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Data article

Data on nitrogen-containing derivatives of fumaropimaric acid

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ABSTRACT

The data presented here are related to the research paper entitled "Levopimaric Acid Derived 1,2-Diamines and Their Application in the Copper-Catalyzed Asymmetric Henry Reaction" [1]. In this data article, we provide ^{1}H, ^{13}C NMR and IR data for the diterpene derivatives described in [1]. The GC–MS analysis of pine oleoresin used as a starting material of the syntheses is also included in the data article.

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Specifications table

Subject area	*Chemistry*
More specific subject area	*Organic synthesis, natural products*
Type of data	*Synthetic schemes, NMR and IR spectra, GC-chromatogram*
How data was acquired	*NMR spectroscopy: Bruker DRX-500, AM-400 and AV-300; IR spectroscopy: Infralum FT-801 and Shimadzu IRAffinity-1 FT-IR; GC–MS analysis: SHIMADZU GCMS-QP2010 Ultra instrument on the basis of gas chromatograph GC-2010 plus with mass detector*
Data format	*Raw, analyzed.*
Experimental factors	*The new diterpene derivatives were synthesized and purified by column chromatography or crystallization*

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Experimental features	*The synthesized compounds were characterized by NMR and IR spectroscopy*
Data source location	*Novosibirsk, Russian Federation*
Data accessibility	*Data are available with this article*

Value of the data

- The data presents NMR, IR spectra of newly synthesized diterpene derivatives and GC–MS analysis of methylated pine oleoresin and could be used by other researchers.
- The provided information on the structural data of diterpenes could be useful for the analysis of spectra and determination of the structure of other diterpene derivatives.
- The data could be helpful for other researchers to identify the compounds described in the research article [1] and to reproduce the experiments reported therein.

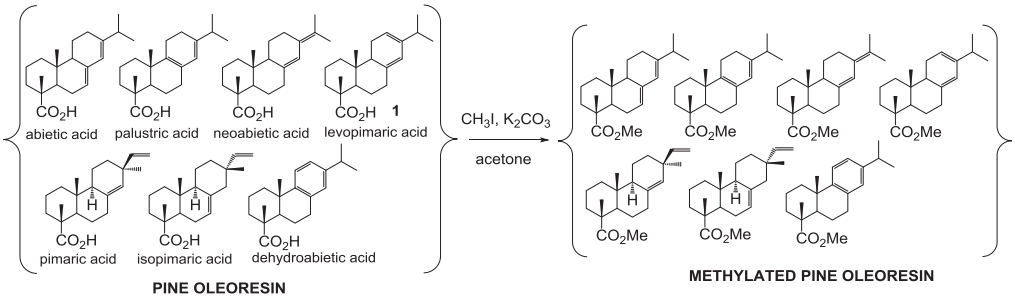
1. Data

The dataset presented in this article focuses on characterization of the new diterpene derivatives described in [1]. The article provides the information on the composition of natural raw material (pine oleoresin) and the structural data of the functionalized diterpenes. Scheme 1 illustrates the preparation of mixture of methylated resin acids. The GC–MS analysis of this mixture is given in Fig. 1. Scheme 2 illustrates the method of preparation and isolation of monomethyl ester of fumaropimaric acid **2**. The compound **2** was characterized using ^{1}H, ^{13}C NMR and IR (Figs. 2-1, 2-2 and 2–3). Scheme 3 illustrates the synthetic route to the 1,2-diisocyanate **3**, which was characterized using ^{1}H, ^{13}C NMR and IR (Figs. 3-1, 3-2 and 3-3). Scheme 4 illustrates the synthetic route to the 1,2-diamine **4**, which was characterized using ^{1}H, ^{13}C NMR and IR (Figs. 4-1, 4-2 and 4-3). Scheme 5 illustrates the method of preparation of imines **5a-f** and aminophenols **6a-f.** Figs. 5a-f and 6a-f shows ^{1}H, ^{13}C NMR and IR spectra of the compounds **5a-f** and **6a-f**. Analyses of the spectra of the compounds **2** and **4** are provided in [2]. Analyses of the spectra of the compounds **3**, **5a-f** and **6a-f** are provided in [1]. The synthetic procedures for the compounds **2**–**6** are described in the research article [1].

2. Experimental design, materials and methods

2.1. General information

The chemicals were of reagent purity grade, obtained from commercial sources, and used without further purification. Pine oleoresin OST 13-128-93 (Russian industry standard; oleoresin contains at least 80% of abietic-type acids) was obtained from Orgsyntez OJSC (available on request at http://



Scheme 1. Methylation of resin acids.

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