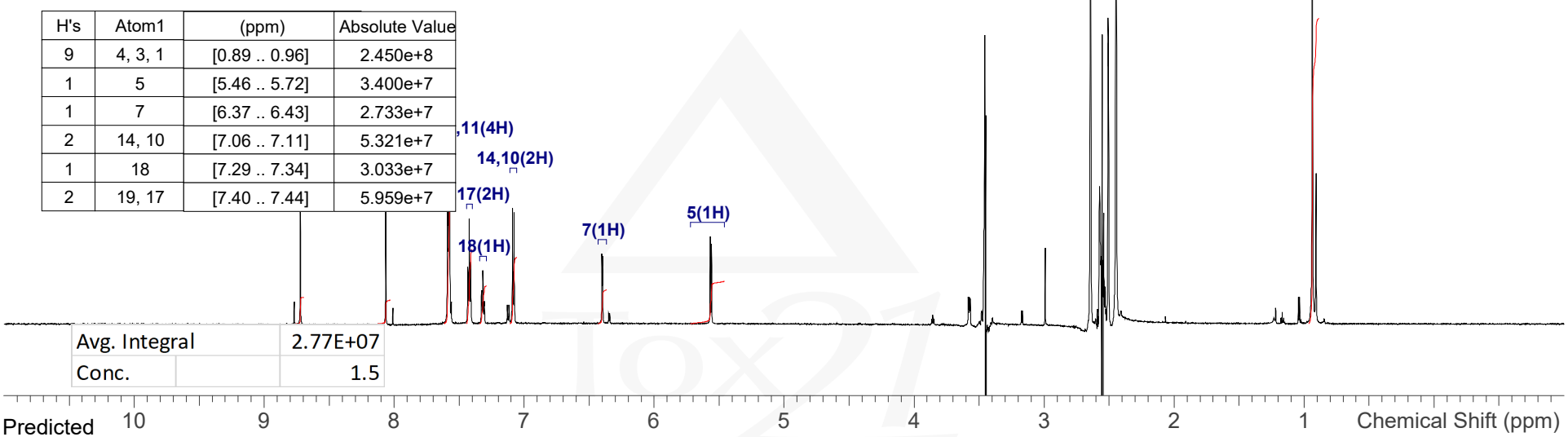
ISOMERS
Two or more isomers detected

Plate44_8nov2016.002.esp
$C_{20}H_{23}N_3O_2$
Tox21_303756
NMRConc (mM): 2.2

Date Stamp 11 Nov 2016 15:29:21

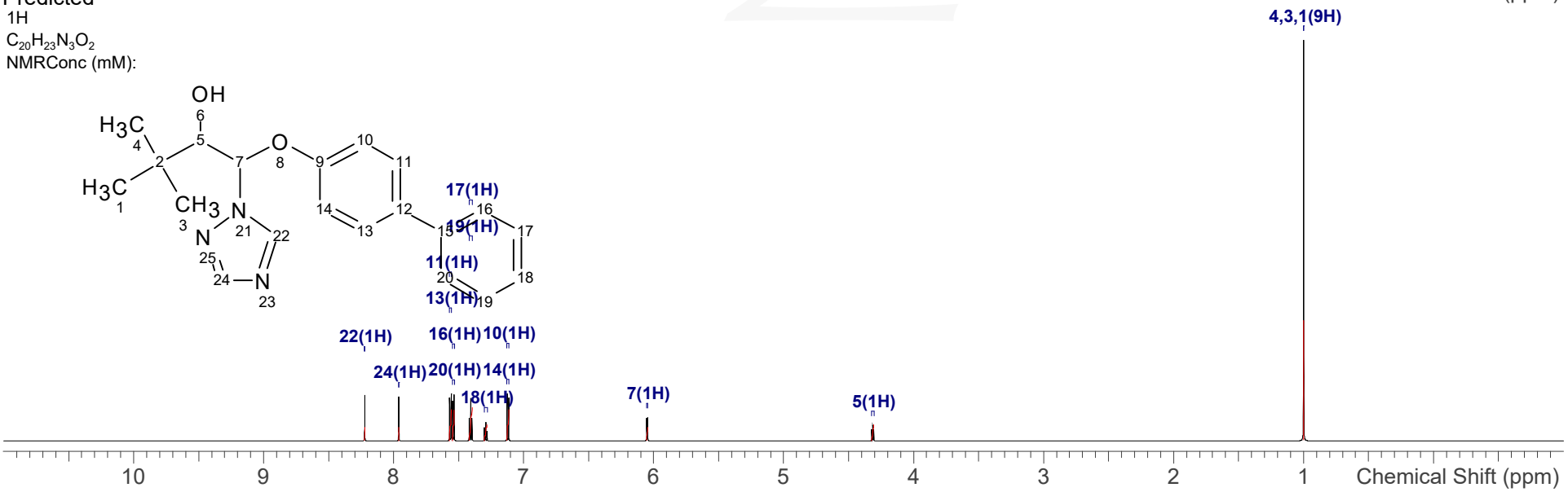
Tox21ID	Tox21_303756
Destination	Plate44
DestWell	A02
Structure Consistency	Yes
Purity Statement	Acceptable
Conc. Measured	1.5
Conc. Alert LOW/HIGH	None
Comments	stereoisomers present
Pass/Fail	PASS

H's	Atom1	(ppm)	Absolute Value
9	4, 3, 1	[0.89 .. 0.96]	2.450e+8
1	5	[5.46 .. 5.72]	3.400e+7
1	7	[6.37 .. 6.43]	2.733e+7
2	14, 10	[7.06 .. 7.11]	5.321e+7
1	18	[7.29 .. 7.34]	3.033e+7
2	19, 17	[7.40 .. 7.44]	5.959e+7



Avg. Integral	2.77E+07
Conc.	1.5

Predicted
1H
$C_{20}H_{23}N_3O_2$
NMRConc (mM):



PubChem