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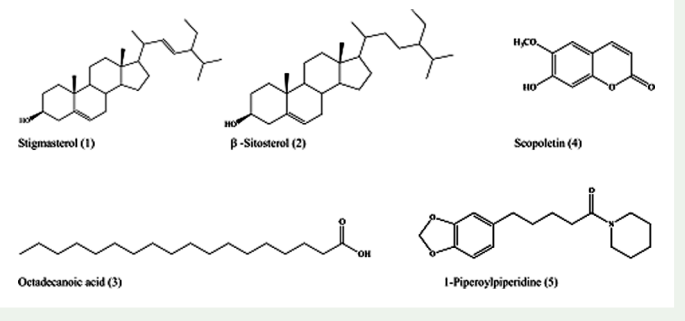
Phytochemical characterisation of an important medicinal plant, *Chenopodium ambrosioides* Linn.

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ABSTRACT

The project was intended to the phytochemical characterisation from the rudimentary methanolic extract of *Chenopodium ambrosioides* Linn., which escorts to the isolation of stigmasterol (1), β-sitosterol (2), octadecanoic acid (3), scopoletin (4) and 1-piperoylpiperidine (5). Literature validates the medicinal authentication of these compounds extorted from other sources, while our previous findings regarding microbial activities of different solvent systems fractions are favouring the presence of medicinally important compounds in this species. Herein, however, we report these natural products for the first time from this species.



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1. Introduction

Chenopodium ambrosioides Linn., is a medicinal species (Podolak et al. 2016) of Chenopodiaceae (Gómez-Caravaca et al. 2011) found in Asia, Europe and America (Kiuchi et al.2002). The plant is widely distributed in Pakistan (Nisar et al. 2013, Shah 2014, Shah et al. 2014). An annual or perennial shrub, with simple leaves, alternate, opposite, lacking stipules (MacDonald et al. 2004). The bracts of the fruits are green or brown (Cavalli et al. 2004).

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This species is used as a vermifuge and against stomach discomfort caused due to intestinal worms (Rossier 2006) and in women's problem of pregnancy (Coutts et al. 2011). Many *ambrosioides* have carminative effect and are used for dietary purpose (Quinlan et al. 2002). The essential oil of *C. ambrosioides* is included in the United States National Formulary and in the British Pharmacopoeia. It is a pale yellow to orange yellow liquid, having a peculiar, unpleasant odour, and a bitter, burning taste (DellaGreca et al. 2005, Harraz et al. 2015). Its insecticidal (Tapondjou et al. 2002) and antimicrobial potency has been explored (Pandey et al. 2012, 2013). It has a burning taste and causes salivation and gastric irritations if used improperly by children or aged and malnourished person (Elseviers & De Broe 1996). Previously, we succeeded to some extent in elucidating the antimicrobial potential of different crude fractions (Nisar et al. 2013, Shah 2014, Shah et al. 2014) from this plant, which motivated us to carry out phytochemical screening of this plant, the details of which are given below.

2. Results and discussion

Different fractions of methanol extract were investigated phytochemically, which succeeded us in isolation and characterization of five compounds viz. Stigmasterol (1), β-sitosterol (2) and Octadecanoic acid (3) from ethyl acetate, while scopoletin (4) from dichloromethane and 1-Piperoylpiperidine (5) from n-butanol sub fraction. The physical and chemical data for these compounds are given as under. (NMR data are uploaded as supporting information).

2.1. *Stigmasterol* (1)

The structure of stigmasetosterol (Figure S1) was characterised from the given data.

Physical state: Colourless crystals. Melting Point: 170°C. R_f: 0.8 (ethyl acetate : hexane; 1:4). IR ($CHCl_3$) V_{max} cm^{-1}: 3432 (OH), 3025, 1648 (C = C). HREI-MS (*m/z*): 412.3920 (calcd. for $C_{29}H_{48}O$, 412.3926). EI-MS *m/z* (rel.int %): [M^+] 412 (8), 397 (12), 394 (20), 379 (27), 369 (35), 351 (71), 327 (60), 301 (18), 300 (18), 300 (67), 273 (30), 270 (24).

2.2. *β-Sitosterol* (2)

The following data were obtained for β-Sitosterol structure (Figure S2) determination.

Physical state: Colourless crystals. Melting Point: 135°C. R_f: 0.67 (ethyl acetate: hexane; 1:4). IR ($CHCl_3$) V_{max} cm^{-1}: 3450 (OH), 3050, 1650 (C = C). HREI-MS *m/z*: 414.3845 (calcd. for $C_{29}H_{50}O$, 414.3861). EIMS *m/z* (rel.int %): [M^+] 414 (15), 399 (10), 396 (12), 381 (72), 329 (28), 275 (12), 273 (17), 255 (36).

2.3. *Octadecanoic acid* (3)

Octadecanoic acid (Figure S3) was characterised using the following data.

Physical state: polymorphic crystals. Melting point: 69.7°C, R_f. 0.67 (ethyl acetate: hexane; 1:9), IR ($CHCl_3$) V_{max} cm^{-1}. 2500 (OH of COOH), 2960 (C-H str). HREI-MS (*m/z*), 284.26834 (Calcd for $C_{18}H_{36}O_2$, 284.26). EIMS *m/z* (rel.int %), [M^+] 284 (100), 286 (20), 286 (2).

2.4. *Scopoletin* (4)

The following data were used to determine the structure (Figure S4) of Scopoletin.

Physical state: colourless crystals, mp: 206°C. R_f: 0.44 (dichloromethane : methanol; 7:3). IR ($CHCl_3$) V_{max} cm^{-1}: 3450 (OH), 3050, 1650 (C=C). HREI-MS (*m/z*): 192.06 (Calcd for $C_{10}H_8O_4$, 192.0468). EIMS *m/z* (rel.int %): [M^+] 192 (100), 193 (10), 194 (2).

2.5. *1-Piperoylpiperidine* (5)

Below is given the spectroscopic and physical data of the 1-Piperoylpiperidine (Figure S5).

Physical state: Yellowish needle-like crystals. Melting Point: 130°C. R_f: 0.47 (dichloro methane: methanol (9:1)). IR ($CHCl_3$) V_{max} cm^{-1}: 3050, 1650 (C=C). HREI-MS (*m/z*): 285.1462 (Calcd for $C_{17}H_{19}NO_3$, 285.3461). EIMS *m/z* (rel.int %): [M^+] 285.14 (100), 286.14 (30), 396 (8).

Chenopodium oil has been the main component of this plant used for killing round and hook worms as well as an abortifacient, and is available commercially, although there are still concerns of side effects by its use (Conway & Slocumb 1979). It may be the combination of essential oil and fixed oil of this plant. The crude hydroalcoholic extract (HCE) has been reported for antimalarial activity (Cysne et al. 2016).

Stigmasterol and β-sitosterol have been reported for antifungal, additive, cholesterol lowering, antitumour and hypoglycaemic properties (Mbambo et al. 2012), stearic acid for Xylene replacement in tissue staining (Guo et al. 2008; Sane et al. 2012),scopolitine for effecting cytokine production, as constituent in Ayurveda medicinal system and for analgesic effects (Moon et al. 2007). 1-piperoylpiperidine has also been reported for its therapeutic applications (Khom et al. 2013). Additionally, the charisma of these compounds goes in favour of verdict of more important molecules/drugs among these or other classes of compounds.

3. Conclusion

The exertion offered at this juncture verify that this plant have incredible healing standards due to the incidence of classes of compounds competent for using as imperative drugs against assorted pathogens. Still these studies are not adequate and advanced research is obligatory for discovering the significance of this plant.

Disclosure statement

No potential conflict of interest was reported by the authors.

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