Phase Transfer Catalyzed Enantioselective Strecker Reactions of α -Amido Sulfones with Cyanohydrins.

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Supporting Information

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General experimental information.

All starting materials and solvents were obtained from commercial suppliers and used without purification. α -Amido sulfones¹ **4a-l** and cyanohydrins² **3b,c** were obtained following literature procedures. ¹H and ¹³C NMR spectra were recorded at 300 MHz and 100 MHz, respectively, in CDCl₃ as the solvent, at 25 °C. Chemical shifts are reported in the δ scale relative to residual CHCl₃ (7.26 ppm) for ¹H NMR and to the central line of CDCl₃ (77.0 ppm) for ¹³C NMR. ¹³C NMR were recorded on a broad band decoupled mode. Mass spectra were recorded on a micromass spectrometer using electrospray (ES+) ionization techniques. Optical rotations were measured on a polarimeter at 25 °C. The enantiomeric excess (ee) of the products was determined by chiral stationary phase HPLC or GC. HPLC and GC traces were compared to racemic samples prepared with tetrabutylammonium bromide as the catalyst. Melting points were measured on an apparatus and are uncorrected.

¹ (a) Pearson, W. H.; Lindbeck, A. C.; Kampf, J. W. *J. Am. Chem. Soc.* **1993**, *115*, 2622-2636. (b) Wenzel, A. G.; Jacobsen, E. N. *J. Am. Chem. Soc.* **2002**, *124*, 12964-12965. (c) Bernacka, E.; Klepacz, A.; Zwierzak, A. *Tetrahedron Lett.* **2001**, *42*, 5093-5094.

² Gassman, P. G.; Talley, J. J. *Tetrahedron Lett.* **1978**, *19*, 3773-3776.

Preparation of catalyst **1a**.

***N*-(*o*-Trifluoromethylbenzyl)quininium bromide (**1a**).** A mixture of (-)-quinine (648 mg, 2 mmol) and *o*-trifluoromethylbenzyl bromide (400 μ L, 2.6 mmol) in toluene (6 mL) was stirred at reflux over night. After cooling to room temperature the precipitated product was isolated through filtration over Büchner, washed with pentane and dried *in vacuo* to afford **1a** as a white solid in 89% yield (1.00 g). m.p. 198-200 °C; ^1H NMR (300 MHz, CDCl_3): δ (ppm) 8.83 (d, $J = 4.7$ Hz, 1H), 8.52 (d, $J = 8.1$ Hz, 1H), 8.10 (d, $J = 8.8$ Hz, 1H), 7.88-7.80 (m, 3H), 7.70 (t, $J = 7.4$ Hz, 1H), 7.43 (dd, $J = 9.4, 2.5$ Hz, 1H), 7.06 (d, $J = 2.5$ Hz, 1H), 6.94 (d, $J = 12.8$ Hz, 1H), 6.78 (d, $J = 7.4$ Hz, 1H), 6.60 (d, $J = 7.4$ Hz, 1H), 5.64-5.45 (m, 2H), 5.11 (d, $J = 10.4$ Hz, 1H), 5.00 (d, $J = 17.2$ Hz, 1H), 4.68 (d, $J = 13.1$, 1H), 3.97 (s, 3H), 3.68-3.62 (m, 1H), 3.33-3.30 (m, 1H), 3.14 (t, $J = 11.8$ Hz, 1H), 2.91 (t, $J = 9.0$ Hz, 1H), 2.60-2.53 (m, 2H), 2.34 (d, $J = 12.5$, 1H), 2.09 (br s, 1H), 1.87 (t, $J = 13.3$ Hz, 1H), 1.52 (t, $J = 12.1$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 158.4, 147.5, 144.0, 142.8, 137.1, 135.8, 133.2, 132.3, 131.3, 130.6, 127.9, 127.8, 125.5, 124.8, 121.7, 120.9, 118.1, 100.0, 72.8, 63.1, 61.8, 60.7, 55.6, 52.2, 37.8, 26.1, 24.9, 21.8; ESIMS m/z 483 [$M\text{-Br}$] $^+$; Anal. Calcd. for $\text{C}_{28}\text{H}_{30}\text{BrF}_3\text{N}_2\text{O}_2$: C, 59.69; H, 5.37; N, 4.97. Found: C, 59.58; H, 5.39; N, 4.98. $[\alpha]_{\text{D}}^{25}$ -138 ($c = 0.34$, CHCl_3).

Copy of the ^1H NMR spectrum of catalyst **1a**.

Copy of the ^1H NMR spectrum of compound **4a**.

Copy of the ^1H NMR spectrum of compound **4b**.

Copy of the ^1H NMR spectrum of compound **4c**.

Copy of the ^1H NMR spectrum of compound **4d**.

Copy of the ^1H NMR spectrum of compound **4e**.

Copy of the ^1H NMR spectrum of compound **4f**.

Copy of the ^1H NMR spectrum of compound **4g**.

Copy of the ^1H NMR spectrum of compound **4h**.

Copy of the ^1H NMR spectrum of compound **4i**.

Copy of the ^1H NMR spectrum of compound **4I**.