Antioxidant activity and enzymatic of lichen substances: A study based on cyclic voltammetry and theoretical

Yañez, Osvaldoa, b
Osorio, Manuel I.c, d;
Osorio, Edisone;
Tiznado, Williamf;
Ruíz, Linag;
García, Camiloh;
Nagles, Orlandoi;
Simirgiotis, Mario J.j;
Castañeta, Groverk;
Areche, Carlosk
García-Beltrán, Olimpo

Abstract
The antioxidant activity of nine lichen substances, including methylatrarate (1), methyl haematommate (2), lobaric acid (3), fumarprotocetraric acid (4), sphaerophorin (5), subsphaeric acid (6), diffractaic acid (7), barbatolic acid (8) and salazinic acid (9) has been determined through cyclic voltammetry. The compounds 1–4 presented slopes close to the Nernst constant of 0.059 V, indicating a 2H+/2e− relation between protons and electrons, as long as the compounds 5, 6, 7, 8, and 9 present slopes between 0.037 V and 0.032 V, indicating a 1H+/2e− relation between protons and electrons. These results show a high free radical scavenging activity by means of the release of H+, suggesting an important antioxidant capacity of these molecules. Theoretical calculations of hydrogen bond dissociation enthalpies (BDE), proton affinities (PA), and Proton Transfer (PT) mechanisms, at M06-2x/6-311+G(d,p) level complement the experimental results. Computations support that the best antioxidant activity is obtained for the molecules (3, 4, 5, 6, 7 and 8), that have a carboxylic acid group close to a phenolic hydroxyl group, through hydrogen atomic transfer (HAT) and sequential proton loss electron transfer (SPLET) mechanisms. Additional computations were performed for modelling binding affinity of the lichen substances with CYPs enzymes, mainly CYP1A2, CYP51, and CYP2C9*2 isoforms, showing strong affinity for all the compounds described in this study. 

Author keywords
Antioxidant; Cyclic voltamperograms; CYPs enzymes; DFT methods; Lichenic substances; Natural products