Use of *Saccharomyces cerevisiae* Yeasts in the Chemoselective Bioreduction of (1E,4E)-1,5-Bis(4-Methoxyphenyl)-1,4-Pentadien-3-one in Biphasic System

**César A. Schaefer**,*a* **Vanessa D. Silva,**,*a* **Boris U. Stambuk**,*b* and **Maria da G. Nascimento**,*a*,*a*

*Departamento de Química and †Departamento de Bioquímica, Universidade Federal de Santa Catarina, 88040-900 Florianópolis-SC, Brazil*

Preparation of (1E,4E)-1,5-bis(4-methoxyphenyl)-1,4-pentadien-3-one (1)

The α,β-unsaturated carbonyl compound 1 was prepared by aldol condensation in a medium with 50% (m/v) of KOH using two equivalents of 4-methoxybenzaldehyde with one equivalent of acetone according to a commonly applied procedure described in the literature. This compound was obtained as a yellow solid in 60% yield after 4 h of reaction. Retention time on GC R, of 12.5 min; m.p. 116-118 °C (115-117 °C); (KBr) IV ν<sub>max</sub>/cm<sup>−1</sup> 3434, 1653, 1630, 1600, 1511, 1256, 1175, 823; ¹H NMR (CDCl<sub>3</sub>, 400 MHz) δ (ppm) 7.7 (d, 2H, J 16 Hz), 7.5 (d, 4H, J 8 Hz), 6.9 (m, 6H), 3.8 (s,6H, –OCH₃).

Figure S1. IR spectrum (KBr) of (1E,4E)-1,5-bis(4-methoxyphenyl)-1,4-pentadien-3-one.
Use of *Saccharomyces cerevisiae* Yeasts in the Chemoselective Bioreduction

Preparation of 1,5-bis(4-methoxyphenyl)-3-pentanone (2)

The saturated ketone 2 was prepared by baker’s yeast-catalyzed bioreduction of 1 in an aqueous/organic solvent biphasic system. This compound was isolated and characterized by $^1$H NMR and GC. $^1$H NMR (CDCl$_3$, 400 MHz) $\delta$ (ppm) 7.1 (m, 4H), 6.8 (m, 4H), 3.8 (s, 6H, –OCH$_3$), 2.8 (t, 4H, CH$_2$) 2.6 (t, 4H, CH$_2$). Retention time on GC $R_t$ of 4.1 min.

Figure S2. $^1$H NMR spectrum (CDCl$_3$, 400 MHz) of (1E,4E)-1,5-bis(4-methoxyphenyl)-1,4-pentadien-3-one.

Figure S3. $^1$H NMR spectrum (CDCl$_3$, 400 MHz) of 1,5-bis(4-methoxyphenyl)-3-pentanone.
Preparation of (1E,4E)-1,5-bis(4-methoxyphenyl)-1,4-pentadien-3-ol (3)

Compound 3 was prepared from (1E,4E)-1,5-bis(4-methoxyphenyl)-1,4-pentadien-3-one by the reduction with NaBH$_4$/wet SiO$_2$ as described in the literature with some modifications, and was used as a standard in the $^1$H NMR and GC analysis. The alcohol 3 was obtained as a pale yellow solid in 49% yield after 1 h of reaction. Retention time on GC R$_t$ of 5.1 min; m.p. 77-80 °C (85-87 °C)$^4$; IV $\nu_{\text{max}}$/cm$^{-1}$(KBr): 3538, 2957, 1605, 1513, 1250, 1174, 1030, 971, 817; $^1$H NMR (CDCl$_3$, 400 MHz) $\delta$ (ppm) 7.3 (d, 4H, $J$ 8 Hz), 6.8 (d, 4H, $J$ 8 Hz), 6.5 (d, 2H, $J$ 16Hz), 6.1 (dd, 2H), 4.9 (m, 1H), 3.7 (s, 6H, –OCH$_3$).

References