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Data Article

The spectrogram data of quinazoline derivatives containing a dithioacetal moiety



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ABSTRACT

The nuclear magnetic resonance, and high-resolution mass spectrometry of quinazoline derivatives containing a dithioacetal moiety, which was hosted in the research article entitled "Syntheses, antiviral activities and induced resistance mechanisms of novel quinazoline derivatives containing a dithioacetal moiety". The data include ^1H nuclear magnetic resonance (^1H NMR), ^{13}C nuclear magnetic resonance (^{13}C NMR), and high-resolution mass spectrometry. In this article, a more comprehensive data interpretation and analysis is explained.

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Specifications table

Subject area	Organic chemistry
More specific subject area	pesticide
Type of data	figures

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How data was acquired	The nuclear magnetic resonance spectra were acquired by JEOL-ECX500 MHz (JEOL, Tokyo, Japan) or Bruker DPX 400 MHz (Bruker BioSpin GmbH, Rheinstetten, Germany). The high-resolution mass spectrometry was acquired through Thermo Scientific Q Exactive (Thermo Fisher Scientific, Massachusetts, America).
Data format	Analyzed
Experimental factors	The quinazoline derivatives were synthesized and purified <i>via</i> chemistry route. The ^1H NMR and ^{13}C NMR were acquired by instruments with CDCl_3 or dimethyl sulfoxide (DMSO) as the solvent with tetramethylsilane (TMS) as an internal standard, and chemical shifts are expressed in δ (ppm).
Experimental features	Through the sharing of nuclear magnetic resonance and high-resolution mass spectrometry, the chemical structure of the compounds can be determined.
Data source location	Guiyang city, China
Data accessibility	The data are included with this article

Value of the data

- The data confirmed the correct structure of these first time synthesized compounds **4a–4x**.
- The data as a background for the bioassay and quantitative structure-activity relationship analysis of compounds **4a–4x**.
- The data serves as a benchmark for other researchers synthesize this type of compound in the future.

1. Data

The dataset of this article provide information on the spectra of 22 quinazoline derivatives contain a dithioacetal moiety. The ^1H NMR, ^{13}C NMR and HRMS spectra of compound **4a** were shown in Figs. 1–3, respectively.

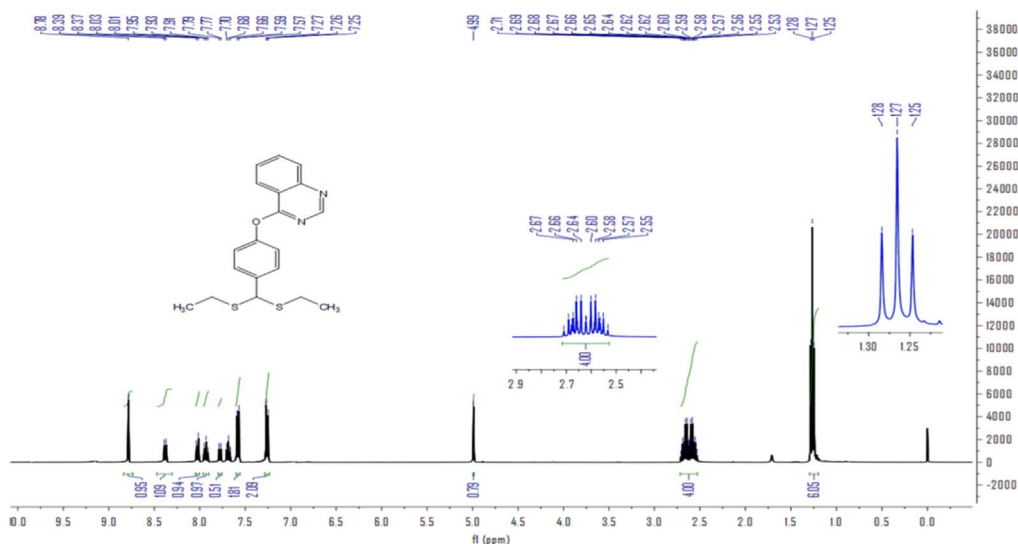


Fig. 1. ^1H NMR of Compound **4a**.

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