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Ethyl (E)-2-Methyl-5-phenyl-2-pentenoate

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The general part of the experimental section [1] has been presented elsewhere. To a solution of (1-carbethoxyethylidene)triphenylphosphorane (5.76 g, 15.7 mmol) in dry benzene (100 ml) was added 3-phenylpropanal (2 g, 14.9 mmol). The mixture was refluxed for 6 hours and the solvent was removed. The residue was purified by flash chromatography (ethyl acetate/light petroleum 5:95), followed by preparative HPLC (ethyl acetate/light petroleum 1:99) to yield ethyl(*E*)-3-methyl-5-phenyl-2-pentenoate (2.71 g, 83%) as a colourless oil.

B.p. 130°/0.4 mmHg (Kugelrohr)

Anal. calc. for C₁₄H₁₈O₂ (218.29): C 77.0, H 8.3; found: C 77.0, H 7.9.

IR (film) 2983, 2933, 1710 (s, C=O), 1619, 1452, 1364, 1266(s), 1177, 1118(s), 1082, 1029, 741 cm⁻¹.

¹H-NMR (400 MHz, CDCl₃) 1.28 (3H, t, *J* 7.1 Hz, -OCH₂C*H*₃), 1.79 (3H, dt, *J* 1.5, 1.0 Hz, CH₃), 2.48 (2H, m, CH₂), 2.75 (2H, bt, *J* 7.6 Hz, Ph-C*H*₂), 4.19 (2H, q, *J* 7.1 Hz, -OC*H*₂CH₃), 6.81 (1H, tq, *J* 7.35, 1.5 Hz, =CH), 7.14-7.35 (5H, m, ArH). Stereochemistry confirmed by n.O.e. difference spectroscopy. Irradiation at 1.79 produced no n.O.e. at 6.81, and irradiation at 6.81 produced no n.O.e. at 1.79.

¹³C-NMR (15 MHz, CDCl₃) 12.27, 14.22 (CH₃), 30.52, 34.74, 60.32, (CH₂), 126.0, 128.1, 128.2 (CH), 128.4 (quat, C2), 140.8 (=CH), 141.2 (quat, C1'), 168.0 (quat, C1).

EI-MS 218(M⁺, 12%), 173(5), 91(100).

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References and Notes

1. Moloney, M.G.; Pinhey, J.T.; Stoermer, M.J. "Vinyl Cation Formation by Decomposition of Vinyl-lead

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Triacetates. The reactions of Vinylmercury and Vinyltin Compounds with Lead Tetraacetate." *J. Chem. Soc. Perkin Trans. 1* **1990**, *10*, 2645.

Sample Availability: No sample available.

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