

# A mechanistic investigation of H/D scrambling processes in flavonoids

Several classes of flavonoids, such as anthocyanins, flavonols, flavanols and flavones, undergo a slow H/D exchange on aromatic ring A, leading to full deuteration at positions C(6) and C(8). Within the flavanol class, H-C(6) and H-C(8) of catechin and epicatechin are slowly exchanged in D<sub>2</sub>O to the corresponding deuterated analogues; even quercetin, a relevant flavonol representative, shows the same behaviour in a D<sub>2</sub>O/DMSO-d<sub>6</sub> 1:1 solution. Detailed kinetic measurements of these H/D scrambling processes are here reported by exploiting the time-dependent changes of their peak areas in the <sup>1</sup>H-NMR spectra taken at different temperatures. A unifying reaction mechanism is also proposed based on our detailed kinetic observations, even taking into account pH and solvent effects. Molecular modelling and QM calculations were also carried out to shed more light on several molecular details of the proposed mechanism.

**Authors:** Graziano Guella – Biorganic Chemistry Lab/Dept. of Physics/University of Trento, Federico Bonaldo<sup>1</sup>, Fulvio Mattivi<sup>2</sup>, Daniele Catorci\*, & Panagiotis Arapitsas<sup>3</sup>, Graziano Guella<sup>1</sup>, \* <sup>1</sup> Bioorganic Chemistry Laboratory, Department of Physics, University of Trento, Trento, Italy; federico.bonaldo@alumni.unitn.it <sup>2</sup> Department of Cellular, Computational and Integrative Biology – CIBIO and C3A, University of Trento, Trento, Italy; fulvio.mattivi@unitn.it <sup>3</sup> Department of Food Quality and Nutrition, Research and Innovation Centre, Fondazione Edmund Mach (FEM), San Michele all'Adige, Italy; panagiotis.arapitsas@fmach.it \* D. Catorci passed away on June 27th, 2020

**Email:** [graziano.guella@unitn.it](mailto:graziano.guella@unitn.it)

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