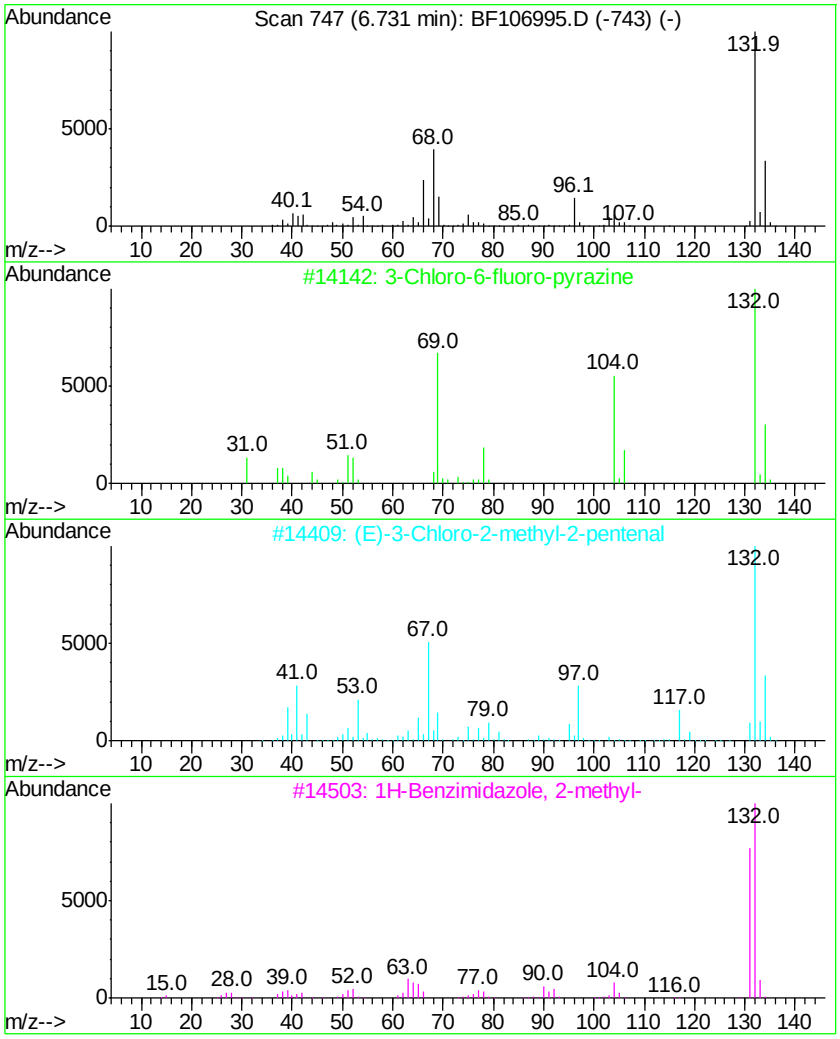
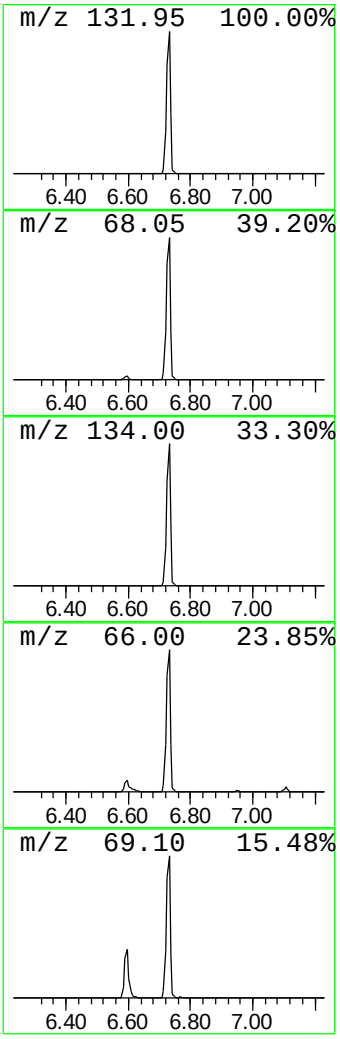
Peak Number 2 unknown6.73 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.73 | 70.08 ng | 1405320 | 1,4-Dichlorobenzene-d4 | 6.95 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 12 |
| 3 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 10 |
| 4 | 4-Chloro-2-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-00-5 | 9 |
| 5 | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2 | 022291-85-6 | 9 |



Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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 |
| 2-Pentanone, 4-hy... | 5.18 | 4.3 | ng | 85337 | 1 | 6.95 | 401072 | 20.0 |
| unknown6.73 | 6.73 | 70.1 | ng | 1405320 | 1 | 6.95 | 401072 | 20.0 |