Designing Novel Carotenoids for Improved Antioxidant Activity and Conducting Organic Molecular Wires

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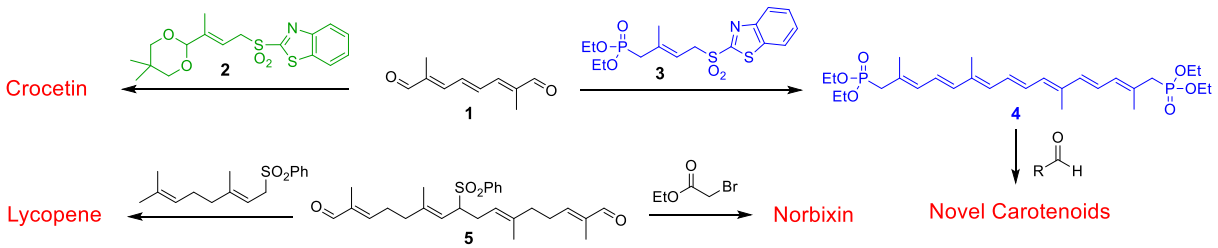
Carotenoids are structurally characterized by the conjugated polyene chains, which exhibit anti-oxidant activity by scavenging reactive oxygen species. These health-benefit nutraceuticals find wide applications in colorant, food additive, cosmetics and drug industries. Synthesis of the polyene chain of carotenoids mostly relied on the Wittig olefination reaction. Sulfone-mediated method, known as Julia olefination, has been applied only to the production of retinol derivatives. We extended the synthetic repertoires of the carotenoid polyene chains by use of organo-sulfur chemistry.[1]

Various building blocks containing a sulfone group were devised for efficient construction of the polyene chains of carotenoids. Benzothiazolyl (BT) sulfone **2** containing an acetal moiety was devised for iterative chain extension of apocarotenoids from C_{10} dial **1**, and crocetin was efficiently prepared.[2] BT-sulfone **3** with a phosphonate moiety reacted with C_{10} dial **1** to produce C_{20} diphosphonate **4**, which provided novel carotenoids upon olefination with various aldehydes (R-CHO). High throughput screening and hierarchical clustering analysis were applied to the novel carotenoids for evaluation of their antioxidant activities utilizing DPPH and ABTS assays.[3] Lycopene synthesis was demonstrated by the sulfone olefination protocol from geranyl sulfone and C_{20} dial **5**,[4] which was also applied to norbixin synthesis by olefination with readily available ethyl bromoacetate.[5]



Carotenoids are also known to play a critical role in photosynthesis to transfer the excited energy of chlorophyll to the reaction center for ATP generation. It could be excellent conducting molecular wires. We designed the stabilized carotenoids by incorporating phenyl substituents to the polyene chain, which controlled conductance of the polyene chain by electronic nature of the phenyl substituents.[6] Electron-donating substituents in phenyl group increase the conductance of carotenoid molecular wires, whereas electron-withdrawing groups decrease it. We also found that all-*E* carotene conducts twice more than 9-Z counterpart.[7]

References:

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