



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

Plate14	B01	Tox21_200518	19.3	27
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Expected concentration = 19.3 mM x 0.15 dilution = 2.895 mM

PASSED

Molecular Formula: C_9H_{12}

Plate14_NFU002035_B1.esp

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low conc.

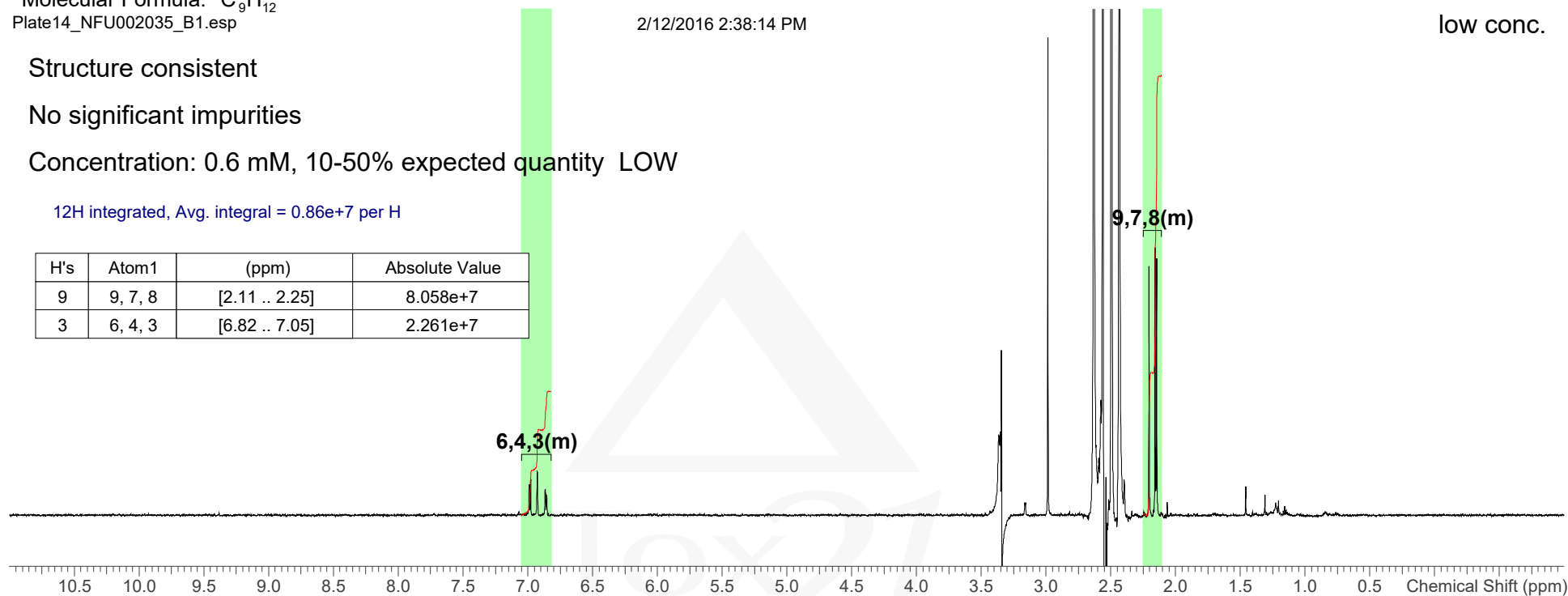
Structure consistent

No significant impurities

Concentration: 0.6 mM, 10-50% expected quantity LOW

12H integrated, Avg. integral = 0.86e+7 per H

H's	Atom1	(ppm)	Absolute Value
9	9, 7, 8	[2.11 .. 2.25]	8.058e+7
3	6, 4, 3	[6.82 .. 7.05]	2.261e+7



11/Feb/2016 19:12:10 ACD/C+H NMR Predictors 2014 (v.14.00)

