

Supplementary Information

Chiroptical activity of chiral hydroxycarboxylic acids: implications for the origin of biological homochirality

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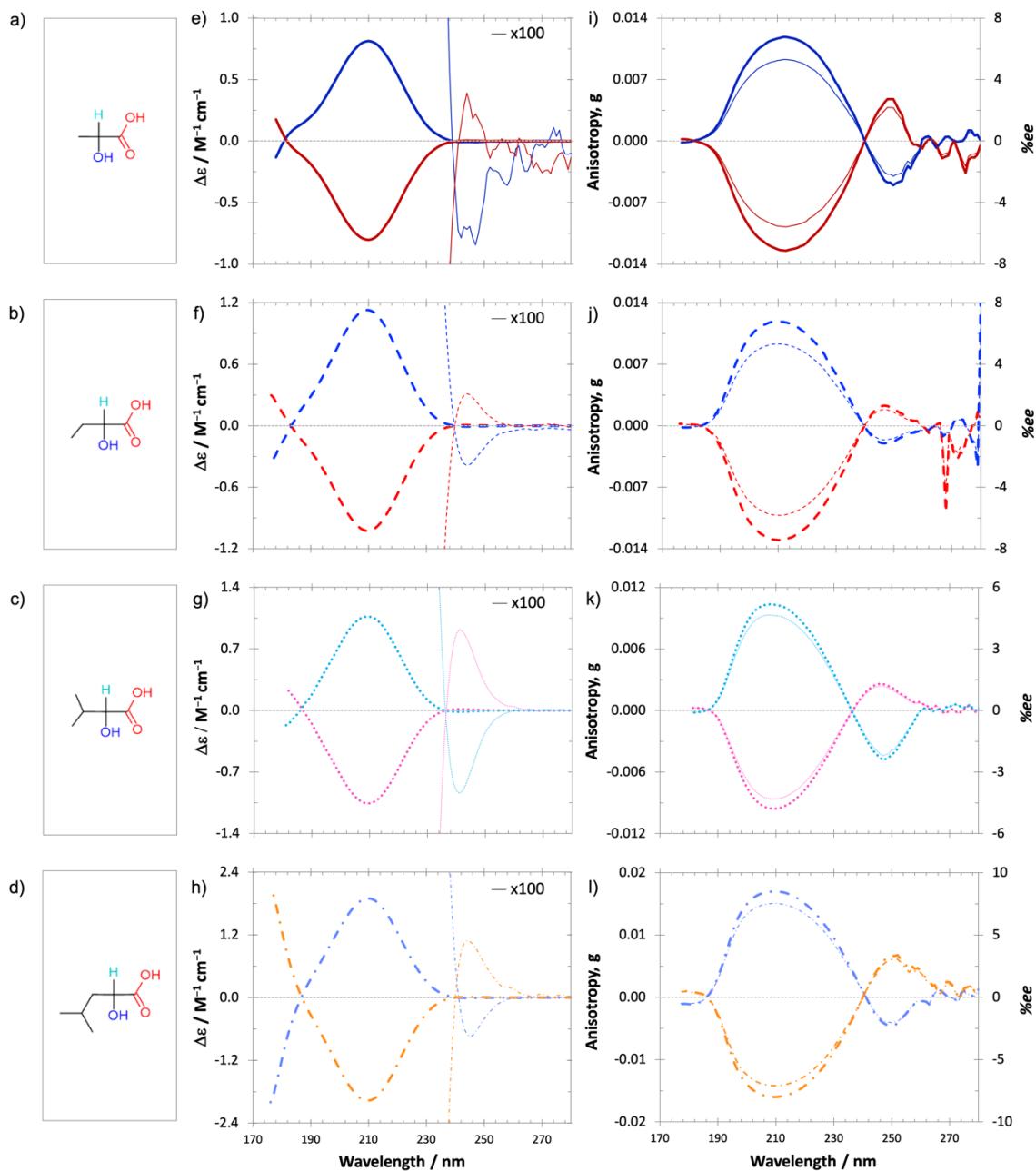
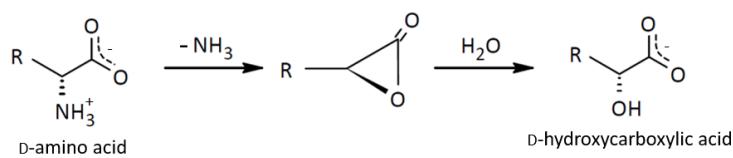
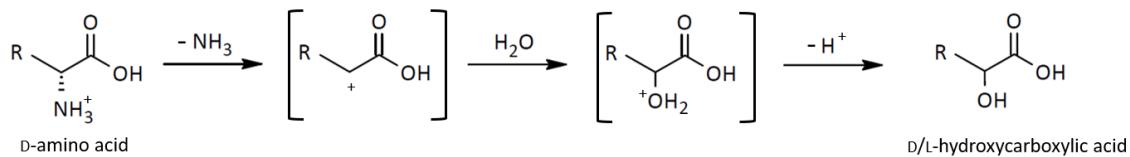


Fig. S1: CD and anisotropy spectra of chiral aliphatic chain hydroxycarboxylic acids in aqueous solution. Schematic structures of a) lactic; b) 2-hydroxybutanoic; c) 2-hydroxy-3-methylbutanoic and d) 2-hydroxy-4-methylpentanoic acid. e) to h) Corresponding electronic circular dichroism spectra of the HCAs in aqueous solution. i) to l) Corresponding anisotropy spectra of the HCAs in aqueous solution (thick) and inducible enantiomeric excess (%ee) by either left- or right-circularly polarised light (thin) as a function of wavelength at the extent of reaction $\xi = 0.9999$ calculated based on relation (1). The D-enantiomers (R-) are in shades of red and the L-enantiomers (S-) are in shades of blue. Note that due to the uncertainties induced by low absorbance and ECD signals, the values of the anisotropy factor g are less reliable above 260 nm for 2-hydroxybutanoic acid, above 270 nm for 2-hydroxy-3-methylbutanoic acid and D-2-hydroxy-4-methylpentanoic acid.

a) pH 7

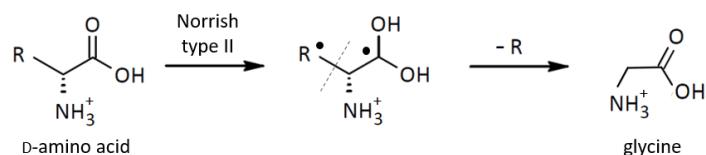


b) pH 1



with R = H, CH₃, etc.; linear side chain,

or



with R = i-Pr, i-Bu, sec-Bu, etc.; branched alkyl side chain.

Fig. S2: The major photodecomposition mechanisms of aliphatic chain amino acids following $n\pi^*$ excitation of the carboxyl chromophore upon UV irradiation in aqueous solution at a) pH 7 and b) pH 1¹.

Supplementary References:

1. Nishino, H. *et al.* Absolute asymmetric photoreactions of aliphatic amino acids by circularly polarized synchrotron radiation: Critically pH-dependent photobehavior. *J. Am. Chem. Soc.* **124**, 11618–11627 (2002).