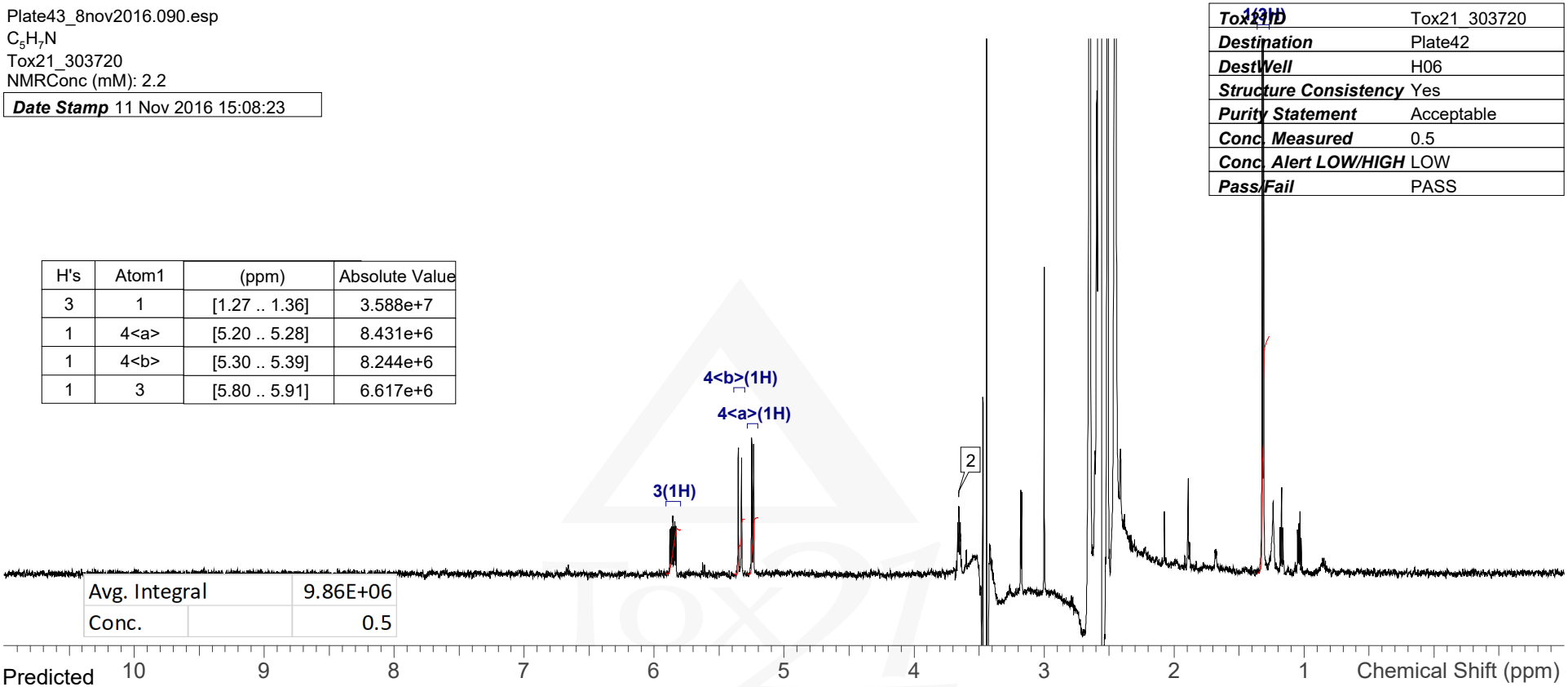
CAUTION, Low Concentration
*Concentration 5-30% of expected value*

Plate43_8nov2016.090.esp
$C_5H_7N$
Tox21_303720
NMRConc (mM): 2.2

***Date Stamp*** 11 Nov 2016 15:08:23

| | |
|---|---|
| ***Tox21 ID*** | Tox21_303720 |
| ***Destination*** | Plate42 |
| ***DestWell*** | H06 |
| ***Structure Consistency*** | Yes |
| ***Purity Statement*** | Acceptable |
| ***Conc. Measured*** | 0.5 |
| ***Conc. Alert LOW/HIGH*** | LOW |
| ***Pass/Fail*** | PASS |

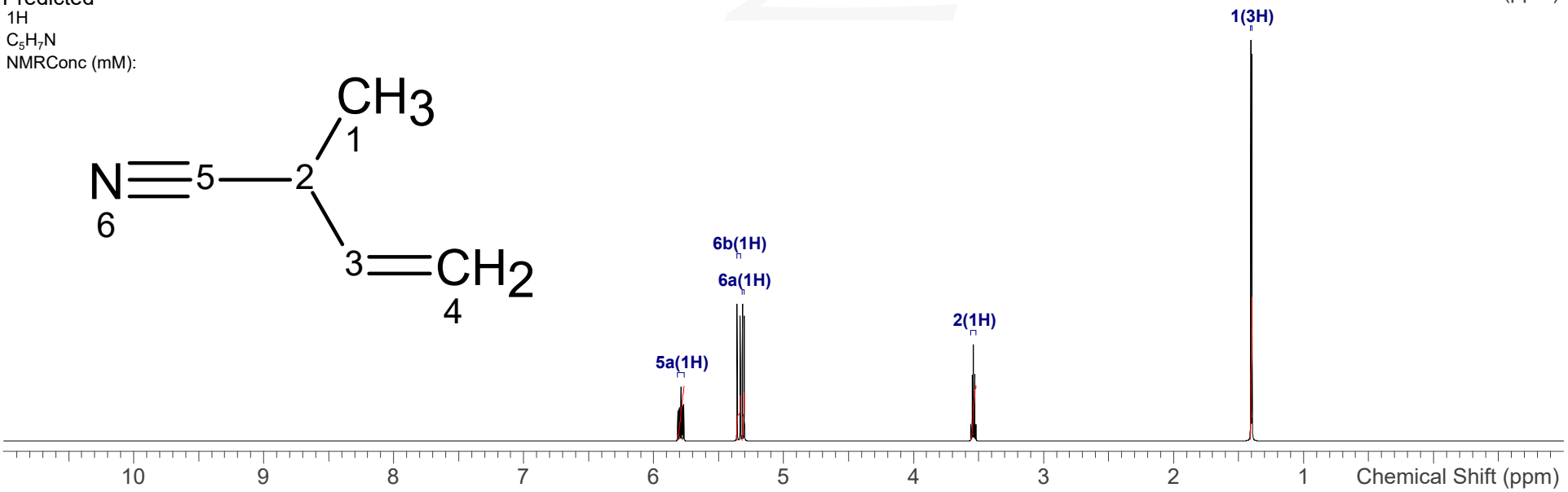
| H's | Atom1 | (ppm) | Absolute Value |
|---|---|---|---|
| 3 | 1 | [1.27 .. 1.36] | 3.588e+7 |
| 1 | 4<a> | [5.20 .. 5.28] | 8.431e+6 |
| 1 | 4<b> | [5.30 .. 5.39] | 8.244e+6 |
| 1 | 3 | [5.80 .. 5.91] | 6.617e+6 |




| | |
|---|---|
| Avg. Integral | 9.86E+06 |
| Conc. | 0.5 |

Predicted
1H
$C_5H_7N$
NMRConc (mM):




PubChem