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Steering the color of the *retro*-carotenoid rhodoxanthin by (*E/Z*)-isomeric ratios, controlled aggregation, and formulation technology

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Food and beverage processors are urgently calling for new sources of vibrant red to purple colorants to replace the increasingly rejected artificial dyes and the insect-derived carmine. Finding alternative solutions to fill this unmet market need based on equipotent natural or nature-identical pigments, such as carotenoids that impart yellow to red colors to plants, is a continuing challenge. The color of colloidally stabilized formulations of carotenoids can be modulated by manipulating (*E/Z*)-isomeric ratios, deposition states, and particle sizes. To date, none of the commercial carotenoid formulations conveys bright red to purple color hues. The yet scarcely studied *retro*-carotenoids commonly feature enlarged chromophores and exceptional light absorption properties that offer new opportunities to yield such color shades. Therefore, this doctoral thesis presents analytical investigations of *retro*-carotenoids and practically feasible formulation approaches to exploit rhodoxanthin as promising pigment for conveying intense red and purple colors to foods and beverages.

Recent trends regarding the development of carotenoid formulations were reviewed to compile the currently available knowledge on formulation technologies and naturally-derived raw materials (CHAPTER 1). Genuine carotenoid profiles of red- and yellow-colored arils of seven cultivars of *Taxus baccata* L. and *Taxus* × *media* Rehder were determined using high performance liquid chromatography-diode array detection-electrospray ionization/atmospheric pressure chemical ionization-multi-stage mass spectrometry (HPLC-DAD-ESI/APCI-MS^n) analyses (CHAPTER 2). To facilitate efficient screenings of *retro*-carotenoids in natural sources in future, APCI-quadrupole time-of-flight-high-resolution mass spectrometry (QTOF-HRMS) analyses were performed to search for typical ion species of rhodoxanthin, eschscholtzxanthone, and eschscholtzxanthin for the first time (CHAPTER 3). In addition to these in-depth analytical studies, a detailed understanding of kinetic and thermodynamic fundamentals of the thermally induced (*E/Z*)-isomerization of rhodoxanthin was generated and then applied to steer the color of techno-functional rhodoxanthin formulations (CHAPTERS 4–5). Extensive kinetic data was gathered by determining rhodoxanthin (*E/Z*)-isomeric ratios after isothermal heating at 40, 50, 60, and 70 °C until the equilibrium states were reached to also derive thermodynamic parameters of the reactions, such as enthalpies, entropies, and Gibbs energies (CHAPTER 4). Consequently, color shades of rhodoxanthin were manipulated by taking advantage of its peculiar (*E/Z*)-isomerization (CHAPTER 5).

In brief, carotenoid profiles of *Taxus* arils were elucidated and identified as an abundant natural source of *retro*-carotenoids. A detailed description of kinetic and thermodynamic parameters of the complex (*E/Z*)-isomerization reactions of rhodoxanthin enabled defining technological measures to modulate the color of rhodoxanthin formulations by tailoring (*E/Z*)-isomeric ratios and controlling aggregations. This body of research on rhodoxanthin paves the way for the replacement of red- and purple-colored artificial dyes and carmine in food industry, addressing their increasing rejection by consumers around the globe.