Antioxidant activity of myricetin-like compounds

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It is well known that the antioxidant potential of flavonols can be probed through the determination of the bond dissociation enthalpies (BDEs) for OH groups and ionization potentials (IPs), related to the hydrogen-atom transfer mechanism (HAT) and single electron transfer mechanism (SET), respectively¹.

In this work, the structures and energetics of myricetin 4'-O-alpha-L-rhamnopyranoside and myricetin 3-O-alpha-L-rhamnopyranoside (see Figure 1 for structures) were examined with density functional theory, using B3LYP² and LC- ω PBE³ functionals with both the 6-311G(d,p) and 6-311+G(d,p) basis sets⁴. In addition, BDEs and IPs were determined in gas-phase, water, and methanol. The computations were performed using the Gaussian 09 software suite⁵.

Figure 1. Chemical structures: (a) myricetin 4'-O-alpha-L-rhamnopyranoside and (b) myricetin 3-O-alpha-L-rhamnopyranoside.

The smallest BDEs among the five OH groups of each compound were determined (using LC- ω PBE/6-311G(d,p) in water, for instance) to be 79.54 kcal/mol for myricetin 4'-O-alpha-L-rhamnopyranoside and 75.21 kcal/mol for myricetin 3-O-alpha-L-rhamnoside while the IPs (at the same level of theory) were obtained as 142.56 and 141.27 kcal/mol, respectively. By comparing with known antioxidants, these values for the BDEs indicate both compounds show promise for antioxidant activity, especially myricetin 3-O-alpha-L-rhamnopyranoside. In addition, the position of the sugar moiety in myricetin has a moderate effect on the BDEs for all OH groups. Interestingly, the BDEs suggest that (depending on the position of inclusion) the sugar moiety can lead to an increase in the antioxidant activity. Therefore, further experimental tests are encouraged. Additional results will be presented and discussed during the Conference.

Acknowledgments

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