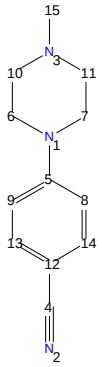
CMC-assist

P1_53



Consistency: NOT OK

Data set 1H: P1_53 1 1 C:\data\iNEXT-G2\nmr
Structure: C:/data/iNEXT-G2/nmr/P1_53/1/37.mol
Acquisition date: May 6, 2019 6:49:57 PM CEST
Solvent: H2O+D2O
Probe: Z129773_0008 (CPP TCI 600S3 H&F-C/N-D-05 Z)
Eretic reference:

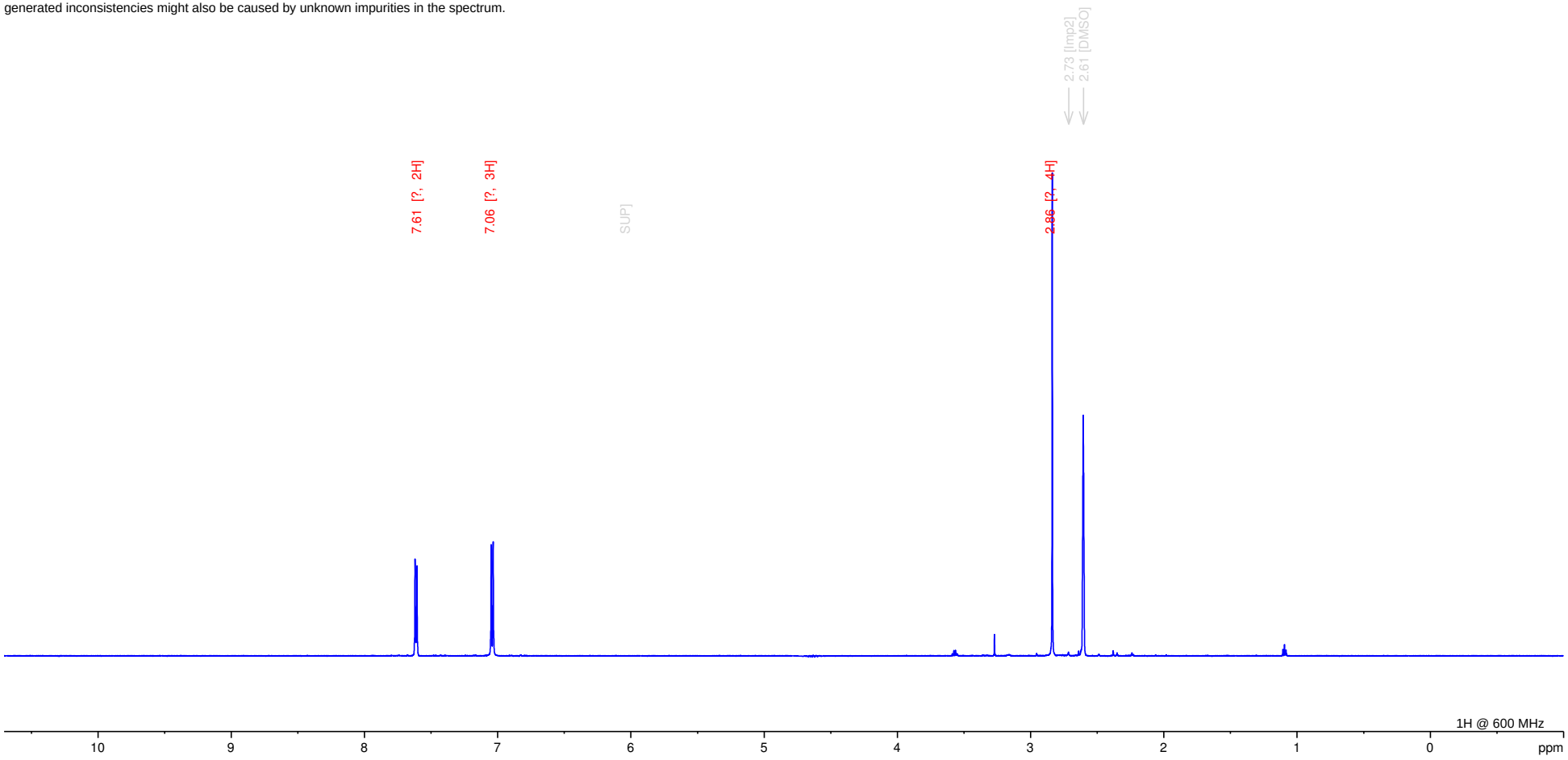
Sum formula: $C_{12}H_{15}N_3$

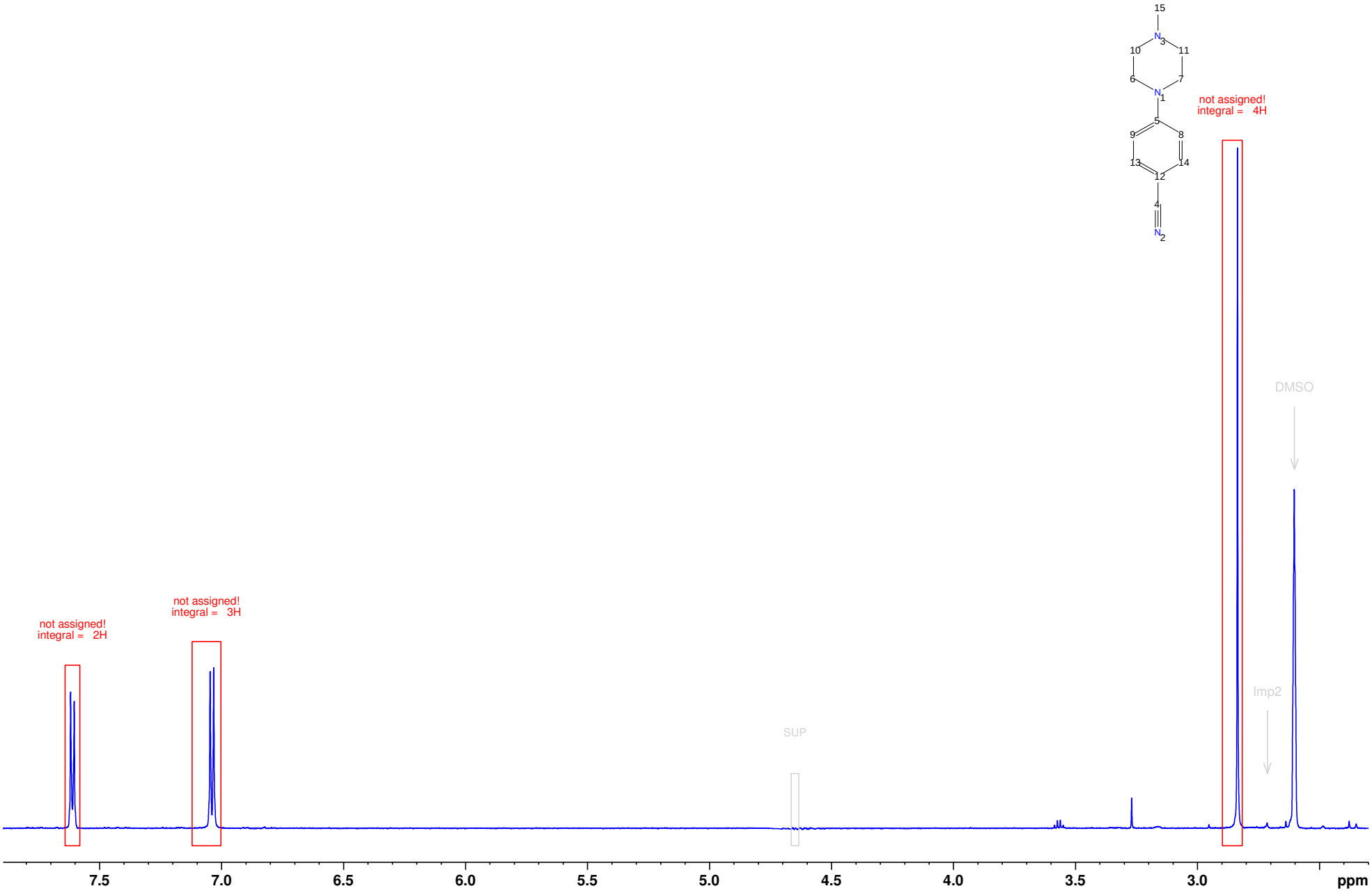
Molecular Mass: 201.13 Da

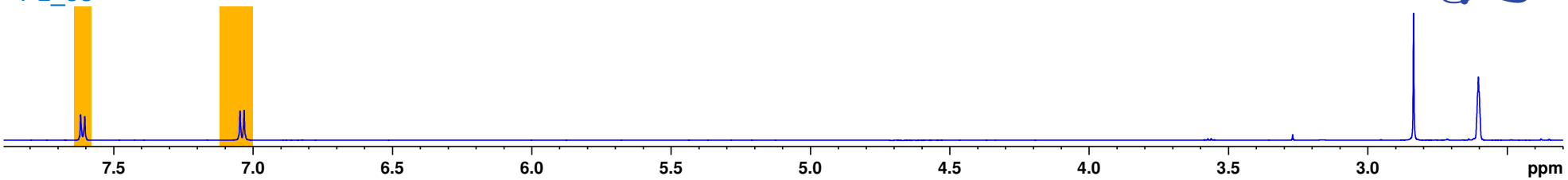
Comments:
Automatic evaluation was aborted.Automatic evaluation: Spectrum and structure do not match. Only invalid solutions were found.
The automatic evaluation ended due to technical problems. No results are available.No assignment could be found for the combination of the structure and spectrum. Please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

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 4.0.5 (of 2018-08-08 23:08:44), on 'X1' as 'ric'




not assigned!
integral = 2H
not assigned!
integral = 3H
SUP
not assigned!
integral = 4H
DMSO
Imp2
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
ppm



not assigned!
integral = 2H

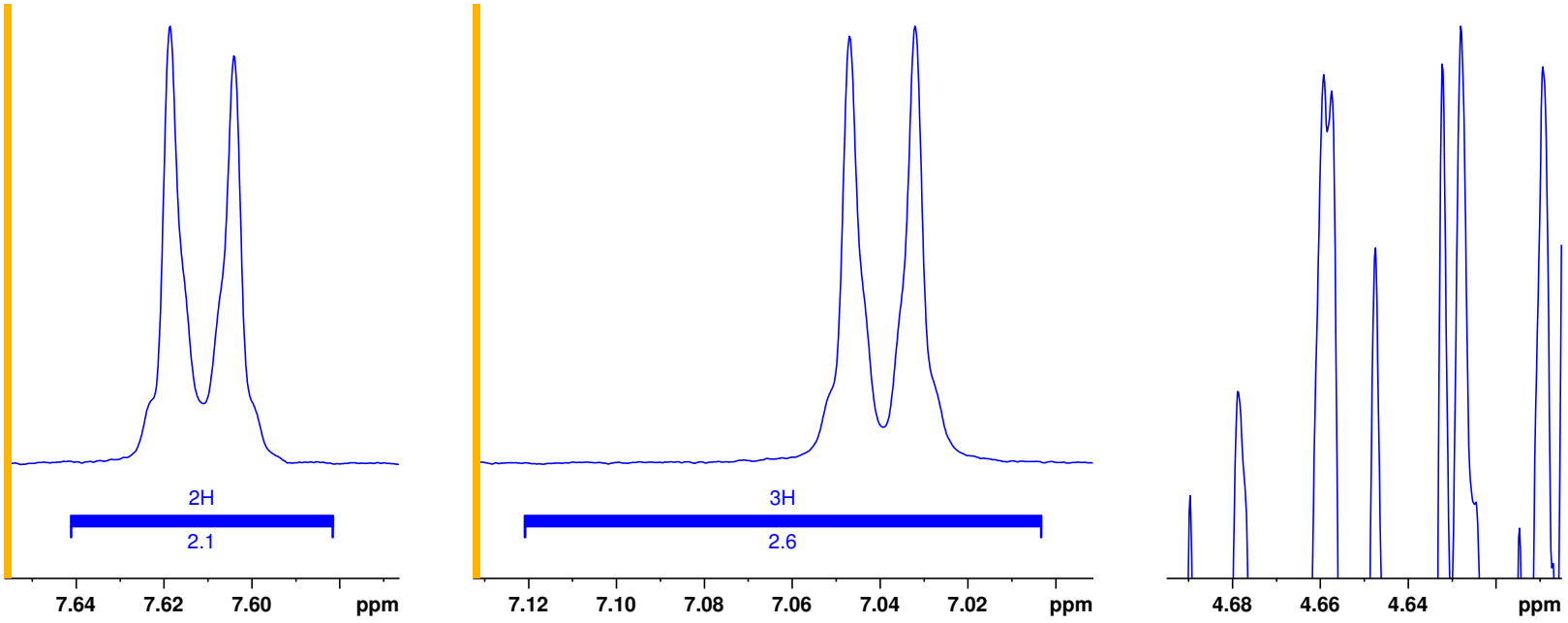
not assigned!
integral = 3H

SUP

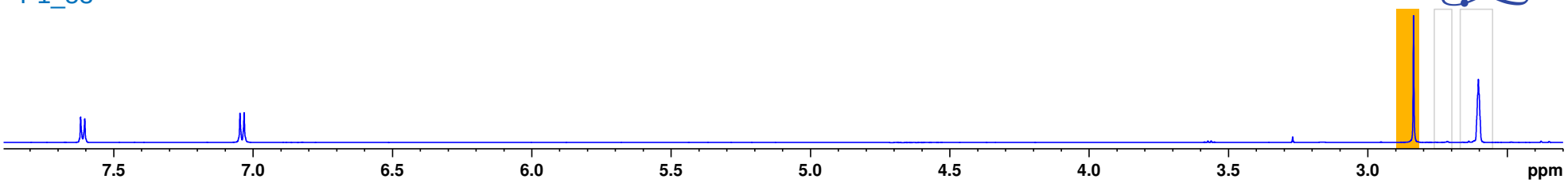
m_2H_Q1
(m)
at 7.611 ppm

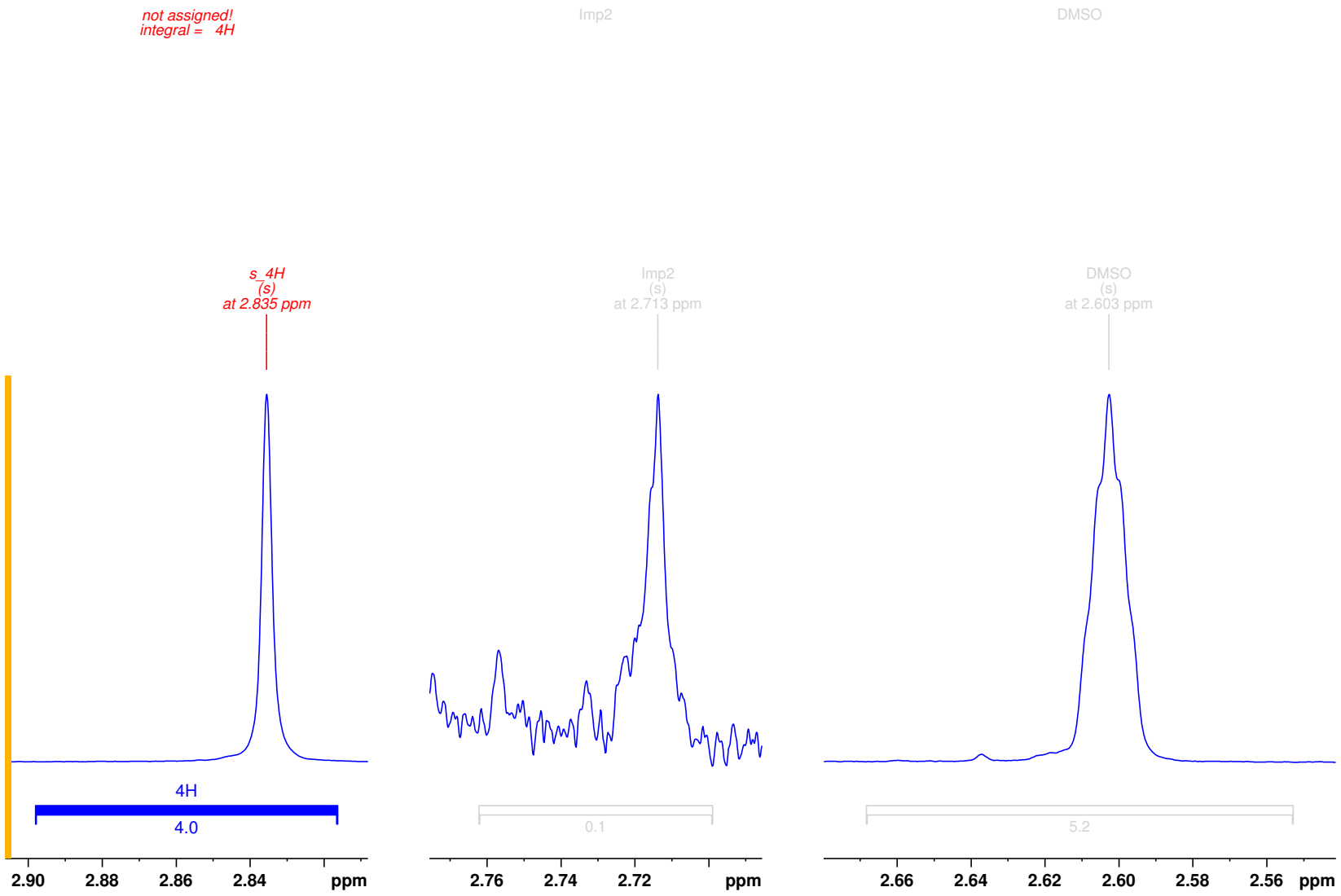
m_3H
(m)
at 7.040 ppm

SUP
(s)
at 4.650 ppm



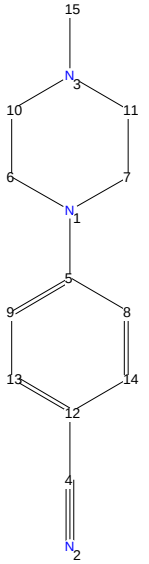
Scale: 0.01666 ppm/cm, 10.00 Hz/cm


7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
ppm


not assigned!
integral = 4H
Imp2
DMSO
s_4H
(s)
at 2.835 ppm
Imp2
(s)
at 2.713 ppm
DMSO
(s)
at 2.603 ppm
4H
4.0
0.1
5.2
2.90
2.88
2.86
2.84
ppm
2.76
2.74
2.72
ppm
2.66
2.64
2.62
2.60
2.58
2.56
ppm
Scale: 0.01666 ppm/cm, 10.00 Hz/cm

1D1H Assignments

Position, coupling, integral	Assignment
2.60 ppm, s, 0H	- not assigned -
2.71 ppm, s, 0H	- not assigned -
7.61 ppm, m, 2H	- not assigned -
2.84 ppm, s, 4H	- not assigned -
7.04 ppm, m, 3H	- not assigned -
4.65 ppm, s	- not assigned -



The spectral description in various Journal formats:

Journal of Organic Chemistry (JOC)

^{1}H NMR (600 MHz, H_2O+D_2O) 7.62 - 7.60 (2H, m), 7.06 - 7.02 (3H, m), 2.84 (4H, s);

Journal of Medicinal Chemistry

^{1}H NMR (600 MHz, H_2O+D_2O) δ 7.62 - 7.60 (m, 2H), 7.06 - 7.02 (m, 3H), 2.84 (s, 4H).

Journal of the American Chemical Society (JACS)

^{1}H NMR (600 MHz, H_2O+D_2O): δ, ppm 7.62 - 7.60 (2H, m), 7.06 - 7.02 (3H, m), 2.84 (4H, s).

Angewandte Chemie

^{1}H-NMR (600 MHz, H_2O+D_2O): δ 7.62 - 7.60 (m, 2H), 7.06 - 7.02 (m, 3H), 2.84 (s, 4H).

Chemistry, a European Journal

^{1}H-NMR (600 MHz, H_2O+D_2O) δ= 7.62 - 7.60 (m, 2H), 7.06 - 7.02 (m, 3H), 2.84 (s, 4H);

Helvetica Chimica Acta

^{1}H-NMR: 7.62 - 7.60 (m, 2 H), 7.06 - 7.02 (m, 3 H), 2.84 (s, 4 H)

Tetrahedron Letters

^{1}H-NMR (600 MHz, H_2O+D_2O) δ 7.62 - 7.60 (m, 2H), 7.06 - 7.02 (m, 3H), 2.84 (s, 4H).