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Chemical constituents from the fruits of *Solanum incanum* L

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ABSTRACT

Phytochemical investigation of the fruits of *Solanum incanum* L. resulted in the isolation of nine compounds, including three steroidal glycoalkaloids (**1-3**), two neolignans (**4–5**), two simple phenolics (**6–7**), one monoterpene glycoside (**8**), and one coumarin glucoside (**9**). The structure elucidation of isolated compounds was determined based on NMR and mass spectral data. Compounds **4** and **9** were isolated for the first time from the genus *Solanum* and their chemotaxonomic significance was discussed.

1. Subject and source

The genus *Solanum* is regarded to be one of the largest among the Angiosperms and the most representative and largest genus of the family Solanaceae (Kaunda and Zhang, 2019). It is comprised of about 1500 species distributed across subtropical and tropical regions of Asia, tropical Africa, non-arid Africa, Americas, and Australia. Many species belonging to this genus possess a rich repertoire of medicinal, economic, and ornamental importance (Kaunda and Zhang, 2019; Yohara et al., 1996). Within the past 30 years, *Solanum* has attracted significant attention in chemical and biological studies. Previous phytochemical investigations on *Solanum* species led to the identification of steroidal saponins, steroidal alkaloids, terpenes, flavonoids, lignans, sterols, phenolics, and coumarins (Kaunda and Zhang, 2019).

Solanum incanum L. or Sodom/bitter apple (English), is a perennial, wild shrub distributed mainly in Kenya, Uganda, Tanzania, Middle East, India, Australia, Madagascar, Mauritius, Saudi Arabia, and Taiwan (Kaunda and Zhang, 2019; Mwonjoria et al., 2014). The leaves and stems have periodically small thorns, and the fruits are often 2–3 cm in diameter with yellowish orange or brown in color when ripe (Mwonjoria et al., 2014). It has been widely used as a folk medicine for managing hepatitis in Taiwan (Lin et al., 2000, Lin et al., 1988), and various ailments such as angina, ear inflammation, sore throat stomach ache, snake bites, wounds, liver disorders, ringworms, warts, inflammatory conditions, painful periods and fever in Africa. Pharmacological studies on this plant have indicated antibacterial, antileishmanial, cytotoxic, and anti-inflammatory activities (Kaunda and Zhang, 2019). The plant was taxonomically identified by Dr. Peter Githaiga Mwitari (Centre for Traditional Medicine Drug Research, Kenya Medical Research Institute (CTMDR-KEMRI) and a voucher specimen (KEMRI/CTMDR/PGM/1/2017) was deposited at the laboratory of phytochemistry, KEMRI.

2. Previous work

Previous chemical investigations on *S. incanum* revealed the presence of 16 flavonoids and 2 vitamins from the aerial parts (Lin et al., 2000 et al., 2000 Mwonjora et al., 2014), 4 steroidal glycoalkaloids (Fukuhara et al., 1991; Manase et al., 2012) and 7 spirostanol saponins (Fukuhara et al., 1991; Manase et al., 2012) from the roots, and 2 sterols from fresh berries. In total, 31 compounds had been isolated from the roots and aerial parts of *S. incanum*, prior to this study.

3. Present study

This study focused on the fruits of the titled plant. The freeze-dried fruit juice of *S. incanum* (156 g) was extracted with 95% ethanol (3 × 4 L × 48 h) at room temperature. The extracts were filtered and evaporated under reduced pressure at 45 °C before adding water and partitioning with EtOAc, to afford H_2O (42.0 g) and EtOAc (34.0 g) fractions, which were separately subjected to column chromatography (CC) over a Diaion HP-20SS, eluting with MeOH: H_2O (0:1 → 1:0) to give six fractions (W1–W6) from H_2O and five fractions (E1-E5) from EtOAc fractions, respectively. Fr. E4 (6.8 g) was further applied to MCI-gel CHP20P and RP-18 CC, eluting with MeOH: H_2O (0:1 → 1:0) to give sub-fractions, E4B1-E4B8. Sub-fr. E4B4 (300 mg) was subjected to

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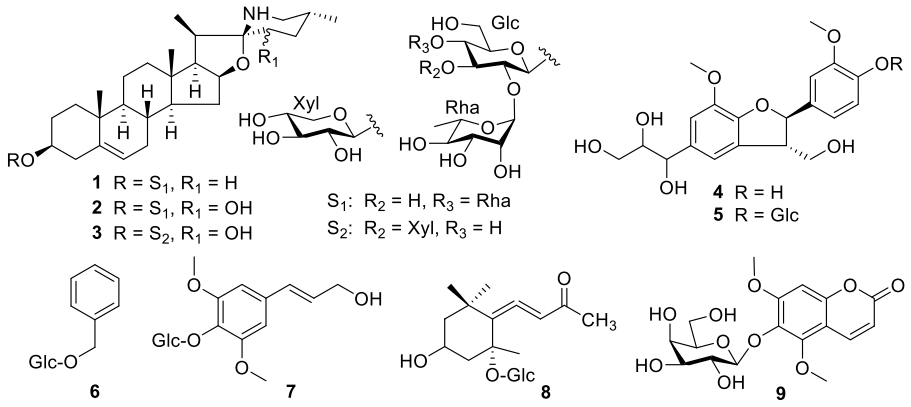

Fig. 1. Chemical Structures of Compounds, 1–9, isolated from the fruits of *S. incanum*.

repeated CC of silica gel, eluting with chloroform/methanol/water (100:0:0, 98:2:0, 96:4:0, 94:6:0, 92:8:0, 90:10:0, 90:10:1, 85:15:1, 80:20:2, 75:25:2, 70:30:5 v/v) to generate four sub-fractions, E4B4A-E4B4D. Sub-fr. E4B4C (109 mg) was further subjected to silica gel, eluted as mentioned above to furnish compound **1** (9 mg). Sub-fr. E4B8 (150 mg) was applied to a silica gel CC, eluting as outlined above to bring forth compound **2** (59 mg). Sub-fr. E4B4A (46 mg) was further subjected to MCI-gel CHP20P (MeOH: H_2O, 0:1 → 1:0) and purified by preparative HPLC with an isocratic mobile phase system of acetonitrile: water (11:89) to furnish compounds **4** (t_R = 34.0 min, 1.0 mg), **8** (t_R = 48.2 min, 2.0 mg) and **9** (t_R = 36.4 min, 1.0 mg).

Repeated CC of Fr. W5 (11 g) over RP-18 (MeOH:H_2O, 0:1 → 1:0) and silica gel (chloroform/methanol/water, 90:10:0, 90:10:1, 85:15:1, 80:20:2, 75:25:2, 70:30:5 v/v) generated compound **3** (3.0 mg). Fr. W6 (8 g) was applied successively to CC over MCI-gel CHP20P (MeOH:H_2O, 0:1 → 1:0), silica gel (chloroform/methanol/water, 90:10:0, 90:10:1, 85:15:1, 80:20:2, 75:25:2, 70:30:5 v/v) and RP-18 (MeOH:H_2O, 0:1 → 1:0) to give compound **5** (10 mg).

Fr. W2 (568 mg) was chromatographed repeatedly over silica gel (chloroform/methanol/water, 85:15:1, 80:20:2, 75:25:2, 70:30:5 v/v) to afford two sub-fractions, W2C1–W2C2. Sub-fr. W2C2 (52 mg) was purified by preparative HPLC with an isocratic mobile phase system of acetonitrile: water (9:91) to furnish compounds **6** (t_R = 23.1 min, 2.0 mg) and **7** (t_R = 26.6 min, 3.0 mg).

The isolated compounds (Fig. 1) were identified as solamargine (**1**) (Tian et al., 1997), solaverine I (**2**) (Yamashita et al., 1990), (23S)-23-hydroxyanguivine (**3**) (Ripperger, 1997), sisymbrifolin (**4**) (Li et al., 2019a,b; Chakravarty et al., 1996), sisymbrifolin 4-*O*-glucopyranoside (**5**) (Eom et al., 2016), benzyl-glucopyranoside (**6**) (Li et al., 2019a,b), syringin (**7**) (Zhou et al., 2019), citroside B (**8**) (Osorio et al., 1999), fraxinol-6-*β*-D-galactopyranoside (9) (Yu et al., 2015), by comparison of their spectroscopic data with literature values.

4. Chemotaxonomic significance

The isolated compounds from *S. incanum* are classified as steroidal alkaloids (**1–3**), lignans (**4–5**), and simple phenolic compounds (**6–9**). Compounds **2–9** were obtained for the first time from the titled plant. Among them, compounds **5** and **9** are new from the genus *Solanum*, and are hereby reported from the family Solanaceae for the first time. The family Solanaceae is hallmarked by steroidal alkaloids and steroidal saponins as the main chemical constituents (Kaunda and Zhang, 2019). Lignans too have been characterized in the genus *Solanum*. The isolation of steroidal alkaloids (**1–3**), sisymbrifolin (**4**), previously obtained from *S. sisymbriifolium* Lam. (Chakravarty et al., 1996), and citroside B, hitherto sourced from *S. quitoense* Lam (Osorio et al., 1999). underscored the taxonomic position of *S. incanum* under the family Solanaceae in regards to chemotaxonomy. Moreover, benzyl-glucopyranoside (**6**) was previously isolated from the fruit pulp of lulo del Choco (*S. topiro* Dunal) (Morales et al., 2000) and the existence of syringin (**7**) in *S. tuberosum* L. is well reported (Pushpa et al., 2014). Sisymbrifolin 4-*O*-glucoside (**5**), has been reported only from *Lycium radicis* cortex Mill. (Eom et al., 2016). The results illustrate that *S. incanum* has identical steroidal alkaloids, lignans, and simple phenolics with other species of *Solanum*. Therefore, steroidal alkaloids, lignans, and simple phenolics can represent the chemosystematic markers of the genus *Solanum*.

CRediT authorship contribution statement

Joseph Sakah Kaunda: Investigation, Data curation, Writing - original draft. **Ying-Jun Zhang:** Writing - review & editing, Supervision.

Declaration of competing interest

The authors declare no conflict of interest.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.bse.2020.104031.

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