Supplementary Material (ESI) for Photochemical & Photobiological Sciences

Supporting Information

Effect of spontaneous emulsification on the photochemistry of *trans*-Anethole

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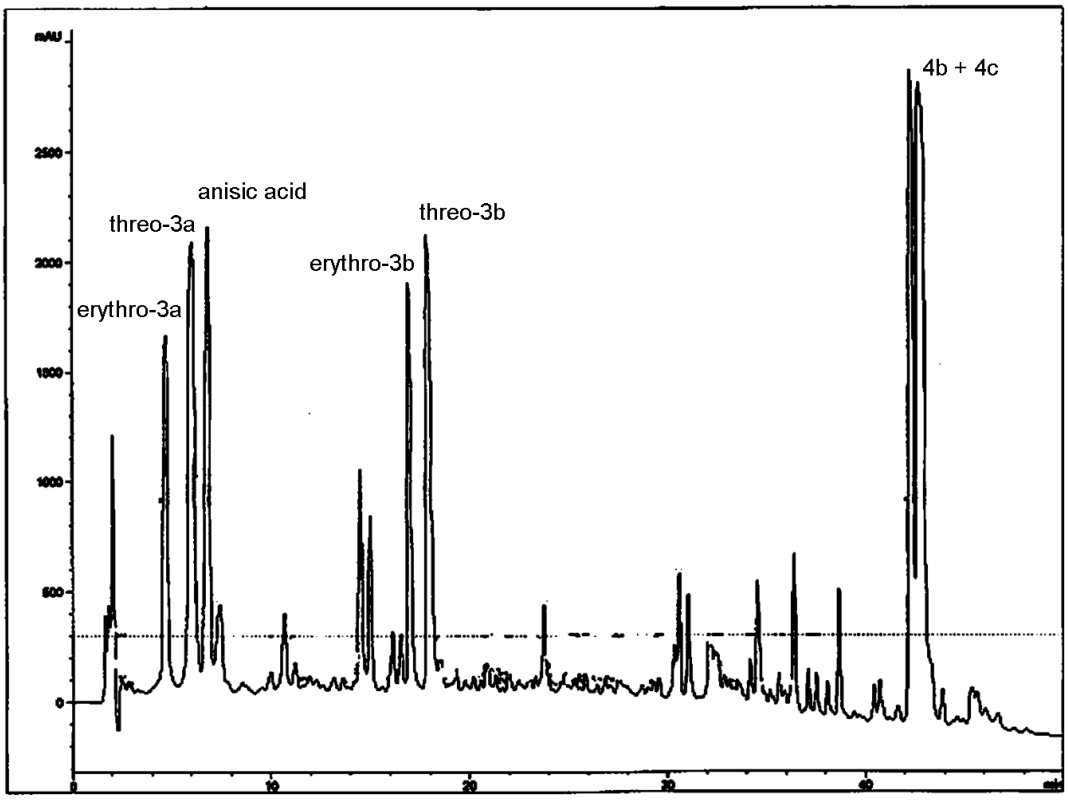

Figure S1. Preparative HPLC isolation of photoproducts obtained by irradiation of *trans*-anethole in 100 % EtOH and 20 % EtOH / 80 % H_2O showing **3a**, **3b**, **4b**, **4c** and **anisic acid**. Chromatographic separations were performed using a Zorbax SB C-18 column (7μm, 250 × 21.2 mm) running a solvent gradient : eluant A, water pH 4.6; eluant B, acetonitrile, t = 0 – 5 min, 20 % (*v/v*) B; t = 40 – 45 min, 78 % (*v/v*) B; t = 55 – 60 min, 100 % (*v/v*) B at a flow rate of 28 $mL.min^{-1}$. Compounds were detected bu UV at 230 nm.

erythro-1-(4-methoxyphenyl)-1,2-dihydroxypropane (3a). ^1H NMR (250 MHz, $CDCl_3$). δ 1.10 (d, *J* = 6.4 Hz, 3H), 3.80 (s, 3H), 4.00 (m, 1H), 4.60 (d, *J* = 4.5, 1H), 6.9 (d, *J* = 8.7 Hz, 2H), 7.3 (d, *J* = 8.7 Hz, 2H); MS (EI) m/z (%) 182 (M^+, 3.9), 164 (18.9), 137 (73.2), 121 (100), 109 (14.5).

threo-1-(4-methoxyphenyl)-1,2-dihydroxypropane (3a). ^{1}H NMR (300 MHz, $CDCl_3$) δ 1.03 (d, *J* = 6.0 Hz, 3H), 3.80 (s, 3H), 3.82 (m, 1H), 4.30 (d, *J* = 7.5 Hz, 1H), 6.9 (d, *J* = 8.6 Hz, 2H), 7.2 (d, *J* = 8.6 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 18.9, 55.4, 72.4, 79.3, 114.0, 128.2, 133.3, 159.6; MS (EI) m/z (%) 182 (M^+, 3.5), 164 (17.7), 137 (93.1), 121 (100), 109 (17.7).

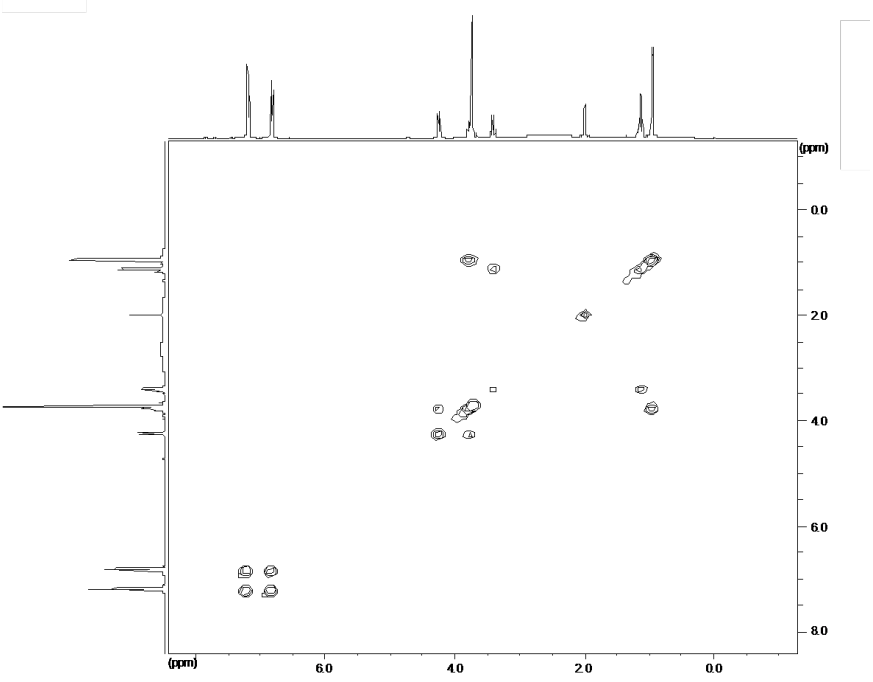

Figure S2. 2D proton-proton correlation spectra (COSY) of **threo-3a**.

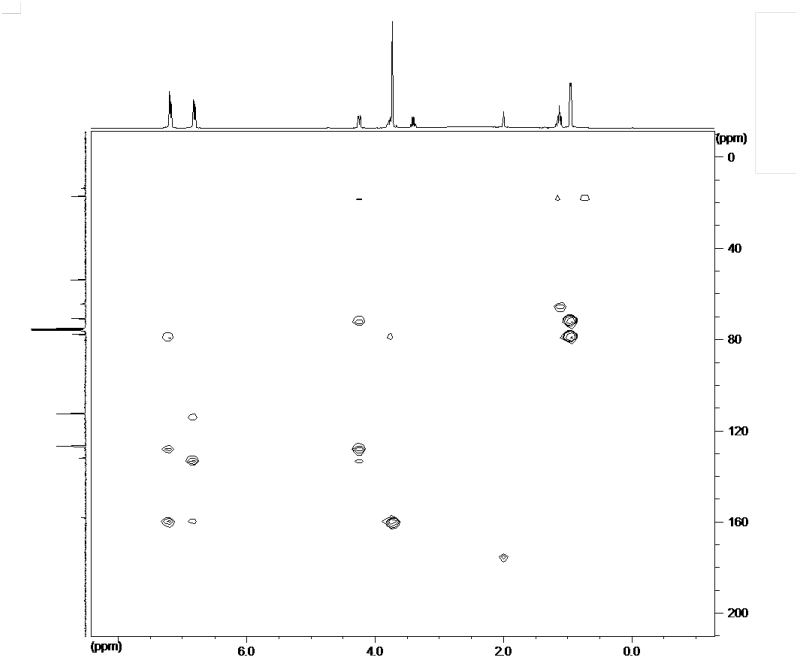

Figure S3. 2D proton-carbon correlation spectra (HMBC) of **threo-3a**.

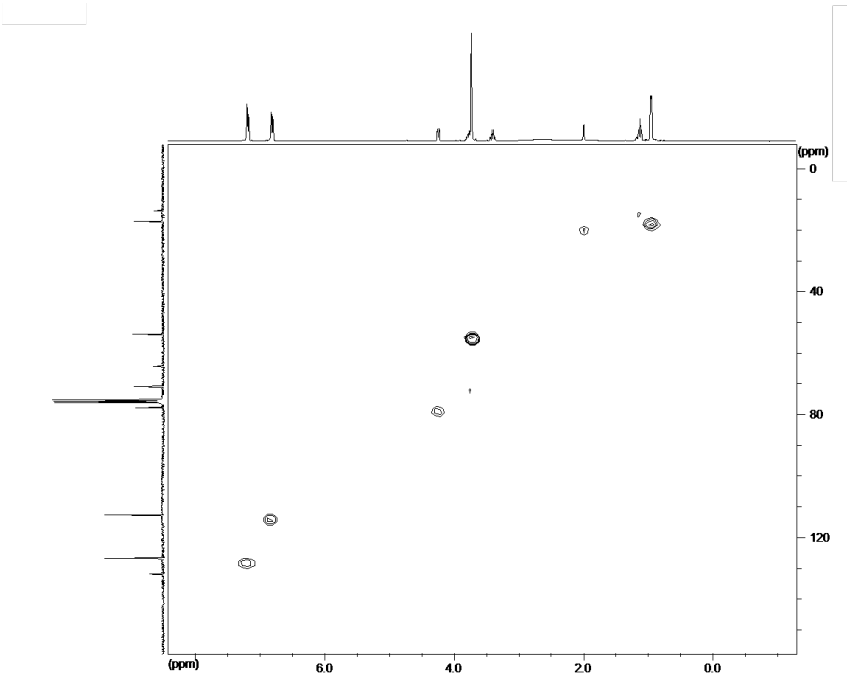

Figure S4. 2D proton-carbon correlation spectra (HMQC) of **threo-3a**.

anisic acid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 3.88 (s, 3H), 6.94 (d, *J* = 9.0 Hz, 2H), 8.06 (d, *J* = 9.0 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 56.0, 114.3, 122.2, 132.9, 164.6; MS (EI) m/z (%) 152 (M+, 86.6), 135 (100), 117 (1.3).

erythro-1-ethoxy-1-(4-methoxyphenyl)-2-propanol (3b). ^{1}H NMR (300 MHz, $CDCl_3$) δ 1.11 (d, *J* = 6.4 Hz, 3H), 1.16 (t, *J* = 6.8 Hz, 3H), 3.34 (q, *J* = 6.8 Hz, 2H), 3.80 (s, 3H), 3.90 (m, 1H), 4.12 (d, *J* = 4.9 Hz, 1H), 6.9 (d, *J* = 9.0 Hz, 2H), 7.2 (d, *J* = 9.0 Hz, 2H); MS (EI) m/z (%) 210 (M+, 0.9), 165 (100), 137 (73.4), 121 (61.0), 109 (21.2).

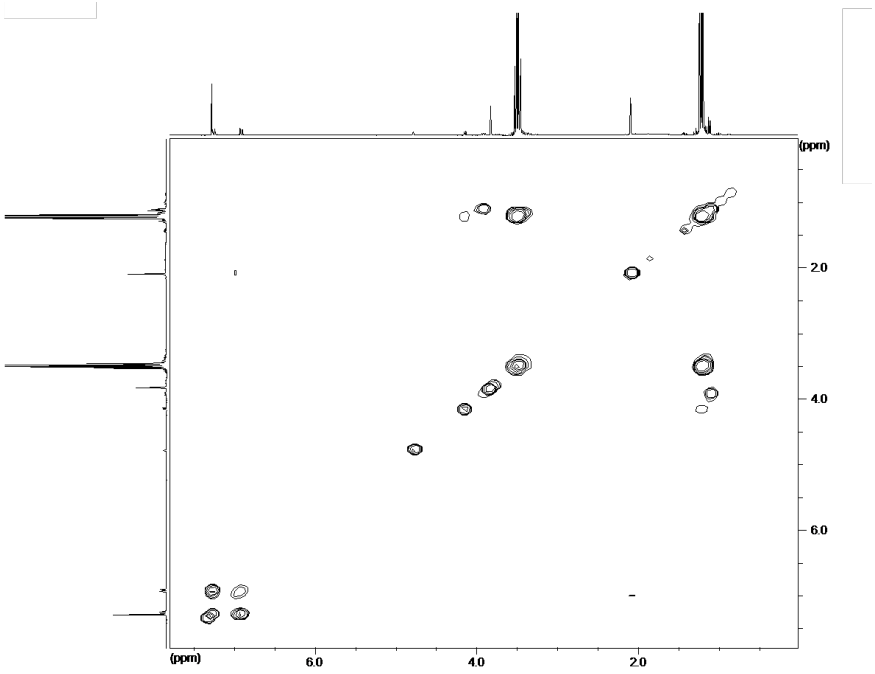

Figure S5. 2D proton-proton correlation spectra (COSY) of **erythro-3b**.

threo-1-ethoxy-1-(4-methoxyphenyl)-2-propanol (3b). ^{1}H NMR (300 MHz, $CDCl_3$) δ 0.94 (d, *J* = 6.4 Hz, 3H), 1.14 (t, *J* = 7.1 Hz, 3H), 3.32 (q, *J* = 7.1, 2H), 3.76 (m, 1H), 3.80 (s, 3H), 3.88 (d, *J* = 8.2 Hz, 1H), 6.8 (d, *J* = 8.7 Hz, 2H), 7.2 (d, *J* = 8.7 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 15.4, 18.0, 55.4, 64.2, 71.5, 87.3, 113.9, 128.8,

131.2, 159.6; MS (EI) m/z (%) 210 (M^+, 0.7), 165 (100), 137 (80.8), 121 (100), 109 (25.9).

(1α,2α,3α,4β)-1,2-bis(4-methoxyphenyl)-3,4-dimethylcyclobutane (4b). ^{13}C NMR (75 MHz, $CDCl_3$) δ 14.7, 20.5, 39.6, 41.9, 47.2, 47.6, 55.1, 55.3, 112.9, 113.5, 127.9, 131.4, 134.1, 157.3, 157.4.

(1α,2β,3α,4β)-1,2-bis(4-methoxyphenyl)-3,4-dimethylcyclobutane (4c). ^{13}C NMR (75 MHz, $CDCl_3$) δ 19.0, 43.3, 52.6, 55.4, 113.9, 128.0, 136.1, 158.1.

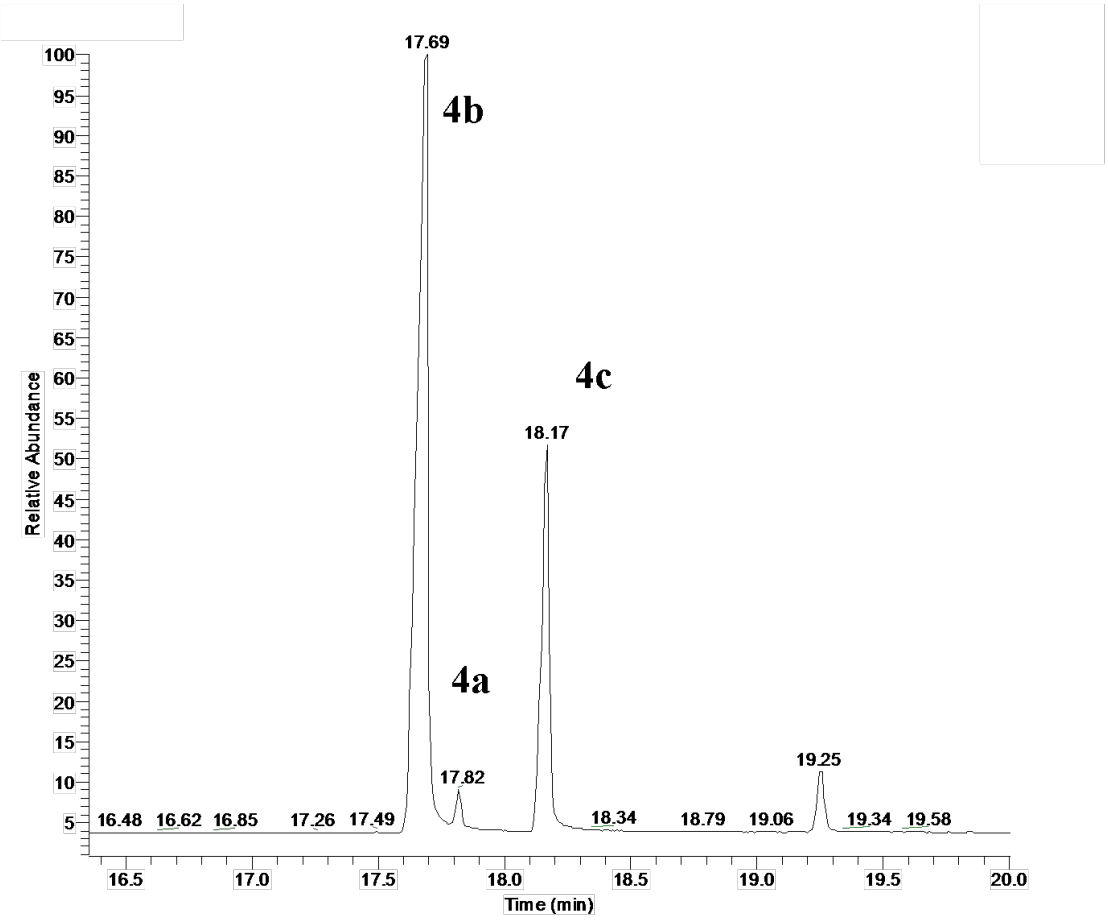

Figure S6. Chromatogram obtained by GC / MS equipped with a 30 m DB5-MS 0.25 mm i.d. capillary column. Carrier gaz : He (Flow rate : 0.6 $mL.min^{-1}$). Temperature gradient : 120°C, 5 min, 10°C / min, 250°C, 2 min. Injector temperature : 250°C.

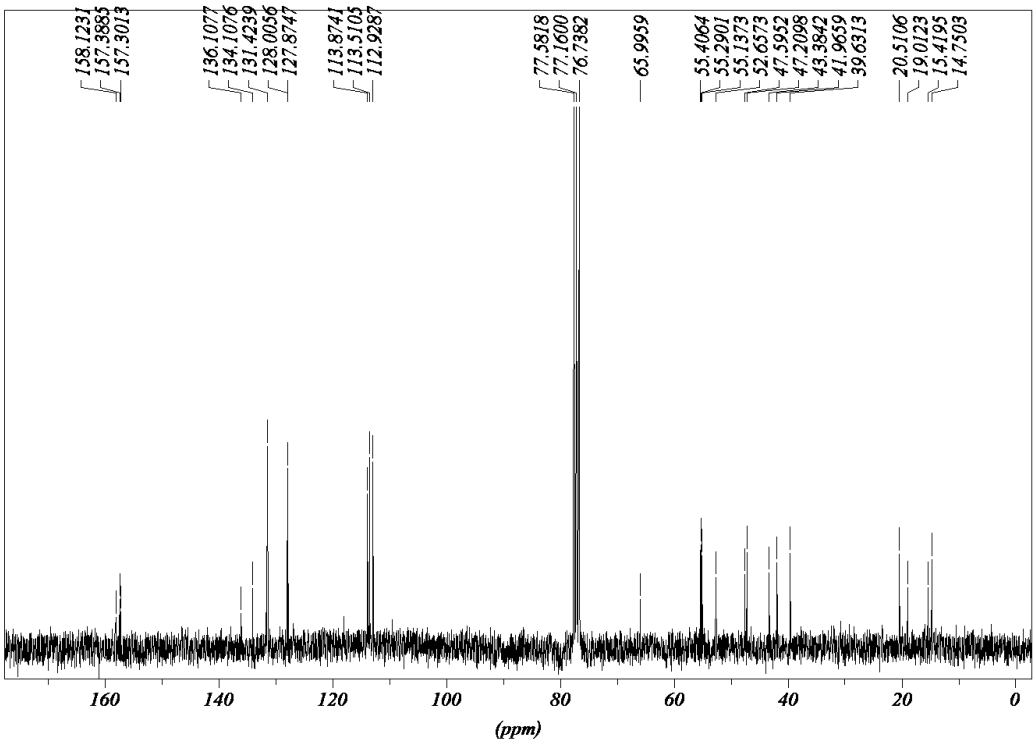

Figure S7. ^{13}C NMR ($CDCl_3$) of a **4b** and **4c** mixture.

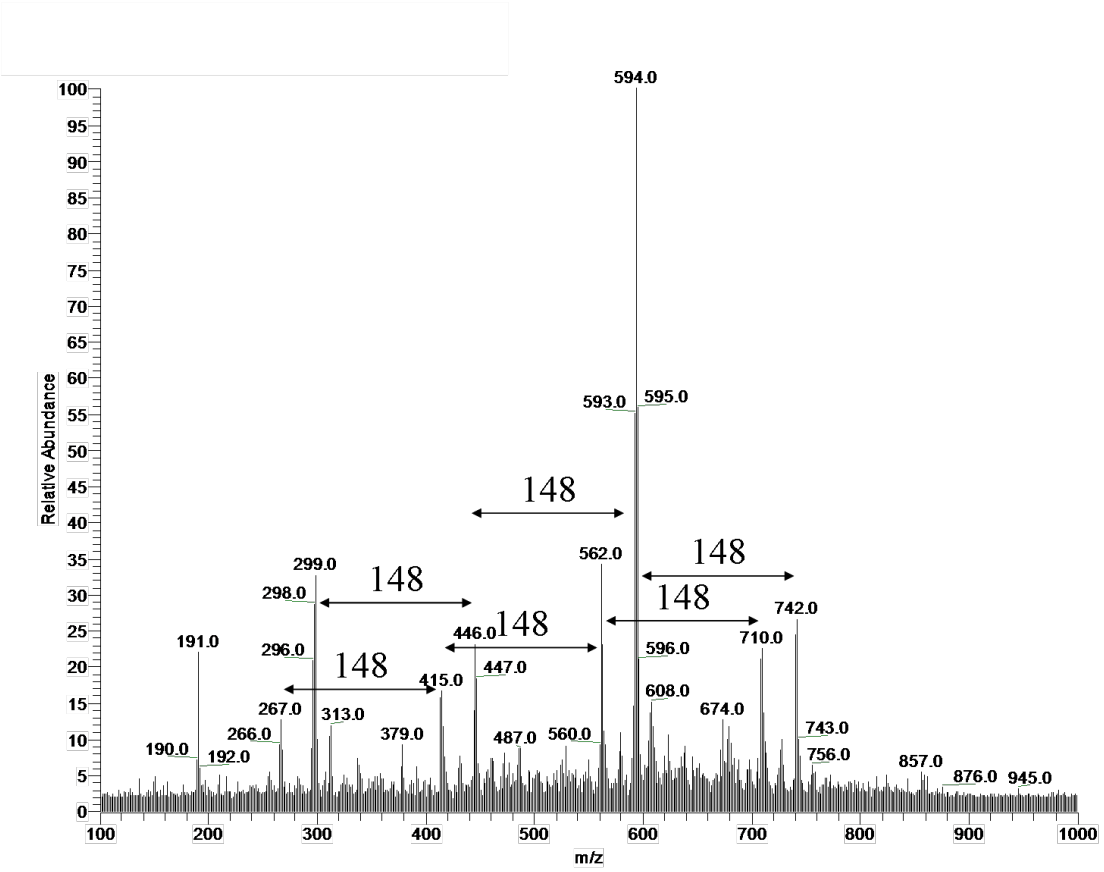

Figure S8. APCI Mass spectrum of polymers obtained by irradiation of *trans*-anethole in 40 % EtOH / 60 % H_2O in deaerated solution. The heated capillary temperature was set at 350°C, cone voltage at 26 V and corona needle at 3080 V.

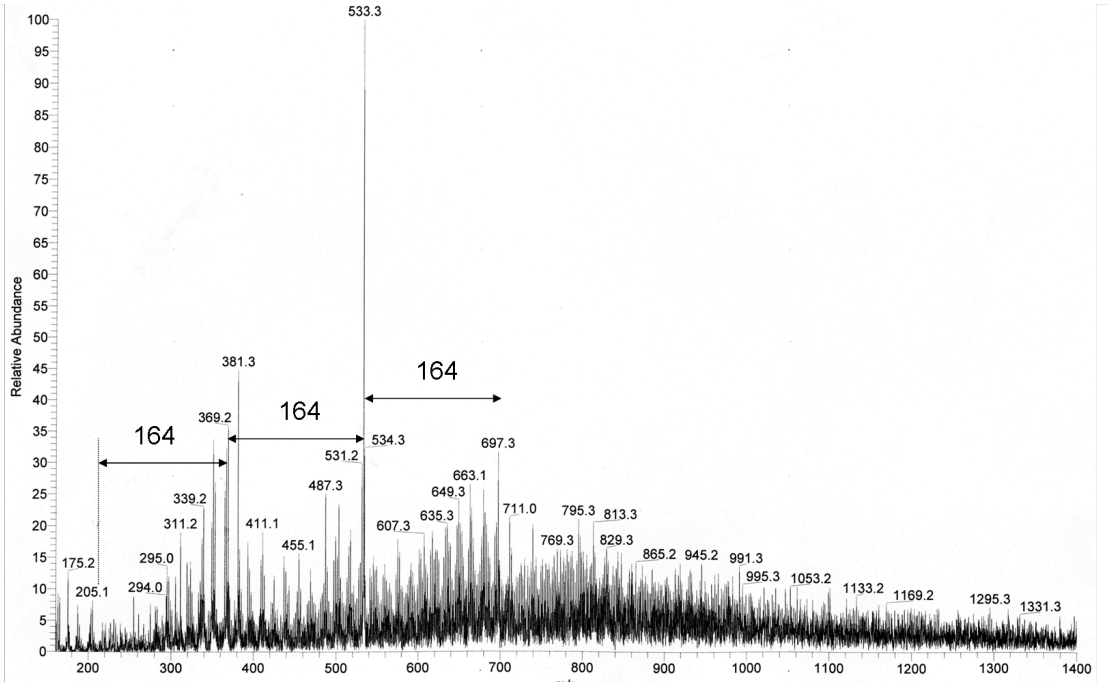

Figure S9. ESI Mass spectrum of polymers obtained by irradiation of trans-anethole in 5 % EtOH / 95 % H_2O in aerated solution.

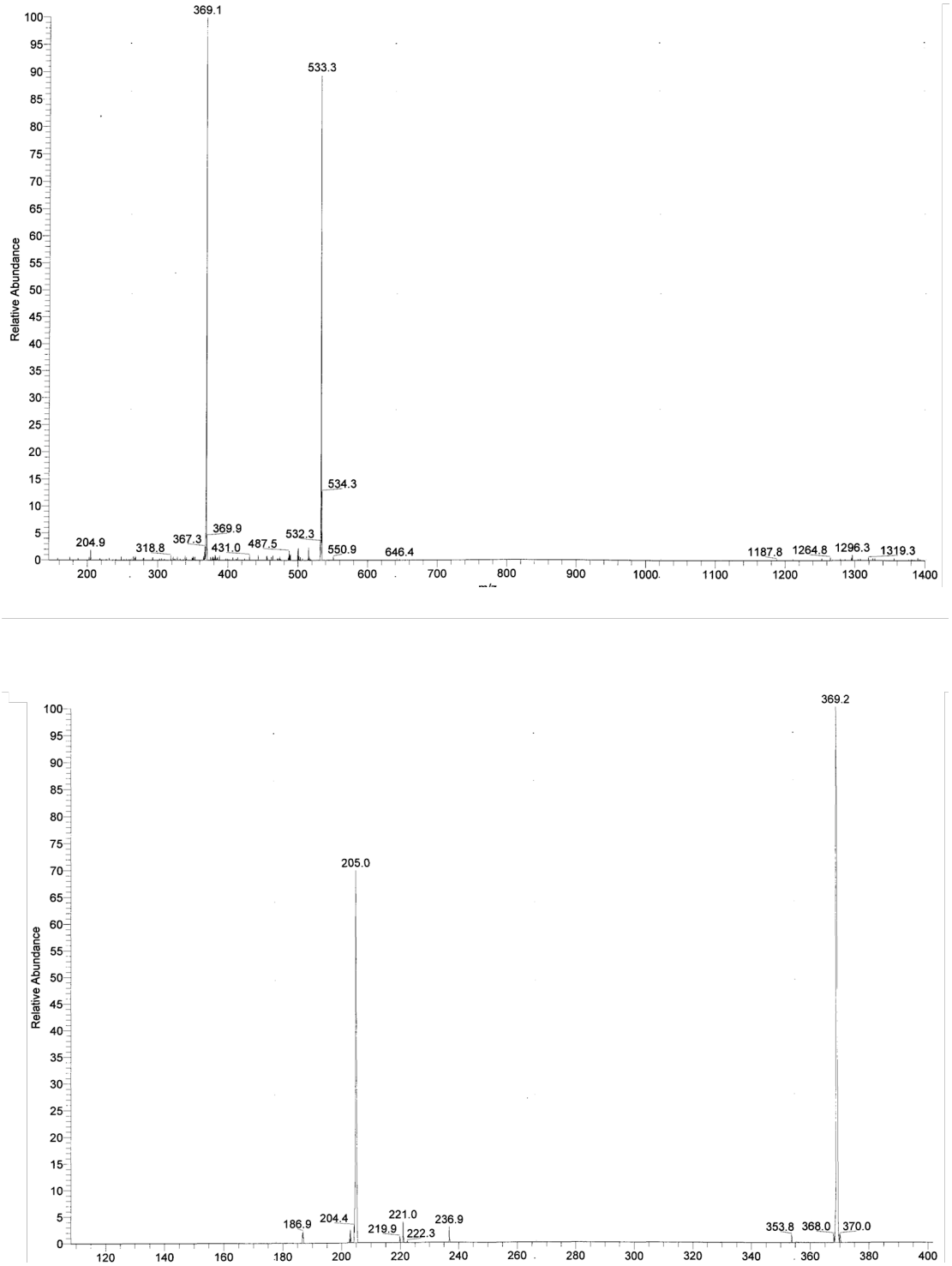

Figure S10. ESI MS / MS mass spectrum of polymers obtained by irradiation of trans-anethole in 5 % EtOH / 95 % H_2O in aerated solution.