

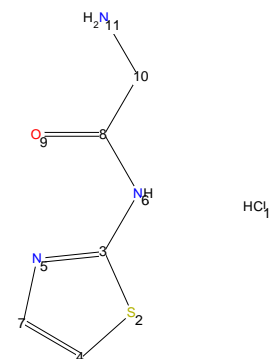
A10\_OS\_Plate01\_A10

Consistency: OK\*, unknown purity\*

Data set 1H: A10\_OS\_Plate01\_A10\_1\_1  
 Structure: E:\TopSpin4.0.8\data\EU\_OpenScreen\CMCq\Franzi\_CMCq\nmr\Plate01  
 Acquisition date: May 7, 2021 5:00:05 AM CEST  
 Solvent: 5%DMSOinH2O\_1.7mm  
 Probe: Z150329\_0015 (CP TCI 600S3 H-C/N-D-01.7 Z)  
 Eretic reference:

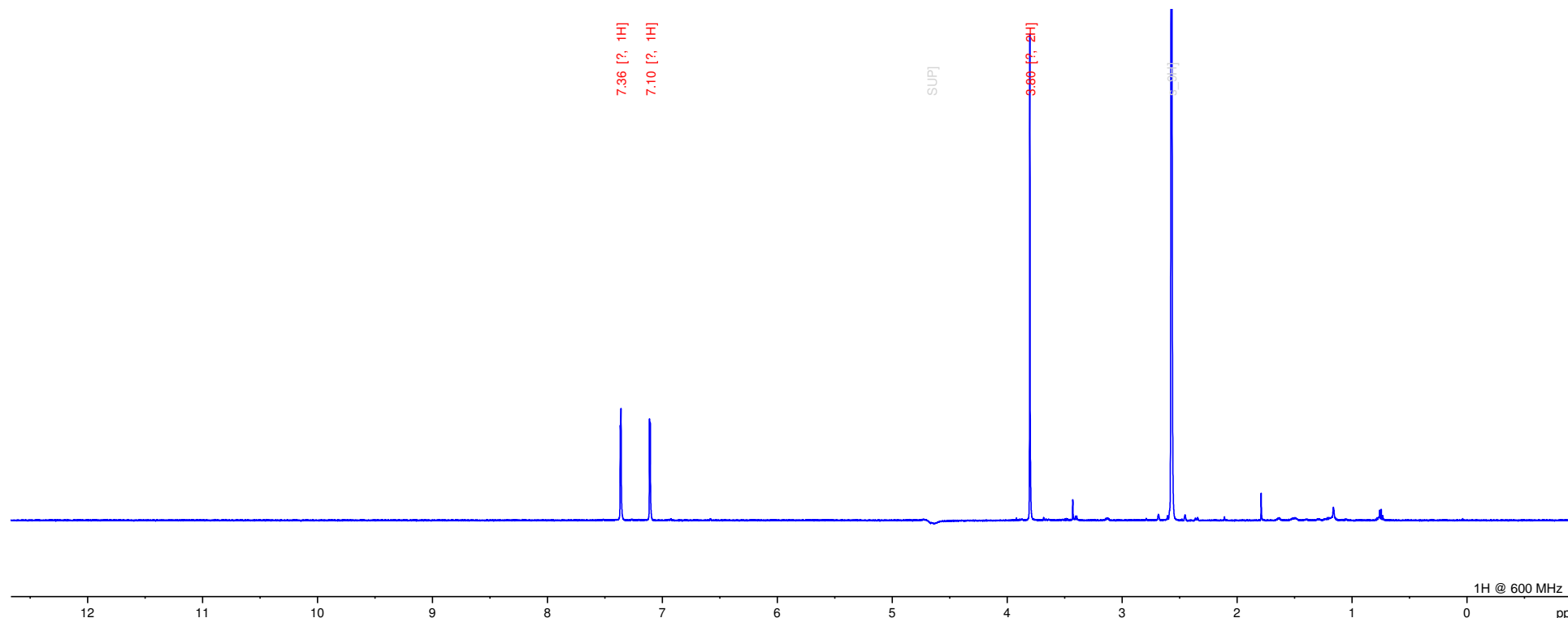
**Comments:**  
 Automatic evaluation was aborted. Automatic evaluation: Spectrum and structure do not match. Only invalid solutions were found. Automatic evaluation: Spectrum and structure do not match. Only invalid solutions were found. Automatic evaluation: Spectrum and structure do not match. Only invalid solutions were found. The automatic evaluation ended due to technical problems. No results are available. No assignment could be found for the combination of the structure and spectrum. Please check manually if the structure is in agreement with the spectrum. Automatically generated inconsistencies might also be caused by unknown impurities in the spectrum. No assignment could be found for the combination of the structure and spectrum. Please check manually if the structure is in agreement with the spectrum.

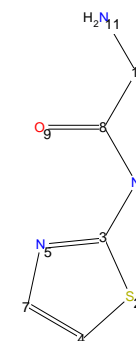
Signature:



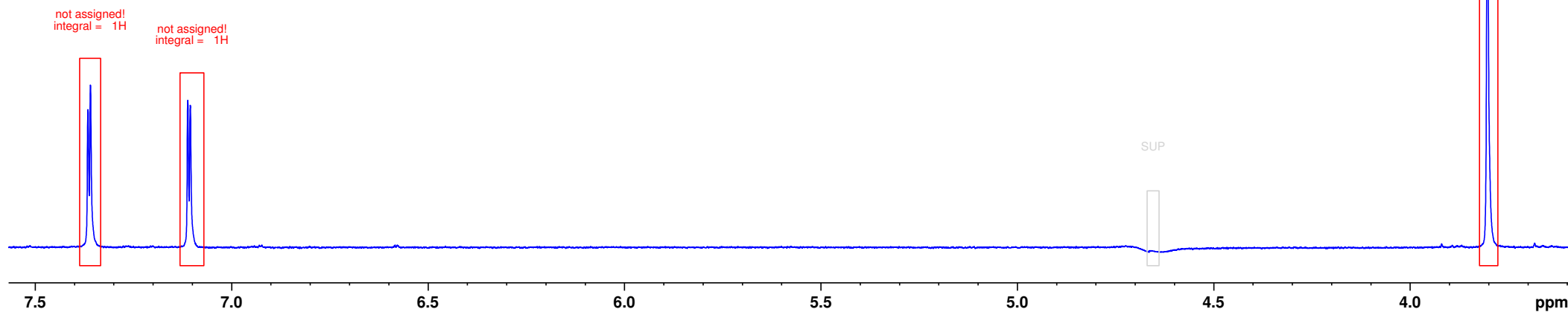
Sum formula:  
 C<sub>5</sub>H<sub>6</sub>ClN<sub>3</sub>OS  
 Molecular Mass:  
 193.01 Da

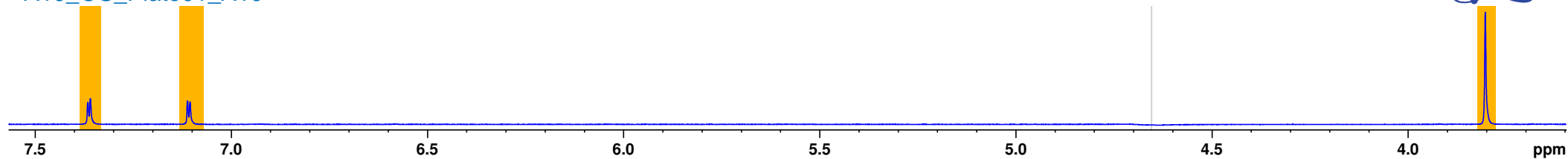
Automatic analysis generated by Bruker CMC (b:17).  
 One or more results have not been created by automatic analysis, or edited manually: marked by '\*'.  
 Report generated by Bruker CMC-assist TopSpin 4.1.3 (of 2021-06-28 13:00:50), on 'HANNESDESKTOP' as 'hanne'





not assigned!  
integral = 2H  
HCl<sub>1</sub>



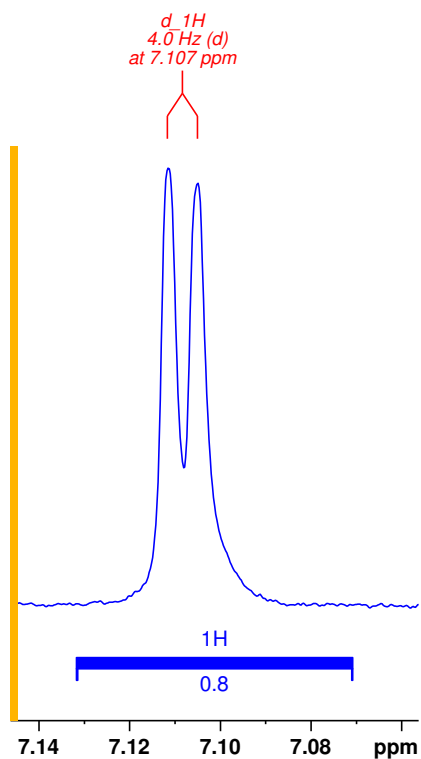
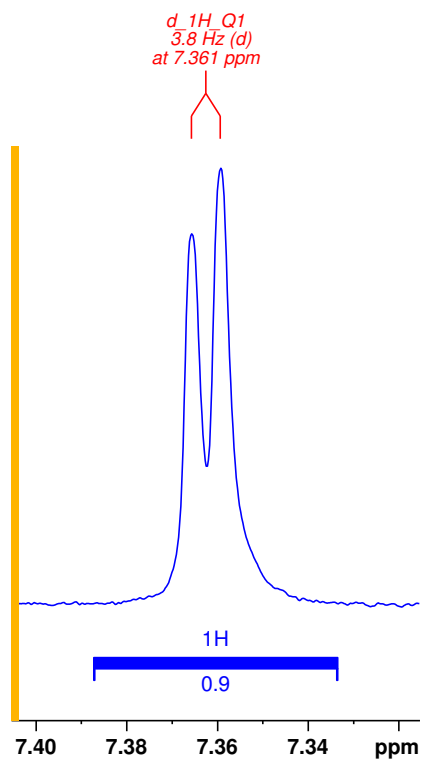


not assigned!  
integral = 1H

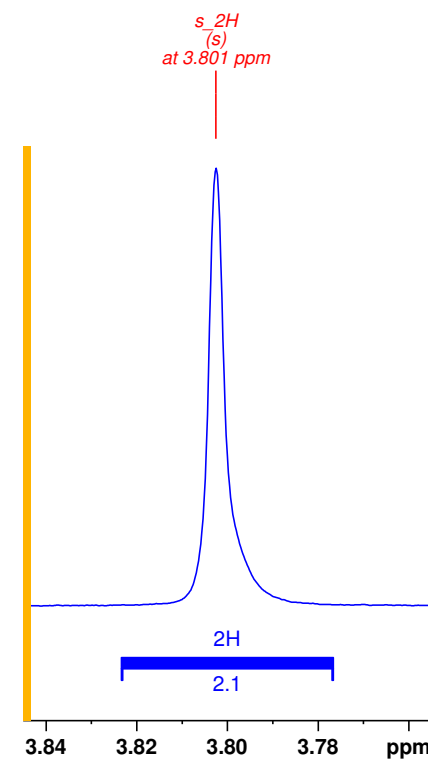
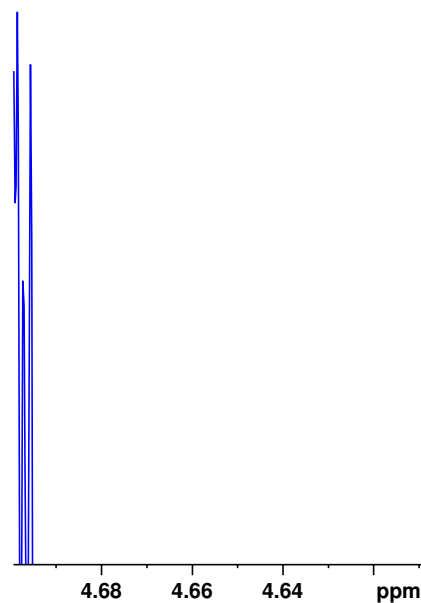
not assigned!  
integral = 1H

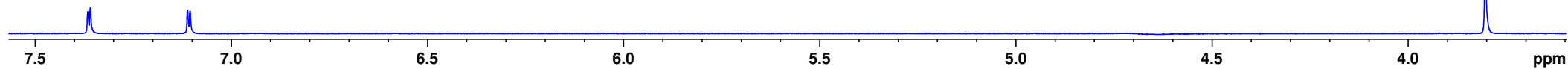
SUP

not assigned!  
integral = 2H

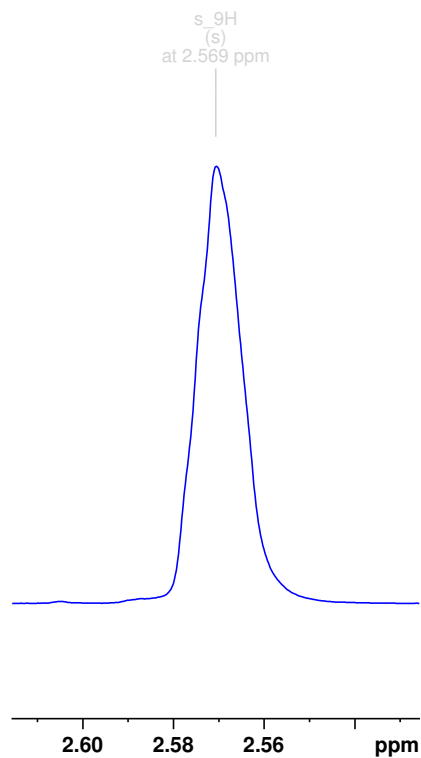


SUP  
(s)  
at 4.655 ppm





s\_9H



## 1D1H Assignments

Position, coupling, integral

7.36 ppm, d (3.8Hz), 1H

2.57 ppm, s

3.80 ppm, s, 2H

7.11 ppm, d (4.0Hz), 1H

4.65 ppm, s

Assignment

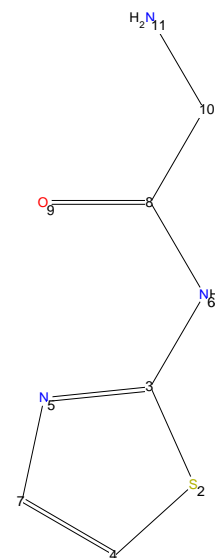
- not assigned -

- not assigned -

- not assigned -

- not assigned -

- not assigned -



HCl

## The spectral description in various Journal formats:

### Journal of Organic Chemistry (JOC)

$^1\text{H}$  NMR ( $\delta$ %DMSO in  $\text{H}_2\text{O}$ , 1.7 mm, 600 MHz):  $\delta_{\text{H}}$  7.36 (1H, d,  $J$  = 3.8 Hz), 7.11 (1H, d,  $J$  = 4.0 Hz), 3.80 (2H, s).

### Journal of Medicinal Chemistry

$^1\text{H}$  NMR (600 MHz,  $\delta$ %DMSO in  $\text{H}_2\text{O}$ , 1.7 mm):  $\delta$  = 7.36 (d,  $J$  = 3.8 Hz, 1H), 7.11 (d,  $J$  = 4.0 Hz, 1H), 3.80 ppm (s, 2H).

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

$^1\text{H}$  NMR (600 MHz,  $\delta$ %DMSO in  $\text{H}_2\text{O}$ , 1.7 mm):  $\delta$ , ppm 7.36 (d,  $J$  = 3.8 Hz, 1H), 7.11 (d,  $J$  = 4.0 Hz, 1H), 3.80 (s, 2H).

### Angewandte Chemie

$^1\text{H}$  NMR (600 MHz,  $\delta$ %DMSO in  $\text{H}_2\text{O}$ , 1.7 mm):  $\delta$ =7.36 (d,  $J$ =3.8 Hz, 1H), 7.11 (d,  $J$ =4.0 Hz, 1H), 3.80 ppm (s, 2H);

### Chemistry, a European Journal

$^1\text{H}$  NMR (600 MHz,  $\delta$ %DMSO in  $\text{H}_2\text{O}$ , 1.7 mm):  $\delta$ =7.36 (d,  $J$ =3.8 Hz, 1H), 7.11 (d,  $J$ =4.0 Hz, 1H), 3.80 ppm (s, 2H);

### Helvetica Chimica Acta

$^1\text{H}$ -NMR (600 MHz,  $\delta$ %DMSO in  $\text{H}_2\text{O}$ , 1.7 mm):  $\delta$  7.36 (d,  $J$  = 3.8 Hz); 7.11 (d,  $J$  = 4.0 Hz); 3.80 (s).

### Tetrahedron Letters

$^1\text{H}$  NMR (600 MHz,  $\delta$ %DMSO in  $\text{H}_2\text{O}$ , 1.7 mm)  $\delta$  7.36 (d,  $J$  = 3.8 Hz, 1H), 7.11 (d,  $J$  = 4.0 Hz, 1H), 3.80 (s, 2H).

### Journal of Natural Products

$^1\text{H}$  NMR ( $\delta$ %DMSO in  $\text{H}_2\text{O}$ , 1.7 mm, 600 MHz)  $\delta$  7.36 (1H, d,  $J$  = 3.8 Hz), 7.11 (1H, d,  $J$  = 4.0 Hz), 3.80 (2H, s);

### Analytical Chemistry

$^1\text{H}$  NMR ( $\delta$ %DMSO in  $\text{H}_2\text{O}$ , 1.7 mm, 600 MHz):  $\delta_{\text{H}}$  7.36 (1H, d,  $J$  = 3.8 Hz), 7.11 (1H, d,  $J$  = 4.0 Hz), 3.80 (2H, s).

#### Planta Medica

$^1\text{H}$  NMR ( $\delta$ %DMSO in  $\text{H}_2\text{O}$ , 1.7 mm, 600 MHz)  $\delta$  7.36 (1H, d,  $J$  = 3.8 Hz), 7.11 (1H, d,  $J$  = 4.0 Hz), 3.80 (2H, s);

#### Organic Letters

$^1\text{H}$  NMR (600 MHz,  $\delta$ %DMSO in  $\text{H}_2\text{O}$ , 1.7 mm)  $\delta$  7.36 (d,  $J$  = 3.8 Hz, 1H), 7.11 (d,  $J$  = 4.0 Hz, 1H), 3.80 (s, 2H).

#### Phytochemistry

$^1\text{H}$  NMR ( $\delta$ %DMSO in  $\text{H}_2\text{O}$ , 1.7 mm, 600 MHz):  $\delta_{\text{H}}$  7.36 (1H, d,  $J$  = 3.8 Hz), 7.11 (1H, d,  $J$  = 4.0 Hz), 3.80 (2H, s);

#### Fitoterapia

$^1\text{H}$  NMR ( $\delta$ %DMSO in  $\text{H}_2\text{O}$ , 1.7 mm, 600 MHz):  $\delta$  7.36 (1H, d,  $J$  = 3.8 Hz), 7.11 (1H, d,  $J$  = 4.0 Hz), 3.80 (2H, s);

#### Bioorganic and Medicinal Chemistry Letters

$^1\text{H}$  NMR (600 MHz,  $\delta$ %DMSO in  $\text{H}_2\text{O}$ , 1.7 mm)  $\delta$  7.36 (d,  $J$  = 3.8 Hz, 1H), 7.11 (d,  $J$  = 4.0 Hz, 1H), 3.80 (s, 2H).