# CMC-assist

## SRL-1134-026

# **Consistency: OK**

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Acquisition date:

Solvent:

Z163739\_0060 (PI HR-400-S1-BBF/H/D-5.0-Z SP) Probe:

Eretic reference:



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.

13

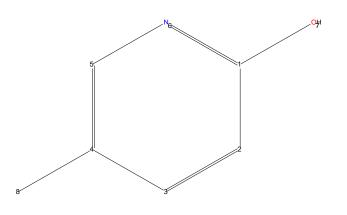
12

11

10

Chemical Formula: C<sub>6</sub>H<sub>7</sub>NO Molecular Weight: 109.1



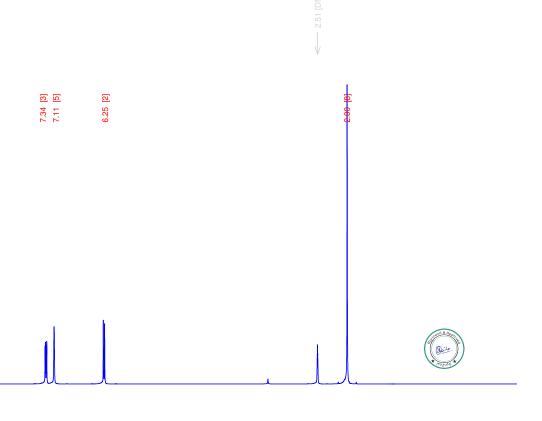




Sum formula: C<sub>6</sub>H<sub>7</sub>NO

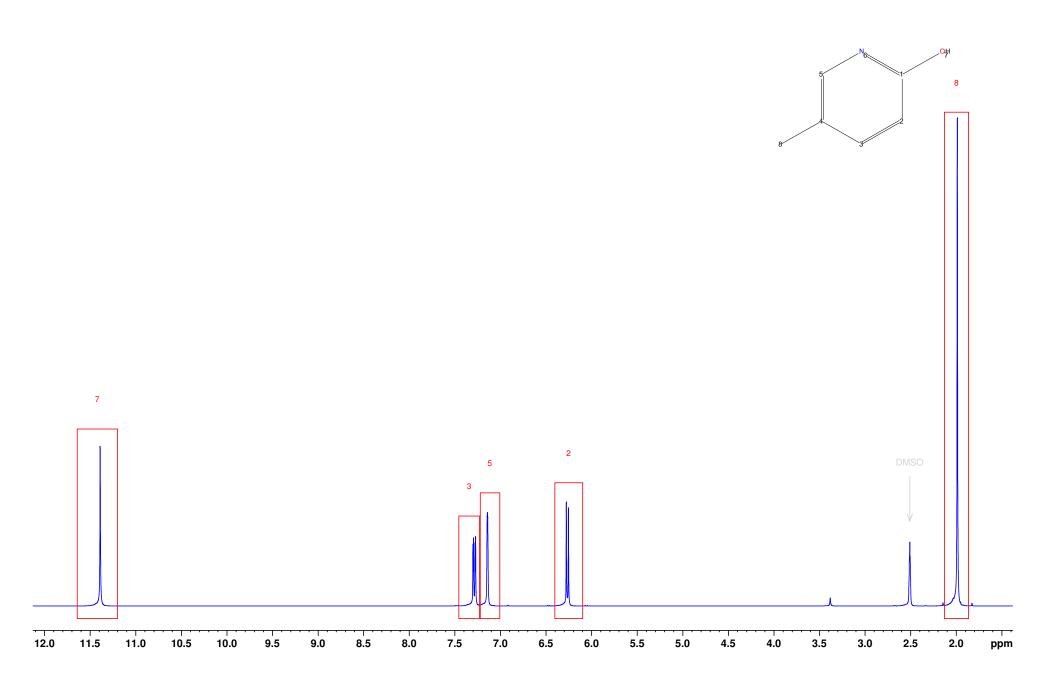
Molecular Mass: 109.05 Da

Automatic analysis generated by Bruker CMC (b:105). All results have been created exlusively by automatic analysis. Report generated by Bruker CMC-assist TopSpin 4.1.1 (of 2020-12-02 01:36:53), on 'CZC84970T5' as 'root'

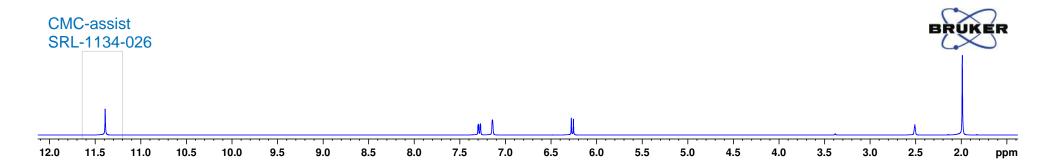


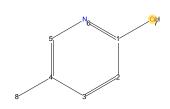


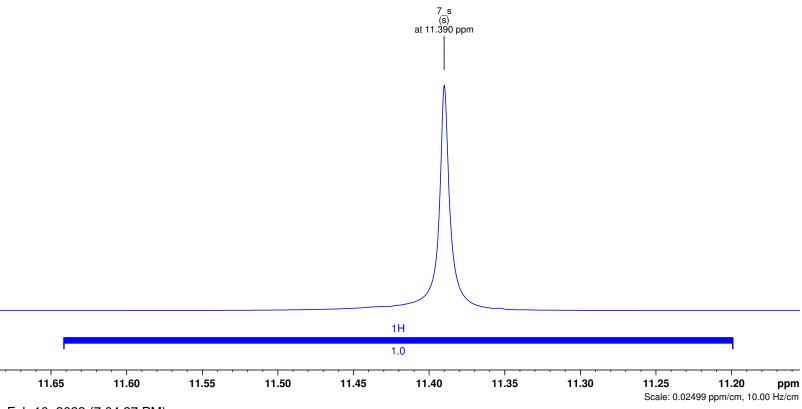




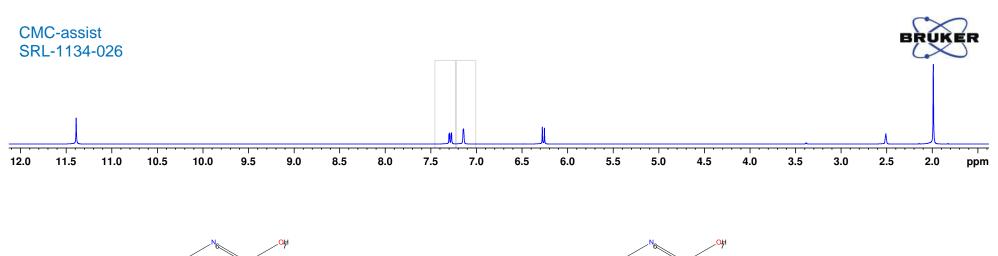
Feb 10, 2022 (7:04:27 PM) Page 2 of 9

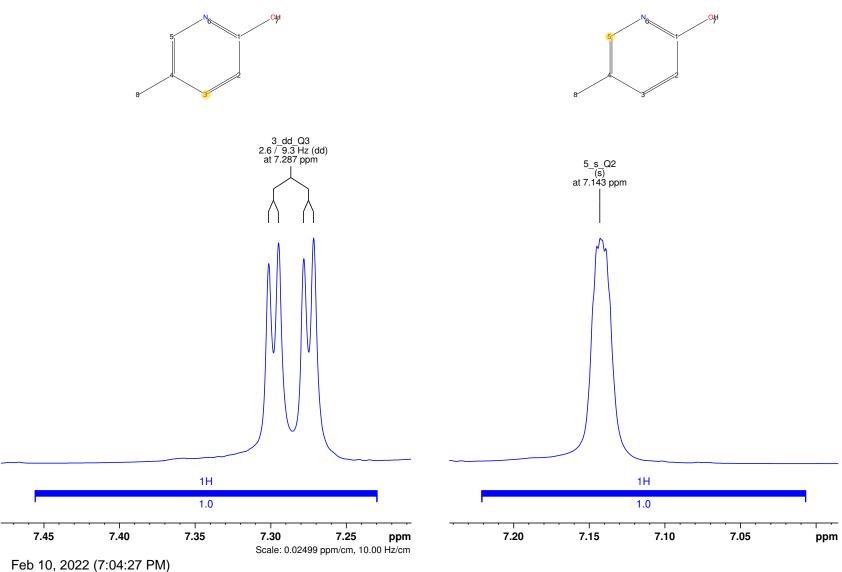




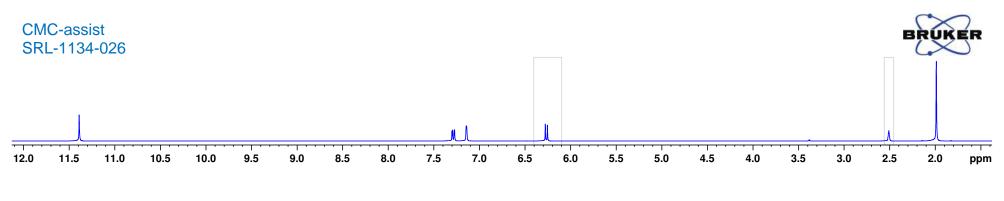


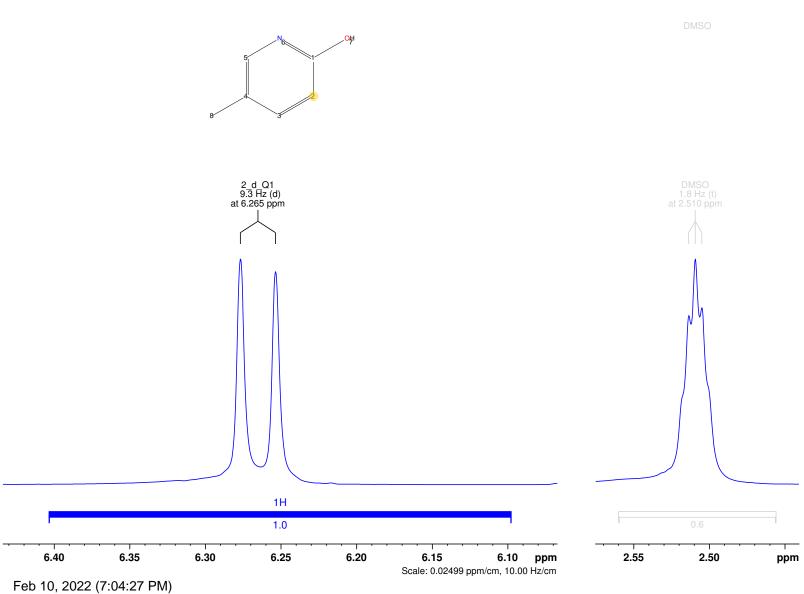
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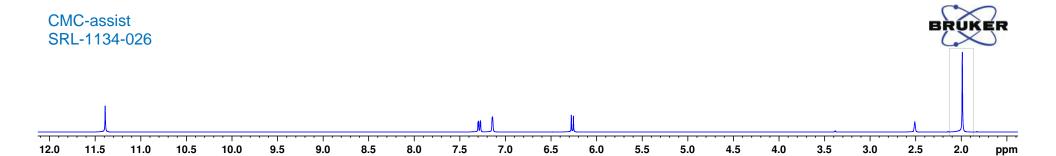


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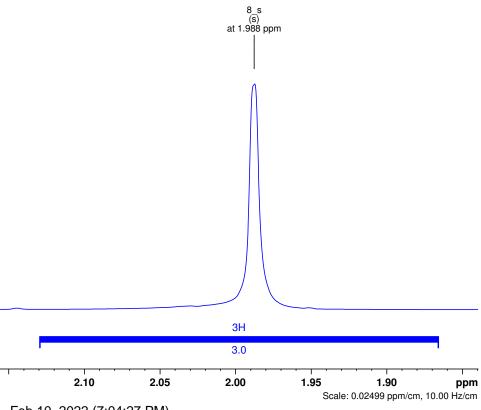




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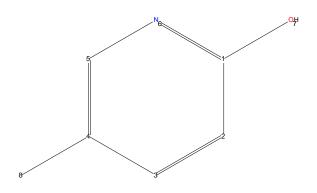


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# 1D1H Assignments

Position, coupling, integral
1.99 ppm, s, 3H
8
6.26 ppm, d (9.3Hz), 1H
2.7.14 ppm, s, 1H
7.29 ppm, dd (2.6, 9.3Hz), 1H
311.39 ppm, s, 1H
2.51 ppm, t (1.8Hz), 0H
Assignment
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7
- not assigned -



Feb 10, 2022 (7:04:27 PM) Page 7 of 9



# The spectral description in various Journal formats:

# **Journal of Organic Chemistry (JOC)**

<sup>1</sup>H NMR (DMSO, 400 MHz):  $\delta_{H}$  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**

<sup>1</sup>H 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).

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<sup>1</sup>H-NMR (400 MHz, DMSO):  $\delta$  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).

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<sup>1</sup>H 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 (s, 3H, H-8).

#### **Journal of Natural Products**

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Feb 10, 2022 (7:04:27 PM)
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#### **Planta Medica**

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<sup>1</sup>H NMR (DMSO, 400 MHz):  $\delta_{H}$  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);

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<sup>1</sup>H 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 (s, 3H, H-8).

Feb 10, 2022 (7:04:27 PM)
Page 9 of 9

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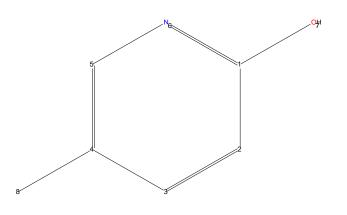
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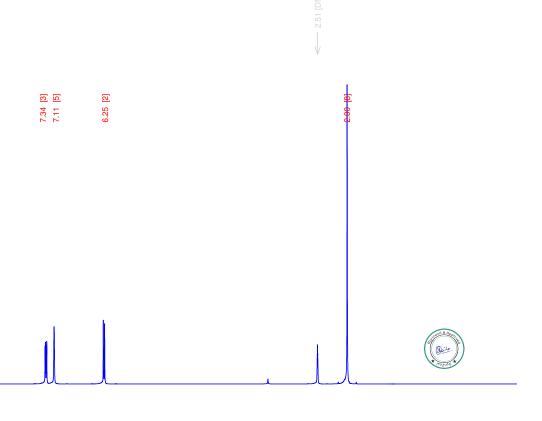




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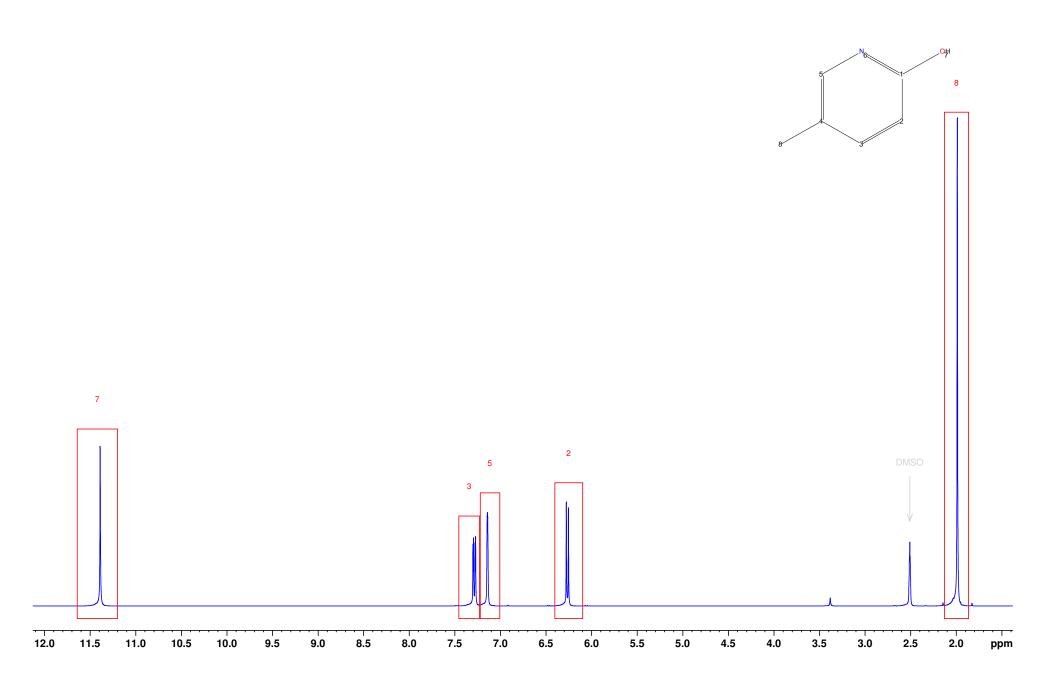
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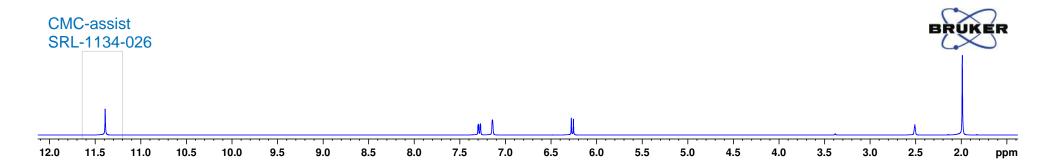


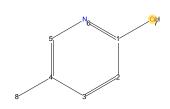


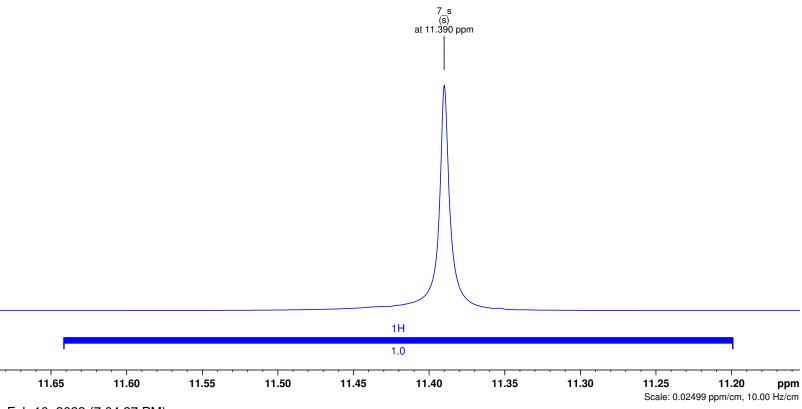




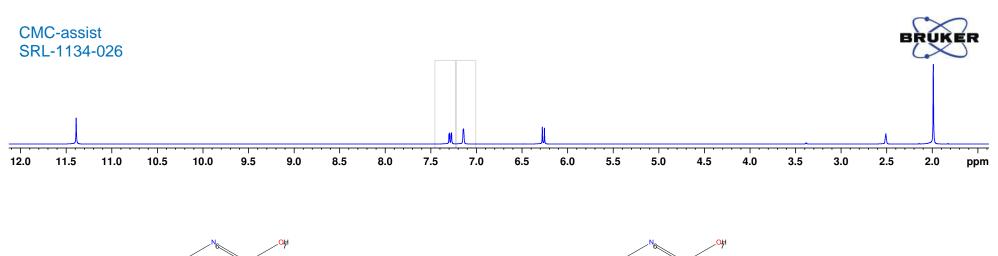
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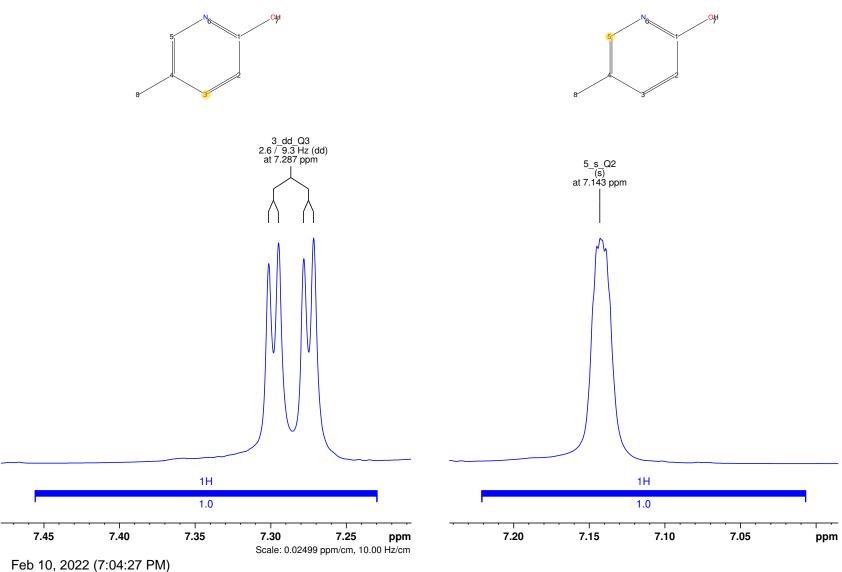




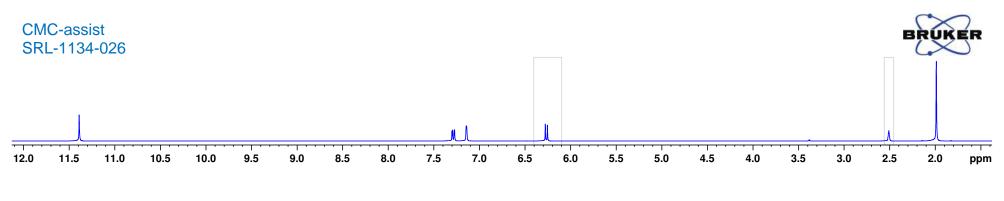


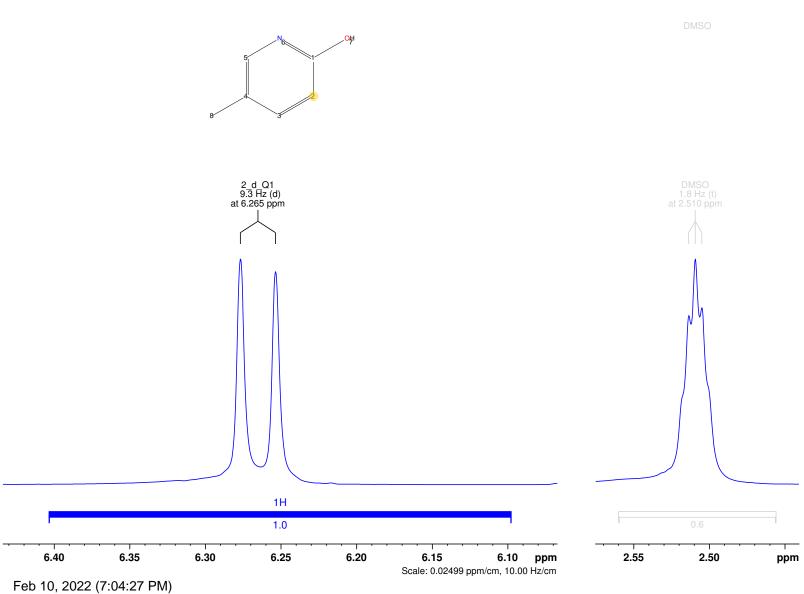
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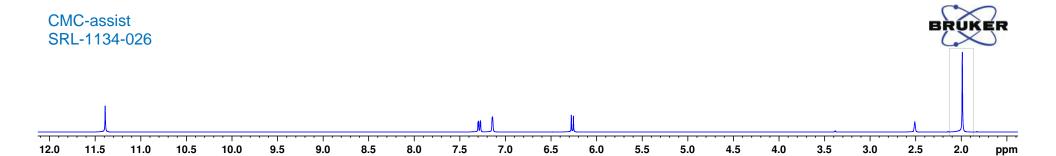


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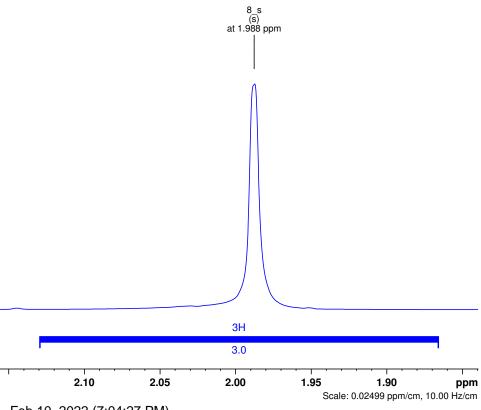




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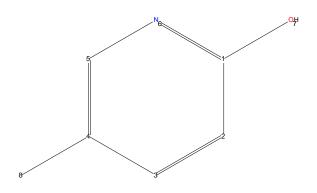


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<sup>1</sup>H NMR (DMSO, 400 MHz):  $\delta_{H}$  11.39 (1H, s, H7), 7.29 (1H, dd, J = 2.6, 9.3 Hz, H3), 7.14 (1H, s, H5), 6.26 (1H, d, J = 9.3 Hz, H2), 1.99 (3H, s, H8).

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#### **Planta Medica**

<sup>1</sup>H NMR (DMSO, 400 MHz)  $\delta$  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);

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# CMC-assist

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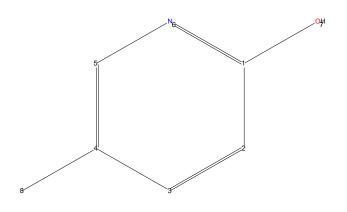
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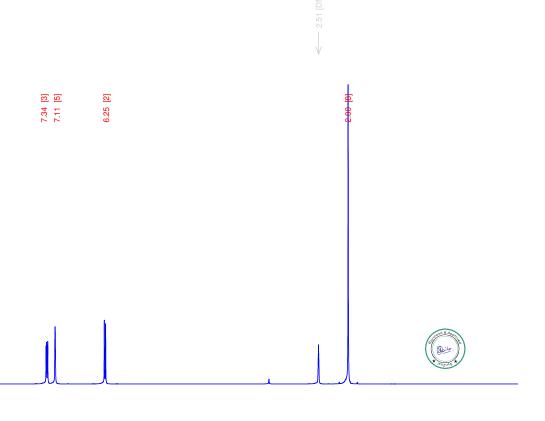




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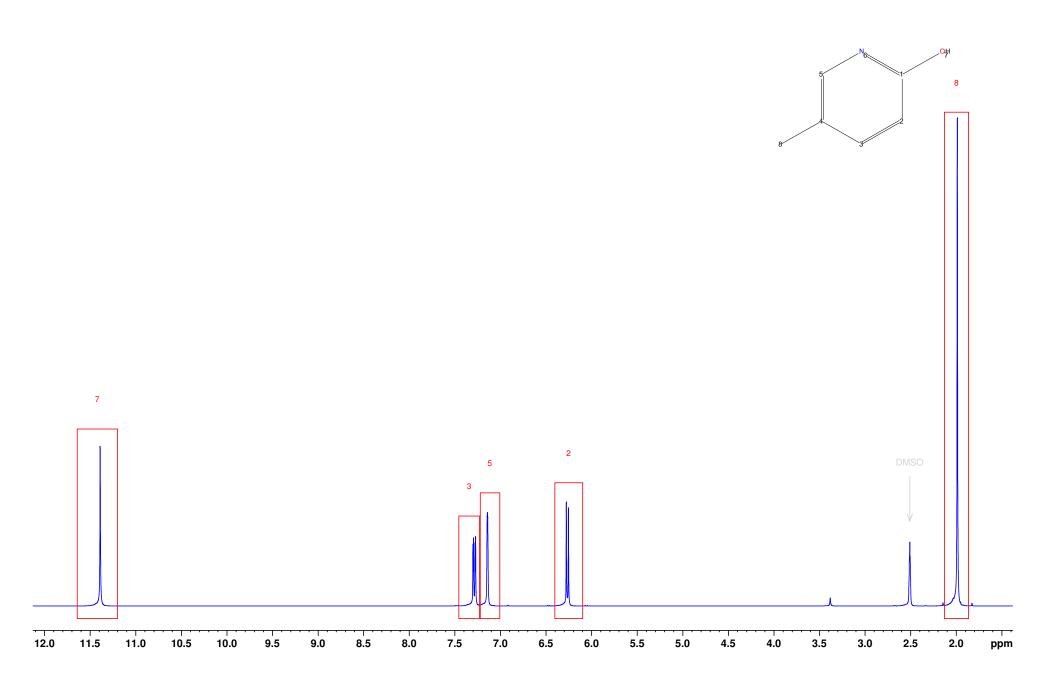
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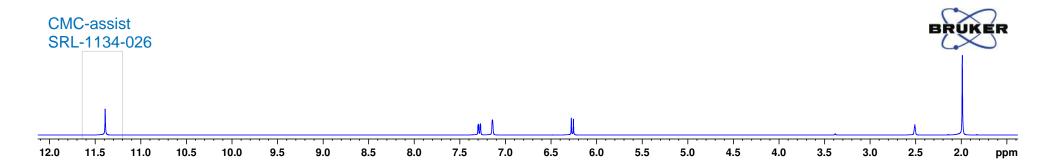


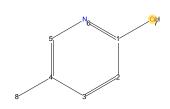


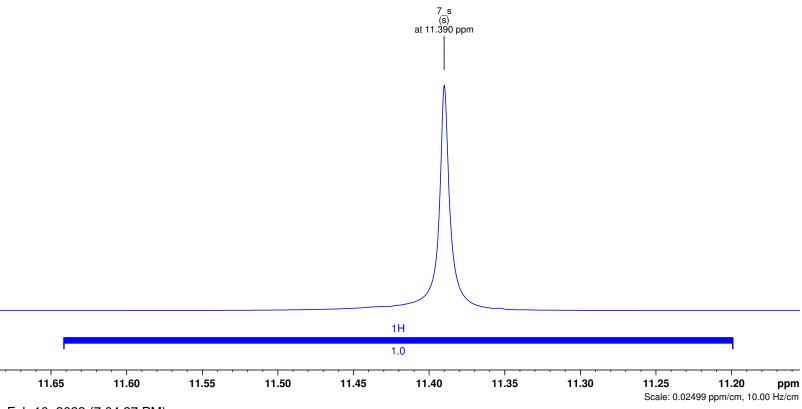




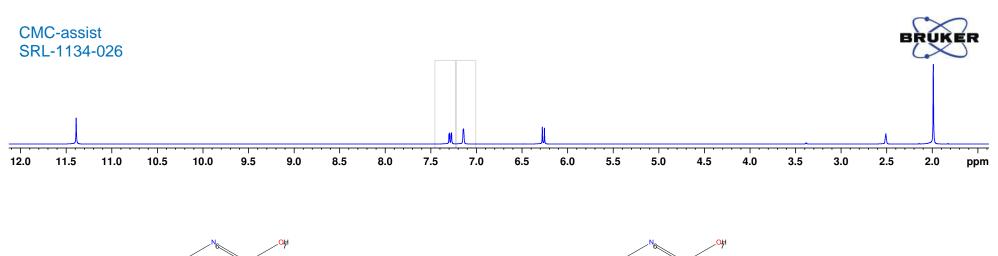
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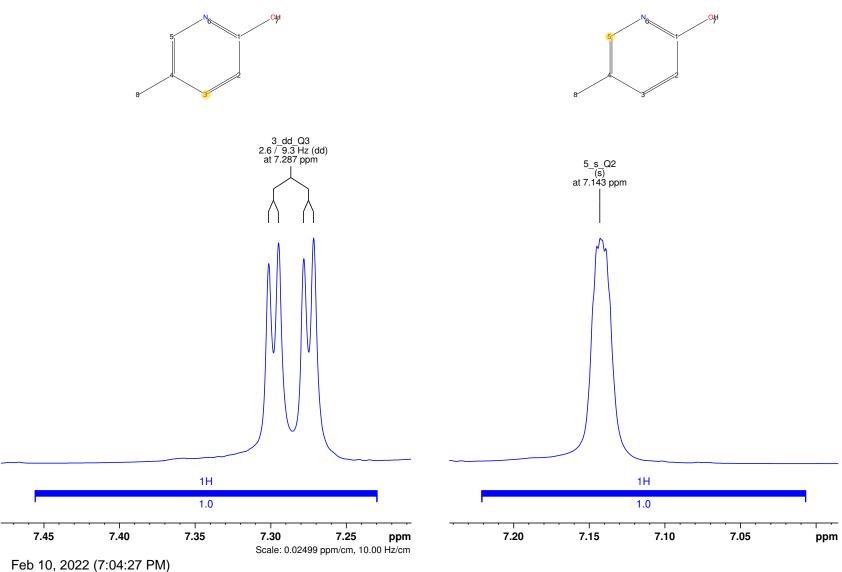




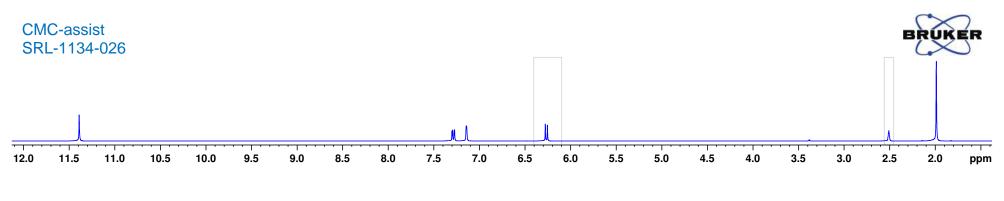


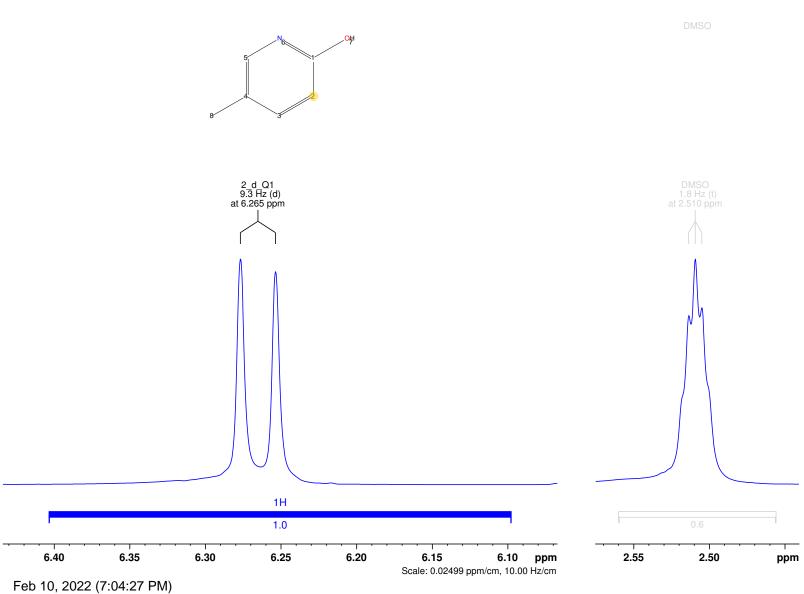
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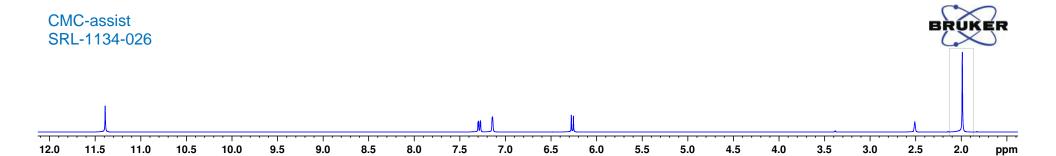


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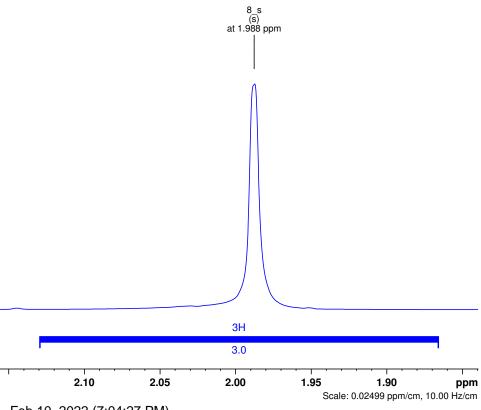




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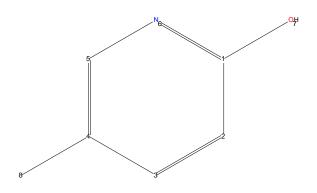


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<sup>1</sup>H NMR (400 MHz, DMSO):  $\delta$  = 11.39 (s, 1H, H-7), 7.29 (dd, J = 2.6, 9.3 Hz, 1H, H-3), 7.14 (s, 1H, H-5), 6.26 (d, J = 9.3 Hz, 1H, H-2), 1.99 ppm (s, 3H, H-8).

#### **Journal of the American Chemical Society (JACS)**

<sup>1</sup>H 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**

<sup>1</sup>H 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

<sup>1</sup>H 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**

<sup>1</sup>H-NMR (400 MHz, DMSO):  $\delta$  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**

<sup>1</sup>H 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 (s, 3H, H-8).

#### **Journal of Natural Products**

<sup>1</sup>H NMR (DMSO, 400 MHz)  $\delta$  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**

<sup>1</sup>H NMR (DMSO, 400 MHz):  $\delta_{H}$  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).

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#### **Planta Medica**

<sup>1</sup>H NMR (DMSO, 400 MHz)  $\delta$  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**

<sup>1</sup>H 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 (s, 3H, H-8).

## **Phytochemistry**

<sup>1</sup>H NMR (DMSO, 400 MHz):  $\delta_{H}$  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**

<sup>1</sup>H NMR (DMSO, 400 MHz):  $\delta$  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**

<sup>1</sup>H 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 (s, 3H, H-8).

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# CMC-assist

## 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 February 10, 2022 6:43:56 PM IST

Acquisition date:

Solvent:

Z163739\_0060 (PI HR-400-S1-BBF/H/D-5.0-Z SP) Probe:

Eretic reference:

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.

13

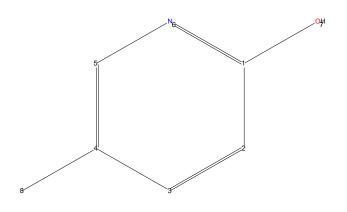
12

11

10

Chemical Formula: C<sub>6</sub>H<sub>7</sub>NO Molecular Weight: 109.1



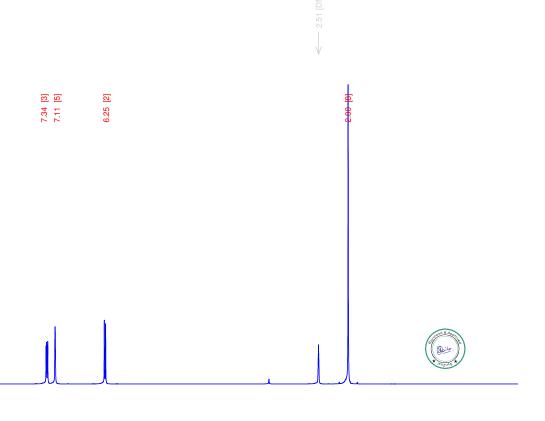




Sum formula: C<sub>6</sub>H<sub>7</sub>NO

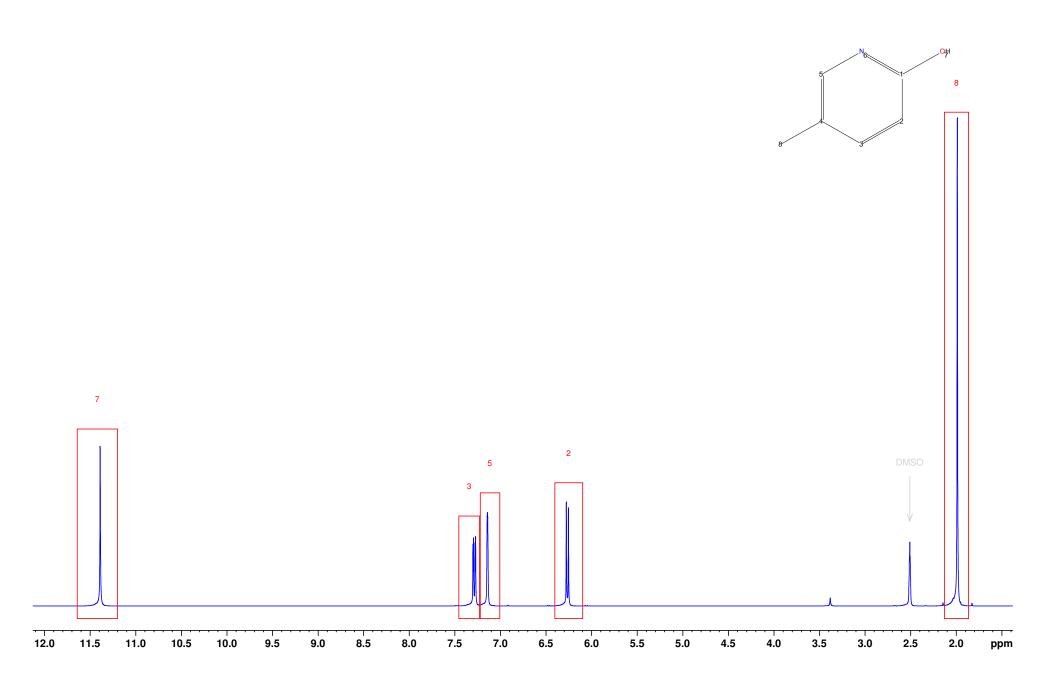
Molecular Mass: 109.05 Da

Automatic analysis generated by Bruker CMC (b:105). All results have been created exlusively by automatic analysis. Report generated by Bruker CMC-assist TopSpin 4.1.1 (of 2020-12-02 01:36:53), on 'CZC84970T5' as 'root'

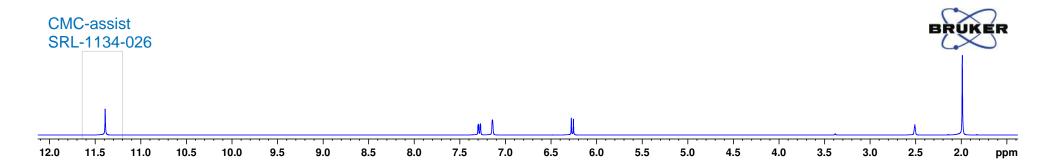


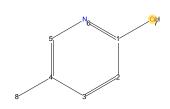


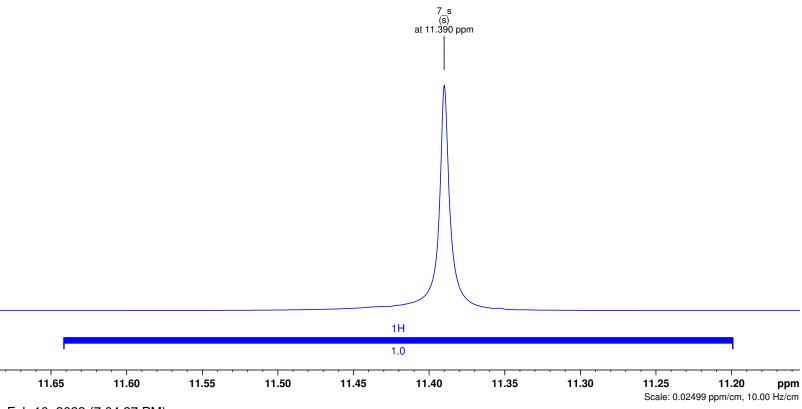




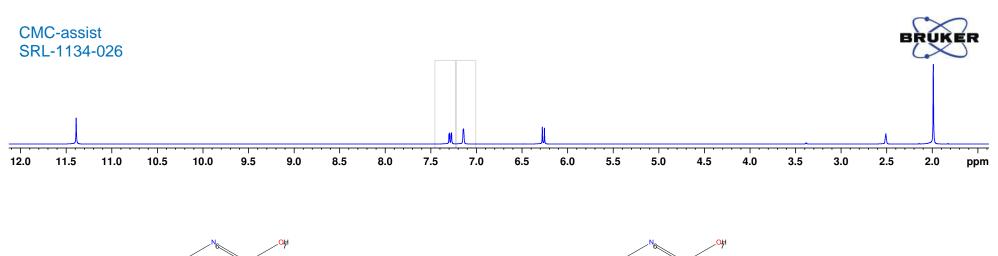
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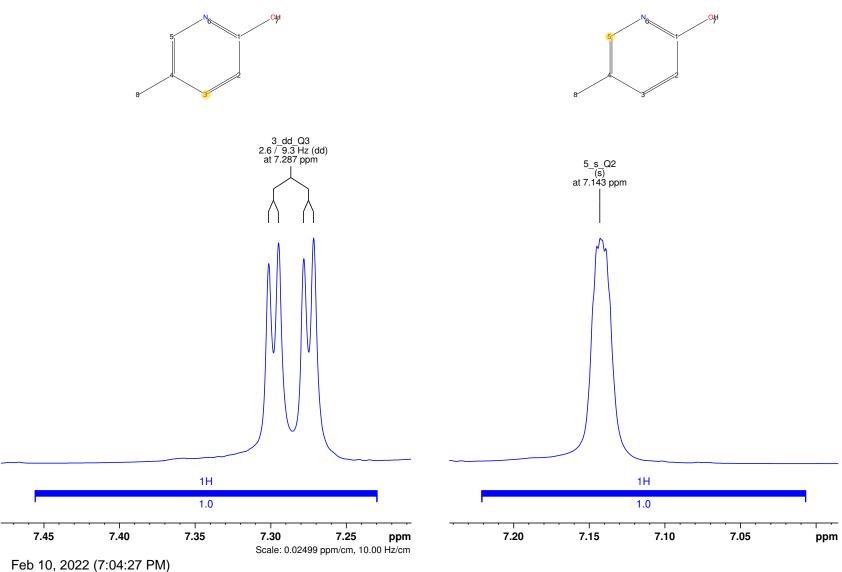




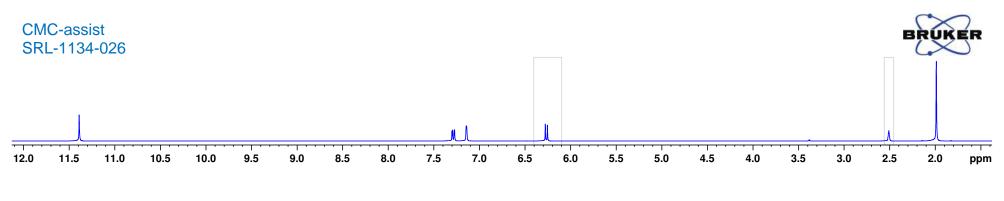


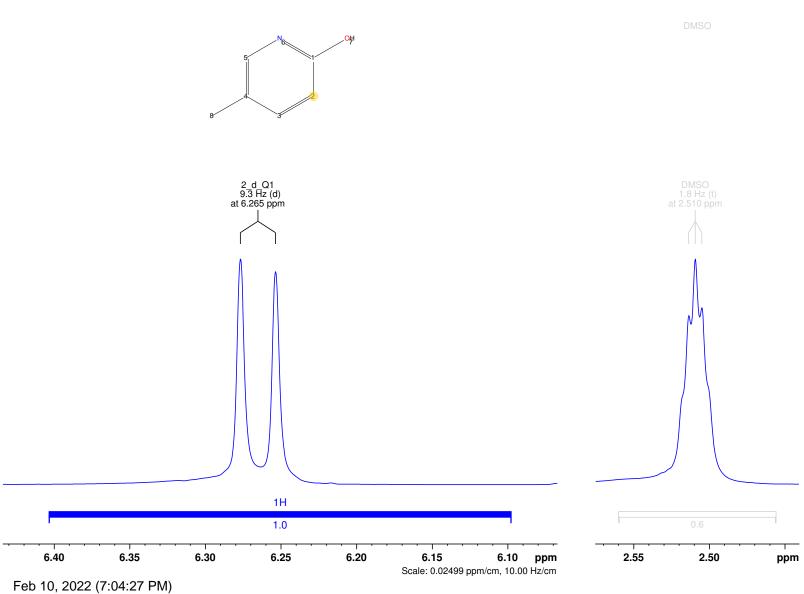
Feb 10, 2022 (7:04:27 PM)



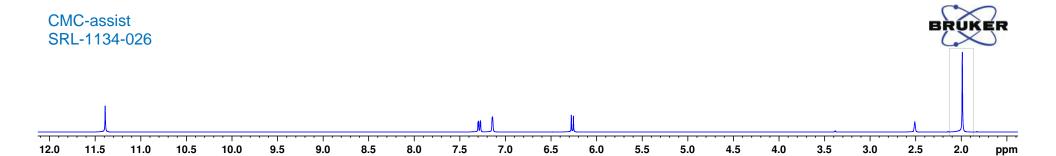


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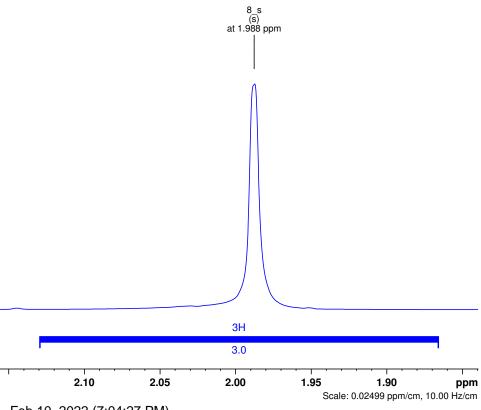




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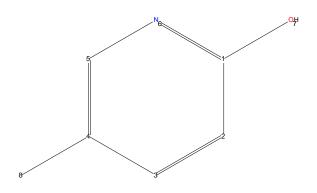


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# 1D1H Assignments

Position, coupling, integral
1.99 ppm, s, 3H
8
6.26 ppm, d (9.3Hz), 1H
2.7.14 ppm, s, 1H
7.29 ppm, dd (2.6, 9.3Hz), 1H
311.39 ppm, s, 1H
2.51 ppm, t (1.8Hz), 0H
Assignment
8
7
- not assigned -



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# The spectral description in various Journal formats:

# **Journal of Organic Chemistry (JOC)**

<sup>1</sup>H NMR (DMSO, 400 MHz):  $\delta_{H}$  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**

<sup>1</sup>H 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)**

<sup>1</sup>H 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**

<sup>1</sup>H 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

<sup>1</sup>H 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**

<sup>1</sup>H-NMR (400 MHz, DMSO):  $\delta$  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**

<sup>1</sup>H 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 (s, 3H, H-8).

#### **Journal of Natural Products**

<sup>1</sup>H NMR (DMSO, 400 MHz)  $\delta$  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**

<sup>1</sup>H NMR (DMSO, 400 MHz):  $\delta_{H}$  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).

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#### **Planta Medica**

<sup>1</sup>H NMR (DMSO, 400 MHz)  $\delta$  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**

<sup>1</sup>H 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 (s, 3H, H-8).

## **Phytochemistry**

<sup>1</sup>H NMR (DMSO, 400 MHz):  $\delta_{H}$  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**

<sup>1</sup>H NMR (DMSO, 400 MHz):  $\delta$  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**

<sup>1</sup>H 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 (s, 3H, H-8).

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