Data in Brief 8 (2016) 308–311

Contents lists available at ScienceDirect

Data in Brief

journal homepage: www.elsevier.com/locate/dib

Data Article

^{1}H-NMR dataset for hydroxycoumarins –Aesculetin, 4-Methylumbelliferone, and umbelliferone

Rui Galhano dos Santos *, João Carlos Moura Bordado, Maria Margarida Mateus

CERENA, Departamento de Engenharia Química e Biológica, Torre Sul, Instituto Superior Técnico, Av. Rovisco Pais, 1049-001 Lisboa, Portugal

ARTICLE INFO

Article history:
Received 18 March 2016
Received in revised form
18 May 2016
Accepted 23 May 2016
Available online 30 May 2016

Keywords:
Coumarins
NMR
Acetone

ABSTRACT

Herein, the integrated raw data regarding the ^{1}H-NMR, experiments of Aesculetin, 4-Methylumbelliferone, and umbelliferone, in Acetone-d^{6} at 25 °C, are presented for further analysis and comparison purposes, for whom may be interested.

Specifications Table

Subject area	*Chemistry*
More specific subject area	*Structural characterization*
Type of data	*Figures, table*
How data was acquired	*The data was acquired on a Bruker Avance 400 spectrometer operating at 400 MHz*
Data format	*Raw*
Experimental factors	*Sample solutions were prepared with deuterated Acetone (Acetone-d^{6}). Residual acetone peak: 2.05*
Experimental features	*Detection temperature was set at 25 °C. Samples were scanned 16 times.*
Data source location	*Lisbon, Portugal, GPS: 38° 44′ 10.31″N; 9° 08′ 19.66″W*
Data accessibility	*Data is provided in the article*

* Corresponding author.
E-mail address: rmglopes@ist.utl.pt (R.G. dos Santos).

http://dx.doi.org/10.1016/j.dib.2016.05.048

Value of the data

- Useful to be used as reference data for chemical shifts for other related compounds.
- Comparison between coumarins with different substitution patterns.
- Helpful in the assignment of signals of molecules containing coumarin backbone residues.

1. Data

The data henceforth described refers to the ^{1}H-NMR experiments of three coumarins, Aesculetin, 4-Methylumbelliferone, and umbelliferone, in deuterated acetone.

The data disclosed regards the ^{1}H-NMR experiments conducted with 4-Methylumbelliferone (Fig. 1), umbelliferone (fig. 2), and Aesculetin (Fig. 3), in deuterated acetone. This data may be helpful for those who intend to compare this data with other from molecules containing the same or related coumarins scaffolds. Table 1 lists all the peaks and their respective intensities.

2. Experimental design, materials, and methods

The coumarins used were chemical grade and purchased from Sigma-Aldrich.

The compounds were subjected to ^{1}H-NMR measurements. The experiments were performed on a Bruker Avance 400 liquid NMR spectrometer, operating at 400 MHz. Detection temperature was set at 25 °C. The samples were loaded in a 5 mm NMR tube. The solvent peak was calibrated according to Gottlieb et al. [1].

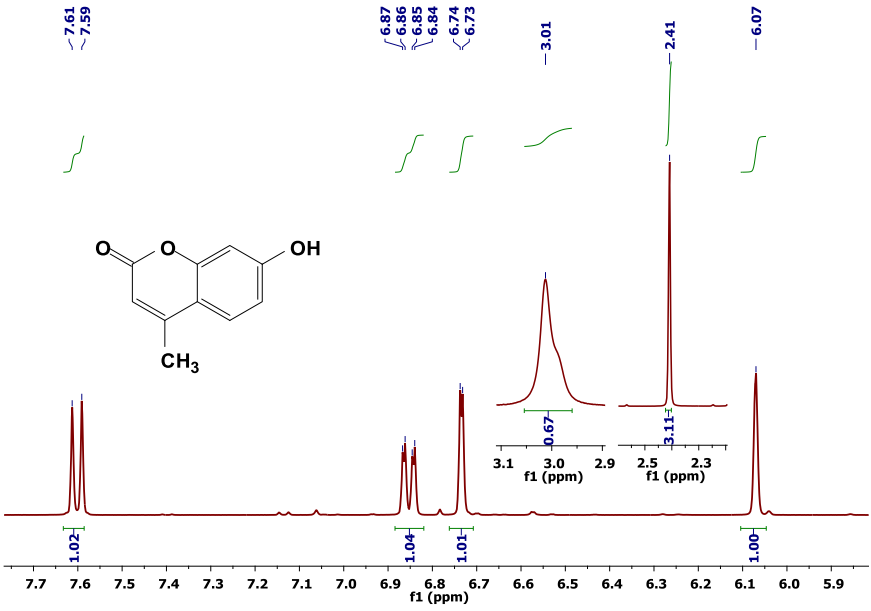

Fig. 1. ^{1}H-NMR spectrum of 4-Methylumbelliferone (acetone-d^{6}, 298 K, 400 MHz).

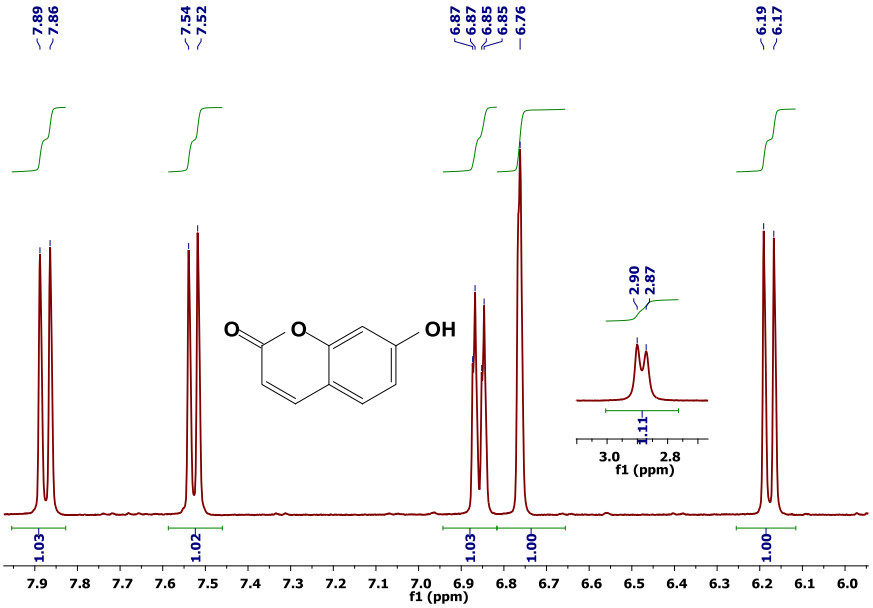

Fig. 2. [1]H-NMR spectrum of umbelliferone (acetone-d[6], 298 K, 400 MHz).

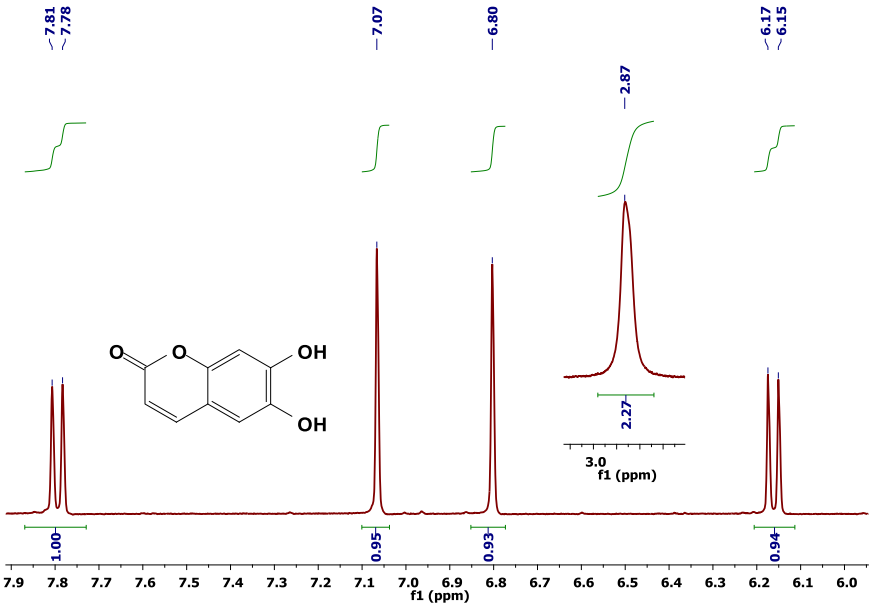

Fig. 3. [1]H-NMR spectrum of Aesculetin (acetone-d[6], 298 K, 400 MHz).

Table 1
Chemicals shifts for 4-methylumbelliferone, umbelliferone, and Aesculetin [1].

Compound					
4-Methylumbelliferone		**Umbelliferone**		**Aesculetin**	
ppm	**Intensity**	**ppm**	**Intensity**	**ppm**	**Intensity**
2.41	2129.6	2.87	171.2	2.87	134.2
3.01	116.5	2.9	194.3	6.15	246.5
6.07	607.4	6.17	501.6	6.17	255.4
6.73	518.7	6.19	515.2	6.8	456
6.74	535.3	6.76	662.3	7.07	484.5
6.84	291.3	6.85	379.1	7.78	237.5
6.85	251.3	6.87	274.9	7.81	233.3
6.86	308.3	7.52	511.3	–	–
6.87	268.4	7.54	479.5	–	–
7.59	489.4	7.86	484.7	–	–
7.61	461.7	7.89	471.7	–	–
9.35	70.5	–	–	–	–

Transparency document. Supplementary material

Transparency document associated with this article can be found in the online version at http://dx.doi.org/10.1016/j.dib.2016.05.048.

Reference

[1] Hugo E. Gottlieb, Vadim Kotlyar, Abraham Nudelman, NMR chemical shifts of common laboratory solvents as trace impurities, J. Org. Chem. 62 (1997) 7512–7515. http://dx.doi.org/10.1021/jo971176v.