

## Supplementary Material

# Analysing the carotenoid composition of Melilot (*Melilotus officinalis* (L.) Pall.) extracts and the effects of isolated (all-*E*)-lutein-5,6-epoxide on primary sensory neurons and macrophages

Györgyi Horváth<sup>1,\*</sup>, Eszter Csikós<sup>1</sup>, Eichertné Violetta Andres<sup>1</sup>, Tímea Bencsik<sup>1</sup>, Anikó Takátsy<sup>2</sup>, Gergely Gulyás-Fekete<sup>2</sup>, Erika Turcsí<sup>2</sup>, József Deli<sup>1,2</sup>, Éva Szőke<sup>3</sup>, Ágnes Kemény<sup>3,4,5</sup>, Maja Payrits<sup>3,5</sup>, Lajos Szente<sup>6</sup>, Marianna Kocsis<sup>7</sup>, Péter Molnár<sup>1</sup>, Zsuzsanna Helyes<sup>3,5</sup>

<sup>1</sup> Department of Pharmacognosy, Faculty of Pharmacy, University of Pécs, Pécs, Hungary

<sup>2</sup> Department of Biochemistry and Medical Chemistry, Medical School, University of Pécs, Pécs, Hungary

<sup>3</sup> Department of Pharmacology and Pharmacotherapy, Medical School, University of Pécs, Pécs, Hungary

<sup>4</sup> Department of Medical Biology and Central Electron Microscope Laboratory, Medical School, University of Pécs, Pécs, Hungary

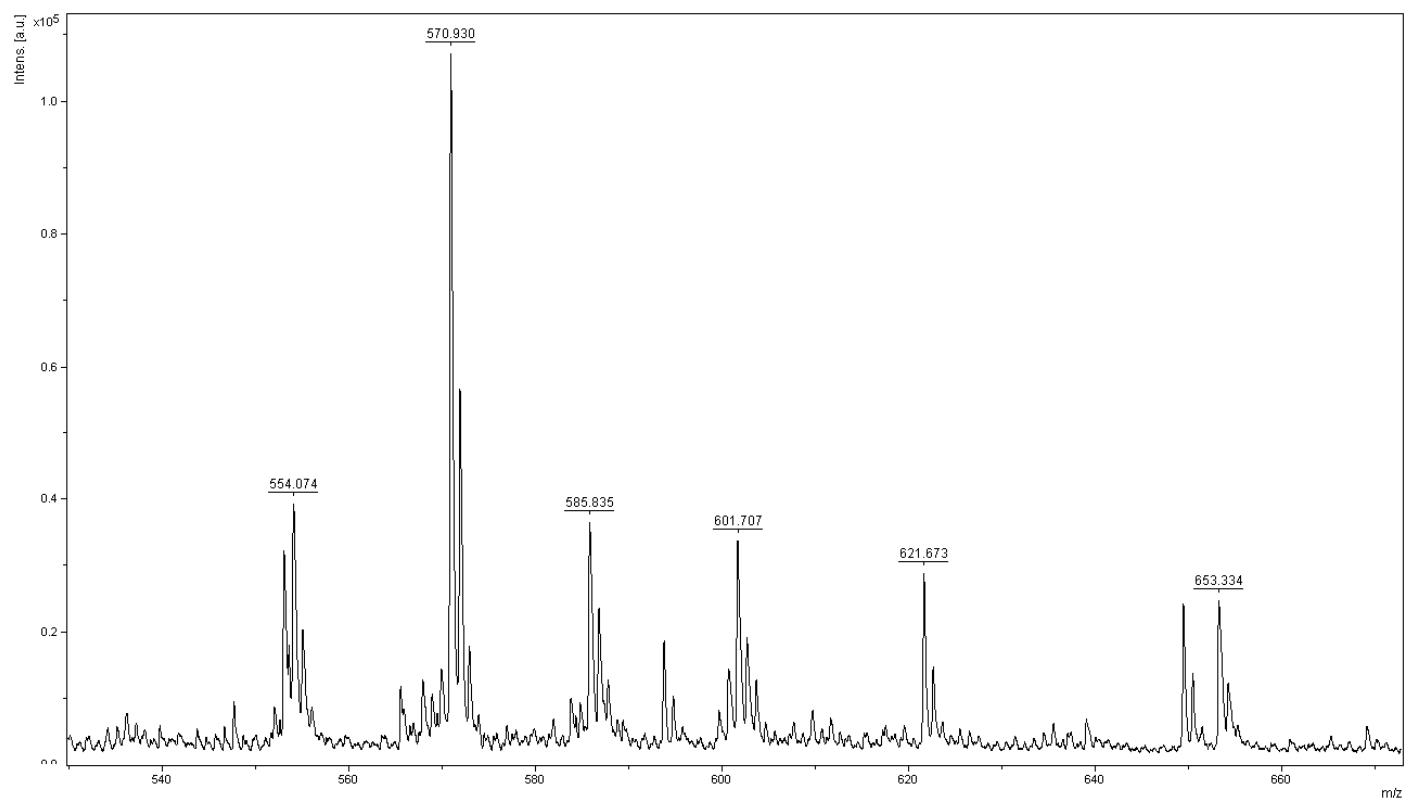
<sup>5</sup> Szentágóthai Research Centre, Centre for Neuroscience, University of Pécs, Pécs, Hungary

<sup>6</sup> Cyclolab Ltd., Budapest, Hungary

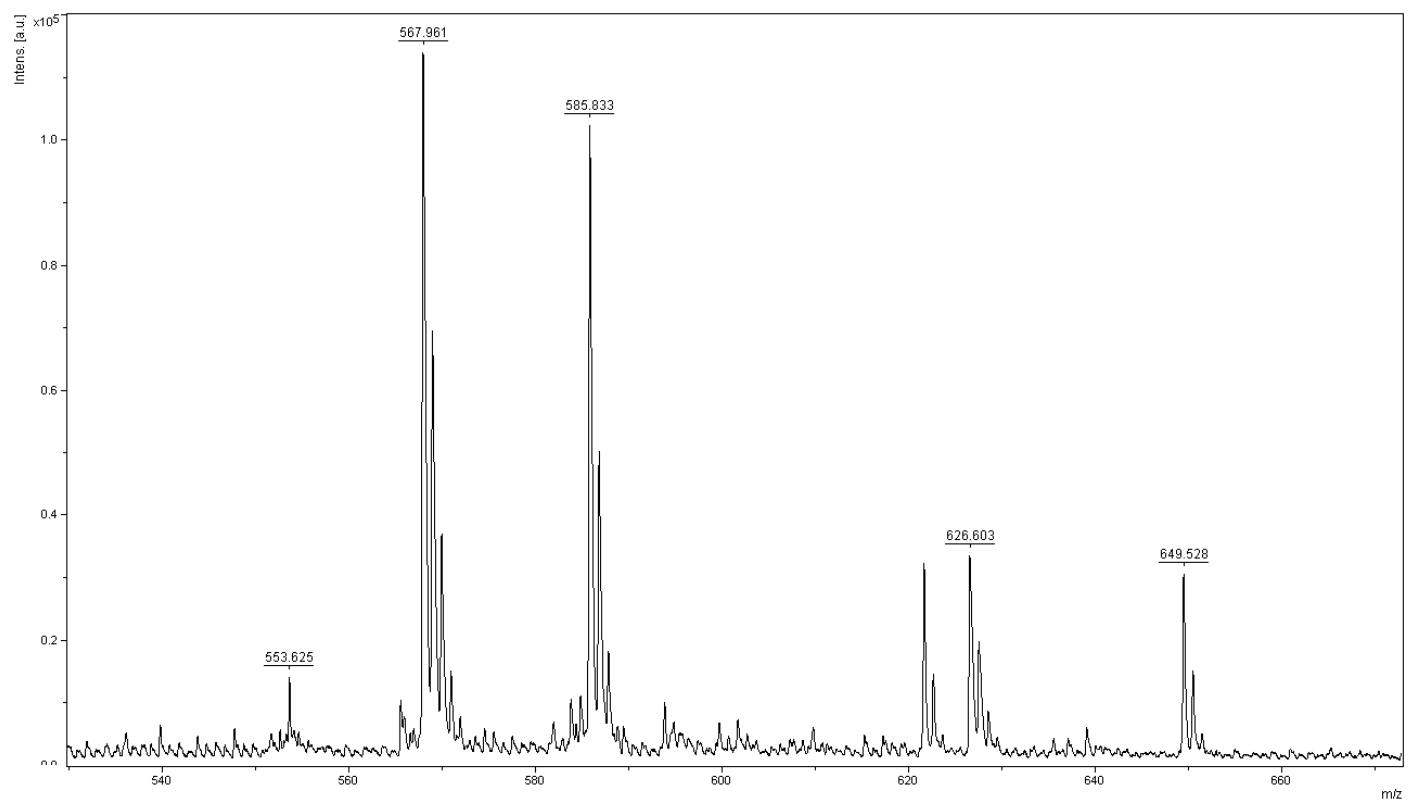
<sup>7</sup> Department of Plant Biology, Institute of Biology, Faculty of Sciences, University of Pécs, Pécs, Hungary

\* Correspondence: [horvath.gyorgyi@gytk.pte.hu](mailto:horvath.gyorgyi@gytk.pte.hu); Tel.: +36-72-503650-28823

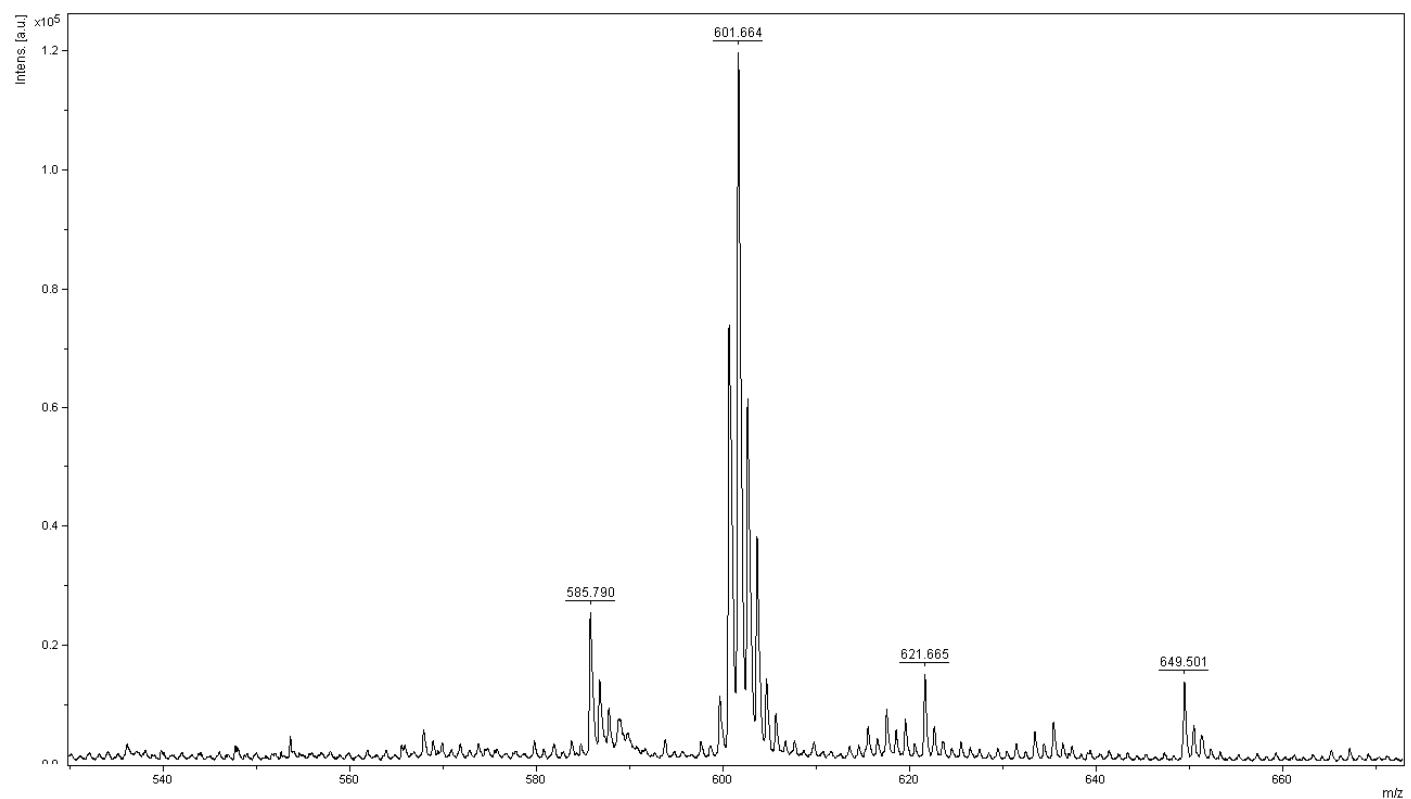
**Figure S1.** Mass spectrum of (all-*E*)-lutein



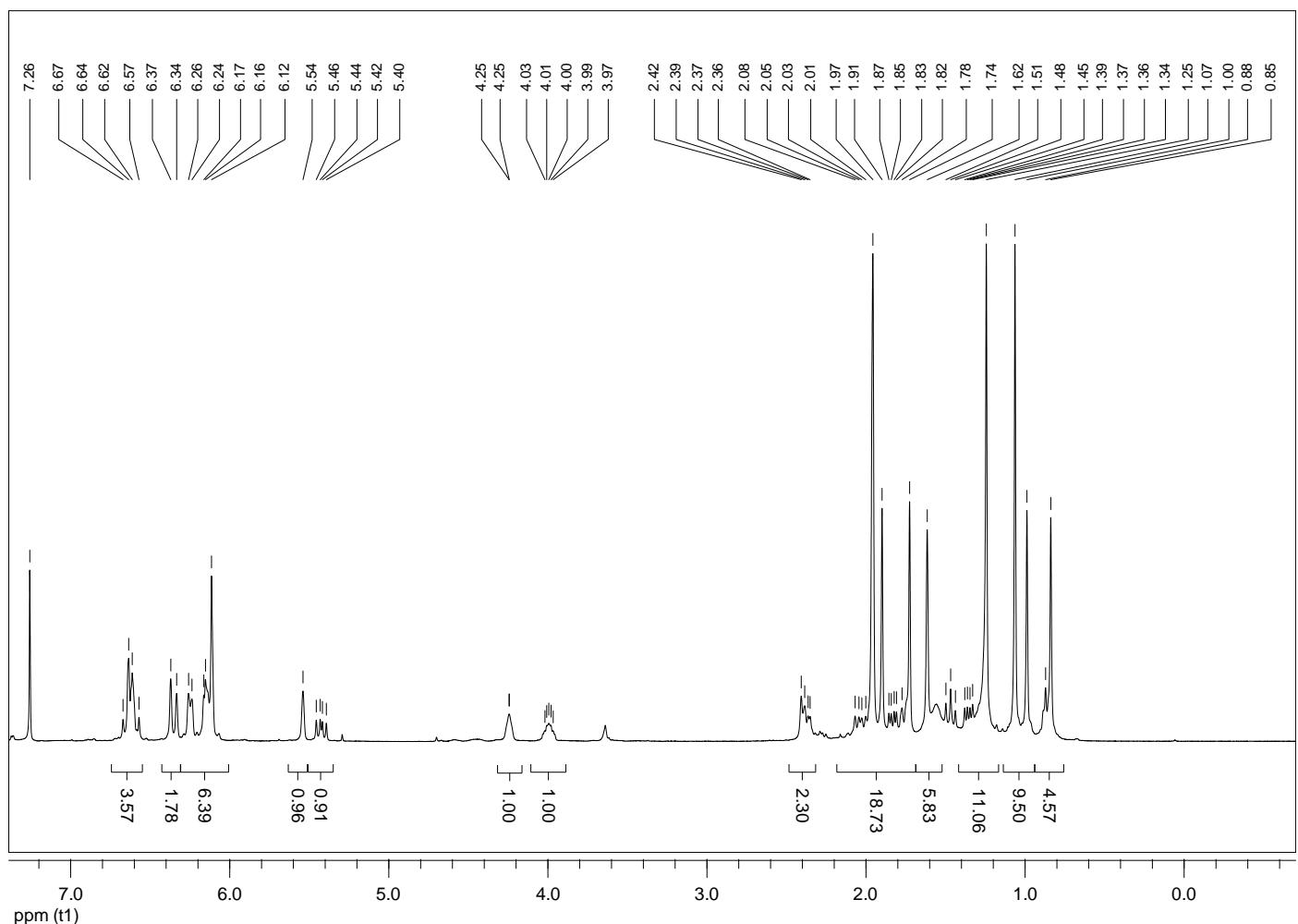
**Figure S2.** Mass spectrum of (all-*E*)-lutein-5,6-epoxide



**Figure S3.** Mass spectrum of (all-*E*)-violaxanthin

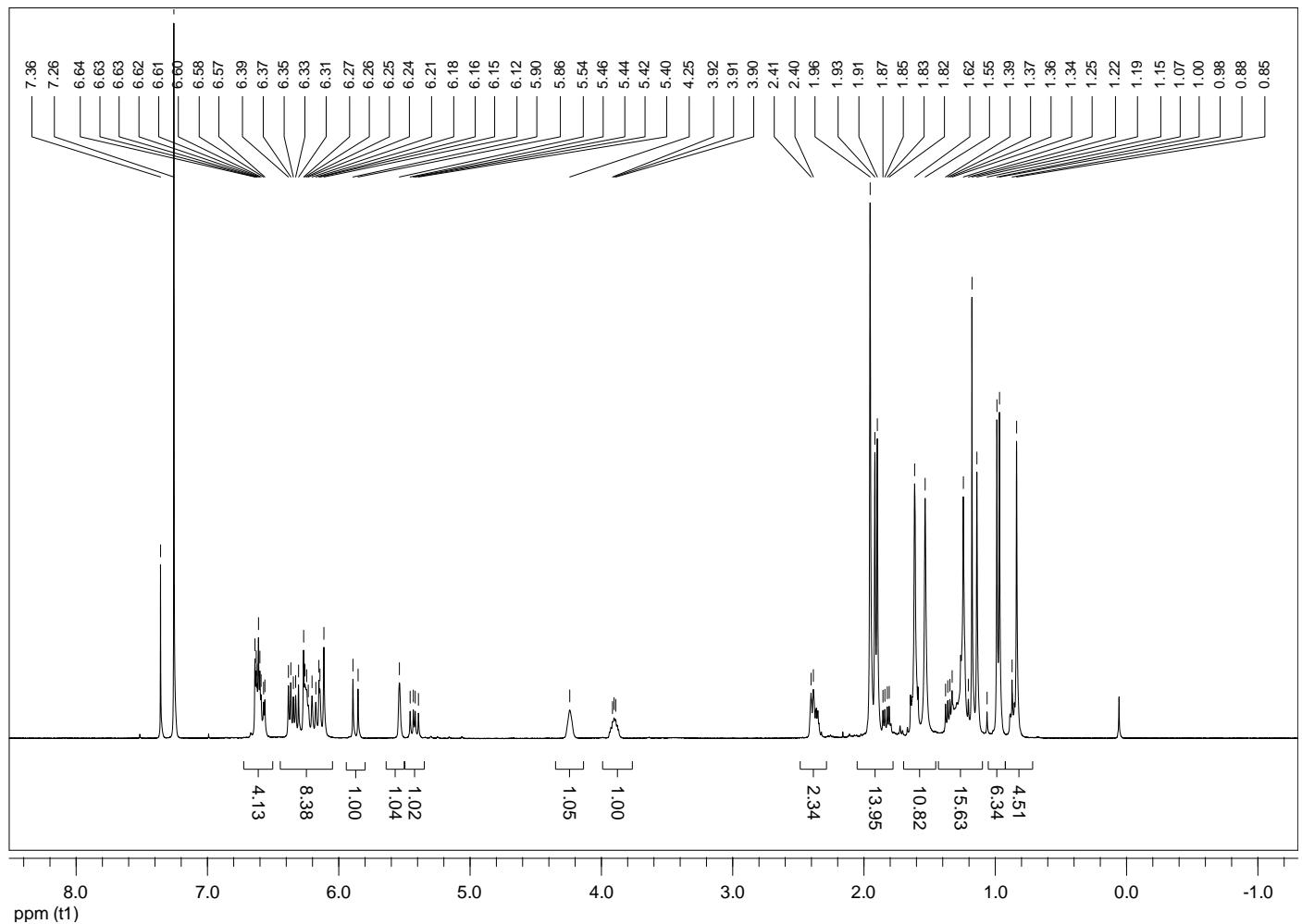


**Figure S4.**  $^1\text{H}$ -NMR spectrum of the isolated (all-*E*)-lutein



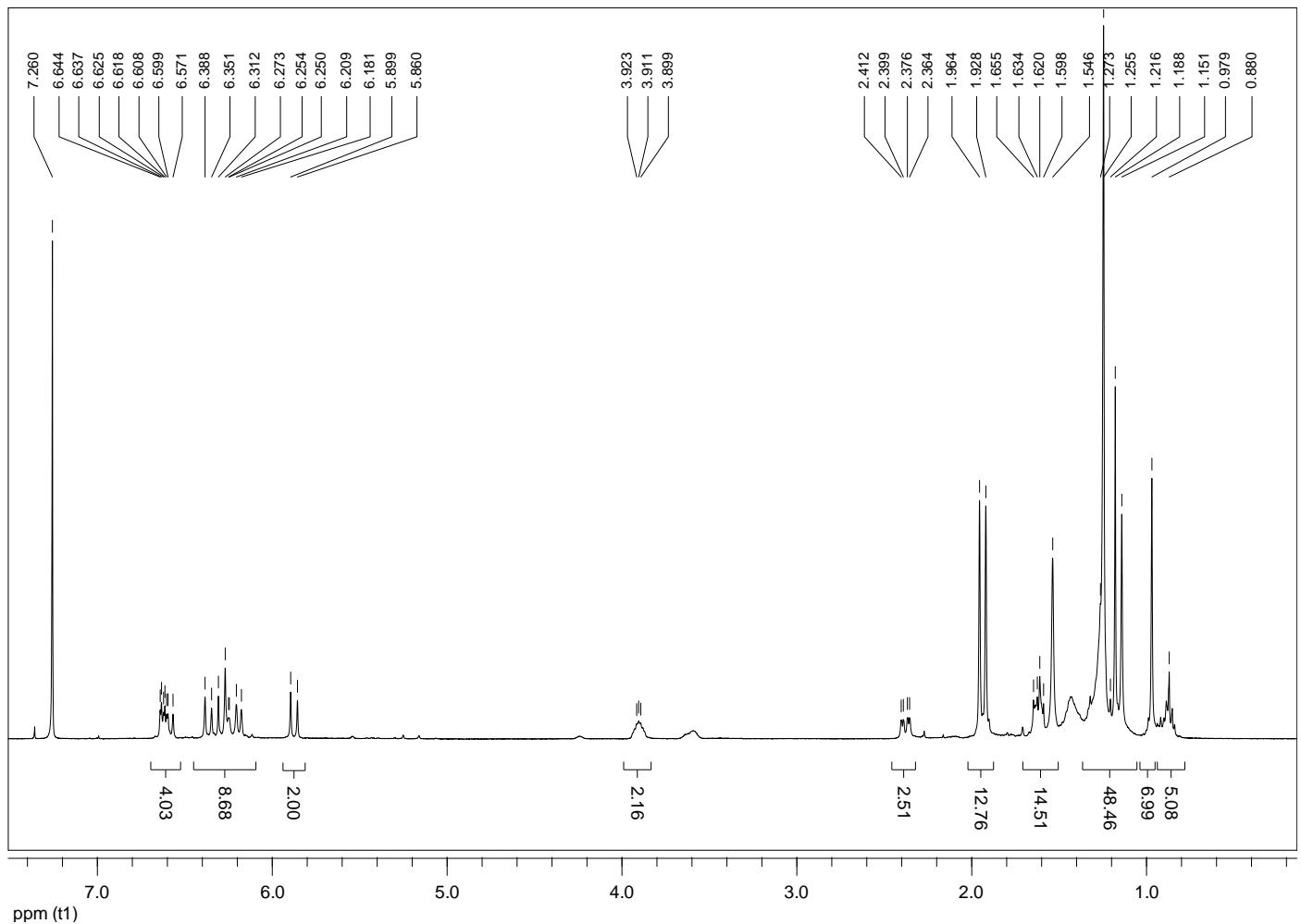
$^1\text{H}$ -NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  6.69 - 6.56 (4H, br m, H-11, H-15, H-11', H-15'), 6.35 (2H, d,  $J$  = 14.8 Hz, H-12, H-12'), 6.28 - 6.22 (2H, br m, H-14, H-14'), 6.18 - 6.13 (3H, br m, H-14, H-8', H-14'), 6.12 (2H, m, H-7, H-8), 5.54 (1H, s, H-4'), 5.43 (1H, dd,  $J$  = 15.3, 9.8 Hz, H-7'), 4.25 (1H, s, H-3'), 4.05 - 3.95 (1H, br m, H-3), 2.44 - 2.34 (2H, br m, H-4, H-6'), 2.04 (1H, dd,  $J$  = 17.0, 9.6 Hz, H-4), 1.97 (12H, s, H-19, H-20, H-19', H-20'), 1.84 (1H, dd,  $J$  = 13.1, 5.8 Hz, H-2), 1.83 - 1.76 (1H, br m, H-2), 1.74 (3H, s, H-18), 1.62 (3H, s, H-18'), 1.48 (1H, t,  $J$  = 11.9 Hz, H-2), 1.36 (1H, dd,  $J$  = 13.1, 6.8 Hz, H-2'), 1.07 (6H, s, H-16, H-17), 0.85 (6H, s, H-16', H-17').

**Figure S5.**  $^1\text{H}$ -NMR spectrum of the isolated (all-*E*)-lutein 5,6-epoxide



<sup>1</sup>H-NMR (500 MHz, CDCl<sub>3</sub>) δ 6.66 – 6.55 (4H, br m, H-11, H-15, H-11', H-15'), 6.37 (1H, d, J = 14.9 Hz, H-12), 6.35 (1H, d, J = 14.9 Hz, H-12'), 6.29 – 6.22 (3H, br m, H-8, H-14, H-14'), 6.20 (2H, d, J = 15.5 Hz, H-10, H-10'), 6.17 – 6.09 (1H, br m, H-8'), 5.88 (1H, d, J = 15.5 Hz, H-7), 5.55 (1H, s, H-4'), 5.43 (1H, dd, J = 15.4, 9.8 Hz, H-7'), 4.25 (1H, s, H-3'), 3.96 – 3.86 (1H, br m, H-3), 2.43 – 2.34 (2H, br m, H-4, H-6'), 1.96 (6H, s, H-20, H-20'), 1.84 (1H, dd, J = 13.2, 5.9 Hz, H-2'), 1.83 (3H, s, H-19), 1.82 (3H, s, H-19'), 1.66 – 1.59 (5H, br m, H-2, H-4, H-18'), 1.36 (1H, dd, J = 13.2, 6.8 Hz, H-2'), 1.31 – 1.21 (1H, br m, H-2), 1.19 (3H, s H-18), 1.15 (3H, s, H-17), 1.00 (3H, s, H-17'), 0.98 (3H, s, H-16), 0.85 (3H, s, H-16').

**Figure S6.**  $^1\text{H}$ -NMR spectrum of the isolated (all-*E*)-violaxanthin



$^1\text{H}$ -NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  6.65 – 6.62 (2H, m, H-15, H-15'), 6.61 (2H, dd,  $J$  = 14.5, 10.7 Hz, H-11, H-11'), 6.37 (2H, d,  $J$  = 14.9 Hz, H-12, H-12'), 6.29 (2H, d,  $J$  = 15.5 Hz, H-8, H-8'), 6.25 (2H, m, H-14, H-14'), 6.20 (2H, d,  $J$  = 15.5 Hz, H-10, H-10'), 5.88 (2H, d,  $J$  = 15.5 Hz, H-7, H-7'), 3.95 – 3.86 (2H, br m, H-3, H-3'), 2.39 (2H, ddd,  $J$  = 14.5, 4.9, 1.3 Hz, H-4, H-4'), 1.96 (6H, s, H-20, H-20'), 1.93 (6H, s, H-19, H-19'), 1.63 – 1.57 (6H, br m, H-2, H-4, H-2', H-4'), 1.19 (6H, s, H-18, H-18'), 1.15 (6H, s, H-17, H-17'), 0.98 (6H, s, H-16, H-16').