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Data Article

Synthesis and characterization of new dialkylacylphosphonylhydrazones

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ABSTRACT

The present work refers to the synthesis of novel dialkylacylphosphonylhydrazones that occurs in three reaction steps: the first one is the synthesis of different dialkyl acetate phosphonoacetates obtained by the reaction of ethyl bromoacetate with the trialkyl phosphite of interest. The second one is the synthesis of acetic diethoxyphosphonylhydrazines which is from the reaction between the synthesized dialkyl phosphonoacetates and hydrazine. The third and final steps is the condensation of acetic diethoxyphosphonylhydrazides with different heterocyclic aldehydes. In total, 17 unpublished compounds, namely 1 to 17 (Table 1) were obtained with a diastereoisomeric mixture of the preferential conformation *E* and all the compounds were characterized by 1-H and 13-C and 31-P NMR, infrared (IR) and mass spectroscopy (MS). This work presents the characterization data of these compounds.

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Specifications Table

Subject area	Chemistry
More specific subject area	Organic chemistry, organophosphorus
Type of data	Text file
How data was acquired	NMR (1H NMR (400 MHz), 13-C (100 MHz) and 31P (162 MHz) Bruker models Avance III 500 / Ultrashield 500 Plus and Avance II 400 / Ultrashield 400 Plus); mass spectroscopy (CG-MS - model QP2010 Plus - Shimadzu); infrared (FT-IR VERTEX 70).
Data format	Analyzed
Experimental factors	For the purification of the synthesized compounds, Biotagedo Isolera ™ Prime was used under the following analysis conditions: Ultra 10 g SNAP Cartridge - 25 μm silica stationary phase; wavelength detection mode; flow rate of 12 ml / min; Baseline correction, UV1 monitor readings at 254 nm and UV2 monitor readings at 365 nm and initial threshold of 20 mAU.
Experimental features	In the first step, in a 50 mL round bottom flask with a reflux condenser and bubbler, ethyl α-bromoacetate and triethyl or tributyl phosphite were reacted in slight excess. The reaction mixture remained under reflux and magnetic stirring for 6 h at 100 °C and was subsequently subjected to vacuum on the rotary evaporator for 5 h at 80 °C to remove excess of the remaining reagent. In the second step the triethyl phosphonoacetate, obtained above, was added to hydrazine monohydrate (64%) in a 50 mL round bottom flask, coupled to the rotary evaporator. The reaction mixture was kept under vacuum at 50 °C for 3 h. In the last step the diethoxyphosphonylhydrazides from step 2 was combined with the corresponding aldehyde, both previously dissolved in 3 mL of EtOH in a 50 mL round bottom flask. Then two 2 drops of 37% HCl were added. The reaction mixture was kept under stirring for 5 h at room temperature. After the reaction time had elapsed, the reaction medium was poured into ice-cold distilled water and left in an ice bath for half-an-hour for precipitation to occur. At the end of this time it was vacuum filtered and air dried. In cases where there was no precipitation, drops of 15% sodium bicarbonate solution were added to reach neutral pH. The resulting aqueous solution was treated with dichloromethane (4 × 15 mL). Finally, anhydrous Na_2SO_4 was added to the organic solution, then it was filtered and evaporated in a rotary evaporator.
Data source location	–
Data accessibility	–

Value of the data

- The synthesis of these dialkylacylphosphonylhydrazones is interesting because of the potential biological activity of the clusters present in the structures as acylidrazones (–CO–NH–N═). The dialkylacylphosphonylhydrazones have applications ranging from medicinal compounds and agrochemicals up to functional materials and considering that organophosphates present effective agricultural protection.
- These compounds have potential drug action to combat Alzheimer's disease, where acetylcholinesterase inhibitor drugs are used. Initial studies have shown inhibition of the enzyme acetylcholinesterase, target of the drugs used for Alzheimer's disease. However, further studies should be conducted in order to verify their action without compromising human health.

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