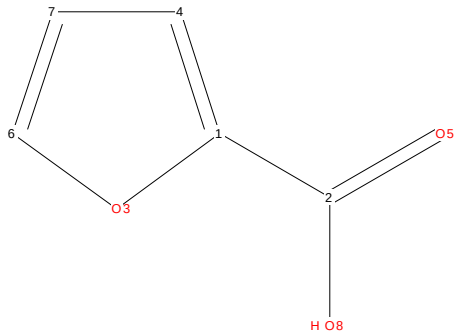


OK, 0.26 mmol/l, very high purity

Data set:	D12_rack9_D12 1 1 /opt/data/singletons/Bionet_g2/mike
Structure:	/opt/data/singletons/Bionet_g2/mike/D12_rack9_D12/1/D12_rack9_D12.mol
Acquisition date:	February 4, 2015 11:29:05 PM EST
Solvent:	H2O+D2O+DMSO
Probe:	5 mm CPQCI 1H/19F-31P/13C/15N/D Z-GRD Z117108/0008
Eretic reference:	

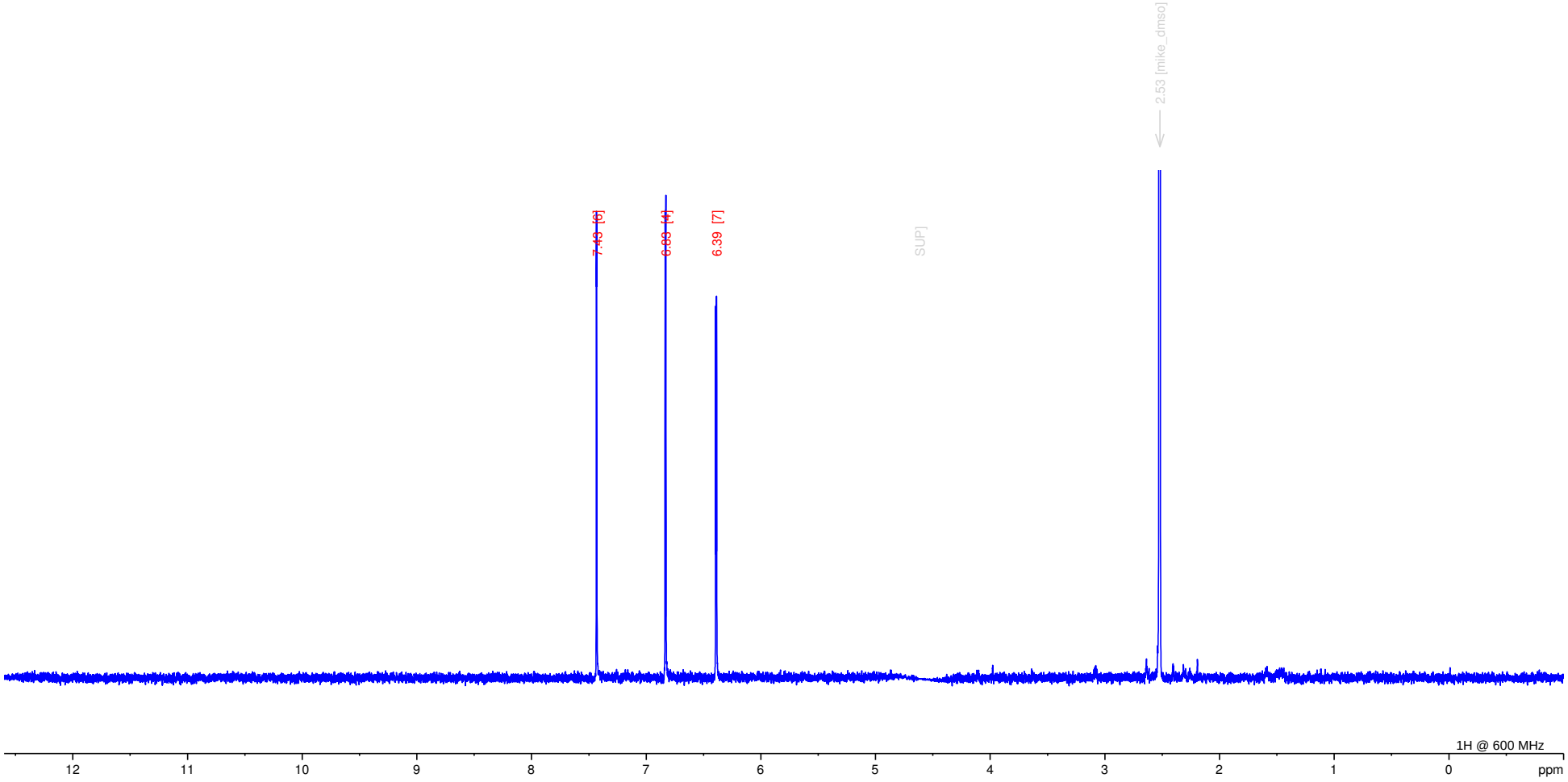
Sum formula:
$C_5H_4O_3$

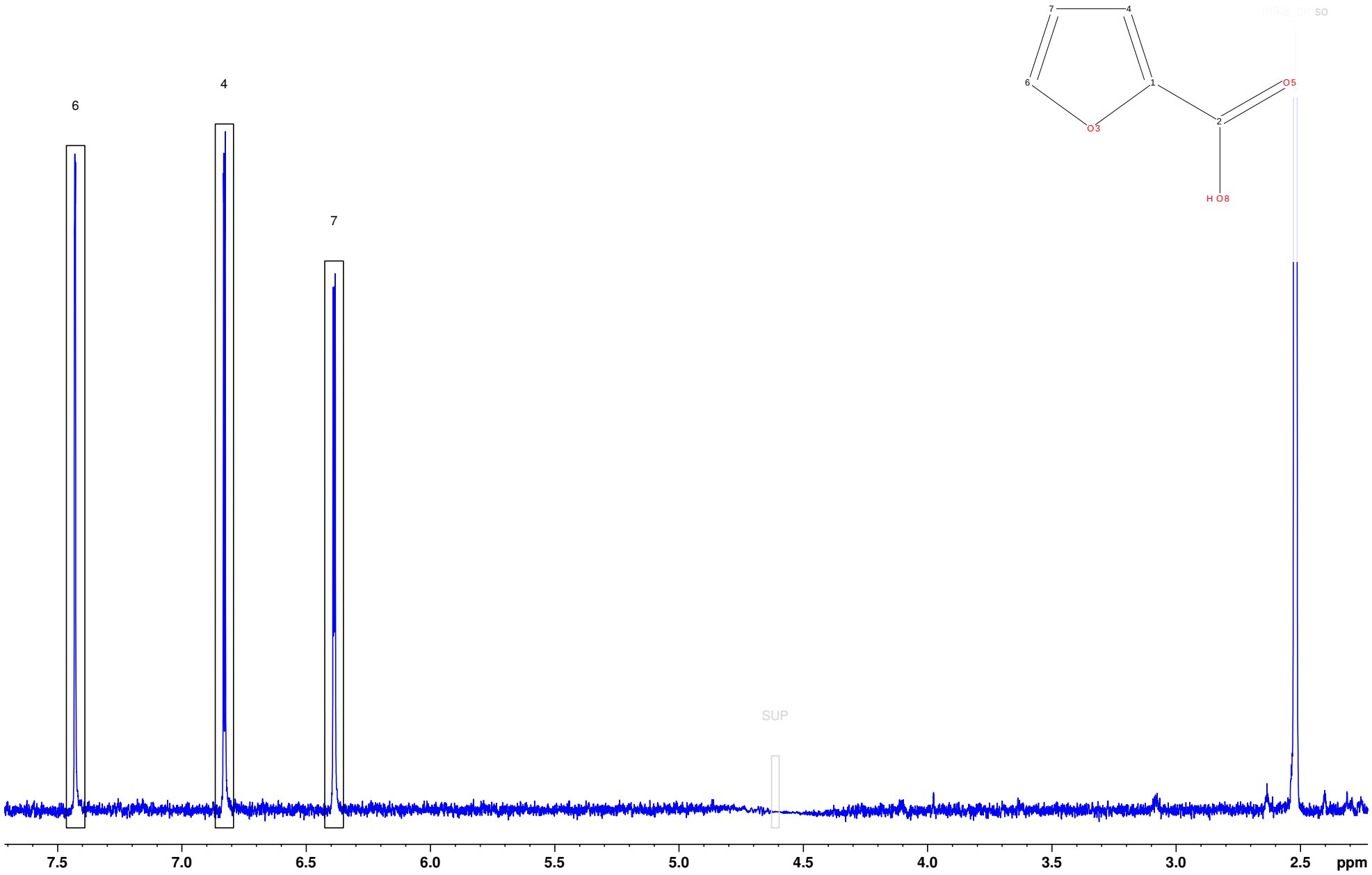
Molecular Mass:
112.02 Da

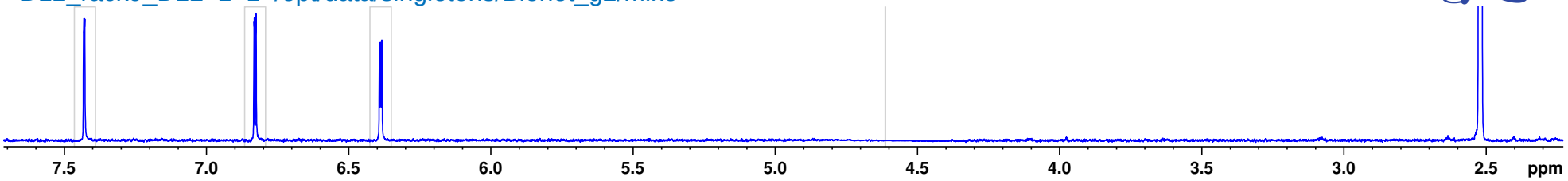
Comments:
Automatic evaluation: Spectrum and structure are in agreement.All major signals in the spectrum could be assigned. Some exchangeable protons have not been assigned . Impurity H2O not assigned.

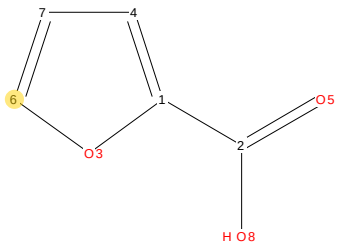
Signature:

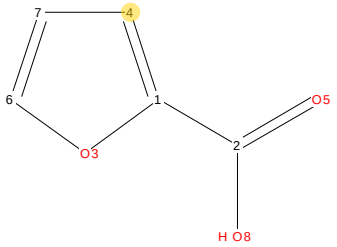
Automatic analysis generated by Bruker CMC (9639).
All results have been created exlusively by automatic analysis.
Report generated by Bruker CMC-assist 2.1, on 'aviii600' as 'nmrsu'

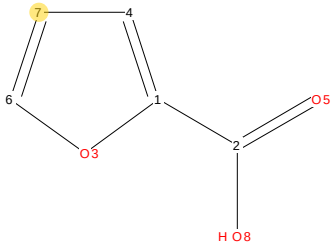



mike_dmso
6
4
7
SUP
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
ppm

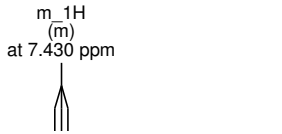


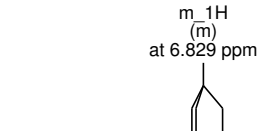


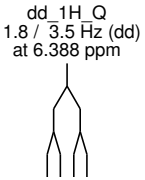




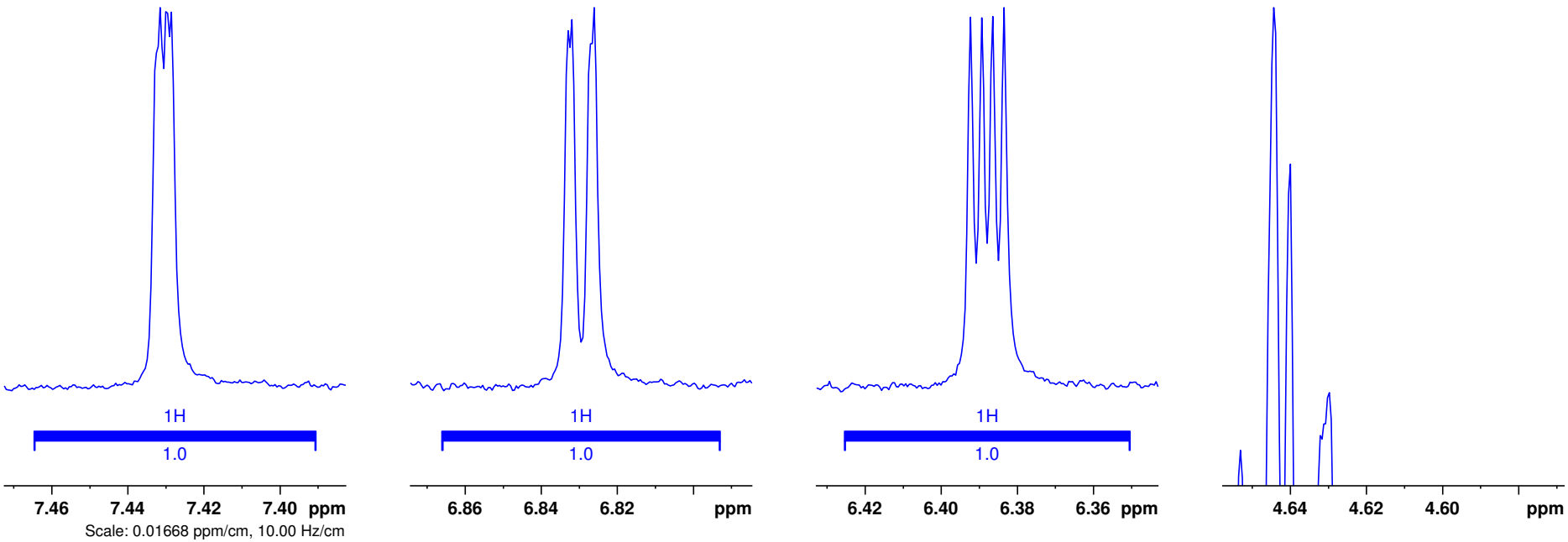
SUP



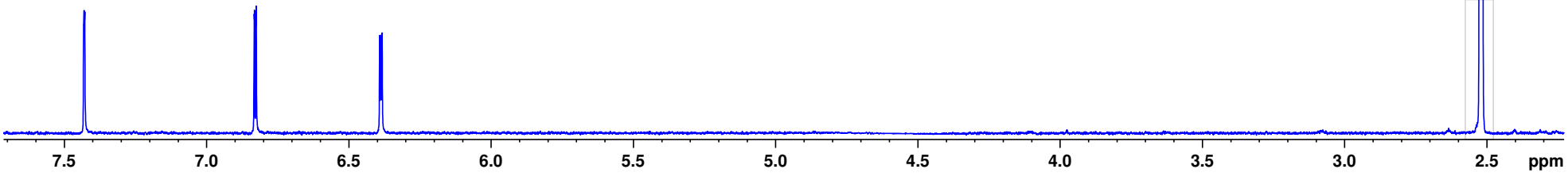




SUP
(m)
at 4.613 ppm

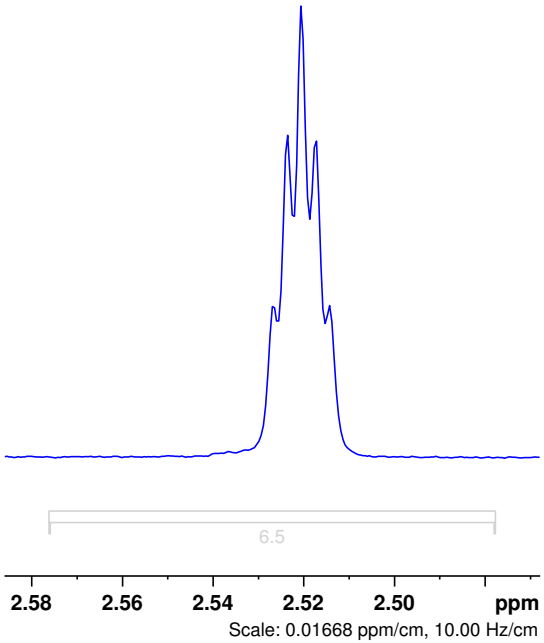


Scale: 0.01668 ppm/cm, 10.00 Hz/cm



mike_dmso

mike_dmso
(m)
at 2.521 ppm



1D1H Assignments

Position, coupling, integral

2.52 ppm, m, 0H

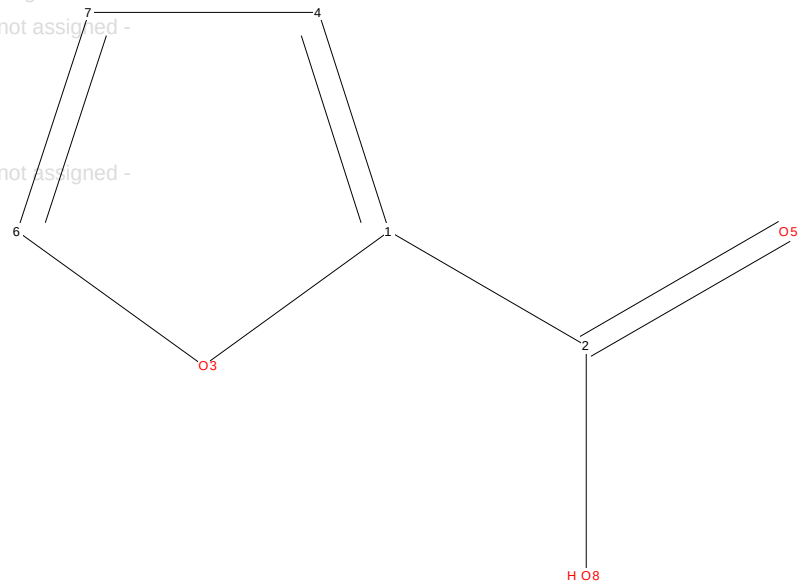
6.39 ppm, dd (1.8, 3.5Hz), 1H

6.83 ppm, m, 1H

7.43 ppm, m, 1H

4.61 ppm, m

Assignment
- not assigned -
7
4
6
- not assigned -



The spectral description in various Journal formats:

Journal of Organic Chemistry (JOC)

^{1}H NMR (600 MHz, H_2O+D_2O+DMSO) 7.44 - 7.43 (1H, m), 6.84 - 6.82 (1H, m), 6.39 (1H, dd, *J*=1.8, 3.5 Hz);

Journal of Medicinal Chemistry

^{1}H NMR (600 MHz, H_2O+D_2O+DMSO) δ 7.44 - 7.43 (m, 1H), 6.84 - 6.82 (m, 1H), 6.39 (dd, *J*=1.8, 3.5 Hz, 1H).

Journal of the American Chemical Society (JACS)

^{1}H NMR (600 MHz, H_2O+D_2O+DMSO): δ, ppm 7.44 - 7.43 (1H, m), 6.84 - 6.82 (1H, m), 6.39 (1H, dd, *J* = 1.8, 3.5 Hz).

Angewandte Chemie

^{1}H-NMR (600 MHz, H_2O+D_2O+DMSO): δ 7.44 - 7.43 (m, 1H), 6.84 - 6.82 (m, 1H), 6.39 (dd, *J*=1.8, 3.5 Hz, 1H).

Chemistry, a European Journal

^{1}H-NMR (600 MHz, H_2O+D_2O+DMSO) δ= 7.44 - 7.43 (m, 1H), 6.84 - 6.82 (m, 1H), 6.39 (dd, *J*=1.8, 3.5 Hz, 1H);

Helvetica Chimica Acta

^{1}H-NMR: 7.44 - 7.43 (m, 1 H), 6.84 - 6.82 (m, 1 H), 6.39 (dd, *J*=1.8, 3.5 Hz, 1 H)

Tetrahedron Letters

^{1}H-NMR (600 MHz, H_2O+D_2O+DMSO) δ 7.44 - 7.43 (m, 1H), 6.84 - 6.82 (m, 1H), 6.39 (dd, 1H, *J* = 1.8, 3.5 Hz).