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Anti-acetylcholinesterase activity potential of *Ocimum* essential oils in comparison to its chemical profile via GC/MS and chemometrics

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Ocimum (sweet basil) is a plant of considerable commercial importance in traditional medicine worldwide as well as for the flavor and sweets industry. The goal of this study was to examine *Ocimum* essential oils anti-acetylcholinesterase activity and to correlate the activity with their chemical profiles using a metabolome based GC-MS approach coupled to chemometrics. Further, molecular docking was adopted to rationalize for activity found in most active essential oil isolates. Essential oil prepared from 4 species including *O. basilicum*, *O. africanum*, *O. americanum* and *O. minimum* exhibited significant inhibitory activity with an IC₅₀ values (0.22, 0.175, 0.57, 0.152 mg/ml) respectively comparable to that of physostigmine with an IC₅₀ value of (0.27 mg/ml). Monoterpene hydrocarbons constituted the most dominant chemical group among *Ocimum* oils: *O. basilicum* 60.8%, *O. africanum* 90.5%, *O. americanum* 95.4% and *O. minimum* 41.7%, with camphor amounting for ca. 50% in *O. africanum* and *O. americanum*, respectively. Monoterpenoid-derived phenolic ethers (i.e. estragole) constituted the most dominant chemical group among *O. basilicum* and *O. minimum*, whereas camphor (a ketone) was the most abundant in *O. africanum* and *americanum*. Supervised and unsupervised multivariate data analysis clearly separated *O. africanum* & *americanum* from other accessions, with estragole, camphor and to less extent β -linalool contributing for species segregation. Estragole was found the most active AchE inhibitor (IC₅₀ 0.05 mg/ml) followed by cineole (IC₅₀ 0.35 mg/ml), eugenol (IC₅₀ 6.62 mg/ml) and camphor (IC₅₀ 3.263 mg/ml). Molecular docking revealed that these monoterpenoids bind to key amino acids in ACE enzyme catalytic domain similar to well known anticholinesterase drugs i.e., huperzine, physostigmine and aricept and posing them as a novel class of AchE inhibitors.

Biography

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