Chemical Data Collections 9–10 (2017) 104–113

Contents lists available at ScienceDirect

Chemical Data Collections

journal homepage: www.elsevier.com/locate/cdc

Data Article

Synthesis, characterization, antifungal activities and crystal structure of thiophene-based heterocyclic chalcones

Liew Suk Ming[a], Joazaizulfazli Jamalis[a,*], Helmi Mohammed Al-Maqtari[a], Mohd Mustaqim Rosli[b], Murugesan Sankaranarayanan[c], Subhash Chander[c], Hoong-Kun Fun[b,d]

[a] Department of Chemistry, Faculty of Science, Universiti Teknologi Malaysia, Johor Bahru, Johor 81310, Malaysia
[b] X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, Penang 11800, Malaysia
[c] Medicinal Chemistry Research Laboratory, Department of Pharmacy, Birla Institute of Technology and Science, Pilani, Rajasthan 333031, India
[d] Department of Pharmaceutical Chemistry, College of Pharmacy, King Saud University, P.O. Box 2457, Riyadh 11451, Saudi Arabia

ARTICLE INFO

Article history:
Received 12 April 2017
Accepted 13 April 2017
Available online 25 April 2017

Keywords:
Antifungal
Heterocycle
Chalcones
Thiophene
Crystal structure

ABSTRACT

Heterocyclic chalcones containing thiophene moiety were synthesized and their chemical structures determined via IR, MS, 1H NMR and 13C NMR spectroscopy. Crystal structure of the compounds was determined using single crystal X-ray diffraction.The chalcones were also screened for in-vitro antifungal activity against two fungal strains; Candida albicans (MTCC 3958) and Aspergillus niger (MTCC 9933)which gave good results.

* Corresponding author.
E-mail addresses: joazaizul@kimia.fs.utm.my, joazaizulfazli@utm.my (J. Jamalis).

http://dx.doi.org/10.1016/j.cdc.2017.04.004
2405-8300/

Specifications Table

Subject area	*Organic chemistry*
Compounds	*1. (E)-1-(5-methylfuran-2-yl)-3-(5-methylthiophen-2-yl)prop-2-en-1-one (**3**)* *2. (E)-1-(5-Chlorothiophen-2-yl)-3-(thiophen-2-yl)-2-propen-1-one (**7**)*
Data category	*Spectral, synthesized, crystallographic*
Data acquisition format	*NMR, IR, Mass spectra*
Data type	*analyzed*
Procedure	*Brief description of procedure (e.g., transformation, simulation, etc.)*
Data accessibility	*State if data is with this article or in public repository. If public repository, please explicitly name repository and data identification number and provide a direct URL to data*

1. Rationale

Chalcones are open-chain flavanoids possessing a basic scaffold of two aromatic rings linked by a three carbon α,β-unsaturated carbonyl system [1] obtained by reacting aromatic aldehydes with aromatic ketones. Synthetic and naturally occurring chalcones have been found to possess a wide range of biological activities such as antibacterial, anticancer, antifungal, anti-inflammatory, antitubercular and antioxidant activity among others [2–6] which is credited to the α,β-unsaturated ketone moiety.

In this study, the Claisen-Schmidt condensation method is employed which can be acid-catalyzed using dry HCl, aluminium trichloride (Al_2Cl_3), ruthenium trichloride ($RuCl_3$) or titanium trichloride ($TiCl_3$) or base-catalyzed using sodium hydroxide (NaOH), potassium hydroxide (KOH), lithium hydroxide ($LiOH.H_2O$) or barium hydroxide (BaOH). Expensive catalysts like Amberlyst-15, bamboo char sulfonic acid, $LiNO_3$/natural phosphate, $SOCl_2$/EtOH or zinc oxide are also applicable but the need for an inert environment, higher temperature and more time for the reaction to take place with resulting yield being lower than the conventional methods [7] does little to promote the use of these catalysts. For my research, the base-catalyzed Claisen–Schmidt condensation method is selected. An advantage of this method is that it specifically generates the (E)-isomers [8].

Drug resistance is a worldwide healthcare problem that is developing rapidly with some examples such as the methicillin-resistant Staphylococcus aureus (MRSA), vancomycin-resistant Enterococci (VRE), multidrug-resistant Neisseria gonorrhoeae (Gonorrhea) and the levofloxacin-resistant pneumococcus. The development of new therapeutic agents with different chemical characteristics from the existing drugs, but are nevertheless equal or even more effective in their activities is thus a priority. This can be done by looking at pre-existing bioactive molecules already used in medicine and modifying their scaffolds to obtain novel molecules with the desired biological properties [9]. Examples are the antibacterial cefoxitin and antifungal tioconazole possessing the thiophene moiety. Heterocyclic chalcones have been found to possess a wide range of biological activities such as antibacterial, antifungal, anticancer, antioxidant and insect antifeedant activity among others [10,11]. The α,β-unsaturated ketone moiety of chalcones is responsible for their bioactivity and losing it often resulted in a major decrease or loss of this property [12] whereas modifying the aromatic rings of chalcones has been found to either boost or diminish the bioactivity of chalcones, depending on the type of modification, e.g.: homocyclic or heterocyclic aromatic ring, or the substituent on the aromatic ring [13]. Attempting the synthesis of novel heterocyclic chalcones containing the thiophene moiety is therefore a logical step towards developing potential new drugs to counter drug resistance as shown in Fig. 1. The crystal structure of chalcones **3** and **7** was also determined using single crystal X-ray diffraction.

2. Procedure

2.1. Materials and methods

All the reagents used were purchased from commercial suppliers without further purification. Melting point determination was done using the Barnstead 9100 Electrothermal digital melting point apparatus and was recorded in °C. Compound purity was confirmed using TLC on silica gel 60 F254. Spectroscopic data were recorded using the FTIR Spectrometer Frontier (ATR-FTIR), Bruker Advancer