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## Data Article

## Data on the synthesis and characterization of two novel polydentate ligands possessing unsymmetrical NH-urea fragment

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## ABSTRACT

The data represent the synthesis and structural characterization of two novel polydentate ligands possessing unsymmetrical NH-urea fragment: an open-chain substituted aromatic compound with unsymmetrical urea and secondary amine units (**S1**) and fused aryloxazinone with unsymmetrical urea fragment (**S2**). The data include the analyzed NMR spectra, turbo-spray mass spectra, melting points and  $R_f$ -values. 1D and 2D NMR spectra are given in the article. The efficiency of the ligands as synergists in the isolation and separation of lanthanoid ions is reported in reference [1].

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## Specifications Table

Subject area	Chemistry
More specific subject area	Organic polydentate ligands
Type of data	Scheme, figures (NMR spectra)
How data was acquired	NMR (1D and 2D), mass spectroscopy, TLC, m.p.
Data format	Analyzed

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E-mail address: [vkurteva@orgchm.bas.bg](mailto:vkurteva@orgchm.bas.bg) (V. Kurteva).<https://doi.org/10.1016/j.dib.2018.08.136>2352-3409/© 2018 The Authors. Published by Elsevier Inc. This is an open access article under the CC BY license (<http://creativecommons.org/licenses/by/4.0/>).

Experimental factors	The ligands were isolated by flash chromatography on silica gel and were then recrystallized
Experimental features	Synthesis and characterization of novel polydentate ligands
Data source location	Sofia, Bulgaria
Data accessibility	The data are available within this article and present a supplementary material to the article “M. Atanassova, S. Todorova, V. Kurteva, N. Todorova, Insights into the synergistic selectivity of 4f-ions implementing 4-acyl-5-pyrazolone and two new unsymmetrical NH-urea ring molecules in an ionic liquid, <i>Sep. Purif. Technol.; In preparation</i> ” [1].

## Value of the data

- The 2D NMR data permit full assignment of the signals in the spectra of the novel compounds.
- The ligands offer unlimited possibilities for NH-derivatization.
- The data can be useful for comparison with similar structures.

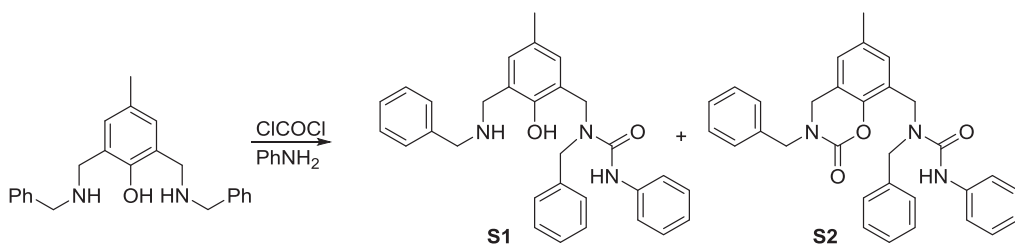
## 1. Data

The data include synthetic details and characterization by 1D and 2D NMR spectra, mass spectrometry, TLC and m.p. of novel organic polydentate ligands.

## 2. Experimental design, materials and methods

### 2.1. General

All reagents were purchased from Aldrich, Merck and Fluka and were used without further purification. The deuterated chloroform was purchased from Deutero GmbH. Fluka silica gel (TLC-cards 60778 with fluorescent indicator 254 nm) were used for TLC chromatography and  $R_f$ -values determination. Merck Silica gel 60 (0.040–0.063 mm) was used for flash chromatography purification of the products. The melting points were determined in capillary tubes on SRS MPA100 OptiMelt (Sunnyvale, CA, USA) automated melting point system. The NMR spectra were recorded on a Bruker Avance II+ 600 spectrometer (Rheinstetten, Germany) in  $CDCl_3$ ; the chemical shifts were quoted in ppm in  $\delta$ -values against tetramethylsilane (TMS) as an internal standard and the coupling constants were calculated in Hz. The spectra were processed with Topspin 2.1 program. The low-resolution mass spectra were taken on a HP 5973 Mass Selective Detector, the turbo spray spectrum on API 150EX (AB/MAS Sciex).



**Scheme 1.** Synthesis of the ligands **S1** and **S2**.

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