Supplementary Information

A PRACTICAL SYNTHESIS OF 2-SUBSTITUTED-5-BROMO-INDOLES

Yang He, a Lianlian Fan, b Haoting Zhu, a Xiaolin Li, a Pu Zhou, a and Yu Luo a, *

a Shanghai Engineering Research Center of Molecular Therapeutics and New Drug Development, School of Chemistry and Molecular Engineering, East China Normal University, Shanghai 200241, China. E-mail: yluo@chem.ecnu.edu.cn
b Department of Pharmacy, China-Japan Union Hospital of Jilin University, Changchun, China

5-Bromo-1-tosyl-1H-indole (3b). To a suspension of sodium hydride (60% in mineral oil, 0.30 g, 7.7 mmol) in DMF (5.0 mL), a solution of compound 2 (1.00 g, 5.1 mmol) in DMF (5.0 mL) was added and the mixture was stirred at 0 °C for 1 h. To the mixture was added a solution of 4-methylbenzenesulfonyl chloride (1.17 g, 6.1 mmol) in DMF (5.0 mL) and the mixture was stirred at room temperature for 4 h. The mixture was poured into water (100 mL) and the resulting precipitate was collected by suction filtration, washed with water (200 mL) and dried. The crude material was purified by flash column chromatography eluting with 5-10% EtOAc/petroleum ether to provide 3b as a white solid (1.63 g, 91%). mp 132-134 °C (lit. 1 134 °C); 1H NMR (CDCl3, 400 MHz), δ 7.77 (d, J = 8.7 Hz, 1H), 7.65 (d, J = 7.7 Hz, 2H), 7.44-7.60 (m, 2H), 7.31 (d, J = 8.6 Hz, 1H), 7.13 (d, J = 7.7 Hz, 2H), 6.50 (s, 1H), 2.25 (s, 3H); 13C NMR (CDCl3, 100 MHz), δ 145.3, 135.0, 133.5, 132.5, 130.0, 127.6, 127.5, 126.8, 124.1, 116.8, 115.0, 108.3, 21.6.

REFERENCES
$^1$H NMR of compound 3b

$^{13}$C NMR of compound 3b
$^1$H NMR of compound 1

$^{13}$C NMR of compound 1
$^1$H NMR of compound 4b

$^{13}$C NMR of compound 4b
IR of compound 4b

[Graph showing IR spectrum with peaks at 3123, 1594, 1433, and 1380 cm\(^{-1}\)].

\(^1\)H NMR of compound 5a

[Graph showing NMR spectrum with peaks at various ppm values].
\[ ^{13} \text{C NMR of compound 5a} \]

\[ \text{IR of compound 5a} \]
$^1$H NMR of compound 5b

$^{13}$C NMR of compound 5b
IR of compound 5b

$\text{Transmittance}\% \quad (\text{a.u.})$

Wavenumber (cm$^{-1}$)

$^1\text{H NMR of compound 5c}$
$^{13}$C NMR of compound 5c

IR of compound 5c
$^1$H NMR of compound 5d

$^{13}$C NMR of compound 5d
IR of compound 5d

\[ \text{Transmittance}\% \text{ (a.u.)} \]

Wavenumber (cm\(^{-1}\))

\(3223, 2989, 1984, 1816, 1753\)

\(^1\)H NMR of compound 5e

\[ 8.2591, 7.8959, 7.6736, 7.4090, 7.4610, 7.3689, 7.3184, 7.3225, 7.1494, 7.1291, 6.3863, 2.2956 \]

T1 (ppm)
$^{13}$C NMR of compound 5e

IR of compound 5e
$^{1}$$H$ NMR of compound $5f$

$^{13}$$C$ NMR of compound $5f$
IR of compound 5f

\[ \text{Wavenumber (cm}^{-1}\text{)} \]

Transmittance (a.u.)

1H NMR of compound 5g
$^{13}$C NMR of compound 5g

IR of compound 5g