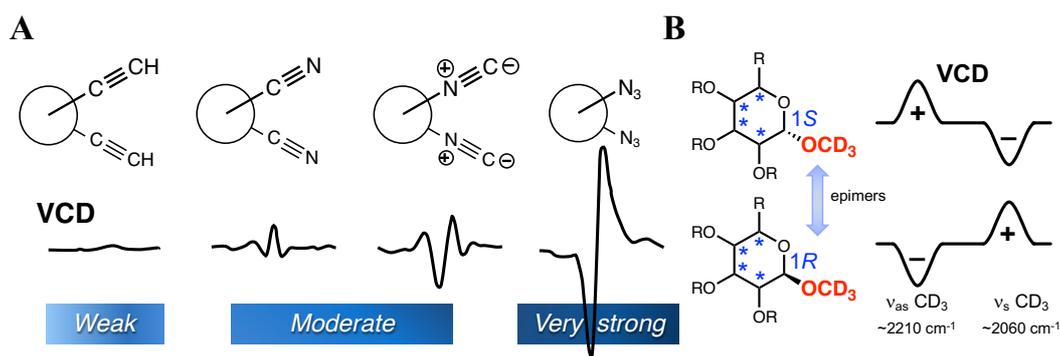


Exploration of Biomolecularly Transparent IR Region for Structural Identification Using VCD

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The stereostructure of biomolecules significantly influences their roles in biological processes. Thus, a comprehensive knowledge of their structural properties is the key to fully understand and regulate their functions. However, stereostructure elucidation of biomolecules is rather challenging because of the limitation of conventional analytical methods. Vibrational circular dichroism (VCD) spectroscopy has proven to be a precise and powerful tool for molecular stereostructural characterization. First, we studied the applicability of nitrile, isonitrile, alkyne, and azido groups to identify suitable chromophores that exhibit VCD couplets in the 2300-1900 cm^{-1} region by using a chiral binaphthyl scaffold. Azido group is the most promising for extracting structural information from biomolecules because it showed the most simple and strong VCD signals whose pattern is readily predicted by harmonic DFT calculations (Figure A).¹ Second, we utilize the C-D stretching in this region to explore the practicality of CD_3 groups for obtaining the local chirality. A series of pyranosides was used as a model study. The epimeric pairs agreeably presented almost mirror-image VCD patterns in the 2300-1900 cm^{-1} region irrespective of other chiral centers (Figure B). The application of this concept was further demonstrated to other complex systems by studying the VCD spectra of the C-1 epimeric pairs of a disaccharide gentiobiose, 6-lauroylated surfactant, and 5-membered glucofuranosides.²



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