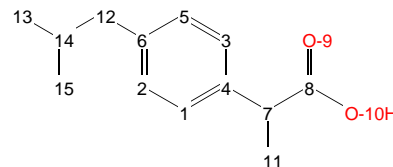


OK, 13.02 mmol/l

Data set: example1_workflow 11 1 C:\Bruker\TopSpin3.2\examdata
 Structure: C:\Bruker\TopSpin3.2\examdata\example1_workflow\11\structure.mol
 Acquisition date: August 22, 2006 7:19:33 AM PDT
 Solvent: DMSO
 Probe: 5 mm PABBI 1H/D-BB Z-GRD Z820201/0131
 Eretic reference: C:\Users\sgn\Desktop\examples\CMC-assist_example1\11\pdata\1\eretic



Sum formula:
 $C_{13}H_{18}O_2$

Molecular Mass:
 206.28 Da

Comments:

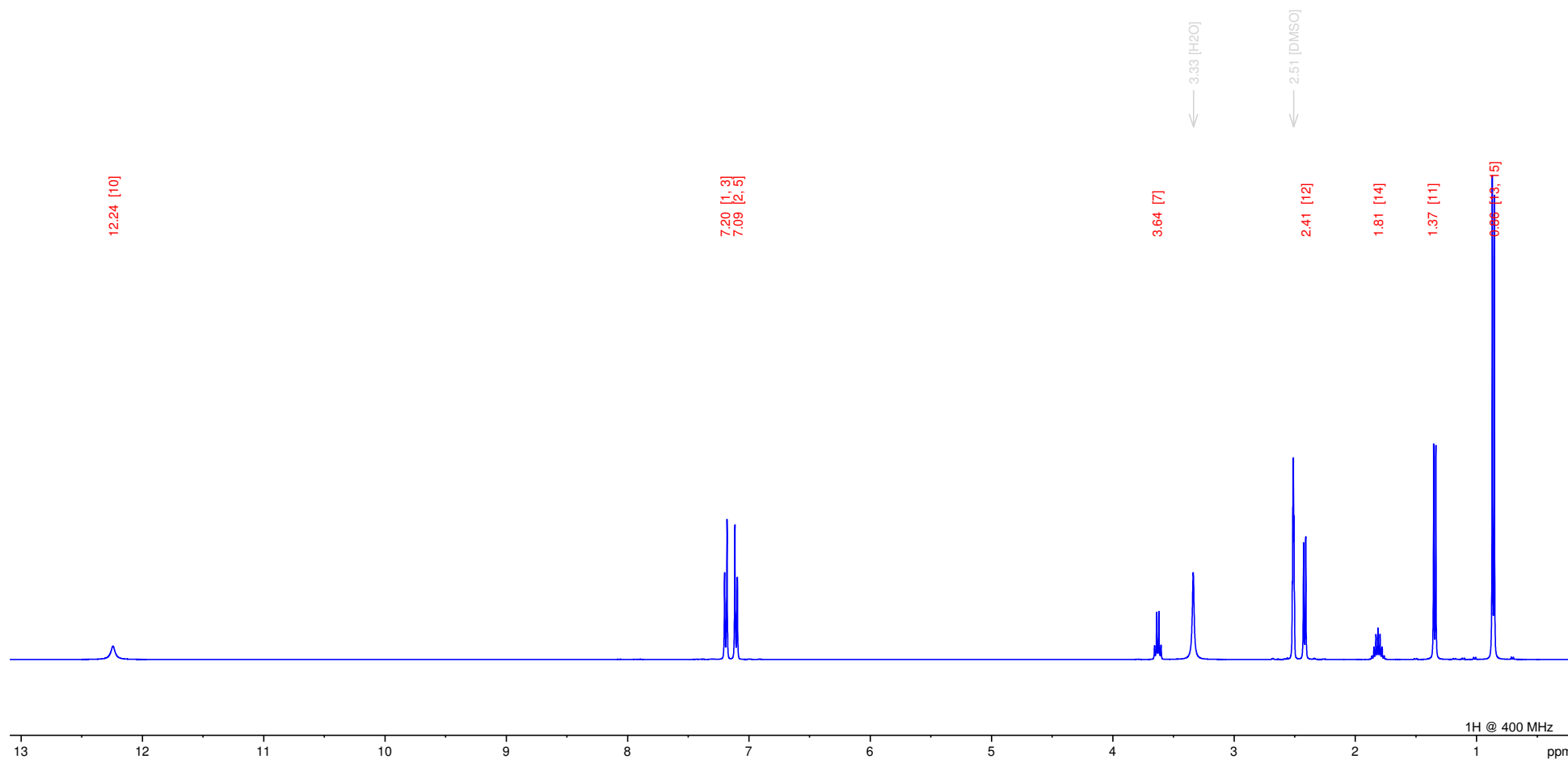
Automatic evaluation: Spectrum and structure are in agreement. The substance within the spectrum has a purity of 98%. All major signals in the spectrum could be assigned. All elements of the structure could be assigned to regions in the spectrum. All given impurities could be assigned to regions in the spectrum.

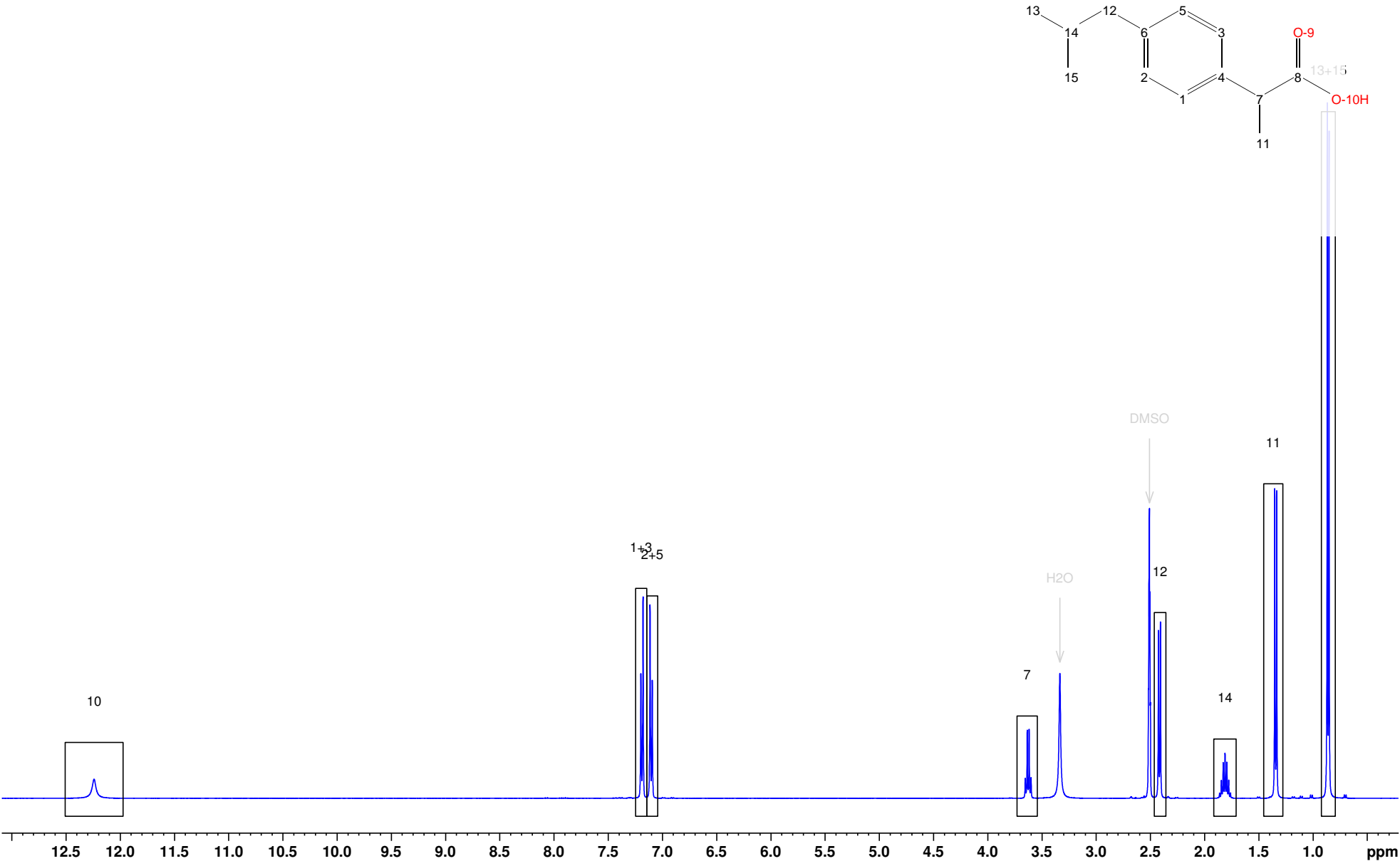
Signature:

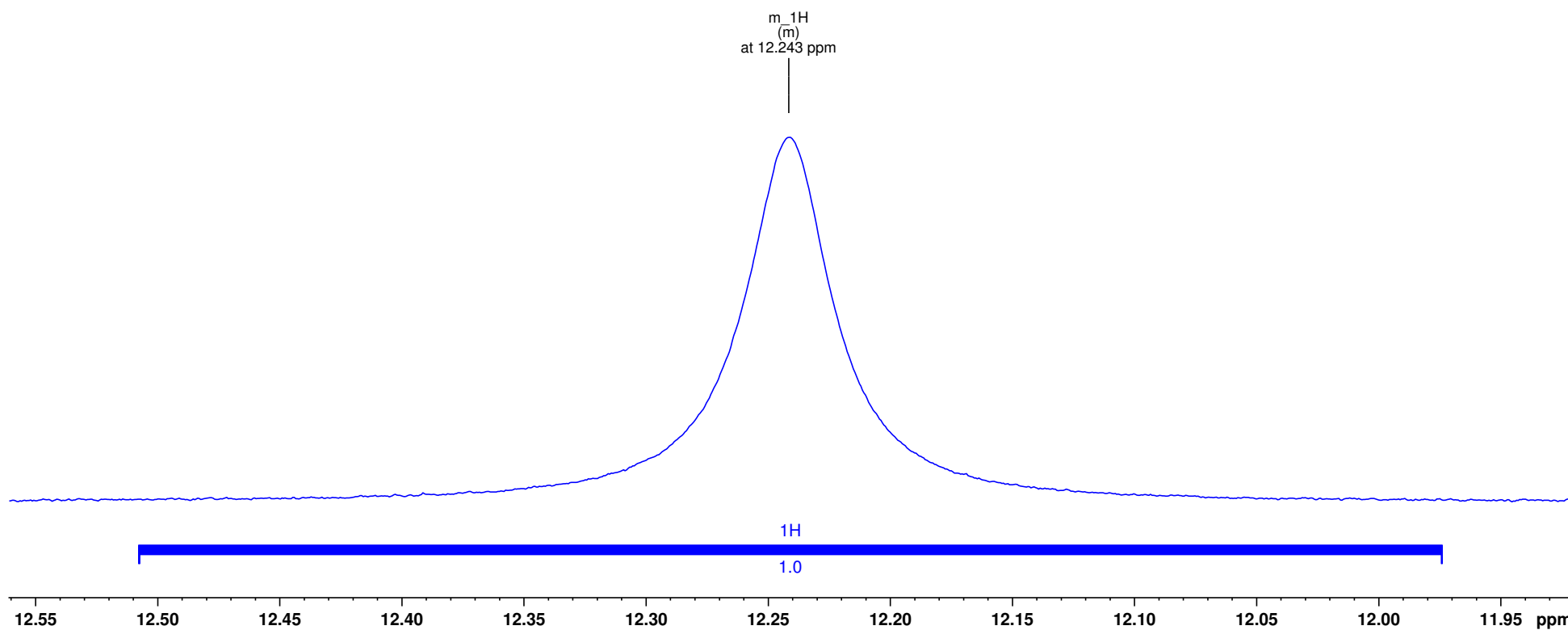
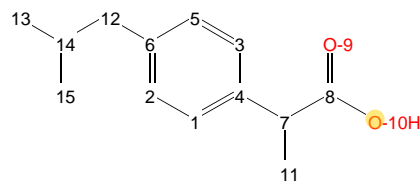
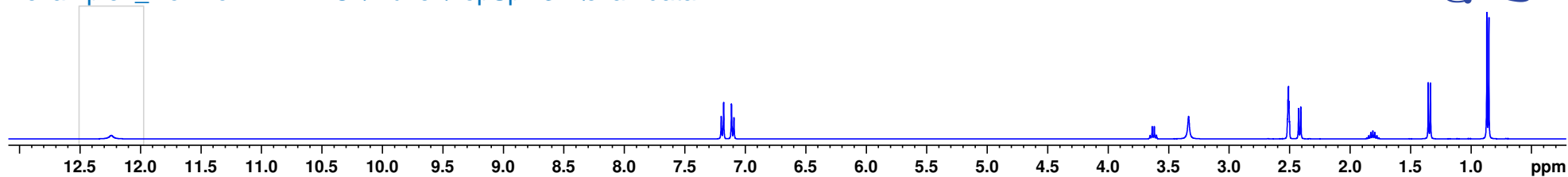
Automatic analysis generated by Bruker CMC (7293).

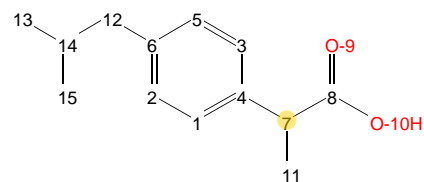
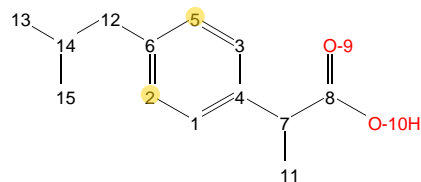
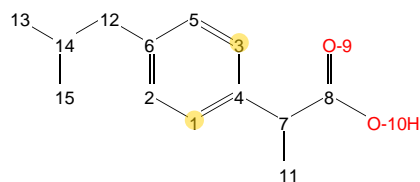
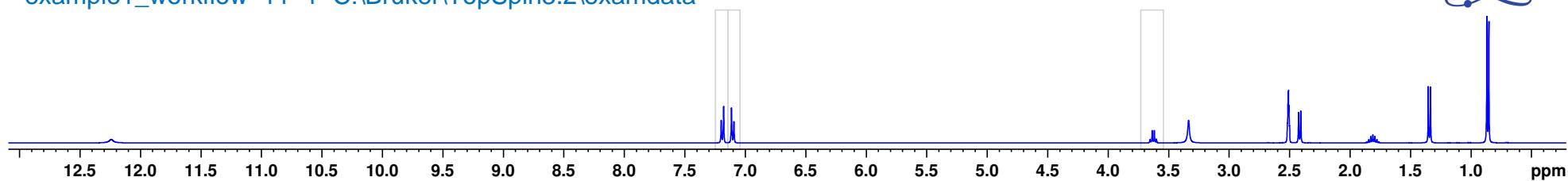
All results have been created exclusively by automatic analysis.

Report generated by Bruker CMC-assist 1.2.pl2, on 'DAVES-ULTRABOOK' as 'Dave'









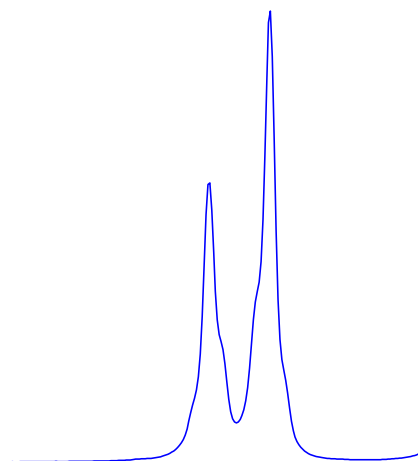
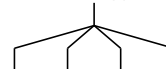
d, 2H, Q
8.0 Hz (d)
at 7.189 ppm



d, 2H
8.0 Hz (d)
at 7.104 ppm



q, 1H
7.0 Hz (q)
at 3.627 ppm

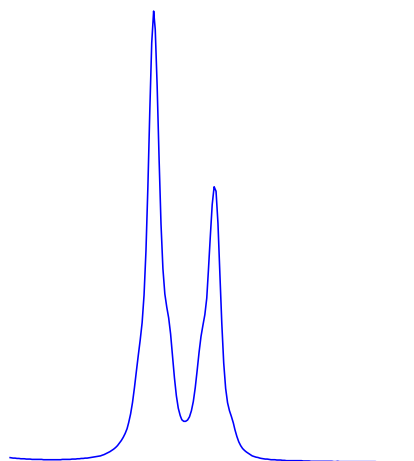


2H

2.0

7.25 7.20 ppm

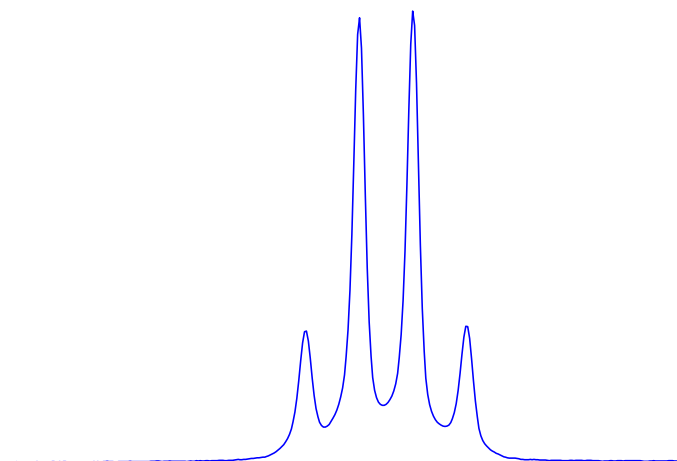
Scale: 0.02499 ppm/cm, 10.00 Hz/cm



2H

2.0

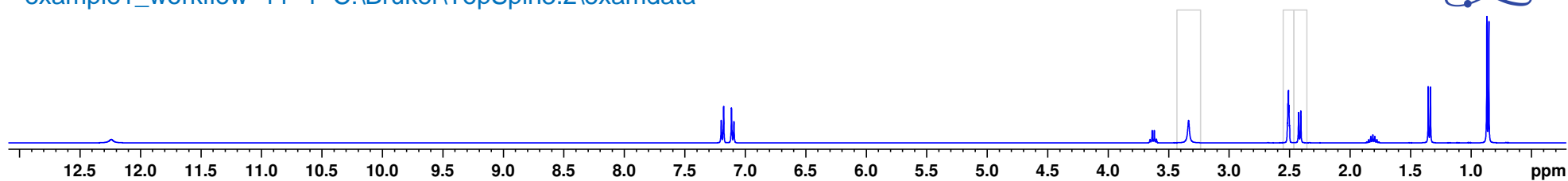
7.15 7.10 ppm



1H

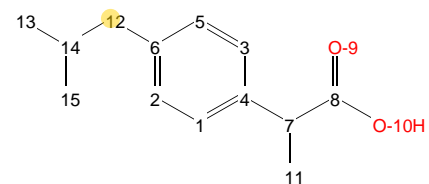
1.0

3.70 3.65 3.60 ppm



H₂O

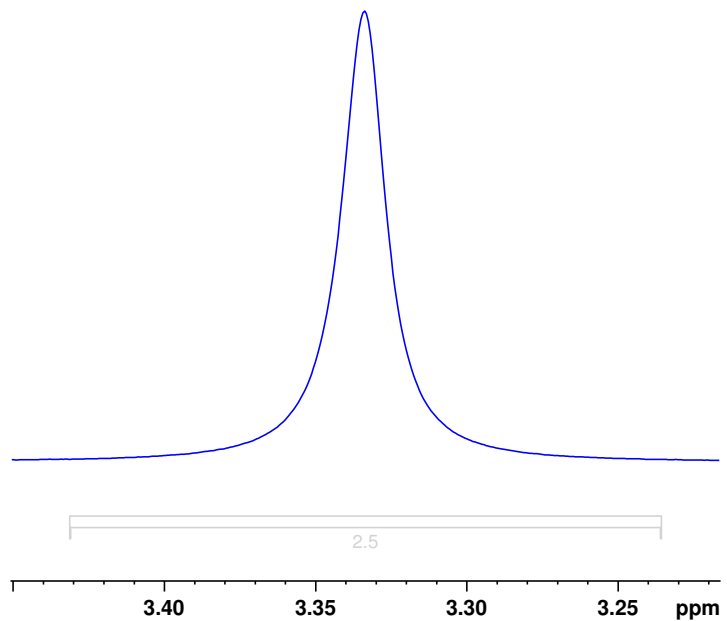
DMSO



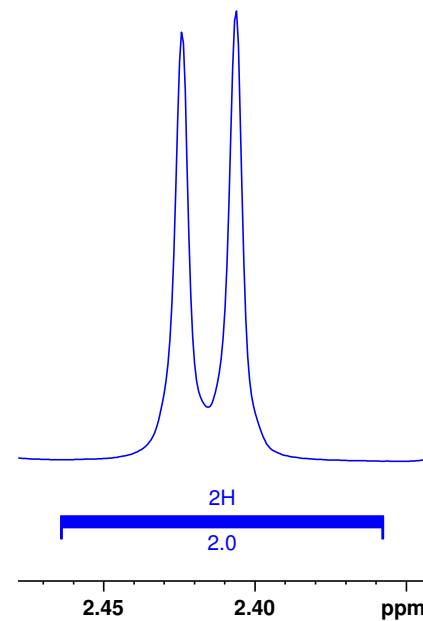
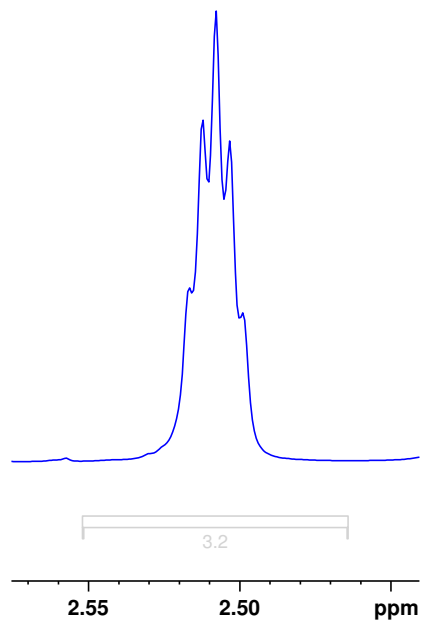
H₂O
(s)
at 3.335 ppm

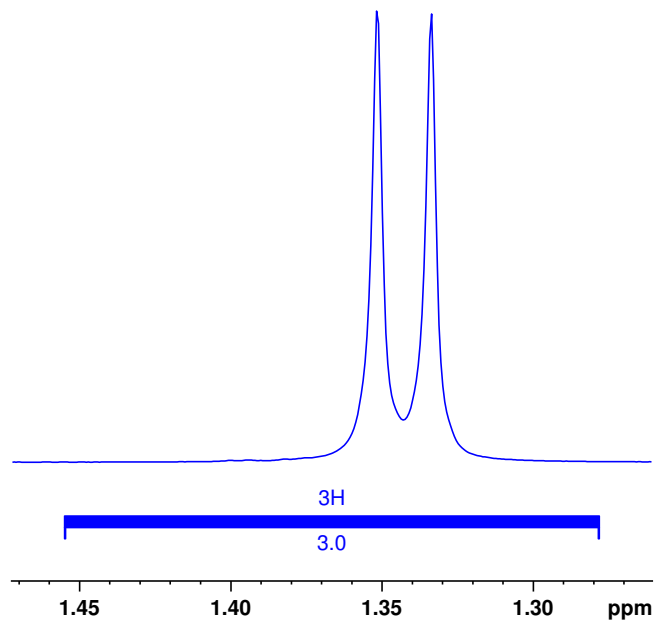
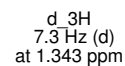
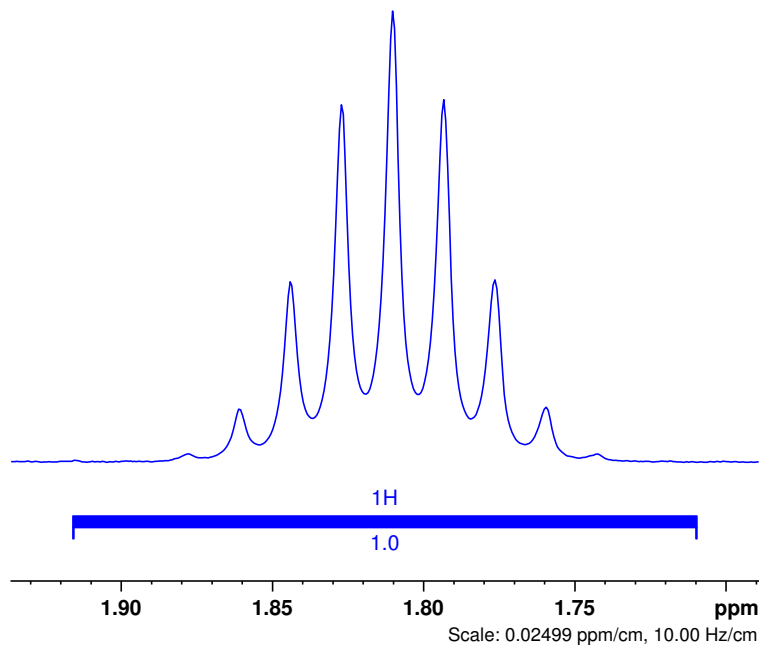
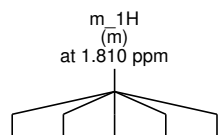
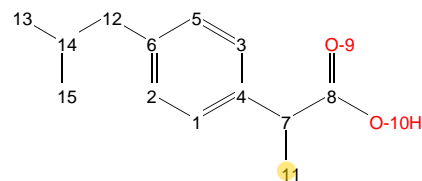
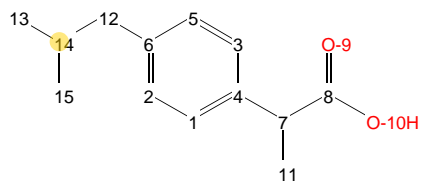
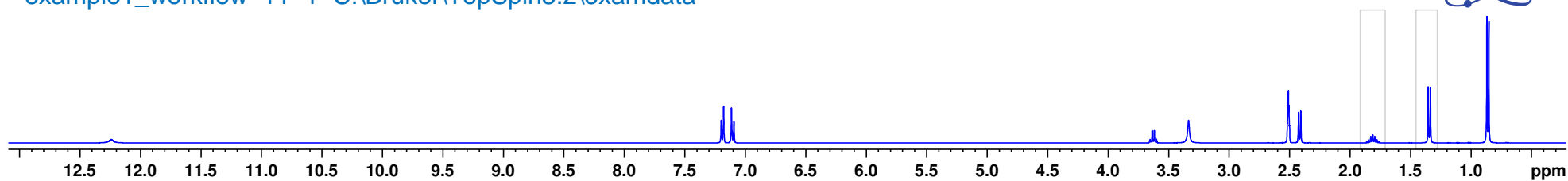
DMSO
(m)
at 2.508 ppm

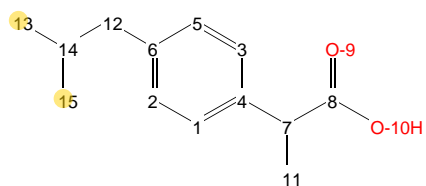
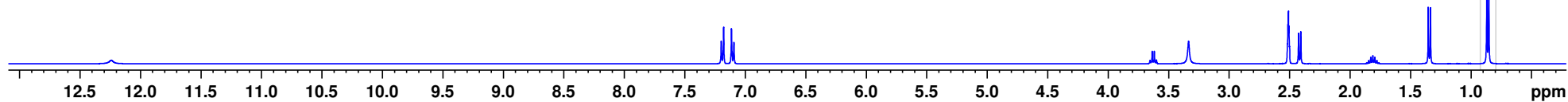
d, 2H
7.3 Hz (d)
at 2.416 ppm



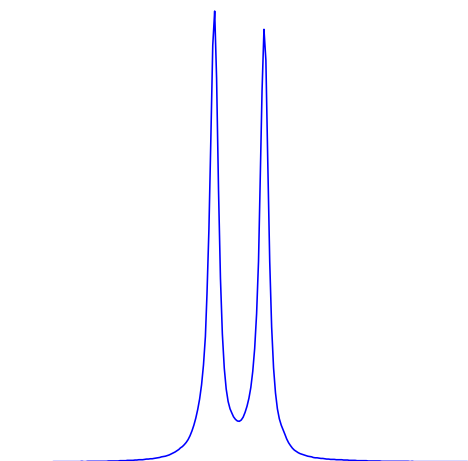
Scale: 0.02499 ppm/cm, 10.00 Hz/cm







d 6H
6.5 Hz (d)
at 0.860 ppm



6H

6.0

0.90 0.85 ppm

Scale: 0.02499 ppm/cm, 10.00 Hz/cm

1D Assignments

Position, coupling, integral

12.24 ppm, m, 1H

7.19 ppm, d (8.0Hz), 2H

7.10 ppm, d (8.0Hz), 2H

3.63 ppm, q (7.0Hz), 1H

3.33 ppm, s, 0H

2.51 ppm, m, 0H

2.42 ppm, d (7.3Hz), 2H

1.81 ppm, m, 1H

1.34 ppm, d (7.3Hz), 3H

0.86 ppm, d (6.5Hz), 6H

Assignment

10

1 + 3

2 + 5

7

- not assigned -

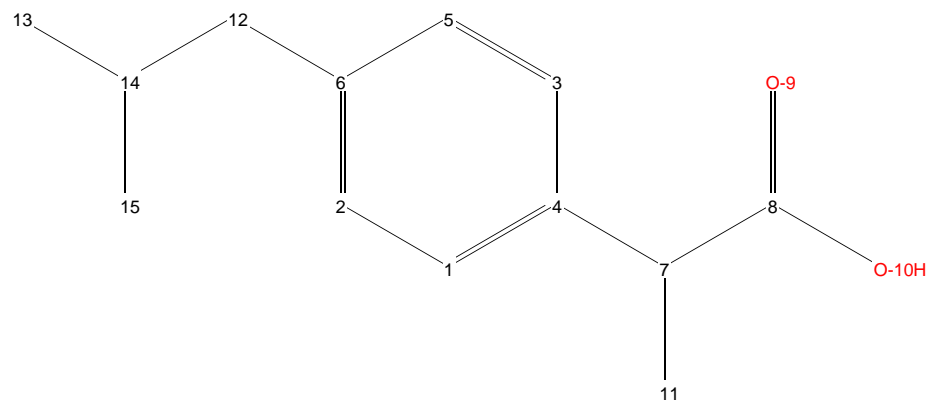
- not assigned -

12

14

11

13 + 15



The assignment in various Journal formats:

Journal of Organic Chemistry (JOC)

¹H NMR (400 MHz, DMSO) 12.30 - 12.18 (1H, m), 7.19 (2H, d, $J=8.0$ Hz), 7.10 (2H, d, $J=8.0$ Hz), 3.63 (1H, q, $J=7.0$ Hz), 2.42 (2H, d, $J=7.3$ Hz), 1.85 - 1.77 (1H, m), 1.34 (3H, d, $J=7.3$ Hz), 0.86 (6H, d, $J=6.5$ Hz);

Journal of Medicinal Chemistry

¹H NMR (400 MHz, DMSO) δ 12.30 - 12.18 (m, 1H), 7.19 (d, $J=8.0$ Hz, 2H), 7.10 (d, $J=8.0$ Hz, 2H), 3.63 (q, $J=7.0$ Hz, 1H), 2.42 (d, $J=7.3$ Hz, 2H), 1.85 - 1.77 (m, 1H), 1.34 (d, $J=7.3$ Hz, 3H), 0.86 (d, $J=6.5$ Hz, 6H).

Journal of the American Chemical Society (JACS)

¹H NMR (400 MHz, DMSO): δ , ppm 12.30 - 12.18 (1H, m), 7.19 (2H, d, $J = 8.0$ Hz), 7.10 (2H, d, $J = 8.0$ Hz), 3.63 (1H, q, $J = 7.0$ Hz), 2.42 (2H, d, $J = 7.3$ Hz), 1.85 - 1.77 (1H, m), 1.34 (3H, d, $J = 7.3$ Hz), 0.86 (6H, d, $J = 6.5$ Hz).

Angewandte Chemie

¹H-NMR (400 MHz, DMSO): δ 12.30 - 12.18 (m, 1H), 7.19 (d, $J=8.0$ Hz, 2H), 7.10 (d, $J=8.0$ Hz, 2H), 3.63 (q, $J=7.0$ Hz, 1H), 2.42 (d, $J=7.3$ Hz, 2H), 1.85 - 1.77 (m, 1H), 1.34 (d, $J=7.3$ Hz, 3H), 0.86 (d, $J=6.5$ Hz, 6H).

Chemistry, a European Journal

¹H-NMR (400 MHz, DMSO) δ = 12.30 - 12.18 (m, 1H), 7.19 (d, $J=8.0$ Hz, 2H), 7.10 (d, $J=8.0$ Hz, 2H), 3.63 (q, $J=7.0$ Hz, 1H), 2.42 (d, $J=7.3$ Hz, 2H), 1.85 - 1.77 (m, 1H), 1.34 (d, $J=7.3$ Hz, 3H), 0.86 (d, $J=6.5$ Hz, 6H);

Helvetica Chimica Acta

¹H-NMR: 12.30 - 12.18 (m, 1 H), 7.19 (d, $J=8.0$ Hz, 2 H), 7.10 (d, $J=8.0$ Hz, 2 H), 3.63 (q, $J=7.0$ Hz, 1 H), 2.42 (d, $J=7.3$ Hz, 2 H), 1.85 - 1.77 (m, 1 H), 1.34 (d, $J=7.3$ Hz, 3 H), 0.86 (d, $J=6.5$ Hz, 6 H)

Tetrahedron Letters

¹H-NMR (400 MHz, DMSO) δ 12.30 - 12.18 (m, 1H), 7.19 (d, 2H, $J = 8.0$ Hz), 7.10 (d, 2H, $J = 8.0$ Hz), 3.63 (q, 1H, $J = 7.0$ Hz), 2.42 (d, 2H, $J = 7.3$ Hz), 1.85 - 1.77

(m, 1H), 1.34 (d, 3H, $J = 7.3$ Hz), 0.86 (d, 6H, $J = 6.5$ Hz).