SUPPORTING INFORMATION

Electrochemically induced N-alkylation of chiral 2-(methylsulfinyl) 1H-benzimidazole

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General

Any commercial available material was purchased from Aldrich or Fluka and used without further purification. Constant current electrolysis were performed using an Hewlett Packard DC Power Supply Mod. E3612A. The NMR spectra were recorded on Bruker DRX 400, 300, 250 spectrometers (400 MHz, 300 MHz, 250 MHz, 1H; 100 MHz, 75 MHz, 62,5 MHz 13C). Spectra were referenced to residual CHCl_3 (7.26 ppm, 1H; 77.00 ppm, 13C). Elemental analyses were performed with FLASH EA 1112 series-Thermo Scientific for CHNS-O apparatus. HPLC analyses were performed with a Waters 1525 HPLC, by calibrating the chiral methods with the corresponding racemic mixtures, using diacel chiralpak ODH and $\lambda = 254$ nm. Optical rotations were measured on a Perkin-Elmer Polarimeter with a sodium lamp at $\lambda = 589$ nm

Computational details

The absolute reduction potential of the **1/A** couple was determined by state of art G3(MP2)-RAD computations further enhanced by the "Full-TZ" approach, including core electrons correlation and using 6-311+G(d,p) as the low level basis set. Solvent (acetonitrile) effects were included by the SMD continuum model. $E^0(\text{Fc}^+/\text{Fc}) = 4.964$ V (consistent with the Fermi-Dirac electron convention) was employed as the absolute potential of the ferricinium/ferrocene (Fc^+/Fc) couple. All calculations were carried out by using the Gaussian program.

3g, HPLC conditions: Daicel Chiralpak ODH, hexane/isopropanol/ (80:20), 0.80 mL/min

3d, HPLC conditions: Daicel Chiralpak ODH, hexane/isopropanol/ (80:20), 0.80 mL/min

3h, HPLC conditions: Daicel Chiralpak ODH, hexane/isopropanol/ (75:25), 0.80 mL/min