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Data Article

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

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ABSTRACT

Herein, the integrated raw data regarding the ¹H-NMR, experiments of Aesculetin, 4-Methylumbelliferone, and umbelliferone, in Acetone-d⁶ at 25 °C, are presented for further analysis and comparison purposes, for whom may be interested.

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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

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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 ^1H -NMR experiments of three coumarins, Aesculetin, 4-Methylumbelliferone, and umbelliferone, in deuterated acetone.

The data disclosed regards the ^1H -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 ^1H -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].

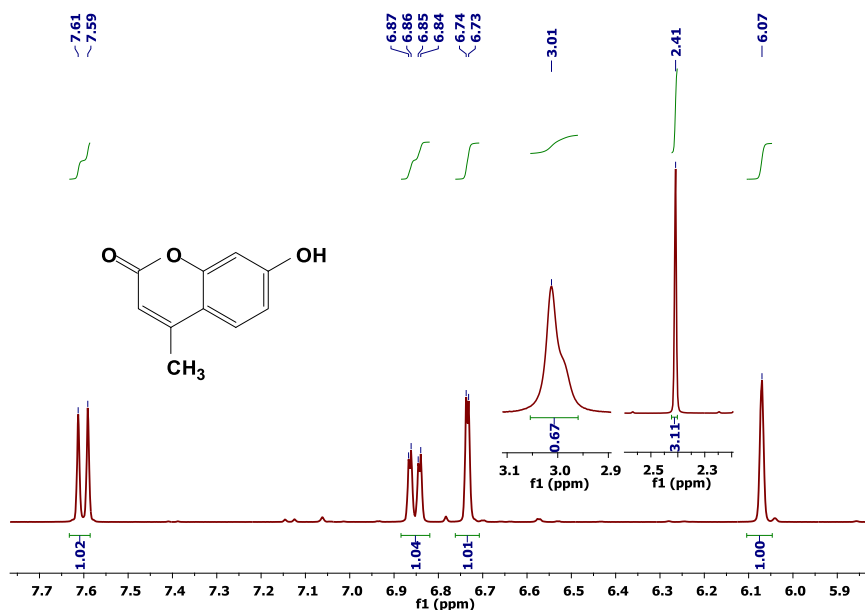


Fig. 1. ^1H -NMR spectrum of 4-Methylumbelliferone (acetone- d_6 , 298 K, 400 MHz).

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