Structure Identification of Compounds Promising Anticancer and Antinematode Extracted From Chinese Traditional Herbs Using NMR

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Plant-parasitic nematodes are a serious threat to crops causing an estimated yield loss worth US$ 100 billion per year. In the European Union (EU), chemical nematicides such as the broad spectrum soil fumigant methyl bromide – for decades the main tool within nematode management – have already been phased out, whilst other soil disinfestants are currently under critical review, as many of them have proved to be hazardous to the environment. In addition, due to consumer and social demands, more and more agricultural land is under organic farming where the application of synthetic nematicides and artificial fertilizers is forbidden. There is, therefore, an urgent need to develop sustainable methods of nematode management (Noling & Becker, 1994; Martin, 2003).

The use of organic amendments, already described by Linford (1938), is seen as one of the most promising solutions to manage plant-parasitic nematodes. Sesame is an important seed and oil crop worldwide. In addition to being a poor host for root-knot nematodes (Rodriguez-Kabana et al., 1988a; 1989), sesame is known to produce several lignin compounds including sesamin and sesamolin which are antioxidants that function as insecticides and insecticidal synergists and are hypothesized to be the active allelopathic compounds in sesame (Bedigian and Harlan,1986).

In order to find more anti-parasites active substances, the sesame's oil cake was phytochemically and pharmacologically investigated to obtain 2 compounds. The nematicidal activity of isolated compounds were tested against J2 of root-knot nematode. The goal of this project is to identify their structures using NMR.

Experimental

Two purified compounds extracted from sesame's oil cake (named ZM-1,2,) promising anti-parasite activity have been analyzed using Bruker Avance-I/III-500 / TXI & BBO Probe, Bruker Avance-I/III-600 / BBO Probe ("Silver 600") and Bruker Avance-II-600 / CryoProbe ("White 600") with conventional 5mm probe, using a 3mg/mL solution of extract dissolved in Meod. The data acquisition have been performed using the DIPSI-2 sequence (Shaka et al., 1998) and, standard 1H, 13CAPT, COSY, HSQC, HMBC, NOESY experiments have been carried out. The data has been processed using Topspin software. All the experiments have been completed with the help of Jim Rocca. Distinguishing differences in the anti-parasite bioactivity of the isolated compounds has been found by bioassay.

Results and Discussion

The two compounds are being identified according to the obtained nmr data. The nematicidal activity of the two compounds were valuated against J2 of root-knot nematodes. Among these two compounds, both ZM-1 and ZM-2 exhibited weak nematicidal activity. However, the two compounds could increase the nematicidal activity of biocontrol fungal product synergistically.

Conclusions

Two compounds were isolated from the sesame's oil cake and all the data of standard 1H, 13CAPT, COSY, HSQC, HMBC, NOESY have been obtained to identify their structures.

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