Electrochemical Study of Astaxanthin and Astaxanthin n-Octanoic Monoester and Diester: Tendency to Form Radicals A. Ligia Focsan,^{1,*} Shalin Pan,² and Lowell D. Kispert,²

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Supporting Information: Energies (in Hartrees) from DFT calculations (B3LYP/6-31G** level) of proton loss from carotenoid dication Car^{2+} to form cations [#]Car⁺ according to eqn. 5.

Table S1. Energies (in Hartrees) from DFT calculations (B3LYP/6-31G** level) of proton loss from carotenoid dication Car^{2+} to form cations ${}^{\#}Car^{+}$ according to eqn. 5.

Car	astaxanthin	β-carotene
Car ²⁺	-1855.103539	-1556.660813
$^{\#}Car^{+}(15)$	-1854.754796	-1556.290962
$^{\#}Car^{+}(14)$	-1854.758050	-1556.294039
$^{\#}Car^{+}(13)$	-1854.771433	-1556.307143
$^{\#}Car^{+}(12)$	-1854.771518	-1556.298418
$^{\#}Car^{+}(11)$	-1854.744605	-1556.284131
$^{\#}Car^{+}(10)$	-1854.768083	-1556.303300
$^{\#}Car^{+}(9)$	-1854.781139	-1556.316283
$^{\#}Car^{+}(8)$	-1854.776194	-1556.310679
$^{\#}Car^{+}(7)$	-1854.740716	-1556.281234
$^{\#}Car^{+}(5)$	-1854.792613	-1556.332971
$^{\#}Car^{+}(4)$	-	-1556.341049
$^{\#}Car^{+}(3)$	-1854.828791	-1556.264855
$^{\#}Car^{+}(3OH)$	-1854.779854	-
$^{\#}Car^{+}(2)$	-1854.773226	-1556.269216
$^{\#}Car^{+}(1)$	-1854.784913	-1556.317354