Supporting Information

Identification of Meliatoxins in *Melia azedarach* Extracts Using Mass Spectrometry for Quality Control

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Fig. 1S $^1$H NMR of ethyl acetate partitions showing proton shifts characteristic of meliatoxins.
The ethyl acetate fraction was submitted to preparative HPLC (Fig. S2A). Two peaks (eluted in ~55% acetonitrile) showed clear and defined signals of limonoids, such as meliatoxins, by $^1$H NMR (Fig. S2B). It can be observed signals of methyl groups between $\delta$ 0.84 and $\delta$ 1.92 ppm corresponding to H-28; H-4'; H-30; H-2' and H-18 of meliatoxins. Signals of methyl of acetate groups at $\delta$ 1.99 and 2.12 ppm (MECOO). Hydrogens linked to the carbons with heteroatoms presented signals between $\delta$ 3.20 and 5.77 ppm. H-17, linked to a carbon that the furan ring is connected, showed a clearly doublet of doublets at $\delta$ 2.85 ppm. Signals related to the furan ring hydrogens were observed around $\delta$ 6.32 and 7.50 ppm (H-21, 22 and 23).

**Fig. 2S**

A prep-HPLC of AcOEt partition showing the elution profile and fractions in which meliatoxins were obtained. B $^1$H NMR (400MHz) of selected fractions showing proton shifts of meliatoxins.