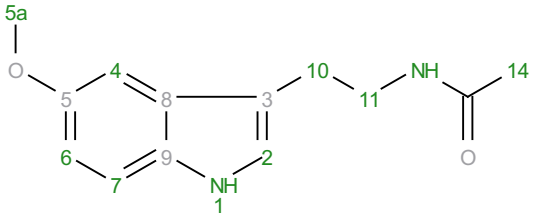
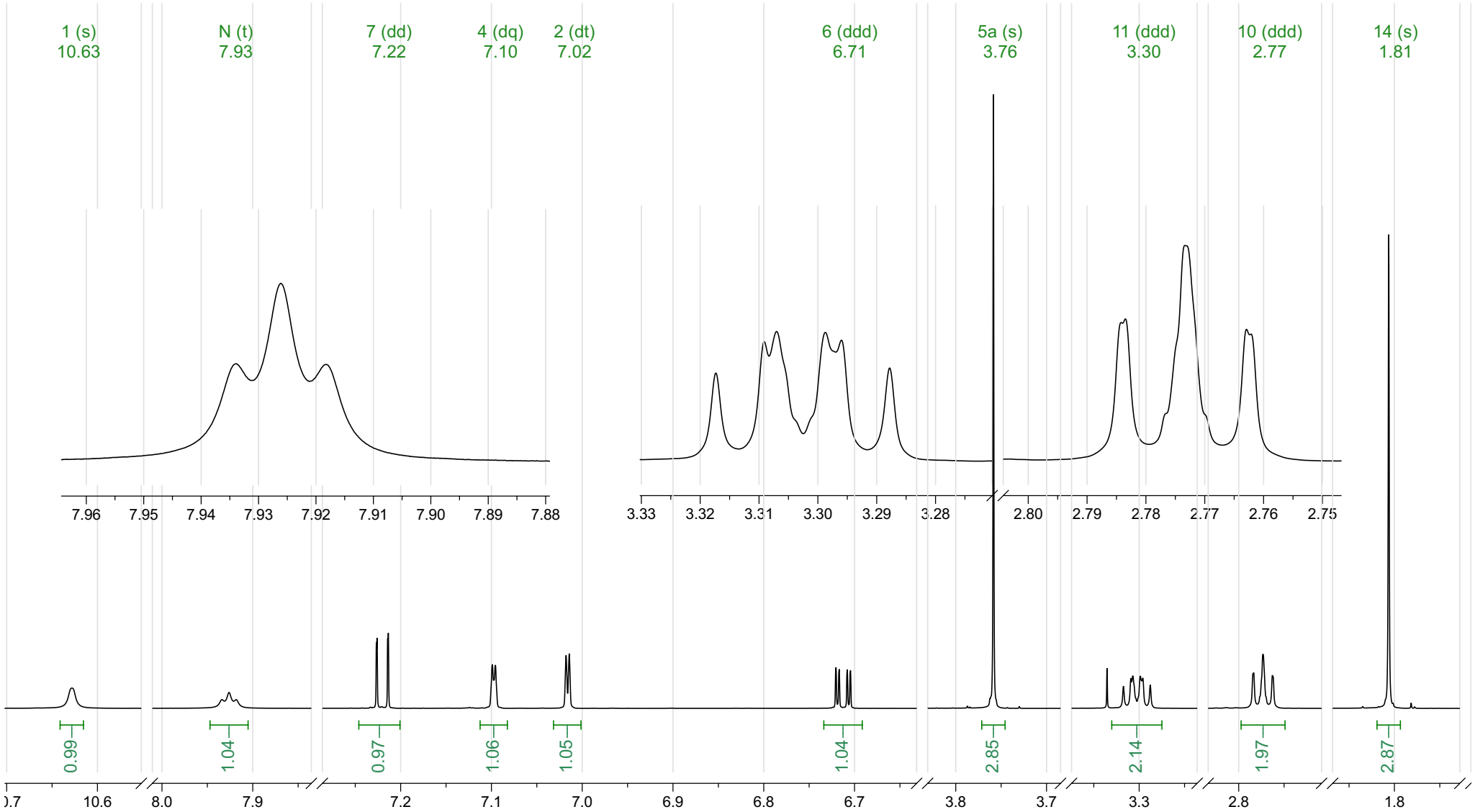
Analyte	X55: Melatonin
Acquisition Date	2018-03-21T15:45:31
Solvent	dmso
Temperature	25
Number of Scans	64
Relaxation Delay	1
Spectrometer Frequency	699.81
Spectral Width	11160.7
Nucleus	1H
Acquired Size	71429



^{1}H NMR (700 MHz, DMSO-d_6) δ 10.63 (s, 1H), 7.93 (t, J = 5.7 Hz, 1H), 7.22 (dd, J = 8.7, 0.5 Hz, 1H), 7.10 (dq, J = 2.2, 0.7 Hz, 1H), 7.02 (dt, J = 2.5, 0.6 Hz, 1H), 6.71 (ddd, J = 8.7, 2.5, 0.4 Hz, 1H), 3.76 (s, 3H), 3.30 (ddd, J = 7.8, 6.9, 5.6 Hz, 2H), 2.77 (ddd, J = 8.3, 6.7, 0.9 Hz, 2H), 1.81 (s, 3H).



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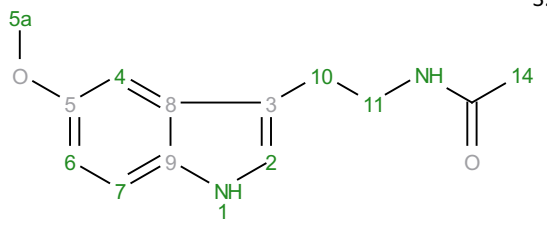
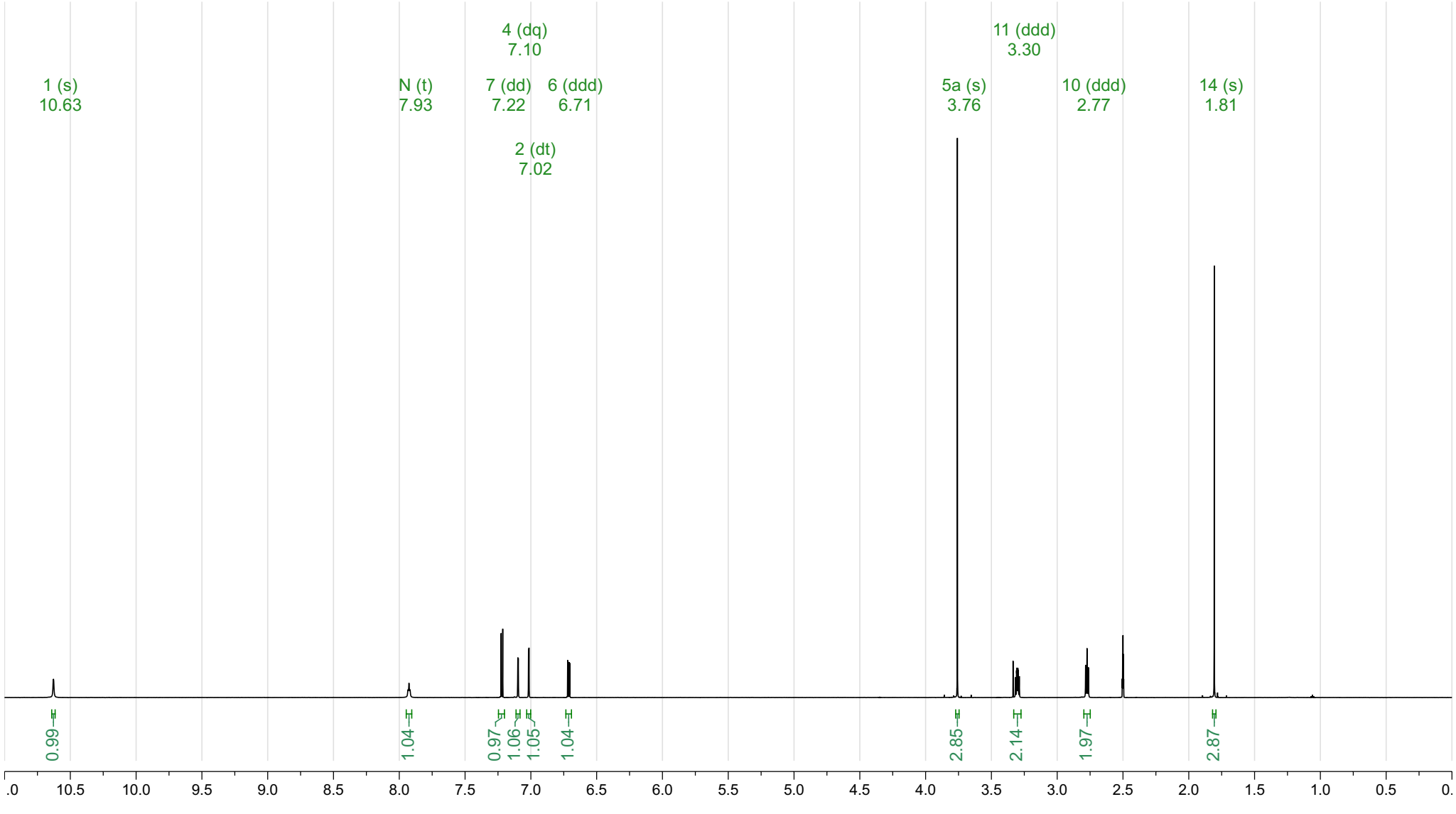
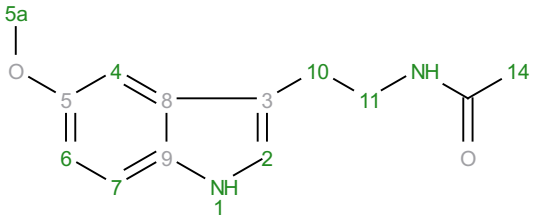


^{1}H NMR (700 MHz, DMSO-d_6) δ 10.63 (s, 1H), 7.93 (t, J = 5.7 Hz, 1H), 7.22 (dd, J = 8.7, 0.5 Hz, 1H), 7.10 (dq, J = 2.2, 0.7 Hz, 1H), 7.02 (dt, J = 2.5, 0.6 Hz, 1H), 6.71 (ddd, J = 8.7, 2.5, 0.4 Hz, 1H), 3.76 (s, 3H), 3.30 (ddd, J = 7.8, 6.9, 5.6 Hz, 2H), 2.77 (ddd, J = 8.3, 6.7, 0.9 Hz, 2H), 1.81 (s, 3H).



Prediction Melatonin
Origin Mnova Best
Solvent DMSO-d6
Version 1.0.0
Frequency 700.00
Nucleus 1H



^{1}H NMR (700 MHz, DMSO-d_6) δ 10.66 (d, J = 8.5 Hz, 1H), 7.82 (t, J = 7.1 Hz, 1H), 7.28 (d, J = 7.6 Hz, 1H), 7.17 – 7.11 (m, 2H), 6.82 (dd, J = 7.3, 1.5 Hz, 1H), 3.80 (s, 3H), 3.44 (q, J = 7.0 Hz, 2H), 3.24 (dt, J = 12.3, 7.1 Hz, 1H), 3.15 (dt, J = 12.3, 7.1 Hz, 1H), 1.82 (s, 3H).