ABSTRACT
The essential oil from different parts of *Datura metel* L. were extracted using hydrodistillation and GC–MS was used to analyse the essential oil. The main components of flowers were ketone (23.61%) and ethyl palmitate (15.84%). The main components of leaves were ketone (18.84%) and phytol (18.71%). Ketone (39.45%) and phytol (31.32%) were the major components of petioles. Palmitic acid (30.60%) and ethyl linoleate (21.56%) were the major components of seeds. The major ingredient of roots was palmitic acid (52.61%). The main ingredients of the stems were palmitic acid (38.38%) and ethyl linoleate (17.38%). All the different parts of essential oil were screened for cytotoxicity. The roots and stems showed the inhibitory effects against HepG-2 with IC$_{50}$ levels of 613.88 and 341.12 mg/L. The leaves and roots showed the inhibitory effects against HeLa with IC$_{50}$ levels of 267.76 and 348.35 mg/L. All the six parts have inhibitory effects against SGC-7901 cell lines.

SHORT COMMUNICATION

Chemical composition and cytotoxicity of the essential oil from different parts of *Datura metel* L.

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1. Introduction

*Datura metel* L. is an annual erect herb distributed mainly in temperate to tropical regions (Fang et al. 2013; Zhang et al. 2014). The flowers, leaves and seeds can be used as medicinal, which can treat cough, asthma, pain, spasm, anaesthesia etc. Recent studies have found that preparations
of *D. metel* L. had a good effect on treatment of psoriasis. Our research group has extensively researched on chemical constituents and pharmacological activities for many years, including multiple parts of *D. metel* L. such as leaves, seeds. A variety of compounds such as alkaloids, flavonoids and withanolides have been isolated from the plant (Yang et al. 2010a, 2010b, 2013; Kuang et al. 2011). We also found that the flowers of *D. metel* L. had effect of anti-inflammatory, anti-itch, anti-proliferative and some other pharmacological effects and the seeds have anti-proliferation and potential immune suppression activities (Yang, Xia, et al. 2014). The compound from the leaves of *D. metel* L. could inhibit the impact of NO production in LPS-induced RAW 264.7 cells (Yang, Guo, et al. 2014). To the best of our knowledge, studies on the essential oil from other parts of *D. metel* L. are very limited, and there are no published reports on the cytotoxicity activity of essential oil from *D. metel* L. In this study, essential oils of flowers, leaves, petiole, seeds, roots and stems of plants were separated and identified by GC–MS method. Using MTT assay tested its cytotoxic activity of the six parts of essential oil against human tumour HepG-2, HeLa and SGC-7901 cell lines in order to make further rational development of medicinal resources.

### 2. Results and discussion

#### 2.1. Chemical composition of the essential oil

Each part of *D. metel* L. was extracted using hydrodistillation to get yellowish oil. The essential oil obtained was qualitatively analysed by GC–MS and quantitatively analysed by GC–FID. A total of 50 components of six parts of plant representing 92.29, 91.20, 95.67, 99.00, 85.72 and 87.66%, respectively, were identified and all constituents are summarised in Table S1.

#### 2.2. Cytotoxicity activity

All the six parts of essential oil were tested for their cytotoxicity against three human cancer cell lines (HepG-2, Hela, and SGC-7901) using the MTT method as described in the literature (Zhang et al. 2015). The IC$_{50}$ values of six parts of essential oil have been shown in Table 1. As observed, in MTT assay, three kinds of cell lines tested were susceptible to the essential oil with IC$_{50}$ from 153.30 to 2623.06 mg/L. The highest activity was observed the stems against SGC-7901 cell lines with IC$_{50}$ 153.3 mg/L, followed by the roots (188.69 mg/L). The roots and stems were found to show cytotoxicity toward HepG-2 cell lines with IC$_{50}$ values of 613.88 and 341.12 mg/L, respectively. The leaves and roots showed cytotoxicity against Hela cell lines with IC$_{50}$ 267.76 and 348.35 mg/L. All the six parts showed cytotoxicity against SGC-7901 cell lines. In all the six parts of essential oil, roots of plant were found to show cytotoxicity.

| IC$_{50}$ (μM) | HepG-2 | HeLa | SGC-7901 |
|---------------|--------|------|----------|
| Flowers       | –      | –    | 221.69 ± 6.54 |
| Leaves        | –      | 267.76 ± 10.12 | 233.94 ± 6.67 |
| Petioles      | –      | –    | 468.45 ± 12.67 |
| Seeds         | –      | –    | 2623.06 ± 90.12 |
| Roots         | 613.88 ± 14.18 | 348.35 ± 11.22 | 188.69 ± 5.31 |
| Stems         | 341.12 ± 12.34 | –    | 153.30 ± 5.20 |

Table 1. The IC$_{50}$ values of HepG-2, Hela, SGC-7901 treated with essential oil from six parts of *D. metel* L. (n = 3).
toward the three cell lines. This is the first report on the cytotoxicity activity of essential oil of six parts from *D. metel* L.

### 3. Conclusion

The data presented above confirm the cytotoxicity activity of essential oil from *D. metel* L. for the first time. The tested oil showed significant cytotoxicity activity with the IC$_{50}$ values in the range of 153.30–2623.06 mg/L. The results of essential oil analysis and cytotoxicity activity can provide some reference and basis for a better and more conducive to the full development and utilisation of *D. metel* L. resources.

### Supplemental data and research materials

Experimental details relating to this paper are available online.

### Disclosure statement

No potential conflict of interest was reported by the authors.

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