Supplementary Material (ESI) for New Journal of Chemistry

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Electronic Supplementary Information

Microwave-enhanced radical reactions at ambient temperature. 3. Highly selective radical synthesis of 3-cyclohexyl-1-phenyl-1-butanone in a microwave double cylindrical cooled reactor

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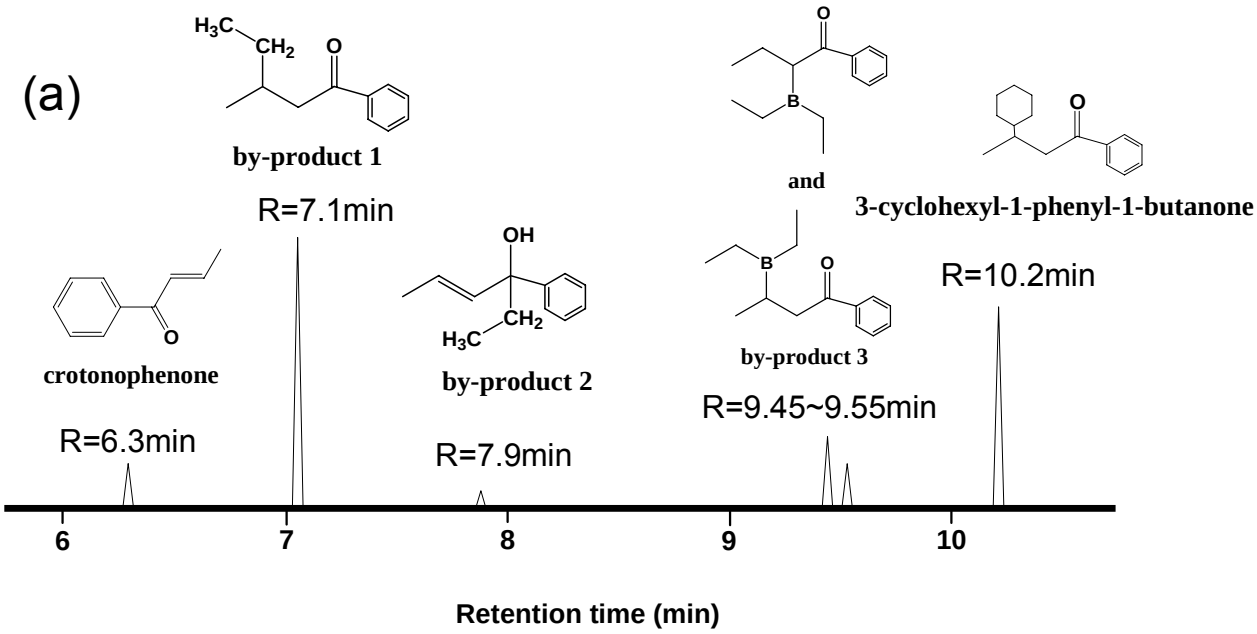

Figure S1a – Gas chromatogram of reactants and products from the synthesis of 3-cyclohexyl-1-phenyl-1-butanone (CPB) by the microwave irradiation alone (MW protocol) after a 120-min period.

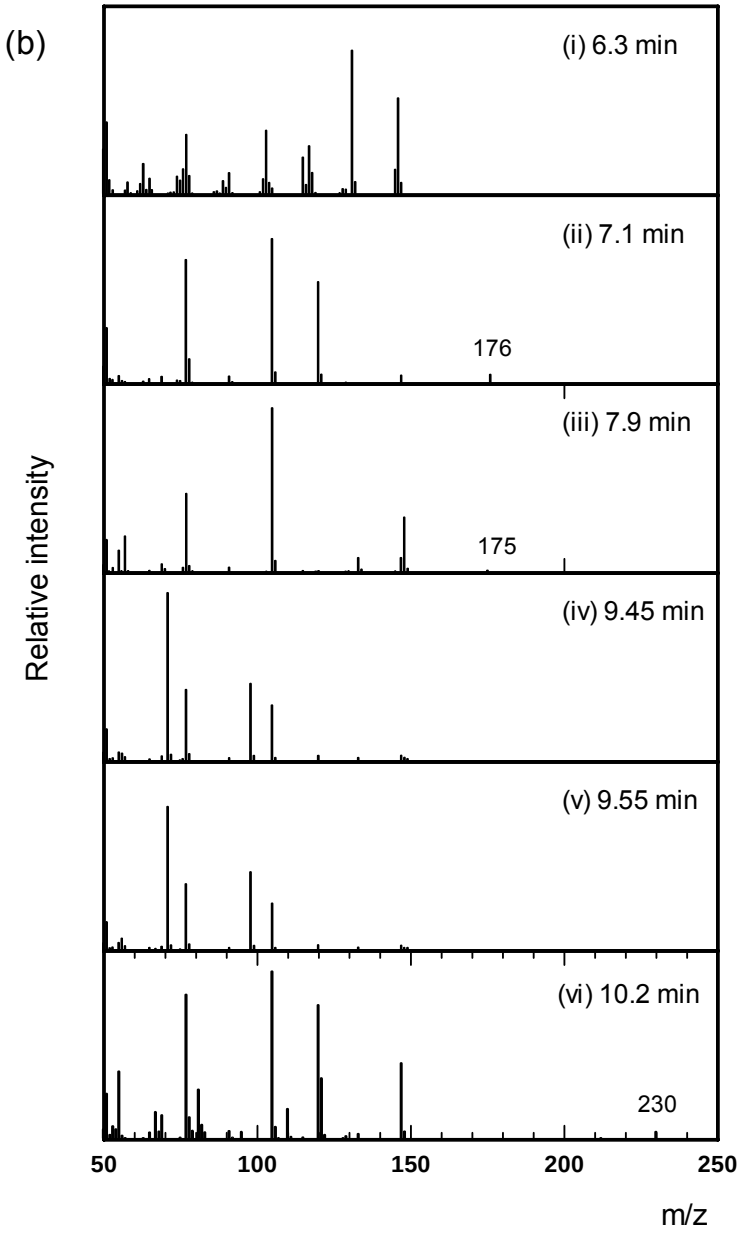

Figure S1b – GC-MS spectra of the product and by-products at the retention times indicated. (i) crotonophenone, molecular mass peak m/z = 146; (ii) by-product 1, molecular mass peak m/z = 176; (iii) by-product 2, molecular mass peak m/z = 175; (iv) and (v) isomers of by-product 3 (see **Scheme 2** and **Figure S1a**) ; and (vi) 3-cyclohexyl-1-phenyl-1-butanone with principal MS peaks occurring at (EI+, 1.3 kV) m/z (peak intensity) = 230 (4, {M}), 147 (41), 120 (83), 105 (100), 91 (6), 77 (91), 67 (16), 55 (41).

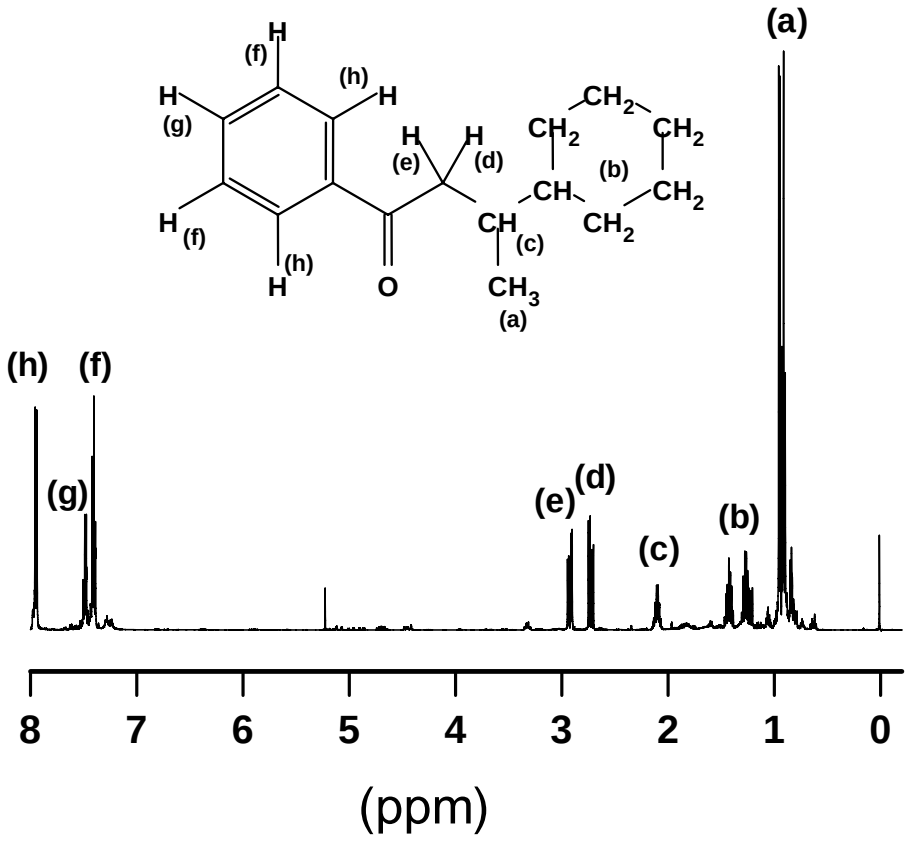

Figure S2 – Proton NMR spectrum of the major fraction from the flash column chromatogram of products obtained in the synthesis and consistent with the major product being 3-cyclohexyl-1- phenyl-1-butanone (CPB): ^{1}H-NMR (500 MHz, $CDCl_3$) δ (ppm): (a) 0.95–0.84 (d, 3H), (b) 1.42–1.24 (m,11H), (c) 2.14–2.08 (m, 1H), (d) 2.74–2.69 (m, 1H), (e) 2.94–2.89 (m, 1H), (f) 7.41–7.38 (m, 2H), (g) 7.48–7.46 (m, 1H), (h) 7.94–7.93 (m, 2H). Note these assignments are consistent with the ones estimated using ChemNMR.