Aggregation-Induced Resonance Raman Optical Activity (AIRROA):

A New Mechanism for Chirality Enhancement

Grzegorz Zajac,^{†,‡} Agnieszka Kaczor,^{*, †,‡} Ana Pallares Zazo,[‡] Jacek Mlynarski,[†] Monika Dudek,[†] Malgorzata Baranska^{*,†,‡}

+ Faculty of Chemistry, Jagiellonian University, Ingardena 3, Krakow 30-060, Poland

‡ Jagiellonian Centre for Experimental Therapeutics (JCET), Jagiellonian University, Bobrzynskiego 14, Krakow 30-348, Poland



Figure S1. RROA spectra of (3R, 3'R), (3S, 3'S) and racemic astaxanthin 3:7 water/acetone aggregates (red, blue and black lines, respectively). A single block (5 minutes acquisition).



Figure S2. RROA spectra of (3R, 3'R), (3S, 3'S) and racemic astaxanthin 3:7 water/acetone aggregates (red, blue and black lines, respectively). Averaged over 12 blocks.



Figure S3. Set of ROA spectra (5 min acquisitions) of $(3R, 3^{\circ}R)$ and $(3S, 3^{\circ}S)$ -astaxanthin J-aggregates without (260 spectra) and with artefacts (10 spectra), that can be clearly distinguished from the true spectra of aggregates due to the high-intensity bands (of the same sign as others) assigned to the solvent (marked with the asterisk).



Figure S4. Zoomed, background subtracted RROA spectra of (3R, 3'R) and (3S, 3'S)-astaxanthin J-aggregates. Marked acetone bands exhibit chirality transfer.



Figure S5. RROA spectra of (3S,3'S)-astaxanthin J-aggregates obtained from two independent measurements from two individual samples.



Figure S6. UV and ECD spectra of lutein aggregates and monomer (red and black lines, respectively).