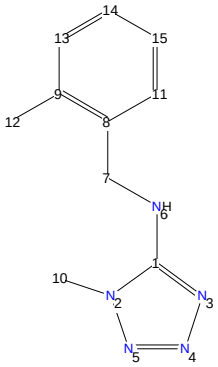
CMC-assist

iNEXT_G2_Plate4



Consistency: OK

Data set 1H:	iNEXT_G2_Plate4 14 1 C:\data\iNEXT-G2\nmr
Structure:	C:/data/iNEXT-G2/nmr/iNEXT_G2_Plate4/14/B02.mol
Acquisition date:	May 3, 2019 12:40:46 PM CEST
Solvent:	H2O+D2O
Probe:	Z129773_0008 (CPP TCI 600S3 H&F-C/N-D-05 Z)
Eretic reference:	

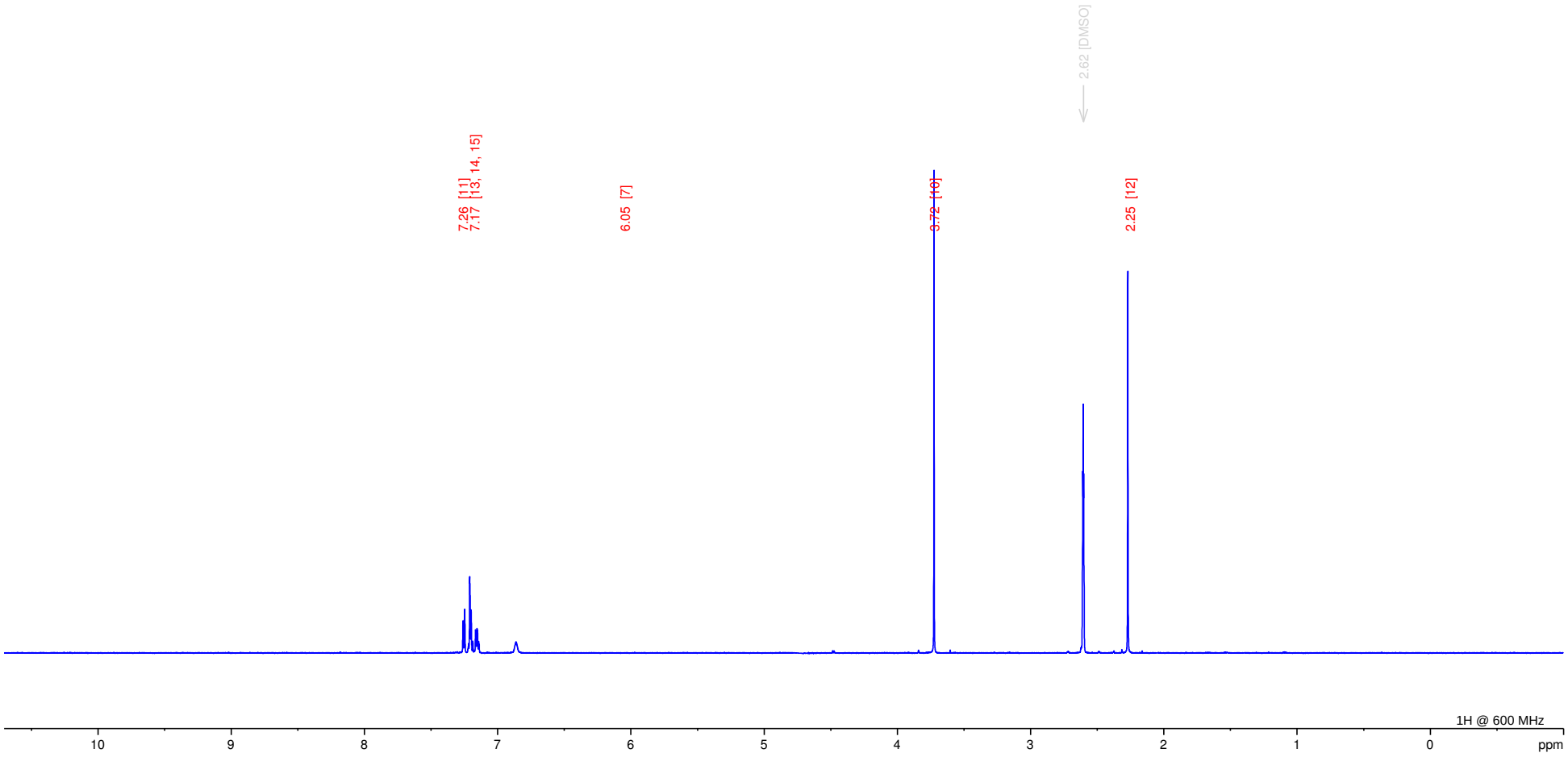
Sum formula:
$C_{10}H_{13}N_5$

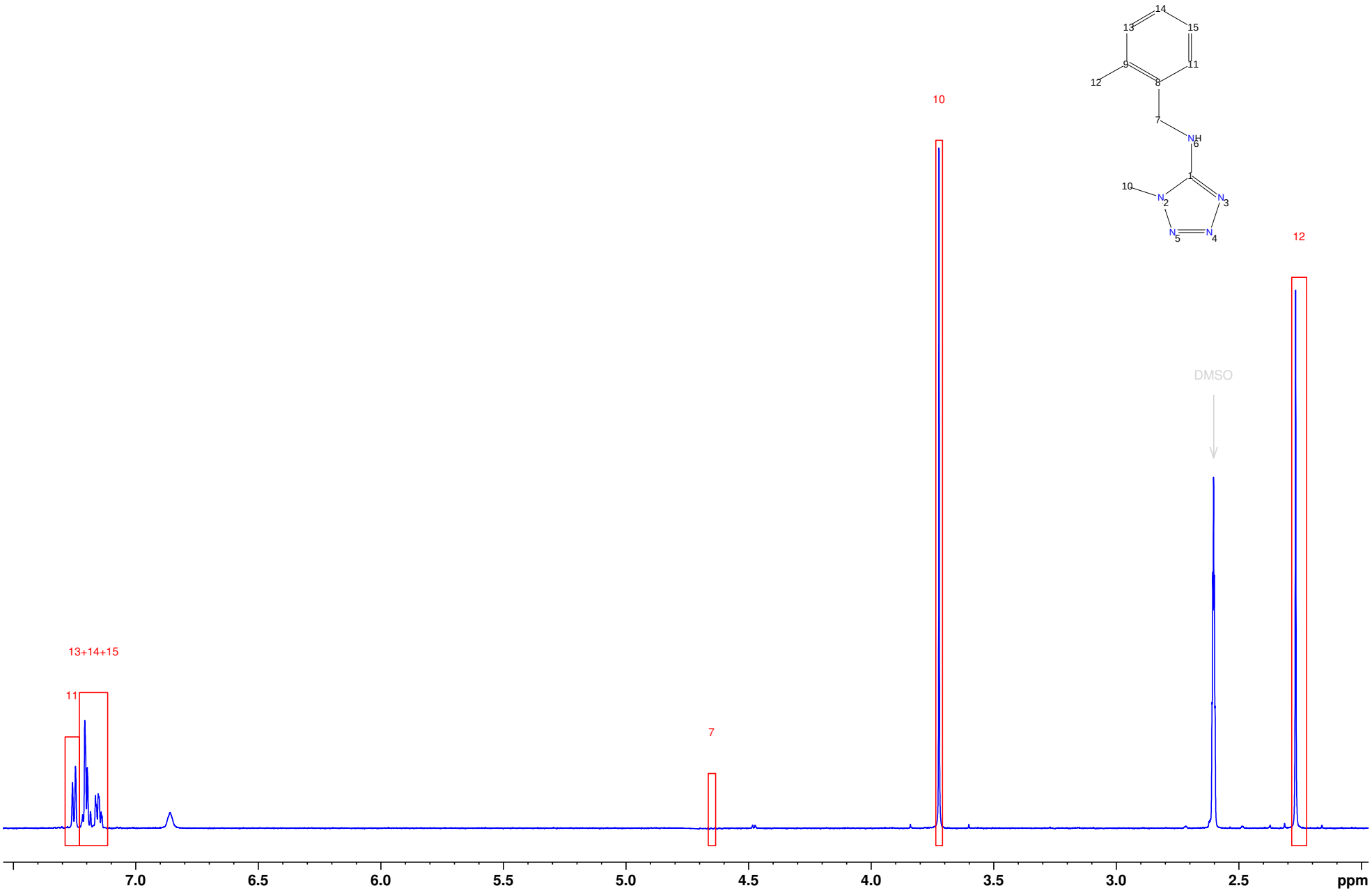
Molecular Mass:
203.12 Da

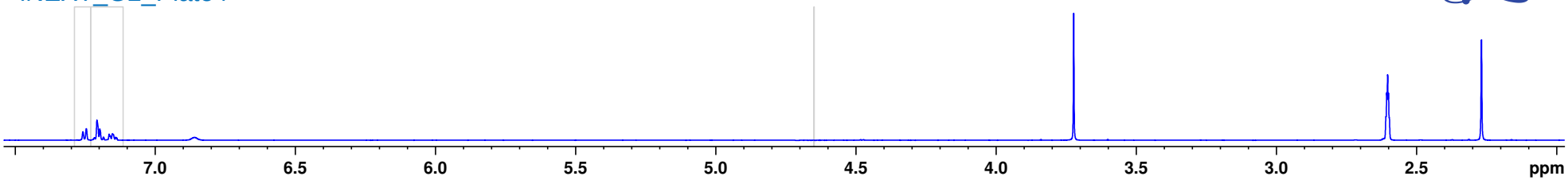
Comments:
Automatic evaluation: Spectrum and structure are in agreement.
All major signals in the spectrum could be assigned. Some exchangeable protons have not been assigned. Satellites of impurity DMSO not assigned. Satellites of impurity DMSO not assigned. Impurity Imp1 not assigned. Impurity Imp2 not assigned.

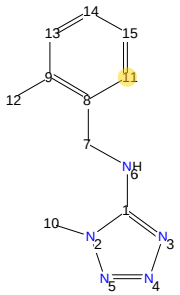
Signature:

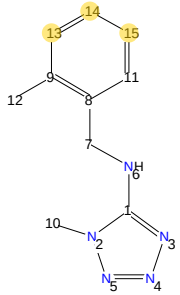
Automatic analysis generated by Bruker CMC (b:143).
All results have been created exlusively by automatic analysis.
Report generated by Bruker CMC-assist TopSpin 3.6.1 (of 2018-12-20 14:06:00), on 'X1' as 'ric'

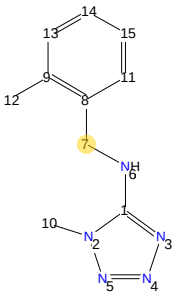


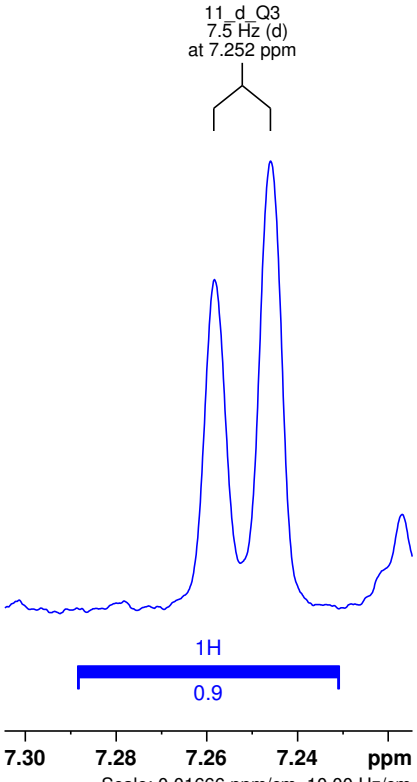

14
13
15
9
11
12
8
7
NH
6
1
10
N
2
N
3
N
5
N
4
10
12
DMSO
13+14+15
11
7
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
ppm

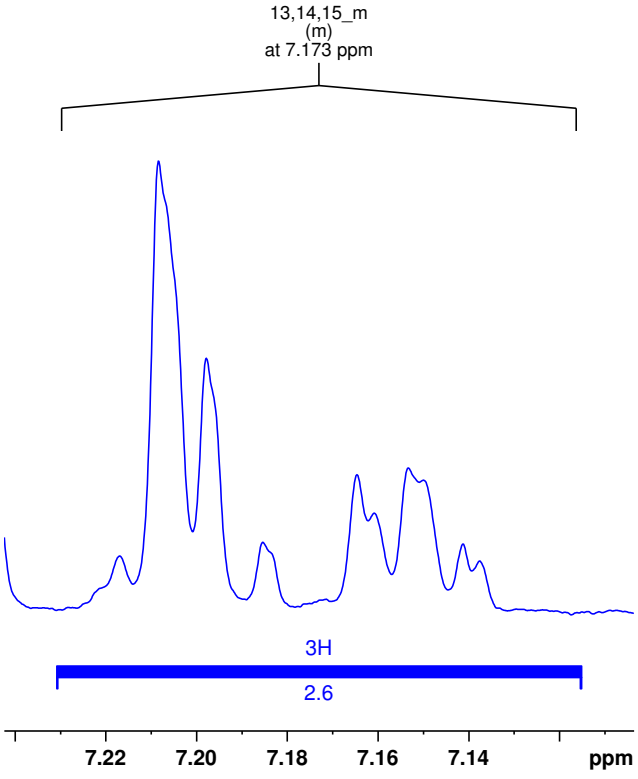


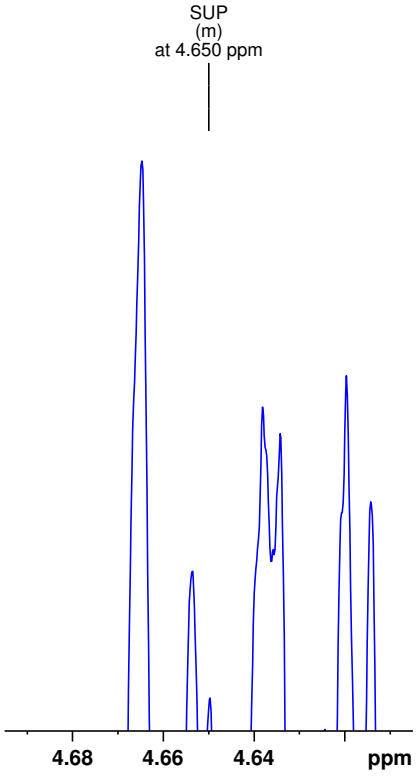




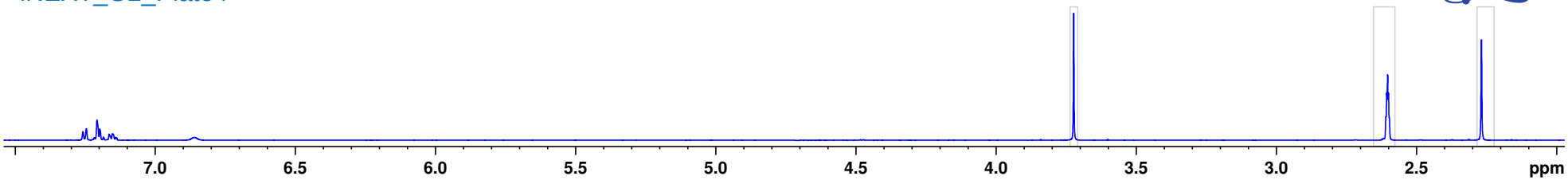


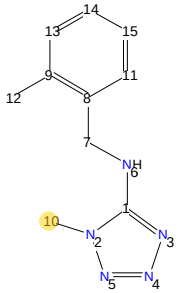




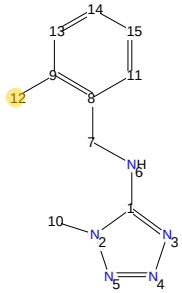


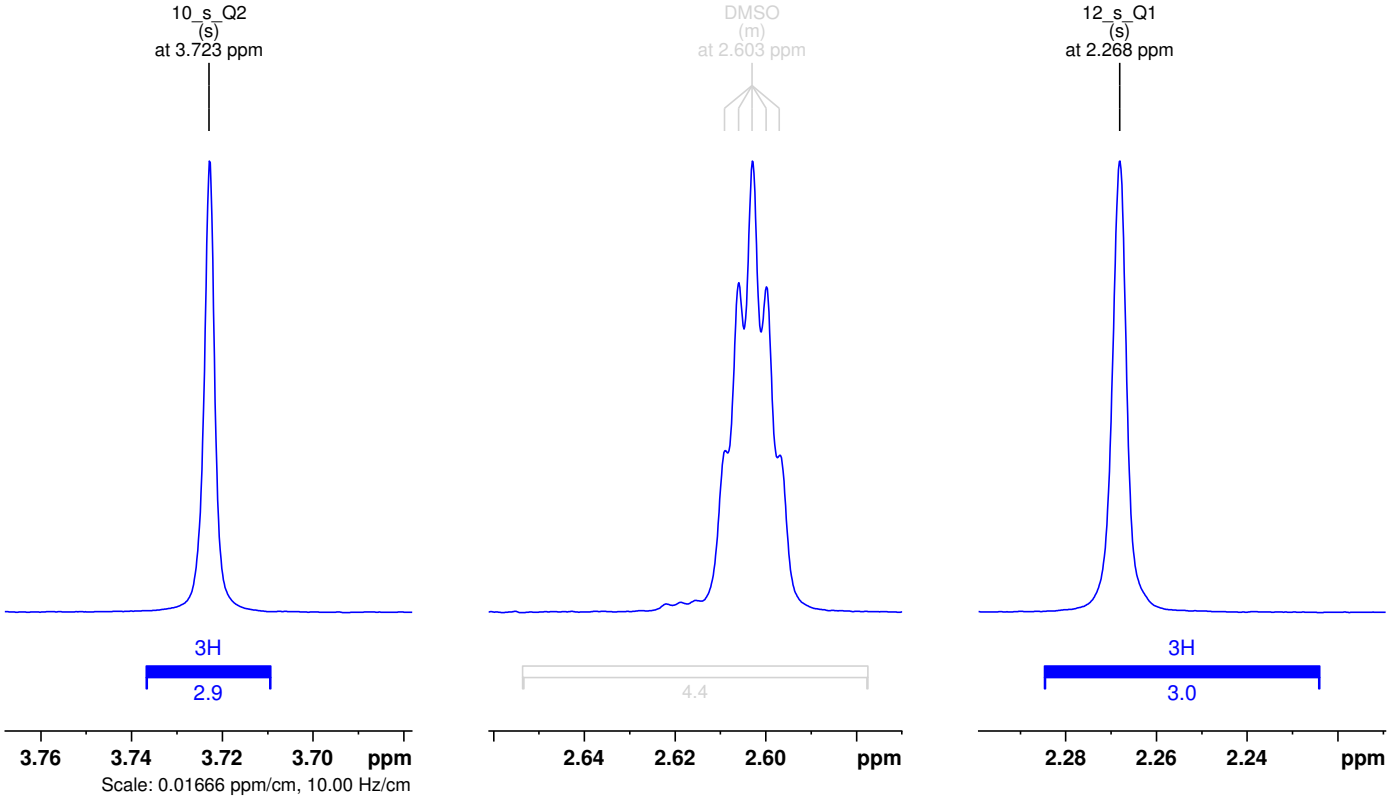
Scale: 0.01666 ppm/cm, 10.00 Hz/cm





DMSO

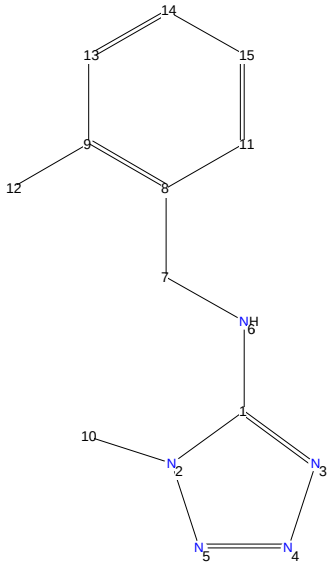




Scale: 0.01666 ppm/cm, 10.00 Hz/cm

1D1H Assignments

Position, coupling, integral	Assignment
2.27 ppm, s, 3H	12
2.60 ppm, m, 0H	- not assigned -
3.72 ppm, s, 3H	10
7.17 ppm, m, 3H	13 + 14 + 15
7.25 ppm, d (7.5Hz), 1H	11
4.65 ppm, m	7



The spectral description in various Journal formats:

Journal of Organic Chemistry (JOC)

^{1}H NMR (600 MHz, H_2O+D_2O) 7.25 (1H, d, *J*=7.5 Hz), 7.23 - 7.12 (3H, m), 3.72 (3H, s), 2.27 (3H, s);

Journal of Medicinal Chemistry

^{1}H NMR (600 MHz, H_2O+D_2O) δ 7.25 (d, *J*=7.5 Hz, 1H), 7.23 - 7.12 (m, 3H), 3.72 (s, 3H), 2.27 (s, 3H).

Journal of the American Chemical Society (JACS)

^{1}H NMR (600 MHz, H_2O+D_2O): δ, ppm 7.25 (1H, d, *J* = 7.5 Hz), 7.23 - 7.12 (3H, m), 3.72 (3H, s), 2.27 (3H, s).

Angewandte Chemie

^{1}H-NMR (600 MHz, H_2O+D_2O): δ 7.25 (d, *J*=7.5 Hz, 1H), 7.23 - 7.12 (m, 3H), 3.72 (s, 3H), 2.27 (s, 3H).

Chemistry, a European Journal

^{1}H-NMR (600 MHz, H_2O+D_2O) δ= 7.25 (d, *J*=7.5 Hz, 1H), 7.23 - 7.12 (m, 3H), 3.72 (s, 3H), 2.27 (s, 3H);

Helvetica Chimica Acta

^{1}H-NMR: 7.25 (d, *J*=7.5 Hz, 1 H), 7.23 - 7.12 (m, 3 H), 3.72 (s, 3 H), 2.27 (s, 3 H)

Tetrahedron Letters

^{1}H-NMR (600 MHz, H_2O+D_2O) δ 7.25 (d, 1H, *J* = 7.5 Hz), 7.23 - 7.12 (m, 3H), 3.72 (s, 3H), 2.27 (s, 3H).