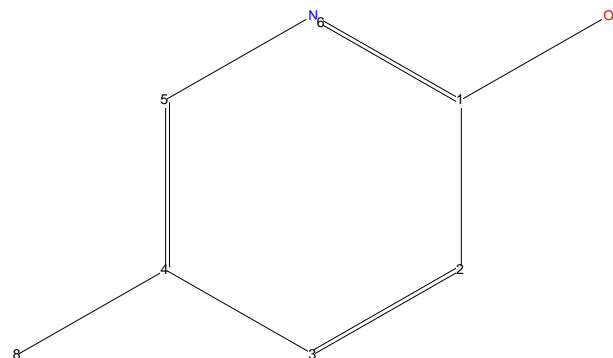


SRL-1134-026

Consistency: OK

Data set 1H: SRL-1134-026 1 1 "D:\Synzeal raw data\2022\2022_02\2022_02_10\data\root\nmr"
 Structure: D:\Synzeal raw data\2022\2022_02\2022_02_10\data\root\nmr\SRL-1134-026\1\structure.mol
 Acquisition date: February 10, 2022 6:43:56 PM IST
 Solvent: DMSO
 Probe: Z163739_0060 (PI HR-400-S1-BBF/H/D-5.0-Z SP)
 Eretic reference:



Sum formula:
C₆H₇NO

Molecular Mass:
109.05 Da

Comments:

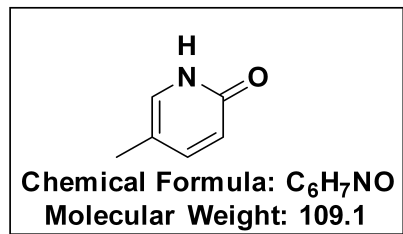
Automatic evaluation: Spectrum and structure are in agreement.
 All major signals in the spectrum could be assigned. All elements of the structure could be assigned to regions in the spectrum. Impurity H₂O not assigned. Impurity CDCl₃ not assigned.

Signature:

Automatic analysis generated by Bruker CMC (b:105).

All results have been created exclusively by automatic analysis.

Report generated by Bruker CMC-assist TopSpin 4.1.1 (of 2020-12-02 01:36:53), on 'CZC84970T5' as 'root'



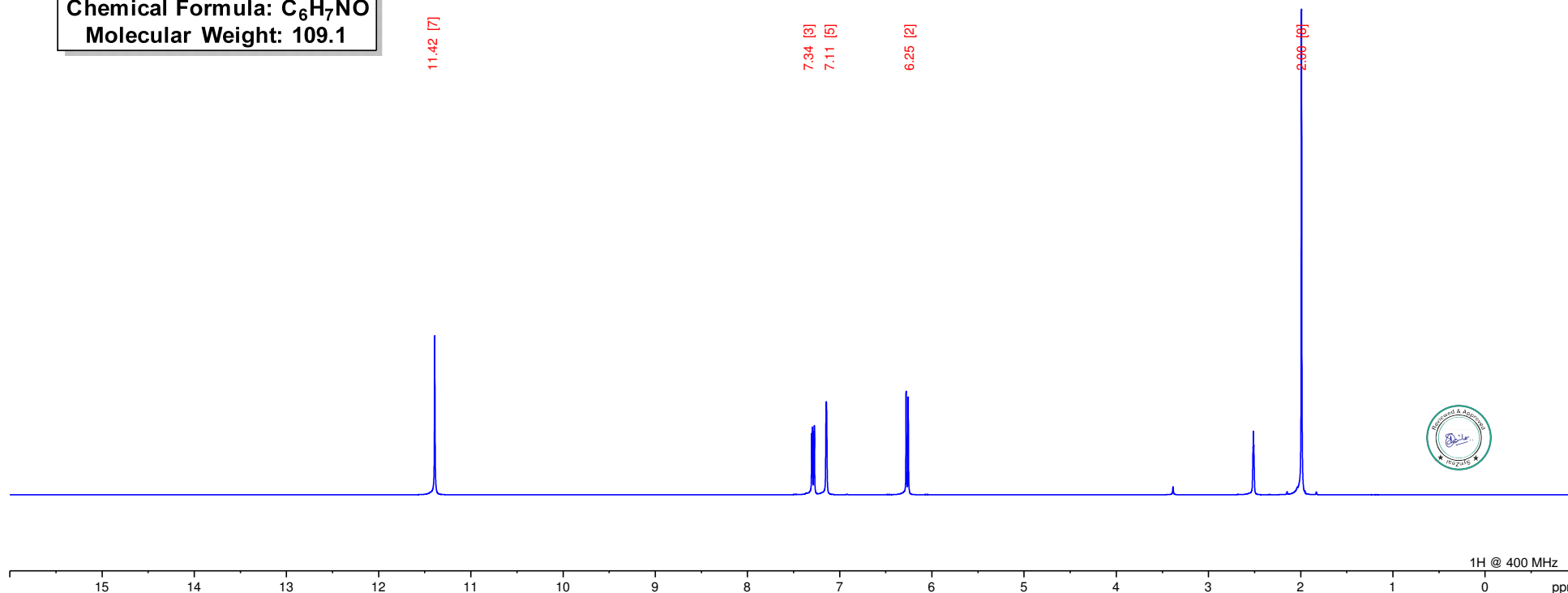
11.42 [7]

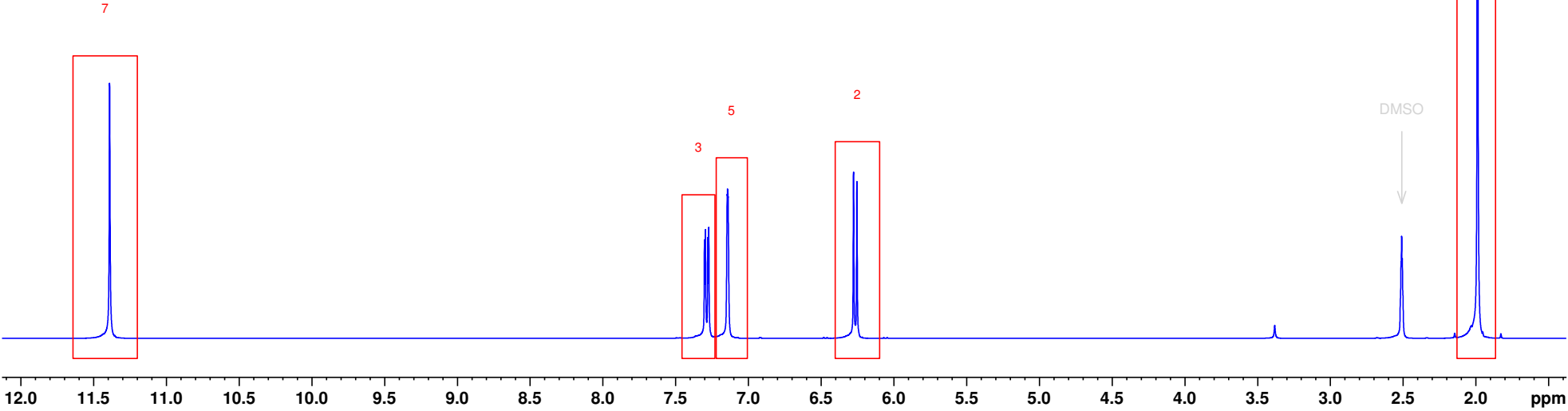
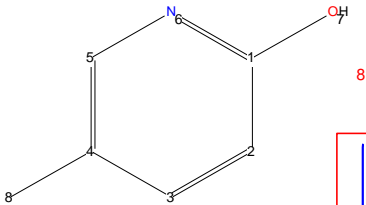
7.34 [3]
7.11 [5]

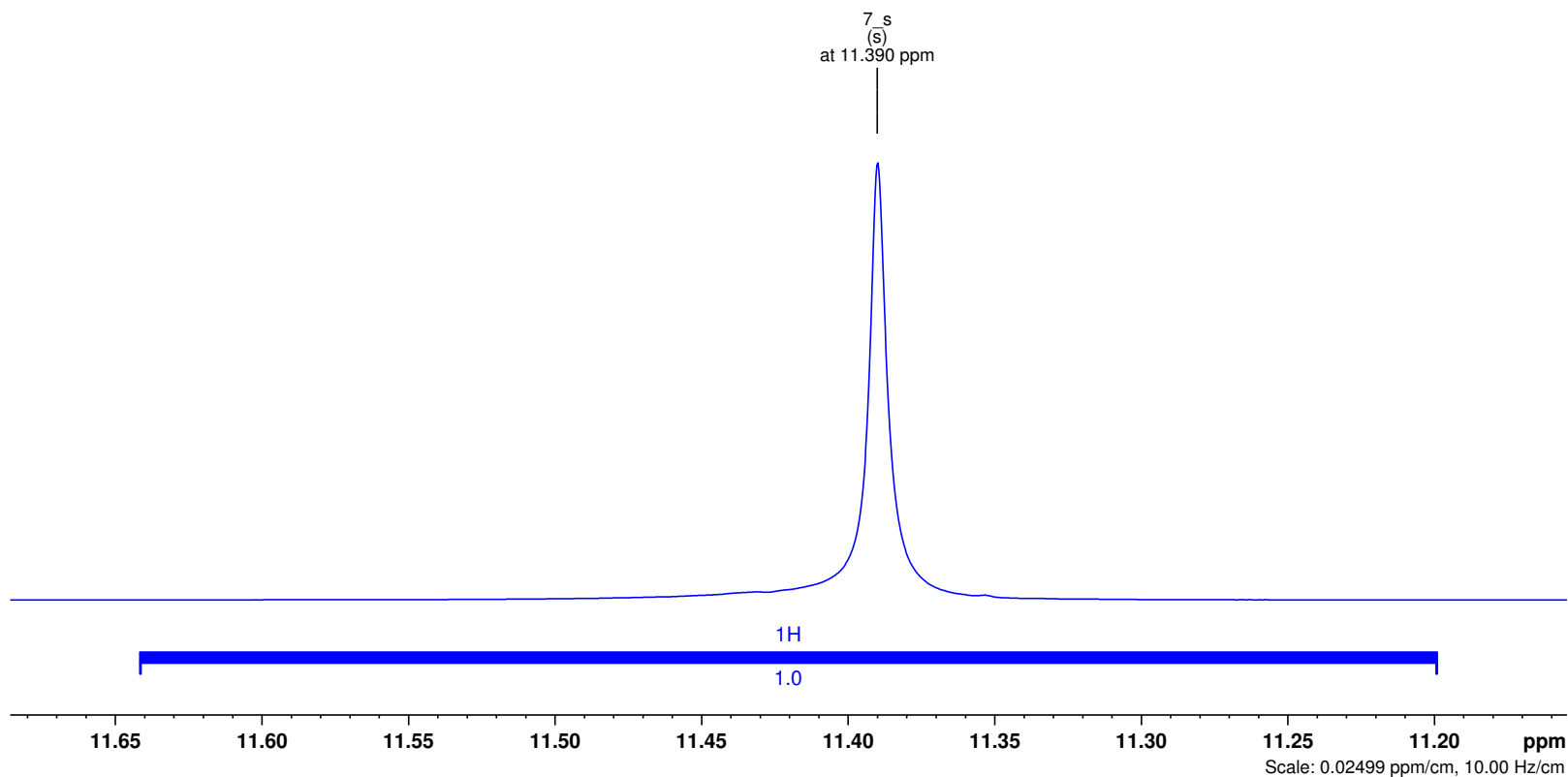
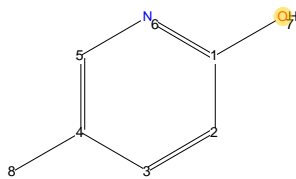
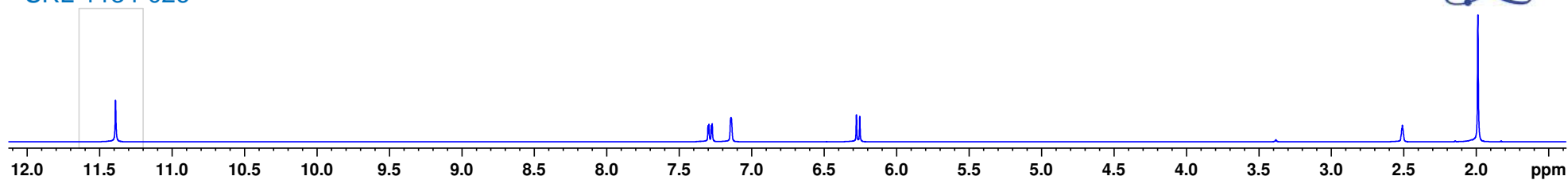
6.25 [2]

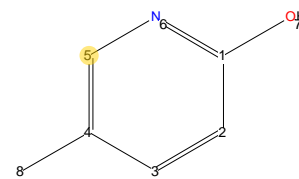
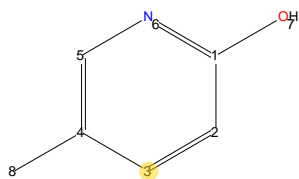
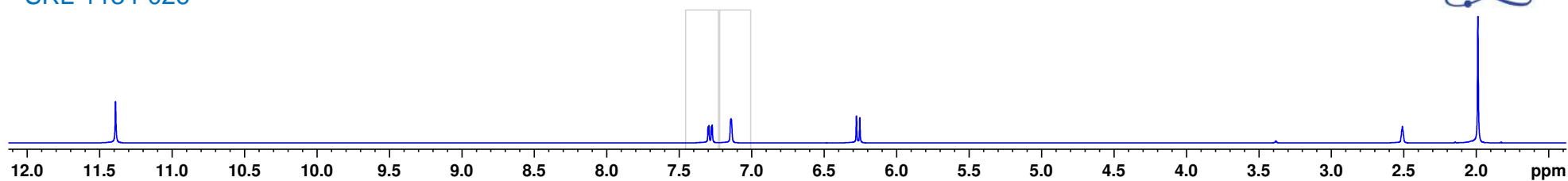
2.51 [DMSO]

2.00 [8]

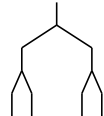




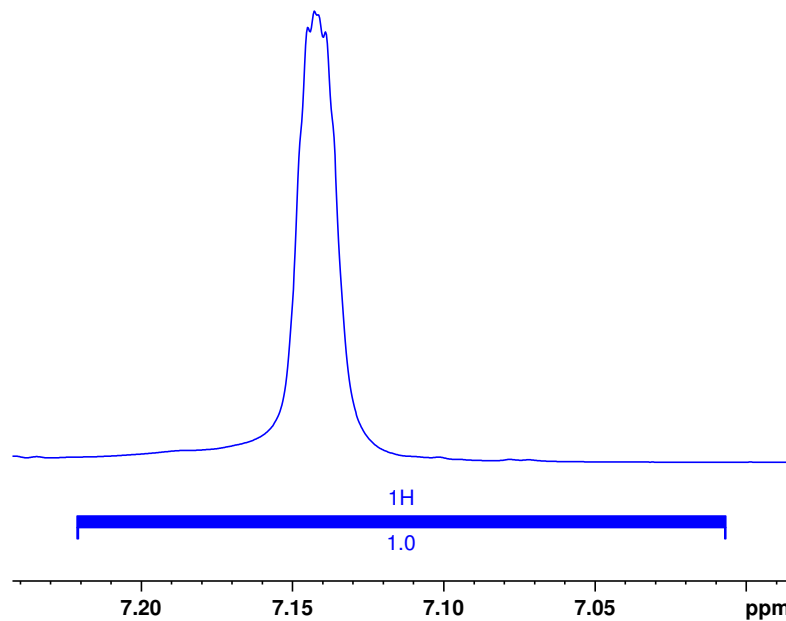
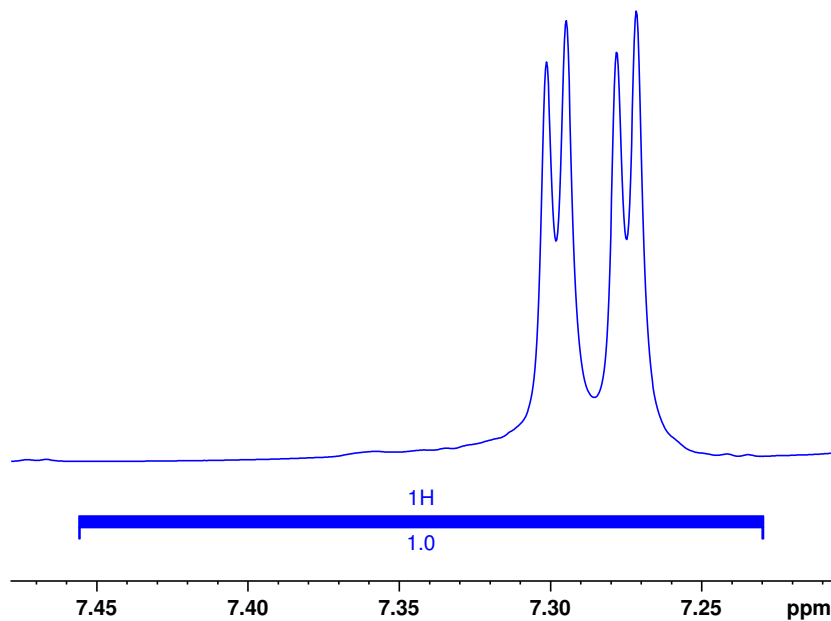




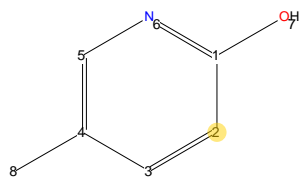
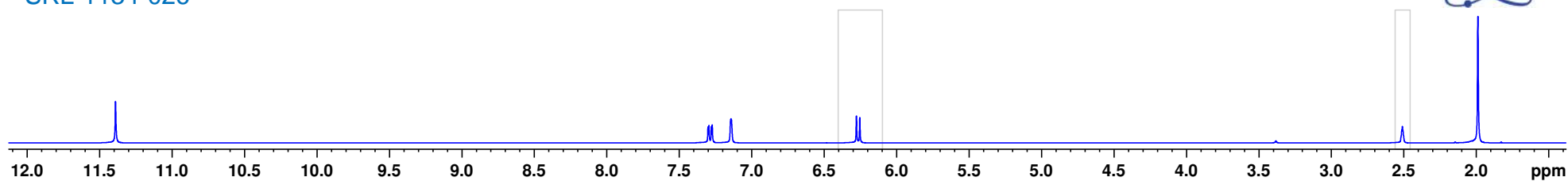
3 dd Q3
2.6 / 9.3 Hz (dd)
at 7.287 ppm



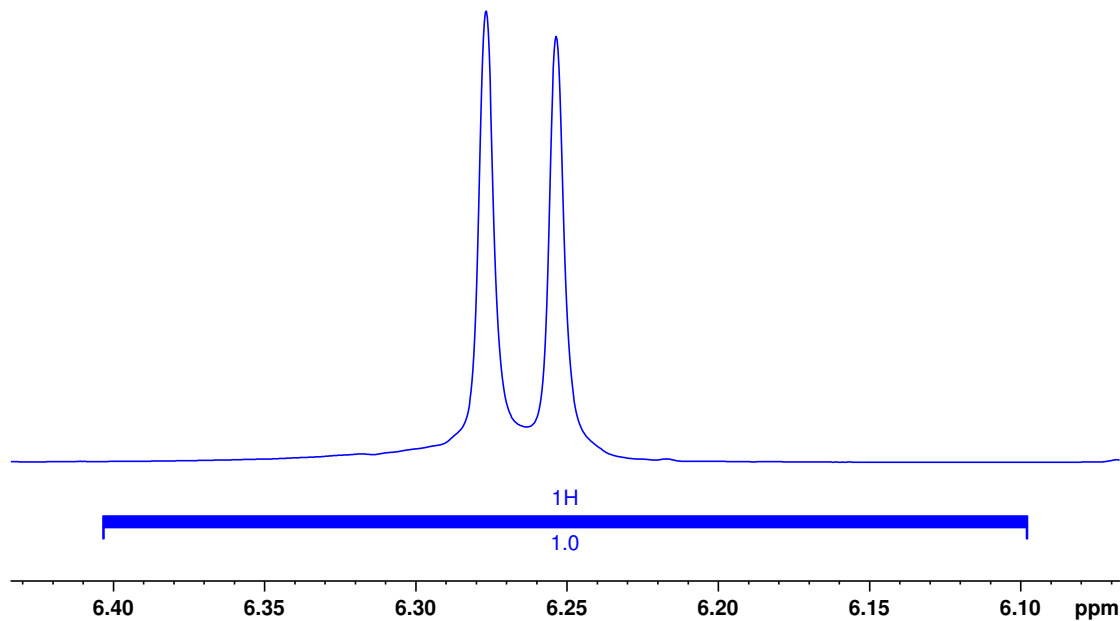
5_s_Q2
(s)
at 7.143 ppm



Scale: 0.02499 ppm/cm, 10.00 Hz/cm

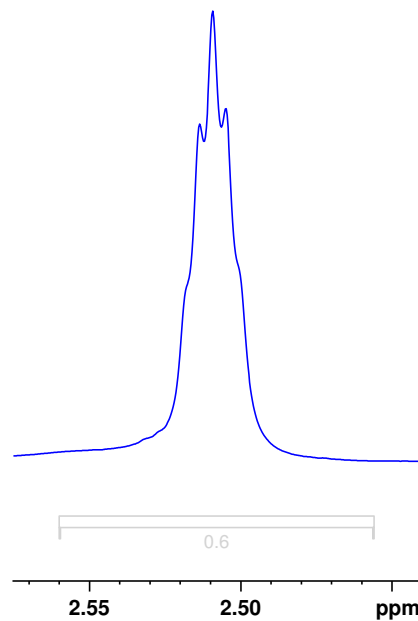


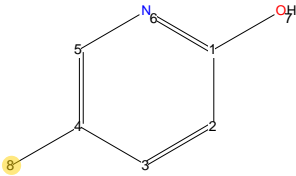
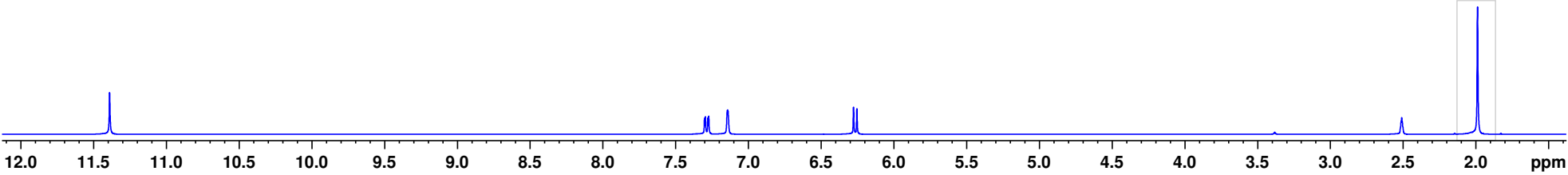
2_d_Q1
9.3 Hz (d)
at 6.265 ppm



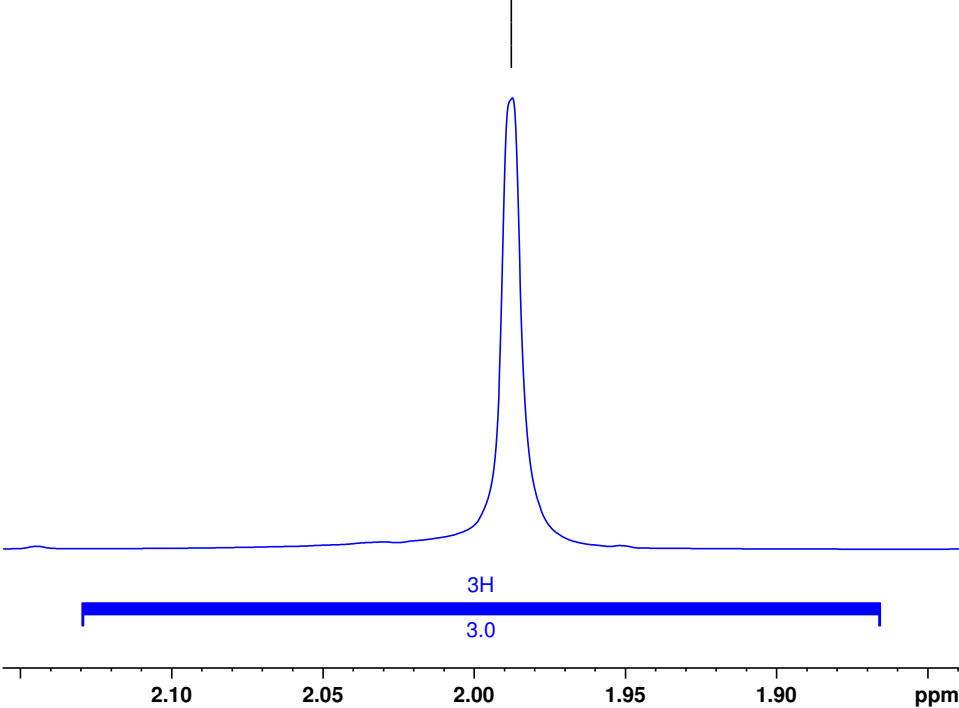
DMSO

DMSO
1.8 Hz (t)
at 2.510 ppm





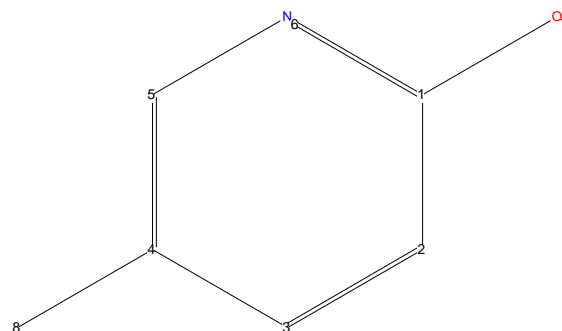
8 s
(s)
at 1.988 ppm



1D1H Assignments

Position, coupling, integral
1.99 ppm, s, 3H
6.26 ppm, d (9.3Hz), 1H
7.14 ppm, s, 1H
7.29 ppm, dd (2.6, 9.3Hz), 1H
11.39 ppm, s, 1H
2.51 ppm, t (1.8Hz), 0H

Assignment
8
2
5
3
7
- not assigned -



The spectral description in various Journal formats:

Journal of Organic Chemistry (JOC)

^1H NMR (DMSO, 400 MHz): δ_{H} 11.39 (1H, s, H7), 7.29 (1H, dd, $J = 2.6, 9.3$ Hz, H3), 7.14 (1H, s, H5), 6.26 (1H, d, $J = 9.3$ Hz, H2), 1.99 (3H, s, H8).

Journal of Medicinal Chemistry

^1H NMR (400 MHz, DMSO): $\delta =$ 11.39 (s, 1H, H-7), 7.29 (dd, $J = 2.6, 9.3$ Hz, 1H, H-3), 7.14 (s, 1H, H-5), 6.26 (d, $J = 9.3$ Hz, 1H, H-2), 1.99 ppm (s, 3H, H-8).

Journal of the American Chemical Society (JACS)

^1H NMR (400 MHz, DMSO): δ , ppm 11.39 (s, 1H, H-7), 7.29 (dd, $J = 2.6, 9.3$ Hz, 1H, H-3), 7.14 (s, 1H, H-5), 6.26 (d, $J = 9.3$ Hz, 1H, H-2), 1.99 (s, 3H, H-8).

Angewandte Chemie

^1H NMR (400 MHz, DMSO): $\delta=$ 11.39 (s, 1H, H-7), 7.29 (dd, $J=2.6, 9.3$ Hz, 1H, H-3), 7.14 (s, 1H, H-5), 6.26 (d, $J=9.3$ Hz, 1H, H-2), 1.99 ppm (s, 3H, H-8);

Chemistry, a European Journal

^1H NMR (400 MHz, DMSO): $\delta=$ 11.39 (s, 1H, H-7), 7.29 (dd, $J=2.6, 9.3$ Hz, 1H, H-3), 7.14 (s, 1H, H-5), 6.26 (d, $J=9.3$ Hz, 1H, H-2), 1.99 ppm (s, 3H, H-8);

Helvetica Chimica Acta

^1H -NMR (400 MHz, DMSO): δ 11.39 (s, H-7); 7.29 (dd, $J = 2.6, 9.3$ Hz, H-3); 7.14 (s, H-5); 6.26 (d, $J = 9.3$ Hz, H-2); 1.99 (s, H-8).

Tetrahedron Letters

^1H NMR (400 MHz, DMSO) δ 11.39 (s, 1H, H-7), 7.29 (dd, $J = 2.6, 9.3$ Hz, 1H, H-3), 7.14 (s, 1H, H-5), 6.26 (d, $J = 9.3$ Hz, 1H, H-2), 1.99 (s, 3H, H-8).

Journal of Natural Products

^1H NMR (DMSO, 400 MHz) δ 11.39 (1H, s, H-7), 7.29 (1H, dd, $J = 2.6, 9.3$ Hz, H-3), 7.14 (1H, s, H-5), 6.26 (1H, d, $J = 9.3$ Hz, H-2), 1.99 (3H, s, H-8);

Analytical Chemistry

^1H NMR (DMSO, 400 MHz): δ_{H} 11.39 (1H, s, H7), 7.29 (1H, dd, $J = 2.6, 9.3$ Hz, H3), 7.14 (1H, s, H5), 6.26 (1H, d, $J = 9.3$ Hz, H2), 1.99 (3H, s, H8).

Planta Medica

^1H NMR (DMSO, 400 MHz) δ 11.39 (1H, s, H-7), 7.29 (1H, dd, J = 2.6, 9.3 Hz, H-3), 7.14 (1H, s, H-5), 6.26 (1H, d, J = 9.3 Hz, H-2), 1.99 (3H, s, H-8);

Organic Letters

^1H NMR (400 MHz, DMSO) δ 11.39 (s, 1H, H-7), 7.29 (dd, J = 2.6, 9.3 Hz, 1H, H-3), 7.14 (s, 1H, H-5), 6.26 (d, J = 9.3 Hz, 1H, H-2), 1.99 (s, 3H, H-8).

Phytochemistry

^1H NMR (DMSO, 400 MHz): δ_{H} 11.39 (1H, s, H-7), 7.29 (1H, dd, J = 2.6, 9.3 Hz, H-3), 7.14 (1H, s, H-5), 6.26 (1H, d, J = 9.3 Hz, H-2), 1.99 (3H, s, H-8);

Fitoterapia

^1H NMR (DMSO, 400 MHz): δ 11.39 (1H, s, H-7), 7.29 (1H, dd, J = 2.6, 9.3 Hz, H-3), 7.14 (1H, s, H-5), 6.26 (1H, d, J = 9.3 Hz, H-2), 1.99 (3H, s, H-8);

Bioorganic and Medicinal Chemistry Letters

^1H NMR (400 MHz, DMSO) δ 11.39 (s, 1H, H-7), 7.29 (dd, J = 2.6, 9.3 Hz, 1H, H-3), 7.14 (s, 1H, H-5), 6.26 (d, J = 9.3 Hz, 1H, H-2), 1.99 (s, 3H, H-8).