Structure and Spasmolytic Activity Relationships of Monoterpene Analogues Found in Many Aromatic Plants

Damião P. de Sousa^{a,*}, Genival A. S. Júnior^a, Luciana N. Andrade^a, Flávia R. Calasans^a, Xirley P. Nunes^b, José M. Barbosa-Filho^b, and Josemar S. Batista^a

- Departamento de Fisiologia, Universidade Federal de Sergipe, CEP 49100-900,
 São Cristóvão, Sergipe, Brazil. E-mail: damiao_desousa@yahoo.com.br
 Laboratório de Tecnologia Farmacêutica, Universidade Federal da Paraíba,
 Caixa Postal 5009, CEP 58051-970, João Pessoa, Paraíba, Brazil
- Z. Naturforsch. **63c**, 808–812 (2008); received March 10/May 23, 2008

* Author for correspondence and reprint requests

Key words: Terpenes, Essential Oils, Smooth Muscle

Rotundifolone, a monoterpene isolated from the essential oil of the leaves of *Mentha* × *villosa*, is a constituent of several essential oils and known to have spasmolytic activity. The present study aimed to investigate the correlation between structure and spasmolytic activity of rotundifolone and its analogues in ileum isolated from guinea-pig. Five of the seven tested analogues were found to have a spasmolytic effect more potent than rotundifolone itself, except for pulegone and (+)-limonene. The comparison between rotundifolone and limonene oxide showed that the absence of the keto group did not decrease the relaxant effect. Comparison of the spasmolytic activity between rotundifolone and (+)-pulegone showed that the absence of the epoxy group did not decrease the relaxation of the ileum. Carvone epoxide was found to be significantly more potent than rotundifolone. The monoterpene (-)-carvone produced ileum relaxation and was more potent than its enantiomer (+)-carvone. (+)-Limonene and pulegone oxide showed a similar effect. The study showed that the functional groups and their position at the ring of rotundifolone contributed to the relaxation activity of the ileum. The absence of the oxygenated molecular structure is not a critical requirement for the molecule to be bioactive.