

Article

Phytochemical Profile and Herbicidal (Phytotoxic), Antioxidants Potential of Essential Oils from *Calycolpus goteanus* (Myrtaceae) Specimens, and in Silico Study

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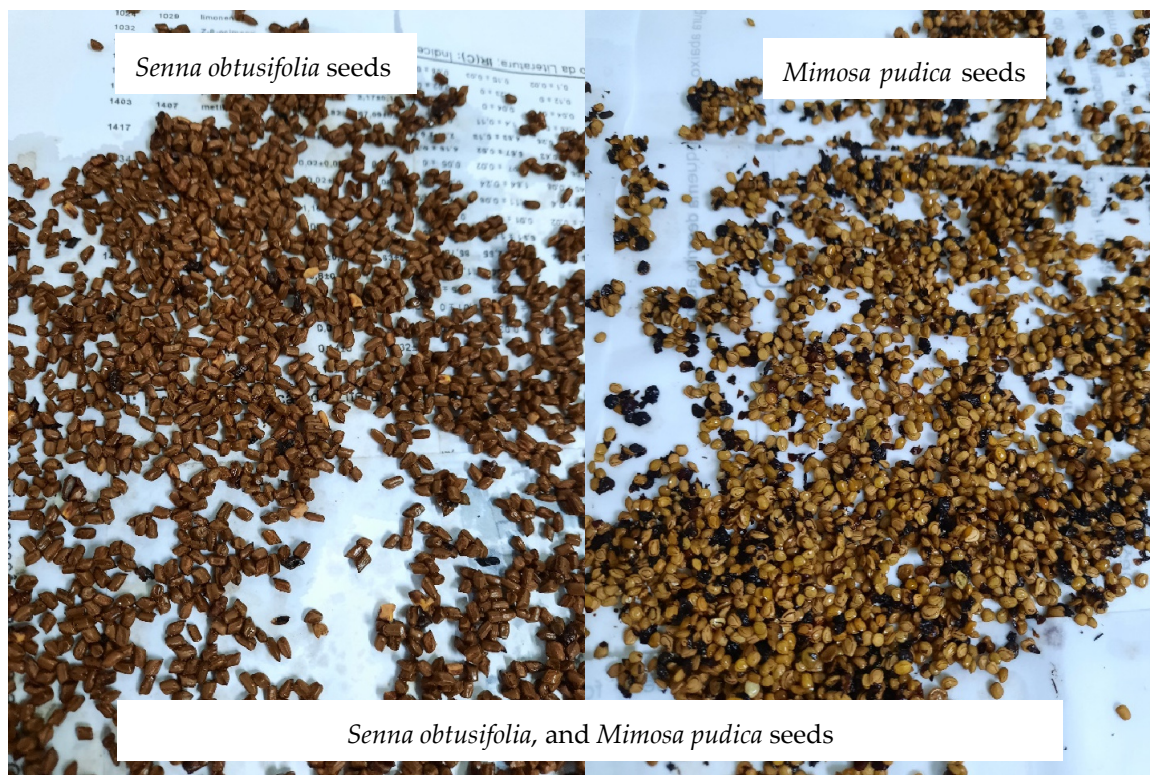
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Abstract: The essential oil (EO) of *Calycolpus goetheanus* (Myrtaceae) specimens (A, B, and C) were obtained through hydrodistillation. The analysis of the chemical composition of the EOs was by gas chromatography coupled with mass spectrometry CG-MS, and gas chromatography coupled with a flame ionization detector CG-FID. The phytotoxic activity of those EOs was evaluated against two weed species from common pasture areas in the Amazon region: *Mimosa pudica* L. and *Senna obtusifolia* (L.) The antioxidant capacity of the EOs was determined by (DPPH•) and (ABTS•+). Using molecular docking, we evaluated the interaction mode of the major EO compounds with the molecular binding protein 4-hydroxyphenylpyruvate dioxygenase (HPPD). The EO of specimen A was characterized by β -eudesmol (22.83%), (*E*)-caryophyllene (14.61%), and γ -eudesmol (13.87%), while compounds 1,8-cineole (8.64%), (*E*)-caryophyllene (5.86%), δ -cadinene (5.78%), and palustrol (4.97%) characterize the chemical profile of specimen B's EOs, and specimen C had α -cadinol (9.03%), δ -cadinene (8.01%), and (*E*)-caryophyllene (6.74%) as the majority. The phytotoxic potential of the EOs was observed in the receptor species *M. pudica* with percentages of inhibition of 30%, and 33.33% for specimens B and C, respectively. The EOs' antioxidant in DPPH• was 0.79 ± 0.08 and 0.83 ± 0.02 mM for specimens A and B, respectively. In the TEAC, was 0.07 ± 0.02 mM for specimen A and 0.12 ± 0.06 mM for specimen B. In the results of the in silico study, we observed that the van der Waals and hydrophobic interactions of the alkyl and pi-alkyl types were the main interactions responsible for the formation of the receptor–ligand complex.

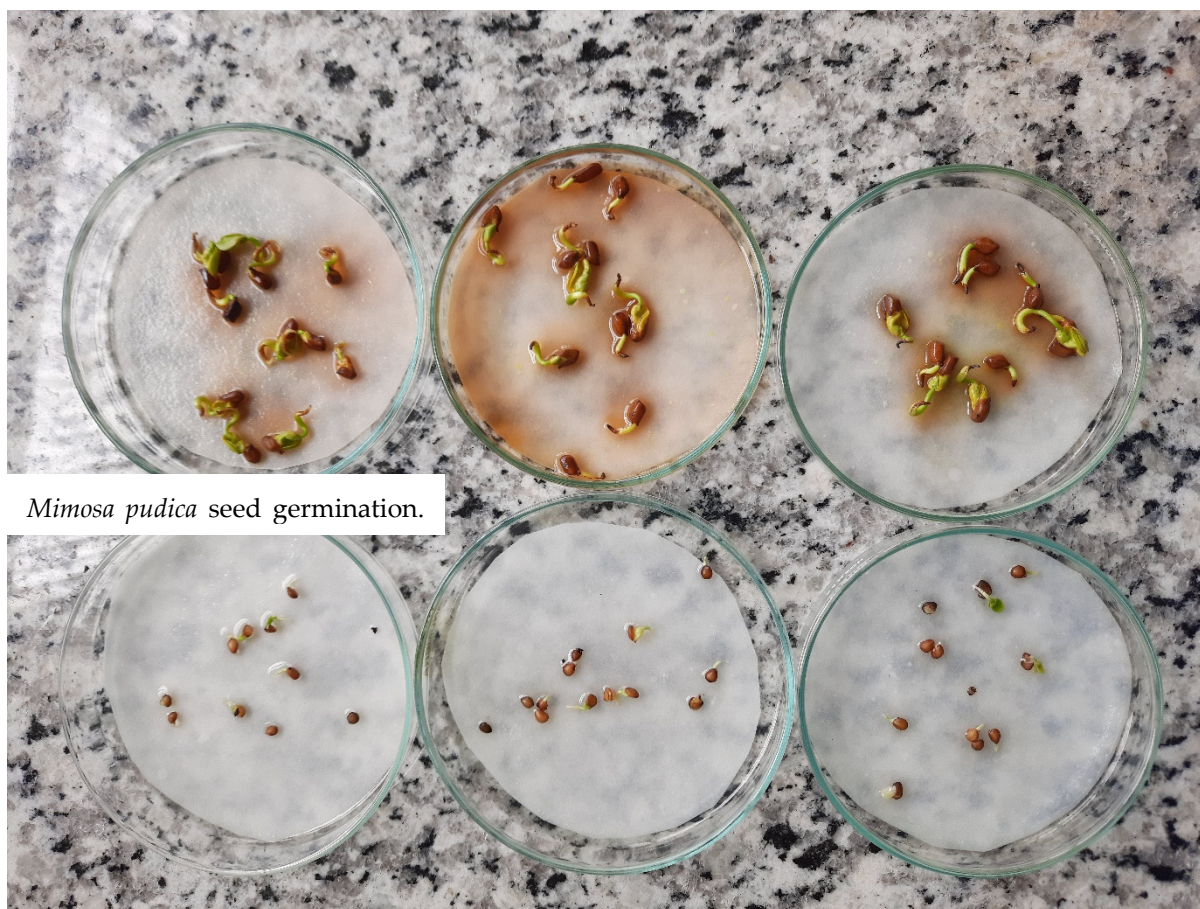
Keywords: natural products; volatile compounds; terpenes; allelopathy; antioxidant capacity

Supplementary material S1

Experiments on the phytotoxic potential of essential oils from *Calycolpus goetheanus*.



Senna obtusifolia seed germination



Mimosa pudica seed germination.



Senna obtusifolia radicle, and hypocotyl.



Mimosa pudica radicle, and hypocotyl.

Seed germination

