

## Antioxidant Activity of Isolated Interglycosidic O-(1→3) Flavonols: a DFT study

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### INTRODUCTION

Many properties of the flavonols are related to their antioxidant activities.<sup>1</sup> Recently, two new Quercetin and Kaempferol derived flavonols presenting the uncommon interglycosidic O-(1→3) linkage were isolated from *Loranthaceae* family plants extracts.<sup>2</sup> In this work, we present a computational study on *Kaempferol 3-O-α-L-arabinofuranosyl-(1→3)-α-L-rhamnoside* (Compound K) and *Quercetin 3-O-α-L-arabinofuranosyl-(1→3)-α-L-rhamnoside* (Compound Q).

The Hydrogen-Atom Transfer and the Single Electron Transfer mechanisms were probed for both compounds through the determination of the Bond Dissociation Enthalpies (BDEs) and Ionization Potentials (IPs), respectively. Present Kaempferol and Quercetin computations along with others results of computational studies on Kaempferol and Quercetin available in the literature as well as solvent effect computations were also used for comparisons.

### METHODS

The geometries of the neutral molecules and all their radicals were fully optimized up to the B3LYP/6-31+G(d,p) level of theory.<sup>3-5</sup> Computations for open-shell species were undertaken with UB3LYP. Vibrational frequencies were computed for both molecules and radicals, to characterize the conformations as minima. All the computations were performed in Gaussian 09 suite of codes.<sup>6</sup>

BDEs were determined as:

$$\text{BDE} = H_f(\text{ArO}\cdot) + H_f(\text{H}\cdot) - H_f(\text{ArOH})$$

where  $H_f(\text{ArO}\cdot)$  is the enthalpy of the radical generated via H-atom abstraction,  $H_f(\text{H}\cdot)$  is the enthalpy of the H atom and  $H_f(\text{ArOH})$  is the enthalpy of neutral molecules. The IPs were determined as the difference between the ArOH

and  $\text{ArOH}^+$  energies (electronic + ZPE) for each compound.

### RESULTS AND DISCUSSION

As we can see in Figure 1, computed BDEs and IPs values for both Compounds K and Q are slightly lower when compared to Kaempferol and Quercetin, respectively. This indicate that the presence of the sugar O-(1→3) linkage moiety can lead to a small increase in the antioxidant activity for the studied compounds, when compared to their respective parental molecules.

Radicals	Compound K	Kaempferol	Compound Q	Quercetin
		BDEs		
3'-ArO	-	-	73.08	75.39
4'-ArO	81.28	81.45	78.14	82.15
7-ArO	87.68	87.19	83.28	87.08
5-ArO	99.13	96.16	95.06	96.26
		IPs		
	169.38	170.35	168.00	168.90

**Figure 1.** BDEs and IPs (in kcal.mol<sup>-1</sup>) at 298 K for Compounds K and Q along with results computed for Kaempferol and Quercetin. All results were computed in the gas phase at B3LYP/6-31+G(d,p) level of theory.

### CONCLUSIONS

BDEs and IPs obtained suggest both compounds studied are promising in presenting antioxidant activity. Thus, further experimental tests (e.g. IC50) are encouraged. Additional results will be presented at the Conference.

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<sup>1</sup> D. Flores *et al.*, Food. Chem., 141, 1497, (2013).

<sup>2</sup> A. C. Guimarães *et al.*, Nat. Prod. Comumm., 7, 1, (2012).

<sup>3</sup> A. D. Becke, J. Chem. Phys., 98, 5648, (1993).

<sup>4</sup> C. Lee *et al.*, Phys. Rev. B, 37, 785, (1988).

<sup>5</sup> J. S. Binkley *et al.*, J. Am. Chem. Soc., 102, 939, (1980)

<sup>6</sup> M. J. Frisch *et al.*, Gaussian 09, Revisions D.01, (2009).