Iron(III)-Catalyzed Aza-Prins-Cyclization: Direct Synthesis of 6-Membered Azacycles

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Material and Methods:

^1H NMR spectra were recorded at 300 and 400 MHz, and ^{13}C NMR were recorded at 75 MHz, VTU 298.0 °K. Chemical shifts were reported in parts per million. The residual solvent peak was used as an internal reference.

For analytical thin-layer chromatography, silica gel ready-foils was used, respectively, being developed with 254 nm UV light and/or spraying with a solution of ninhydrin (10% w/v in EtOH) or vainillin in EtOH:H₂SO₄:AcOH (15:1:1.3) and heating at 200 °C. Column chromatography was performed using silica gel (0.015-0.04 mm) and *n*-hexane/EtOAc solvent systems. All reagents were obtained from commercial sources and used without further purification. Solvents were dried and distilled before use.

General Procedures:

General procedure for a ferric halide promoted aza-Prins cyclization: To a solution of homoallyl tosyl amine or homopropargyl tosyl amine (1 equiv) and aldehyde (1.5 equiv) in dry CH₂Cl₂ was added anhydrous FeX₃ (1.5 equiv) in one portion. The reaction was concluded in approximately 10 min, quenched by addition of water with stirring and extracted with CH₂Cl₂. The combined organic layers were dried over magnesium sulphate, and the solvent was removed under reduced pressure. This crude reaction mixture was purified by flash silica gel column chromatography (*n*-hexane/EtOAc solvent systems).

Starting Materials:

Dimethyl 1-diazo-2-oxopropylphosphonate: To a stirred suspension of NaH (264.8 mg at 60%)¹ in THF:C₆H₆ (5:1, 12 mL) at 0 °C were added *p*-toluenesulfonyl azide² (1.29 g, 6.6 mmol) and dimethyl 2-oxopropylphosphonate (0.83 mL, 6.0 mmol), respectively. The reaction was allowed to proceed for 12 hours at room temperature and then filtered through a pad of Celite to lead the pure Dimethyl 1-diazo-2-oxopropylphosphonate (1.05 g, 5.5 mmol) in 90% yield.

***N*-(but-3-ynyl)-4-methylbenzenesulfonamide:** To a solution of 3-aminopropan-1-ol (5.10 mL, 66.6 mmol) in CH₂Cl₂ (166 mL) at 0 °C were added Et₃N (18.56 mL, 133.1 mmol) and 4-methylbenzene-1-sulfonyl chloride (66.6 mL, 66.6 mmol) respectively. The reaction was allowed to warm to rt. The reaction was diluted with CH₂Cl₂ and washed with H₂O, dried over MgSO₄ and concentrated. The crude obtained was used in the next reaction.

To a solution of the alcohol crude in CH₂Cl₂ (500 mL) at 0 °C were added Et₃N (65.2 mL, 467.0 mmol) and DMSO (43.8 mL, 61.7 mmol) respectively. The mixture was stirred for 15 min, and SO₃Py (31.8 g, 199.7 mmol) was slowly added. The reaction was diluted with CH₂Cl₂ and washed with a HCl aqueous solution (5% w/v), a saturated aqueous solution of NaHCO₃ and brine, dried over MgSO₄ and concentrated. The crude obtained was purified through a flash column of silica gel (*n*-hexane/EtOAc, 80:20) and the aldehyde (11.3 g, 49.93 mmol, 75% 2 steps) was used in the next reaction.

To a stirred solution of the aldehyde (2g, 8.8 mmol) in MeOH (88.0 mL) were added sequentially K₂CO₃ (2.4 g, 17.8 mmol) and dimethyl 1-diazo-2-oxopropylphosphonate (2.0 g, 10.6 mmol) at rt. The reaction was stirred until TLC showed the end of the reaction. The mixture of reaction was filtered

(1) Previously, the NaH was washed with dry THF.

(2) Curphey, Thomas J. *Preparation of p-toluenesulfonyl azide. A cautionary note.* *Org. Prep. Proced. Int.* **1981**, 13, 112-15.

through a pad of Celite and concentrated. This crude reaction mixture was purified by flash silica gel column chromatography (*n*-hexane/EtOAc 40:60) to gave *N*-(but-3-ynyl)-4-methylbenzenesulfonamide (1.4 g, 6.4 mmol) in 72% yield as an oil.

Final products (Table 1 and Table 3):

***trans*-4-chloro-2-cyclohexyl-1-tosylpiperidine** (Table 1, entry 1). ^1H NMR (CDCl_3 , 300 MHz) δ 7.72 (d, J = 8.3 Hz, 2H), 7.30 (d, J = 7.9 Hz, 2H), 4.00 (m, 1H), 3.88 (brdd, J = 4.8 & 15.2 Hz, 1H), 3.75 (brdd, J = 5.2 & 10.7 Hz, 1H), 3.00 (td, J = 2.7 & 13.4 Hz, 1H), 2.43 (s, 3H), 2.20 (brdd, J = 1.9 & 11.5 Hz, 1H), 1.91 (brdd, J = 2.0 & 10.9 Hz, 1H), 1.77 (m, 4H), 1.58 (brs, 1H), 1.45 (m, 3H), 1.16 (m, 3H), 0.93 (m, 2H). ^{13}C NMR (CDCl_3 , 300 MHz) δ 143.0 (C), 138.3 (C), 129.6 (2CH), 126.7 (2CH), 59.1 (CH), 52.9 (CH), 40.6 (CH_2), 35.7 (CH), 35.1 (CH_2), 34.6 (CH_2), 30.0 (CH_2), 29.7 (CH_2), 25.9 (CH_2), 25.8 (CH_2), 25.7 (CH_2), 21.3 (CH_3). FTIR (CHCl_3): 2928.9, 2853.2, 1451.3, 1335.7, 1157.6, 932.3 cm^{-1} . Elemental analysis: $\text{C}_{18}\text{H}_{26}\text{ClNO}_2\text{S}$ calcd.: C 60.74 H 7.36 N 3.94; found: C 60.72 H 7.39 N 3.95.

***trans*-4-chloro-2-isobutyl-1-tosylpiperidine** (Table 1, entry 2). ^1H NMR (CDCl_3 , 300 MHz) δ 7.72 (d, J = 8.3 Hz, 2H) 7.30 (d, J = 8.0 Hz, 2H) 4.21 (m, 1H), 4.05 (m, 1H), 3.86 (brdd, J = 4.7 & 15.0 Hz, 1H), 3.05 (td, J = 2.5 & 13.3 Hz, 1H), 2.41 (s, 3H), 1.97 (brd, J = 9.8 Hz, 2H), 1.70-1.43 (m, 4H), 1.25 (m, 1H), 0.88 (d, J = 6.4 Hz, 3H), 0.86 (d, J = 6.5 Hz, 3H). ^{13}C NMR (CDCl_3 , 300 MHz) δ 143.3 (C), 138.0 (C), 129.6 (2CH), 126.9 (2CH), 53.0 (CH), 52.1 (CH), 40.2 (CH_2), 39.2 (CH_2), 38.6 (CH_2), 35.2 (CH_2), 24.7 (CH), 22.5 (CH_3), 22.2 (CH_3), 21.4 (CH_3). FTIR (CHCl_3): 2957.3, 2870.0, 1338.8, 1158.1, 9352.1 cm^{-1} . Elemental analysis: $\text{C}_{16}\text{H}_{24}\text{ClNO}_2\text{S}$ calcd.: C 58.25 H 7.33 N 4.25; found: C 58.26 H 7.53 N 4.32.

***trans*-4-chloro-2-heptyl-1-tosylpiperidine** (Table 1, entry 3). ^1H NMR (CDCl_3 , 300 MHz) δ 7.69 (d, J = 8.2 Hz, 2H), 7.28 (d, J = 8.2 Hz, 2H), 4.05 (m, 2H), 3.86 (brdd, J = 4.2 & 14.6 Hz, 1H), 3.02 (t, J = 15.0 Hz, 1H), 2.41 (s, 3H), 1.98 (m, 2H), 1.65 (td, J = 2.4 & 12.8 Hz, 1H), 1.51 (m, 2H), 1.36 (m, 1H), 1.21 (brs, 10H), 0.86 (t, J = 6.5 Hz, 3H). ^{13}C NMR (CDCl_3 , 300 MHz) δ 143.1 (C), 138.0 (C), 129.6 (2CH), 126.7 (2CH), 53.8 (CH), 52.9 (CH), 40.1 (CH_2), 38.2 (CH_2), 35.2 (CH_2), 31.5 (CH_2), 30.1 (CH_2), 29.0 (CH_2), 28.9 (CH_2), 26.2 (CH_2), 22.4 (CH_2), 21.3 (CH_3), 13.9 (CH_3). FTIR (CHCl_3): 2928.1, 2856.9, 2360.8, 1454.6, 1338.2, 1157.8 cm^{-1} . Elemental analysis: $\text{C}_{19}\text{H}_{30}\text{ClNO}_2\text{S}$ calcd.: C 61.35 H 8.13 N 3.77; found: C 61.36 H 8.40 N 3.83.

***trans*-4-chloro-2-phenyl-1-tosylpiperidine** (Table 1, entry 4). ^1H NMR (CDCl_3 , 300 MHz) δ 7.77 (d, J = 8.1 Hz, 2H), 7.31 (m, 7H), 5.40 (brs, 1H), 3.94 (m, 2H), 3.04 (dt, J = 2.7 & 12.0 Hz, 1H), 2.74 (brd, J = 13.6 Hz, 1H), 2.46 (s, 3H), 1.89 (m, 2H), 1.57 (dd, J = 4.6 & 12.0 Hz, 1H). ^{13}C NMR (CDCl_3 , 300 MHz) δ 143.4 (C), 137.8 (C), 137.1 (C), 129.7 (2CH), 128.7 (2CH), 127.2 (CH), 126.7 (CH), 126.3 (CH), 55.8 (CH), 52.6 (CH), 41.2 (CH_2), 37.5 (CH_2), 35.0 (CH_2), 21.3 (CH_3). FTIR (CHCl_3): 3030.3, 2956.5, 1452.0, 1323.6, 1159.8 cm^{-1} . Elemental analysis: $\text{C}_{18}\text{H}_{20}\text{ClNO}_2\text{S}$ calcd.: C 61.79 H 5.76 N 4.00; found: C 61.74 H 5.96 N 4.39.

***trans*-2-benzyl-4-chloro-1-tosylpiperidine** (Table 1, entry 5). ^1H NMR (CDCl_3 , 300 MHz) δ 7.55 (d, J = 8.3 Hz, 2H), 7.27 (m, 5H), 7.12 (d, J = 6.2 Hz, 2H), 4.39 (m, 1H), 4.20 (m, 1H), 3.87 (brd, J = 13.5

Hz, 1H), 3.14 (td, $J = 2.6$ & 13.1 Hz, 1H), 2.79 (m, 2H), 2.40 (s, 3H), 2.12 (m, 1H), 2.02 (m, 1H), 1.67 (m, 2H). ^{13}C NMR (CDCl_3 , 300 MHz) δ 143.1 (C), 137.3 (C), 137.3 (C), 129.5 (2 CH), 128.8 (2 CH), 128.6 (2 CH), 126.8 (2 CH), 126.6 (CH), 55.2 (CH), 52.5 (CH), 40.4 (CH_2), 36.8 (CH_2), 36.4 (CH_2), 35.5 (CH_2), 21.3 (CH_3). FTIR (CHCl_3): 3025.2, 2962.0, 1599.3 cm^{-1} . Elemental analysis: $\text{C}_{19}\text{H}_{22}\text{ClNO}_2\text{S}$ calcd.: C 62.71 H 6.09 N 3.85; found: C 62.75 H 6.09 N 3.91.

4-chloro-1-tosylpiperidine (Table 1, entry 6). ^1H NMR (CDCl_3 , 300 MHz) δ 7.62 (d, $J = 8.9$ Hz, 2H), 7.30 (d, $J = 8.1$ Hz, 2H), 4.10 (m, 1H), 3.15 (m, 2H), 3.05 (m, 2H), 2.41 (s, 3H), 2.11 (m, 2H), 1.92 (m, 2H). ^{13}C NMR (CDCl_3 , 300 MHz) δ 143.2 (C), 132.0 (C), 129.3 (2CH), 127.1 (2CH), 54.9 (CH), 42.4 (2CH $_2$), 33.5 (2CH $_2$), 21.1 (CH_3). FTIR (CHCl_3): 2965.5, 2924.5, 1342.1, 1162.6, 930.0 cm^{-1} . Elemental analysis: $\text{C}_{12}\text{H}_{16}\text{ClNO}_2\text{S}$ calcd.: C 52.64 H 5.89 N 5.12; found: C 52.62 H 5.86 N 5.12.

trans-4-bromo-2-cyclohexyl-1-tosylpiperidine (Table 1, entry 7). ^1H NMR (CDCl_3 , 300 MHz) δ 7.70 (d, $J = 8.3$ Hz, 2H), 7.29 (d, $J = 8.0$ Hz, 2H), 4.12 (m, 1H), 3.81 (brdd, $J = 4.7$ & 15.1 Hz, 1H), 3.67 (brdd, $J = 5.0$ & 10.8 Hz, 1H), 2.98 (t, $J = 12.9$ Hz, 1H), 2.42 (s, 3H), 2.30 (brdd, $J = 1.8$ & 13.4 Hz, 1H), 2.02 (brdd, $J = 2.0$ & 11.5 Hz, 1H), 1.78-1.52 (m, 8H), 1.12 (m, 3H), 0.90 (m, 2H). ^{13}C NMR (CDCl_3 , 300 MHz) δ 143.0 (C), 138.2 (C), 129.4 (2CH), 126.4 (2CH), 59.5 (CH), 43.7 (CH), 41.2 (CH_2), 35.8 (CH_2), 35.2 (CH_2), 35.0 (CH), 30.0 (CH_2), 29.4 (CH_2), 25.6 (CH_2), 25.5 (CH_2), 25.4 (CH_2), 21.1 (CH_3). FTIR (CHCl_3): 2928.6, 2852.9, 1335.7, 1156.7, 753.4 cm^{-1} . Elemental analysis: $\text{C}_{18}\text{H}_{26}\text{BrNO}_2\text{S}$ calcd.: C 54.00 H 6.55 N 3.50; found: C 54.31 H 6.64 N 3.67.

trans-4-bromo-2-isobutyl-1-tosylpiperidine (Table 1, entry 8). ^1H NMR (CDCl_3 , 400 MHz) δ 7.72 (d, $J = 8.2$ Hz, 2H), 7.31 (d, $J = 8.0$ Hz, 2H), 4.18 (m, 2H), 3.81 (brdd, $J = 4.4$ & 12.6 Hz, 1H), 3.05 (td, $J = 2.2$ & 14.7 Hz, 1H), 2.44 (s, 3H), 2.08 (m, 2H), 1.87 (td, $J = 5.5$ & 12.8 Hz, 1H), 1.70 (dd, $J = 4.7$ & 12.6 Hz, 1H), 1.57 (m, 1H), 1.46 (m, 1H), 1.26 (qui, $J = 7.1$ Hz, 1H), 0.88 (d, $J = 6.4$ Hz, 3H), 0.87 (d, $J = 6.5$ Hz, 3H). ^{13}C NMR (CDCl_3 , 300 MHz) δ 142.9 (C), 137.6 (C), 129.3 (2CH), 126.5 (2CH), 52.3 (CH), 43.6 (CH), 40.7 (CH_2), 39.1 (CH_2), 38.6 (CH_2), 35.6 (CH_2), 24.3 (CH), 22.1 (CH_3), 21.8 (CH_3), 21.0 (CH_3). FTIR (CHCl_3): 2956.8, 2869.8, 1337.3, 1157.1, 934.7 cm^{-1} . Elemental analysis: $\text{C}_{16}\text{H}_{24}\text{BrNO}_2\text{S}$ calcd.: C 51.34 H 6.46 N 3.74; found: C 51.37 H 6.59 N 3.74.

trans-4-bromo-2-heptyl-1-tosylpiperidine (Table 1, entry 9). ^1H NMR (CDCl_3 , 300 MHz) δ 7.71 (d, $J = 8.1$ Hz, 2H), 7.31 (d, $J = 8.2$ Hz, 2H), 4.18 (m, 1H), 4.04 (m, 1H), 3.82 (brd, $J = 15.0$ Hz, 1H), 3.04 (td, $J = 2.5$ & 15.3 Hz, 1H), 2.44 (s, 3H), 2.11 (m, 2H), 1.86 (ddd, $J = 5.3$, 12.8 & 12.9 Hz, 1H), 1.70 (dd, $J = 4.8$ & 12.8 Hz, 1H), 1.53 (brs, 1H), 1.41 (m, 1H), 1.23 (brs, 10H), 0.89 (t, $J = 6.2$ Hz, 3H). ^{13}C NMR (CDCl_3 , 300 MHz) δ 143.1 (C), 138.0 (C), 129.6 (2CH), 126.7 (2CH), 54.5 (CH), 43.9 (CH), 40.9 (CH_2), 39.1 (CH_2), 36.0 (CH_2), 31.5 (CH_2), 29.8 (CH_2), 28.9 (2 CH_2), 26.1 (CH_2), 22.4 (CH_2), 21.3 (CH_3), 13.9 (CH_3). FTIR (CHCl_3): 2927.6, 2856.3, 1336.9, 1157.2, 934.0 cm^{-1} . Elemental analysis: $\text{C}_{19}\text{H}_{30}\text{BrNO}_2\text{S}$ calcd.: C 54.80 H 7.26 N 3.36; found: C 54.80 H 7.44 N 3.29.

trans-4-bromo-2-phenyl-1-tosylpiperidine (Table 1, entry 10). ^1H NMR (CDCl_3 , 300 MHz) δ 7.77 (d, $J = 8.1$ Hz, 2H), 7.32 (m, 7H), 5.35 (brd, $J = 4.2$ Hz, 1H), 4.01 (m, 1H), 3.90 (dt, $J = 2.3$ & 14.8 Hz, 1H), 3.04 (td, $J = 2.6$ & 15.2 Hz, 1H), 2.85 (brd, $J = 13.7$ Hz, 1H), 2.46 (s, 3H), 2.06 (m, 2H), 1.75 (dd, $J = 4.6$ & 12.5 Hz, 1H). ^{13}C NMR (CDCl_3 , 300 MHz) δ 143.6 (C), 137.9 (C), 137.2 (C), 129.9 (2CH), 128.9 (2CH), 127.4 (CH), 126.9 (2CH), 126.5 (2CH), 56.7 (CH), 43.7 (CH), 42.2 (CH_2), 38.5 (CH_2), 35.9 (CH_2), 21.5 (CH_3). FTIR (CHCl_3): 3029.3, 2928.8, 1338.8, 1157.8, 933.7 cm^{-1} . Elemental analysis: $\text{C}_{18}\text{H}_{20}\text{BrNO}_2\text{S}$ calcd.: C 54.83 H 5.11 N 3.55; found: C 54.80 H 5.15 N 3.52.

cis-4-bromo-2-phenyl-1-tosylpiperidine (Table 1, entry 10). ^1H NMR (CDCl_3 , 300 MHz) δ 7.51 (d, J = 8.2 Hz, 2H), 7.22 (m, 7H), 4.62 (t, J = 6.3 Hz, 1H), 4.16 (sep, J = 3.8 Hz, 1H), 3.88 (m, 1H), 3.42 (m, 1H), 2.50 (m, 1H), 2.41-2.34 (m, 4H), 2.20 (m, 1H), 2.05 (m, 1H). ^{13}C NMR (CDCl_3 , 300 MHz) δ 143.1 (C), 139.1 (C), 136.2 (C), 129.3 (CH), 127.9 (CH), 127.2 (CH), 127.0 (CH), 126.8 (CH), 58.5 (CH), 44.8 (CH), 42.5 (CH_2), 40.7 (CH_2), 34.6 (CH_2), 21.3 (CH_3). FTIR (CHCl_3): 3019.4, 2928.4, 1343.5, 1160.1, 935.6 cm^{-1} . Elemental analysis: $\text{C}_{18}\text{H}_{20}\text{BrNO}_2\text{S}$ calcd.: C 54.83 H 5.11 N 3.55; found: C 54.90 H 5.25 N 3.43.

trans-2-benzyl-4-bromo-1-tosylpiperidine (Table 1, entry 11). ^1H NMR (CDCl_3 , 300 MHz) δ 7.55 (d, J = 8.3 Hz, 2H), 7.27 (m, 5H), 7.11 (d, J = 6.2 Hz, 2H), 4.34 (m, 2H), 3.82 (brd, J = 13.4 Hz, 1H), 3.15 (td, J = 2.6 & 13.0 Hz, 1H), 2.79 (d, J = 8.0 Hz, 2H), 2.40 (s, 3H), 2.23 (m, 1H), 2.13 (dt, J = 2.1 & 13.3 Hz, 1H), 1.89 (ddd, J = 4.9, 12.1 & 17.3 Hz, 2H). ^{13}C NMR (CDCl_3 , 300 MHz) δ 143.1 (C), 137.3 (C), 137.3 (C), 129.5 (2CH), 128.8 (2CH), 128.6 (2CH), 126.8 (2CH), 126.6 (CH), 55.9 (CH), 43.3 (CH), 41.2 (CH_2), 37.7 (CH_2), 36.3 (CH_2), 36.2 (CH_2), 21.3 (CH_3). FTIR (CHCl_3): 3027.6, 2927.5, 1452.5, 1155.9, 937.9 cm^{-1} . Elemental analysis: $\text{C}_{19}\text{H}_{22}\text{BrNO}_2\text{S}$ calcd.: C 55.88 H 5.43 N 3.43; found: C 55.88 H 5.47 N 3.29.

4-bromo-1-tosylpiperidine (Table 1, entry 12). ^1H NMR (CDCl_3 , 300 MHz) δ 7.62 (d, J = 8.3 Hz, 2H), 7.31 (d, J = 8.0 Hz, 2H), 4.21 (qui, J = 3.3 Hz, 1H), 3.18 (m, 2H), 3.04 (m, 2H), 2.41 (s, 3H), 2.15 (m, 2H), 2.03 (m, 2H). ^{13}C NMR (CDCl_3 , 300 MHz) δ 143.6 (C), 133.0 (C), 129.7 (2CH), 127.4 (2CH), 47.7 (CH), 43.7 (2 CH_2), 34.6 (2 CH_2), 21.4 (CH_3). FTIR (CHCl_3): 2964.3, 2925.0, 1343.3, 1163.7, 929.3 cm^{-1} . Elemental analysis: $\text{C}_{12}\text{H}_{16}\text{BrNO}_2\text{S}$ calcd.: C 45.29 H 5.07 N 4.40; found: C 45.40 H 4.96 N 4.28.

4-chloro-2-cyclohexyl-1,2,5,6-tetrahydro-1-tosylpyridine (Table 3, entry 1). ^1H NMR (CDCl_3 , 300 MHz) δ 7.67 (d, J = 8.2 Hz, 2H), 7.26 (d, J = 8.1 Hz, 2H), 5.88 (brs, 1H), 4.12 (brs, 1H), 3.86 (dd, J = 5.1 & 14.0 Hz, 1H), 3.23 (m, 1H), 2.41 (s, 3H), 1.85 (m, 3H), 1.71 (m, 3H), 1.60 (m, 1H), 1.47 (m, 1H), 1.05 (m, 5H). ^{13}C NMR (CDCl_3 , 300 MHz) δ 143.2 (C), 137.8 (C), 129.6 (C), 129.4 (2CH), 126.7 (2CH), 123.7 (CH), 59.2 (CH), 42.6 (CH), 39.4 (CH_2), 30.0 (CH_2), 29.7 (CH_2), 29.5 (CH_2), 25.9 (CH_2), 25.8 (CH_2), 25.7 (CH_2), 21.3 (CH_3). FTIR (CHCl_3): 2928.2, 2853.1, 1339.1, 1161.1, 921.7 cm^{-1} . Elemental analysis: $\text{C}_{18}\text{H}_{24}\text{ClNO}_2\text{S}$ calcd.: C 61.09 H 6.84 N 3.96; found: C 61.33 H 6.80 N 3.78.

4-chloro-1,2,5,6-tetrahydro-2-isobutyl-1-tosylpyridine (Table 3, entry 2). ^1H NMR (CDCl_3 , 300 MHz) δ 7.70 (d, J = 8.2 Hz, 2H), 7.28 (d, J = 7.4 Hz, 2H), 5.77 (brs, 1H), 4.47 (brs, 1H), 3.88 (dd, J = 6.3 & 14.9 Hz, 1H), 3.23 (ddd, J = 5.0, 11.6 & 15.2 Hz, 1H), 2.43 (s, 3H), 2.05 (m, 1H), 1.91 (dd, J = 4.7 & 17.5 Hz, 1H), 1.75 (sep, J = 6.7 Hz, 1H), 1.49 (m, 1H), 1.33 (m, 1H), 0.95 (t, J = 6.0 Hz, 6H). ^{13}C NMR (CDCl_3 , 300 MHz) δ 143.5 (C), 138.0 (C), 129.6 (C), 129.6 (2CH), 127 (2CH), 125.3 (CH), 52.8 (CH), 43.6 (CH_2), 38.5 (CH_2), 30.5 (CH_2), 24.6 (CH), 22.7 (CH_3), 22.6 (CH_3), 21.5 (CH_3). FTIR (CHCl_3): 2957.1, 2869.9, 1338.9, 1158.2, 935.0 cm^{-1} . Elemental analysis: $\text{C}_{16}\text{H}_{22}\text{ClNO}_2\text{S}$ calcd.: C 58.61 H 6.76 N 4.27; found: C 58.83 H 7.08 N 4.29.

4-chloro-2-heptyl-1,2,5,6-tetrahydro-1-tosylpyridine (Table 3, entry 3). ^1H NMR (CDCl_3 , 300 MHz) δ 7.69 (d, J = 8.2 Hz, 2H), 7.27 (d, J = 6.7 Hz, 2H), 5.78 (brs, 1H), 4.37 (brs, 1H), 3.89 (dd, J = 6.2 & 14.7 Hz, 1H), 3.22 (ddd, J = 4.9, 11.6 & 16.3 Hz, 1H), 2.42 (s, 3H), 2.05 (m, 1H), 1.93 (dd, J = 4.7 & 17.4 Hz, 1H), 1.55 (m, 3H), 1.42-1.26 (m, 9H), 0.89 (t, J = 6.1 Hz, 3H). ^{13}C NMR (CDCl_3 ,

300 MHz) δ 143.4 (C), 137.9 (C), 129.7 (C), 129.6 (2CH), 126.9 (2CH), 125.4 (CH), 54.5 (CH), 38.8 (CH₂), 34.7 (CH₂), 31.7 (CH₂), 30.5 (CH₂), 29.2 (CH₂), 29.1 (CH₂), 26.0 (CH₂), 22.6 (CH₂), 21.4 (CH₃), 14.0 (CH₃). FTIR (CHCl₃): 2927.0, 2855.5, 1458.3, 1340.4, 1159.6 cm⁻¹. Elemental analysis: C₁₉H₂₈ClNO₂S calcd.: C 61.69 H 7.63 N 3.79; found: C 61.58 H 7.72 N 3.83.

4-chloro-2-phenyl-1,2,5,6-tetrahydro-1-tosylpyridine (Table 3, entry 4). ¹H NMR (CDCl₃, 300 MHz) δ 7.65 (d, *J* = 8.3 Hz, 2H), 7.31 (m, 7H), 6.00 (brs, 1H), 5.64 (brs, 1H), 3.79 (dd, *J* = 6.4 & 14.6 Hz, 1H), 3.12 (ddd, *J* = 4.8, 11.7 & 14.7 Hz, 1H), 2.42 (s, 3H), 2.26 (m, 1H), 2.06 (ddd, *J* = 0.9, 4.7 & 17.5 Hz, 1H). ¹³C NMR (CDCl₃, 300 MHz) δ 143.4 (C), 138.4 (C), 137.4 (C), 131.3 (C), 129.4 (2 CH), 128.3 (2 CH), 127.9 (2 CH), 126.9 (2 CH), 126.8 (CH), 123.0 (CH), 56.6 (CH), 38.6 (CH₂), 30.6 (CH₂), 21.3 (CH₃). FTIR (CHCl₃): 3062.1, 2924.9, 1339.9, 1160.6, 931.4 cm⁻¹. Elemental analysis: C₁₈H₁₈ClNO₂S calcd.: C 62.15 H 5.22 N 4.03; found: C 62.19 H 5.38 N 3.85.

2-benzyl-4-chloro-1,2,5,6-tetrahydro-1-tosylpyridine (Table 3, entry 5). ¹H NMR (CDCl₃, 300 MHz) δ 7.58 (d, *J* = 8.2 Hz, 2H), 7.26 (m, 7H), 5.68 (brs, 1H), 4.65 (m, 1H), 3.84 (dd, *J* = 6.1 & 14.5 Hz, 1H), 3.07 (m, 1H), 2.91 (ddd, *J* = 5.7, 13.1 & 18.8 Hz, 2H), 2.40 (s, 3H), 2.18 (m, 1H), 1.97 (dd, *J* = 3.9 & 17.3 Hz, 1H). ¹³C NMR (CDCl₃, 300 MHz) δ 143.3 (C), 137.4 (C), 136.5 (C), 130.2 (C), 129.5 (2CH), 129.3 (2CH), 128.3 (2CH), 126.7 (2CH), 126.6 (CH), 123.9 (CH), 55.4 (CH), 41.4 (CH₂), 38.9 (CH₂), 30.7 (CH₂), 21.3 (CH₃). FTIR (CHCl₃): 3028.6, 2925.4, 1339.2, 1158.7 cm⁻¹. Elemental analysis: C₁₉H₂₀ClNO₂S calcd.: C 63.06 H 5.57 N 3.87; found: C 63.03 H 5.53 N 3.89.

4-chloro-1,2,5,6-tetrahydro-1-tosylpyridine (Table 3, entry 6). ¹H NMR (CDCl₃, 400 MHz) δ 7.67 (d, *J* = 8.3 Hz, 2H), 7.33 (d, *J* = 8.0 Hz, 2H), 5.74 (brs, 1H), 3.64 (m, 2H), 3.27 (t, *J* = 5.7 Hz, 2H), 2.47 (m, 5H). ¹³C NMR (CDCl₃, 300 MHz) δ 143.9 (C), 133.2 (C), 129.9 (C), 129.8 (2CH), 127.6 (2CH), 119.8 (CH), 45.2 (CH₂), 43.3 (CH₂), 32.6 (CH₂), 21.5 (CH₃). FTIR (CHCl₃): 2920.5, 2853.9, 1335.8, 1161.3, 929.8 cm⁻¹. Elemental analysis: C₁₂H₁₄ClNO₂S calcd.: C 53.03 H 5.19 N 5.15; found: C 53.09 H 5.24 N 4.96.

4-bromo-2-cyclohexyl-1,2,5,6-tetrahydro-1-tosylpyridine (Table 3, entry 7). ¹H NMR (CDCl₃, 400 MHz) δ 7.69 (d, *J* = 8.2 Hz, 2H), 7.28 (d, *J* = 7.3 Hz, 2H), 6.13 (brs, 1H), 4.07 (brs, 1H), 3.85 (dd, *J* = 3.6 & 11.5 Hz, 1H), 3.26 (m, 1H), 2.43 (s, 3H), 1.98 (m, 3H), 1.77 (brd, *J* = 9.0 Hz, 3H), 1.54 (dd, *J* = 2.9 & 11.4 Hz, 1H), 1.26-1.04 (m, 6H). ¹³C NMR (CDCl₃, 300 MHz) δ 143.0 (C), 137.5 (C), 129.1 (2CH), 127.7 (CH), 126.5 (2CH), 118.7 (C), 59.9 (CH), 42.2 (CH), 39.7 (CH₂), 31.6 (CH₂), 29.7 (CH₂), 29.3 (CH), 25.6 (2CH₂), 25.4 (CH₂), 21.0 (CH₃). FTIR (CHCl₃): 2927.7, 2852.8, 1338.3, 1161.2, 906.1 cm⁻¹. Elemental analysis: C₁₈H₂₄BrNO₂S calcd.: C 54.27 H 6.07 N 3.52; found: C 54.30 H 6.18 N 3.33.

4-bromo-1,2,5,6-tetrahydro-2-isobutyl-1-tosylpyridine (Table 3, entry 8). ¹H NMR (CDCl₃, 400 MHz) δ 7.70 (d, *J* = 8.2 Hz, 2H), 7.28 (d, *J* = 8.0 Hz, 2H), 5.99 (brs, 1H), 4.43 (brs, 1H), 3.84 (dd, *J* = 6.1 & 14.7 Hz, 1H), 3.26 (ddd, *J* = 5.1, 11.5 & 16.2 Hz, 1H), 2.4 (s, 3H), 2.13 (m, 1H), 2.06 (m, 1H), 1.75 (sep, *J* = 6.8 Hz, 1H), 1.50 (m, 1H), 1.38 (m, 1H), 0.95 (t, *J* = 7.3 Hz, 6H). ¹³C NMR (CDCl₃, 300 MHz) δ 143.3 (C), 137.6 (C), 129.4 (2CH), 129.2 (C), 126.8 (2CH), 118.9 (CH), 53.7 (CH), 43.2 (CH₂), 38.9 (CH₂), 32.3 (CH₂), 24.4 (CH), 22.5 (CH₃), 22.0 (CH₃), 21.3 (CH₃). FTIR (CHCl₃): 2955.1, 2869.8, 1338.7, 1158.9, 909.2 cm⁻¹. Elemental analysis: C₁₆H₂₂BrNO₂S calcd.: C 51.61 H 5.96 N 3.76; found: C 51.61 H 5.79 N 3.76.

4-bromo-2-heptyl-1,2,5,6-tetrahydro-1-tosylpyridine (Table 3, entry 9). ^1H NMR (CDCl_3 , 400 MHz) δ 7.69 (d, J = 8.2 Hz, 2H), 7.27 (d, J = 9.6 Hz, 2H), 6.01 (brs, 1H), 4.32 (brs, 1H), 3.85 (dd, J = 6.0 & 14.7 Hz, 1H), 3.24 (ddd, J = 5.0, 11.4 & 16.1 Hz, 1H), 2.42 (s, 3H), 2.15 (m, 1H), 2.06 (dd, J = 4.7 & 18.5 Hz, 1H), 1.54 (m, 3H), 1.33 (m, 9H), 0.88 (t, J = 6.6 Hz, 3H). ^{13}C NMR (CDCl_3 , 300 MHz) δ 143.5 (C), 137.9 (C), 129.6 (2CH), 129.3 (C), 126.9 (2CH), 119.1 (C), 55.7 (CH), 39.4 (CH_2), 34.5 (CH_2), 32.7 (CH_2), 31.7 (CH_2), 29.3 (2 CH_2), 29.1 (CH_2), 26.0 (CH_2), 22.6 (CH_2), 21.5 (CH_3), 14.1 (CH_3). FTIR (CHCl_3): 2927.3, 2855.8, 1339.98, 1160.0, 1095.0 cm^{-1} . Elemental analysis: $\text{C}_{19}\text{H}_{28}\text{BrNO}_2\text{S}$ calcd.: C 55.07 H 6.81 N 3.38; found: C 55.26 H 7.07 N 3.36.

4-bromo-2-phenyl-1,2,5,6-tetrahydro-1-tosylpyridine (Table 3, entry 10). ^1H NMR (CDCl_3 , 300 MHz) δ 7.65 (d, J = 8.2 Hz, 2H), 7.31 (m, 7H), 6.22 (brs, 1H), 5.59 (brs, 1H), 3.75 (dd, J = 6.2 & 14.5 Hz, 1H), 3.14 (m, 1H), 2.42 (s, 3H), 2.34 (m, 1H), 2.19 (dd, J = 4.4 & 17.7 Hz, 1H). ^{13}C NMR (CDCl_3 , 300 MHz) δ 143.4 (C), 138.8 (C), 136.9 (C), 129.6 (C), 128.7 (2 CH), 128.3 (2 CH), 127.7 (2 CH), 127.0 (2 CH), 126.8 (CH), 124.7 (CH), 54.3 (CH), 42.1 (CH_2), 35.4 (CH_2), 21.3 (CH_3). FTIR (CHCl_3): 3061.0, 2923.0, 1344.0, 1160.9 cm^{-1} . Elemental analysis: $\text{C}_{18}\text{H}_{18}\text{BrNO}_2\text{S}$ calcd.: C 55.11 H 4.62 N 3.57; found: C 55.13 H 4.41 N 3.53.

2-benzyl-4-bromo-1,2,5,6-tetrahydro-1-tosylpyridine (Table 3, entry 11). ^1H NMR (CDCl_3 , 300 MHz) δ 7.57 (d, J = 8.3 Hz, 2H), 7.26 (m, 7H), 5.91 (brs, 1H), 4.60 (brs, 1H), 3.9 (dd, J = 6.0 & 14.5 Hz, 1H), 3.08 (td, J = 4.5 & 11.5 Hz, 1H), 2.96 (dd, J = 4.3 & 9.8 Hz, 1H), 2.86 (dd, J = 6.3 & 9.8 Hz, 1H), 2.40 (s, 3H), 2.27 (m, 1H), 2.11 (dd, J = 3.5 & 16.6 Hz, 1H). ^{13}C NMR (CDCl_3 , 300 MHz) δ 143.3 (C), 137.4 (C), 136.5 (C), 129.5 (2CH), 129.3 (2CH), 128.4 (2CH), 128.0 (CH), 126.7 (2CH), 126.6 (CH), 119.5 (C), 56.5 (CH), 41.2 (CH_2), 39.5 (CH_2), 32.9 (CH_2), 21.3 (CH_3). FTIR (CHCl_3): 3028.3, 2924.9, 1338.5, 1158.1, 1096.6 cm^{-1} . Elemental analysis: $\text{C}_{19}\text{H}_{20}\text{BrNO}_2\text{S}$ calcd.: C 56.16 H 4.96 N 3.45; found: C 56.17 H 5.07 N 3.52.

4-bromo-1,2,5,6-tetrahydro-1-tosylpyridine (Table 3, entry 12). ^1H NMR (CDCl_3 , 300 MHz) δ 7.66 (d, J = 8.2 Hz, 2H), 7.33 (d, J = 8.3 Hz, 2H), 5.95 (brs, 1H), 3.61 (dd, J = 2.7 & 5.6 Hz, 2H), 3.26 (t, J = 5.7 Hz, 2H), 2.57 (m, 2H), 2.44 (s, 3H). ^{13}C NMR (CDCl_3 , 300 MHz) δ 143.7 (C), 133.1 (C), 129.5 (2CH), 127.4 (2CH), 123.7 (CH), 118.9 (C), 46.1 (CH_2), 43.6 (CH_2), 34.5 (CH_2), 21.3 (CH_3). FTIR (CHCl_3): 2919.0, 2854.2, 1333.8, 1159.9, 919.5 cm^{-1} . Elemental analysis: $\text{C}_{12}\text{H}_{14}\text{BrNO}_2\text{S}$ calcd.: C 45.58 H 4.46 N 4.43; found: C 45.64 H 4.36 N 4.37.

6-(10-bromodecyl)-4-chloro-1-tosyl-1,2,3,6-tetrahydropyridine (7). To a stirred solution of 100 mg (0.45 mmol) of homopropargyl tosyl amine and 11-bromoundecanal³ (162.2 mg, 0.67 mmol) in dry CH_2Cl_2 (5 mL) was added anhydrous FeCl_3 (100 mg, 0.67 mmol) in one portion at room temperature. The reaction was completed in approximately 10 min, quenched by addition of water with stirring and extracted with CH_2Cl_2 . The combined organic layers were dried over magnesium sulphate, and the solvent was removed under reduced pressure. This crude reaction mixture was purified by flash silica gel column chromatography (EtOAc/n -hexane solvent systems) affording compound **7** as a pale yellow oil (175 mg, 0.36 mmol, 80%). ^1H NMR (CDCl_3 , 300 MHz) δ 7.68 (d, J = 8.2 Hz, 2H), 7.27 (d, J = 8.3 Hz, 2H), 5.77 (brs, 1H), 4.37 (brd, J = 5.7 Hz, 1H), 3.88 (dd, J = 6.1 & 14.6 Hz, 1H), 3.41 (t, J = 6.9 Hz, 2H), 3.22 (ddd, J = 4.8, 11.5 & 15.3 Hz, 1H), 2.42 (s, 3H), 2.03 (m, 1H), 1.95-1.80 (m, 3H), 1.55-1.27 (m, 16H). ^{13}C NMR (CDCl_3 , 300 MHz) δ 143.2 (C), 137.8 (C), 129.5 (C), 129.4 (2CH), 126.7

(3) J. E. Baldwin, R. M. Adlington, S. H. Ramcharitar, *Tetrahedron* **1992**, 48, 3413–3428.

(2CH), 124.9 (CH), 54.4 (CH), 38.6 (CH₂), 34.5 (CH₂), 33.8 (CH₂), 32.6 (CH₂), 30.3 (CH₂), 29.1 (3CH₂), 29.1 (CH₂), 28.5 (CH₂), 27.9 (CH₂), 25.8 (CH₂), 21.3 (CH₃). FTIR (CHCl₃): 2927.2, 2864.2, 1457.1, 1341.0, 1159.8 cm⁻¹. Elemental analysis: C₂₂H₃₃BrClNO₂S calcd.: C 53.82 H 6.78 N 2.85; found: C 53.84 H 6.87 N 2.69.

11-(4-chloro-1-tosyl-1,2,5,6-tetrahydropyridin-2-yl)undecanenitrile (8). To a stirring solution of the corresponding compound **9** (276 mg, 0.56 mmol) in dry DMSO (2 mL) was added NaCN (110 mg, 2.24 mmol) and the reaction mixture was stirred at 70 °C for 3 h. Then it was allowed to cool down to rt, and water was added to quench the reaction. The mixture was diluted with diethyl ether, the combined organic layers were dried over magnesium sulphate, and the solvent was removed under reduced pressure. This crude reaction mixture was purified by flash silica gel column chromatography (EtOAc/*n*-hexane solvent systems) affording compound **8** as a pale yellow oil (171.3 mg, 0.39 mmol, 70%) ¹H NMR (CDCl₃, 300 MHz) δ 7.68 (d, *J* = 8.2 Hz, 2H), 7.28 (d, *J* = 7.9 Hz, 2H), 5.76 (brs, 1H), 4.37 (m, 1H), 3.87 (dd, *J* = 6.0 & 14.7 Hz, 1H), 3.22 (ddd, *J* = 5.0, 11.4 & 16.1 Hz, 1H), 2.42 (s, 3H), 2.33 (t, *J* = 7.1 Hz, 2H), 2.08 (m, 1H), 1.91 (dd, *J* = 4.6 & 17.3 Hz, 1H), 1.68-1.27 (m, 18H). ¹³C NMR (CDCl₃, 300 MHz) δ 143.2 (C), 137.8 (C), 129.5 (C), 129.4 (2CH), 126.7 (2CH), 124.9 (CH), 119.6 (C), 54.4 (CH), 38.6 (CH₂), 34.5 (CH₂), 30.3 (CH₂), 29.1 (2CH₂), 29.0 (CH₂), 28.9 (3CH₂), 28.5 (CH₂), 28.4 (CH₂), 25.8 (CH₂), 25.81 (CH₂), 21.3 (CH₃), 16.9 (CH₂). FTIR (CHCl₃): 2925.3, 2862.2, 1457.1, 1339.1, 1158.5 cm⁻¹. Elemental analysis: C₂₃H₃₃ClN₂O₂S calcd.: C 63.21 H 7.61 N 6.41; found: C 63.28 H 7.62 N 6.37.

4-chloro-2-(10-(-4-chloro-1,2,5,6-tetrahydro-1-tosylpyridin-2-yl)decyl)-1,2,5,6-tetrahydro-1-tosylpyridine (10). A solution of the corresponding nitrile **8** (200 mg, 0.46 mmol) in dry THF (4.6 mL) was cooled to 0 °C, and DIBAL-H (1.37 mL, 1.37 mmol, 1M in cyclohexene) was added. The reaction mixture was stirred until TLC showed complete conversion of the substrate, quenched by the addition of 1 N HCl solution, and filtered through a Celite pad. The precipitate was thoroughly washed with EtOAc. The organic layer was washed with NaHCO₃ saturated solution and dried over MgSO₄ and the solvent was removed under reduced pressure. This crude reaction mixture was purified by flash silica gel column chromatography (EtOAc/*n*-hexane solvent systems) affording compound **9**. The crude obtained was used in the next reaction.

To a stirred solution of the corresponding crude of the aldehyde **9** and homopropargyl tosyl amine (70 mg, 0.307 mmol) in dry CH₂Cl₂ (10 mL) was added anhydrous FeCl₃ (76.2 mg, 0.46 mmol) in one portion at room temperature. The reaction was completed in approximately 10 min, quenched by addition of water with stirring and extracted with CH₂Cl₂. The combined organic layers were dried over magnesium sulphate, and the solvent was removed under reduced pressure. This crude reaction mixture was purified by flash silica gel column chromatography (EtOAc/*n*-hexane solvent systems) to afford compound **10** (178 mg, 0.262 mmol, 57%, 2 steps). ¹H NMR (CDCl₃, 300 MHz) δ 7.67 (d, *J* = 8.2 Hz, 4H), 7.26 (d, *J* = 8.0 Hz, 4H), 5.77 (brs, 2H), 4.36 (brs, 2H), 3.88 (dd, *J* = 6.0 & 14.7 Hz, 2H), 3.21 (ddd, *J* = 4.7, 11.5 & 15.9 Hz, 2H), 2.41 (s, 6H), 2.03 (m, 2H), 1.91 (dd, *J* = 4.4 & 17.4 Hz, 2H), 1.55-1.24 (m, 20H). ¹³C NMR (CDCl₃, 300 MHz) δ 143.2 (C), 137.8 (C), 129.5 (C), 129.4 (2CH), 126.7 (2CH), 124.9 (CH), 54.4 (CH), 38.6 (CH₂), 34.5 (CH₂), 33.8 (CH₂), 32.6 (CH₂), 30.3 (CH₂), 29.3 (3CH₂), 29.2 (2CH₂), 29.1 (3CH₂), 25.8 (CH₂), 21.3 (CH₃). FTIR (CHCl₃): 2926.7, 2854.1, 1339.7, 1159.3, 918.1 cm⁻¹. Elemental analysis: C₃₄H₄₆Cl₂N₂O₄S₂ calcd.: C 59.90 H 6.80 N 4.11; found: C 59.96 H 6.70 N 3.75.

Table 1, Entry 5

Crystal structure analysis:

Data reduction and cell parameters refinement were carried out with the programs COLLECT⁴ and DENZO.⁵ The structure was solved by direct methods using SIR97.⁶ Refinement was performed with SHELXL-97⁷ using full-matrix least squares with anisotropic thermal parameters for all non-H atoms, with the exception of the C16 methyl group. The hydrogen atoms were placed at calculated positions. The refinement converged at $R_1 = 0.0922$ and $wR_2 = 0.242$ with a goodness-of-fit of 1.10 for 3202 reflections with $F_o > 2\sigma(F_o)$ and 185 parameters. The largest peak and hole on the final difference map were 0.53 and $-0.43 \text{ e}/\text{\AA}^3$. The molecular graphics were computed with PLATON.⁸

X-Ray Crystallographic structures

a) X-Ray Crystallographic structure of **trans-2-benzyl-4-chloro-1-tosylpiperidine**. $\text{C}_{19}\text{H}_{22}\text{ClN}_2\text{O}_2\text{S}$, MW= 363.9, orthorhombic, space group $P2_1nb$, $a=7.613(2)$, $b=11.410(2)$, $c=21.452(4) \text{ \AA}$, $V=1863.4(7) \text{ \AA}^3$, $Z=4$, $\rho_c=1.30 \text{ gm.cm}^{-3}$, $F(000)=768.0$, $\mu (\text{Mo K}\alpha)= 0.33\text{mm}^{-1}$, $R=0.0362$, $R_w=0.1011$ and $S=1.01$ for 2123 observed reflections ($\Theta_{\text{max}}=27^\circ$, $I>2s(I)$ criterion and 218 parameters. Maximum and minimal residual in the final difference map: 0.18 and $0.16 \text{ e}/\text{\AA}^3$. Intensity data were collected at 293 °K on a Enraf-Nonius Kappa CCD diffractometer with graphite monochromated Mo $\text{K}\alpha$ radiation ($\lambda= 0.71070 \text{ \AA}$). Crystallographic data (excluding the structure factor tables) have been deposited with the Cambridge Crystallographic Data Center, deposition number 296770. Copies of the data can be obtained free of charge, on application to the CCDC Director: 12 Union Road, Cambridge, CB2, 1EZ, UK [Fax: 44-(0)1223-306033 or e-mail deposit@ccdc.cam.ac.uk].

⁴ Nonius Kappa CCD Server Software; Nonius, R.V.:Delft, The Netherlands, 1998.

⁵ Otwinowsky, Z.; Minor, W. In *Methods in Enymology, Macromolecular Crystallography Part A*; Carter, C. E.; Sweet, R.M. Eds.; Academic Press; University of Texas, Southwestern Medical Centre at Dallas, 1997; Vol.276, pp. 307-326.

⁶ Altomare, A.; Burla, M.C.; Camalli, M.; Cascarano, G.; Giacovazzo, C.; Guagliardi, A.R. *J. Appl. Crystallogr.* **1999**, 32, 115-119.

⁷ Sheldrick, G.M., *SHELXL-97 Program for the Refinement of Crystal Structures*; University of Göttingen: Göttingen, Germany, 1997.

⁸ Spek, A.L., *PLATON*, University of Utrecht, The Netherlands, 1992

X-Ray Crystallographic structures

a) X-Ray Crystallographic structure of ***trans*-4-chloro-2-isobutyl-1-tosylpiperidine**. $C_{16}H_{24}ClNO_2S$, mol. wt.= 329.9, monoclinic, space group $P2_1/c$, $a=7.974(2)$, $b=19.241(4)$, $c=12.584(3)$ Å, $V=1806.8(8)$ Å³, $Z=4$, $D_c=1.21$ g.cm⁻³, $F(000)=704$, $\mu=(Mo\ K_{\alpha})=0.33$ mm⁻¹. A single crystal of approximate dimensions 0.40x0.25x0.20 mm was used for all X-ray measurements. The intensity data of all reflections within the θ range 3.5-26.8° were measured at 293 °K in an Enraf-Nonius KappaCCD diffractometer, using graphite-monochromated $Mo\ K_{\alpha}(\lambda=0.7174\text{ Å})$ radiation. A total of 19502 reflections were collected. From 3729 unique, 3202 with $F_o > 2\sigma(F_o)$ were considered observed and used for structure solution and refinements. Crystallographic data, including atomic coordinates, have been deposited with the Cambridge Crystallographic Data Centre (deposit number CCDC 610469). Copies of the data can be obtained free of charge, on application to the Director, CCDC, 12 Union Road, Cambridge CB2 1EZ, UK [Fax: 44-(0)1223-306033 or e-mail: deposit@ccdc.cam.ac.uk]

“Ab initio” computational data

Optimized Structures using B3LYP/6-31G(d) with the Gaussian G03

Table 2**Table 2: Optimized structures (B3LYP/6-31G(d)) corresponding to the *N*-Sulfonyl-Iminium Intermediates.**Entry 1: R=Me *E*-iminium

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.395728	3.344858	-0.093069
2	1	0	0.789747	3.955277	-0.777788
3	1	0	1.463863	3.730306	0.933820
4	6	0	2.016475	2.238547	-0.498018
5	1	0	1.948210	1.892795	-1.546739
6	6	0	2.896967	1.429887	0.378102
7	1	0	3.962911	1.762537	0.219044
8	1	0	2.655523	1.596016	1.461437
9	6	0	2.856667	-0.060569	0.041831
10	1	0	3.691632	-0.580518	0.596362
11	1	0	3.050391	-0.188309	-1.066783
12	7	0	1.594363	-0.733662	0.342173
13	6	0	1.308039	-1.145891	1.547745
14	1	0	0.331459	-1.683086	1.669949
15	16	0	0.472562	-1.078684	-1.078791
16	8	0	1.005277	-0.333054	-2.115960
17	8	0	0.492269	-2.465393	-1.134480
18	6	0	-0.912052	-0.499735	-0.480588
19	6	0	-1.906116	-1.375091	0.011709
20	6	0	-1.220215	0.875482	-0.529465
21	6	0	-3.139189	-0.903561	0.426083
22	1	0	-1.698638	-2.462043	0.040298
23	6	0	-2.453620	1.353499	-0.115963
24	1	0	-0.459093	1.584770	-0.912758
25	6	0	-3.434079	0.470158	0.363072
26	1	0	-3.903256	-1.607500	0.796697
27	1	0	-2.672689	2.432913	-0.172122
28	6	0	2.112722	-1.019352	2.779553
29	1	0	1.448200	-0.696525	3.624915
30	1	0	2.528450	-2.032905	3.038413
31	1	0	2.962932	-0.297016	2.696405
32	6	0	-4.761386	0.970365	0.776239
33	1	0	-5.461998	0.933176	-0.099587
34	1	0	-5.194641	0.340945	1.593353
35	1	0	-4.704531	2.029738	1.130665

Entry 1: R=Me *Z*-iminium

Center	Atomic	Atomic	Coordinates (Angstroms)		
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Number	Number	Type	X	Y	Z
1	6	0	3.948373	2.652135	0.817273
2	1	0	3.878788	3.440057	1.581205
3	1	0	4.931953	2.166636	0.741867
4	6	0	2.920225	2.336289	0.031599
5	1	0	1.955677	2.865471	0.114692
6	6	0	2.997743	1.328193	-1.052986
7	1	0	3.108595	1.872011	-2.035906
8	1	0	3.905402	0.675685	-0.943609
9	6	0	1.740214	0.478080	-1.174837
10	1	0	1.819761	-0.124188	-2.133309
11	1	0	0.842737	1.163050	-1.251389
12	7	0	1.439758	-0.477346	-0.109525
13	6	0	2.160632	-0.534293	0.981873
14	16	0	0.020900	-1.563256	-0.527215
15	8	0	0.201126	-1.819099	-1.878146
16	8	0	0.141902	-2.594393	0.396401
17	6	0	-1.207992	-0.562434	-0.214241
18	6	0	-1.836659	-0.548928	1.048914
19	6	0	-1.749089	0.265367	-1.221254
20	6	0	-2.941679	0.248333	1.296244
21	1	0	-1.449954	-1.208161	1.848342
22	6	0	-2.854088	1.064798	-0.980808
23	1	0	-1.291621	0.254525	-2.228555
24	6	0	-3.468386	1.067252	0.283029
25	1	0	-3.419849	0.235541	2.290003
26	1	0	-3.263161	1.697166	-1.786631
27	6	0	-4.661373	1.901407	0.535586
28	1	0	-5.584454	1.320840	0.270985
29	1	0	-4.731766	2.193585	1.613052
30	1	0	-4.645210	2.830160	-0.087861
31	6	0	1.959025	-1.476519	2.106893
32	1	0	2.209898	-2.526940	1.784950
33	1	0	2.622847	-1.193575	2.962590
34	1	0	0.894613	-1.497055	2.461779
35	1	0	3.017149	0.178575	1.110166

Entry 2: R= Et E-iminium

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.336940	-3.051483	-1.574817
2	1	0	0.681431	-3.912751	-1.480363
3	1	0	1.384718	-2.584494	-2.556877
4	6	0	2.078053	-2.623600	-0.551023
5	1	0	2.017378	-3.132737	0.409989
6	6	0	3.061302	-1.486692	-0.637335
7	1	0	4.077074	-1.866573	-0.455945
8	1	0	3.064105	-1.061493	-1.647911
9	6	0	2.858473	-0.372460	0.407603
10	1	0	3.670997	0.358164	0.368937
11	1	0	2.833572	-0.795622	1.413190
12	7	0	1.583769	0.373893	0.234649

13	6	0	1.363644	1.287869	-0.640727
14	1	0	0.371696	1.743668	-0.611230
15	16	0	0.234589	0.067312	1.590202
16	8	0	0.610196	-1.254812	2.059851
17	8	0	0.343321	1.274485	2.392391
18	6	0	-1.269050	0.046044	0.672119
19	6	0	-2.113258	1.162959	0.746406
20	6	0	-1.618457	-1.105552	-0.047365
21	6	0	-3.330816	1.114433	0.075192
22	1	0	-1.832153	2.029606	1.335305
23	6	0	-2.839274	-1.120196	-0.709768
24	1	0	-0.952044	-1.960405	-0.084752
25	6	0	-3.715928	-0.020500	-0.657636
26	1	0	-3.999740	1.968172	0.131942
27	1	0	-3.126353	-2.005570	-1.269835
28	6	0	2.305936	1.816785	-1.666882
29	1	0	1.872646	1.570817	-2.647828
30	1	0	3.283200	1.333362	-1.611739
31	6	0	-5.054052	-0.075761	-1.346056
32	1	0	-5.789799	-0.578165	-0.704509
33	1	0	-5.437940	0.924636	-1.563926
34	1	0	-5.001429	-0.640619	-2.281792
35	6	0	2.434973	3.353021	-1.546965
36	1	0	3.083573	3.718571	-2.347148
37	1	0	1.463633	3.847733	-1.646344
38	1	0	2.876590	3.642872	-0.589334

Entry 2: R=Et Z-iminium

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	0.0000001031	-0.000000182	0.000001243
2	1	-0.0000000315	-0.000000222	0.000001988
3	1	-0.0000000139	-0.0000000314	0.000001628
4	6	-0.0000001269	0.000000156	0.000000576
5	1	-0.0000000251	-0.0000000602	0.000001605
6	6	0.0000003275	0.000002453	0.000003230
7	1	0.0000001092	0.000001226	0.000001029
8	1	0.0000000102	0.000000307	0.000000495
9	6	-0.0000001321	-0.000000417	0.000000579
10	1	0.0000000209	0.000000956	-0.000001322
11	1	0.0000000677	0.000001051	-0.000000520
12	7	-0.0000001230	0.000003129	0.000000856
13	6	0.0000002030	-0.000001858	-0.000000059
14	16	0.0000000614	-0.000005574	-0.000000028
15	8	0.0000001252	0.000001687	-0.000000189
16	8	0.0000000334	0.000002804	-0.000001975
17	6	-0.0000000678	0.000002167	0.000001650
18	6	0.0000000957	-0.000000448	-0.000002334
19	6	-0.0000000483	0.000000225	-0.000000539
20	6	0.0000000553	0.000004113	0.000000273
21	1	-0.0000000844	-0.000000935	-0.000000385
22	6	-0.0000001568	-0.000003267	-0.000003106
23	1	0.0000000157	0.000000576	-0.000000389

24	6	0.000000637	-0.000000067	0.000000983
25	1	-0.000000148	-0.000000862	-0.000000504
26	1	0.000000005	0.000001099	-0.000000007
27	6	0.000000137	0.000000498	-0.000000191
28	1	-0.000001164	0.000000556	-0.000004231
29	1	-0.000001744	-0.000003905	0.000000788
30	1	0.000001862	0.000001697	0.000001704
31	6	-0.000000906	0.000001254	0.000001796
32	1	0.000000163	-0.000000513	-0.000002216
33	1	-0.000000666	-0.000002572	-0.000001217
34	1	0.000000024	-0.000000268	-0.000000733
35	6	-0.000001418	-0.000001602	0.000000557
36	1	-0.000000624	-0.000001541	-0.000000681
37	1	0.000000355	-0.000000207	-0.000000316
38	1	-0.000000696	-0.000000597	-0.000000037

Entry 3: R=i-Pr E-iminium

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.294047	-2.643741	2.250641
2	1	0	-0.609846	-3.443103	2.471056
3	1	0	-1.469650	-1.932973	3.040680
4	6	0	-1.910608	-2.568131	1.086691
5	1	0	-1.720624	-3.312822	0.332242
6	6	0	-2.932750	-1.517997	0.743363
7	1	0	-3.901068	-1.993176	0.604974
8	1	0	-3.045649	-0.824383	1.569154
9	6	0	-2.668459	-0.763220	-0.561849
10	1	0	-3.473484	-0.081716	-0.791039
11	1	0	-2.572265	-1.449957	-1.385031
12	7	0	-1.407642	0.051786	-0.543338
13	6	0	-1.300239	1.191403	0.013593
14	1	0	-0.348101	1.684256	-0.093226
15	16	0	-0.060423	-0.519307	-1.604798
16	8	0	-0.318502	-1.907499	-1.697279
17	8	0	-0.150867	0.354275	-2.717133
18	6	0	1.384683	-0.190923	-0.688493
19	6	0	2.185953	0.883250	-1.061737
20	6	0	1.761149	-1.055948	0.337048
21	6	0	3.365024	1.103977	-0.376381
22	1	0	1.903016	1.515695	-1.881703
23	6	0	2.939579	-0.814467	1.007105
24	1	0	1.147798	-1.897241	0.595096
25	6	0	3.758919	0.263590	0.661842
26	1	0	3.991383	1.928100	-0.663581
27	1	0	3.239213	-1.476882	1.798384
28	6	0	-2.334234	1.952385	0.782857
29	1	0	-3.240662	1.372987	0.871666
30	6	0	5.065604	0.484464	1.380617
31	1	0	5.826451	-0.176712	0.977093
32	1	0	5.413981	1.502620	1.265146
33	1	0	4.971145	0.271052	2.438508

34	6	0	-1.784269	2.254882	2.188094
35	1	0	-2.525369	2.815263	2.743960
36	1	0	-1.565933	1.348192	2.741044
37	1	0	-0.881284	2.854108	2.139259
38	6	0	-2.636855	3.245662	-0.000920
39	1	0	-3.384282	3.813982	0.538340
40	1	0	-1.752518	3.865937	-0.099429
41	1	0	-3.023730	3.037849	-0.991998

Entry 3: R=i-Pr Z-iminium

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.770976	3.595910	0.561254
2	1	0	1.292329	4.099794	1.380787
3	1	0	2.846889	3.643058	0.533992
4	6	0	1.070339	2.988518	-0.377231
5	1	0	-0.007009	2.993849	-0.319480
6	6	0	1.662138	2.307662	-1.584207
7	1	0	1.418357	2.877374	-2.477374
8	1	0	2.745683	2.297331	-1.535875
9	6	0	1.089233	0.916781	-1.857182
10	1	0	1.540020	0.462727	-2.725889
11	1	0	0.030748	1.003080	-2.041101
12	7	0	1.227432	-0.072675	-0.730267
13	6	0	2.168147	0.021373	0.133070
14	16	0	0.059310	-1.424378	-0.839756
15	8	0	-0.019982	-1.620601	-2.239242
16	8	0	0.568536	-2.411860	0.037668
17	6	0	-1.418163	-0.729696	-0.228891
18	6	0	-1.640586	-0.683780	1.145830
19	6	0	-2.379933	-0.288400	-1.129519
20	6	0	-2.826848	-0.163570	1.611055
21	1	0	-0.912581	-1.068551	1.834694
22	6	0	-3.565228	0.228046	-0.640717
23	1	0	-2.215370	-0.369385	-2.187025
24	6	0	-3.806087	0.300017	0.727944
25	1	0	-3.007106	-0.129159	2.669867
26	1	0	-4.314313	0.564446	-1.333271
27	6	0	-5.114336	0.830753	1.257091
28	1	0	-5.767047	0.006630	1.528348
29	1	0	-4.960889	1.434872	2.143303
30	1	0	-5.626160	1.431665	0.516740
31	6	0	2.543702	-0.814027	1.322804
32	1	0	1.729855	-1.444557	1.629379
33	1	0	2.826868	0.853350	-0.030351
34	6	0	3.728586	-1.709057	0.899196
35	1	0	4.059740	-2.271269	1.763246
36	1	0	3.437250	-2.412863	0.130543
37	1	0	4.569158	-1.121445	0.543931
38	6	0	2.931929	0.136006	2.467192
39	1	0	3.197628	-0.452420	3.336502
40	1	0	3.789054	0.748981	2.207486
41	1	0	2.114256	0.791746	2.745968

Entry 4: R=s-Bu E-iminium

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.222946	2.828926	-2.437910
2	1	0	0.662994	3.402353	-2.696234
3	1	0	-0.560006	2.101347	-3.174106
4	6	0	-0.885557	3.043299	-1.299776
5	1	0	-0.526676	3.796274	-0.599412
6	6	0	-2.160039	2.338305	-0.918758
7	1	0	-2.978556	3.070066	-0.858265
8	1	0	-2.443582	1.618187	-1.695360
9	6	0	-2.136003	1.650663	0.459904
10	1	0	-3.122491	1.260610	0.723250
11	1	0	-1.838069	2.361413	1.232610
12	7	0	-1.176247	0.516820	0.540945
13	6	0	-1.378204	-0.670404	0.089762
14	1	0	-0.569050	-1.384385	0.259733
15	16	0	0.396153	0.820627	1.614170
16	8	0	0.493308	2.269738	1.568816
17	8	0	0.087787	0.067265	2.818943
18	6	0	1.679098	0.038410	0.691667
19	6	0	2.162805	-1.199249	1.137475
20	6	0	2.231971	0.698025	-0.414992
21	6	0	3.219774	-1.783011	0.446065
22	1	0	1.738753	-1.674130	2.015908
23	6	0	3.283880	0.087215	-1.085601
24	1	0	1.847182	1.659305	-0.736911
25	6	0	3.798543	-1.154295	-0.668498
26	1	0	3.610886	-2.737447	0.786193
27	1	0	3.724858	0.586913	-1.943510
28	6	0	-2.588293	-1.201304	-0.602247
29	1	0	-3.309678	-0.397672	-0.776725
30	6	0	4.968021	-1.776121	-1.385245
31	1	0	5.908132	-1.328111	-1.038020
32	1	0	5.029029	-2.852182	-1.201545
33	1	0	4.910820	-1.609747	-2.465505
34	6	0	-2.162453	-1.807953	-1.958032
35	1	0	-3.043013	-2.182373	-2.485275
36	1	0	-1.680701	-1.063479	-2.599872
37	1	0	-1.469572	-2.645366	-1.818608
38	6	0	-3.236766	-2.252085	0.354151
39	1	0	-2.529528	-3.076785	0.511636
40	1	0	-3.400997	-1.787285	1.334354
41	6	0	-4.569155	-2.796595	-0.174274
42	1	0	-4.445999	-3.365384	-1.100446
43	1	0	-5.009410	-3.469326	0.567952
44	1	0	-5.286860	-1.989539	-0.359393

Entry 4 R=s-Bu Z-iminium

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.384436	3.494474	-1.722502
2	1	0	-2.138615	3.775619	-2.742111
3	1	0	-3.442738	3.376624	-1.494851
4	6	0	-1.440128	3.342914	-0.792005
5	1	0	-0.394287	3.499788	-1.059997
6	6	0	-1.705904	3.016863	0.656647
7	1	0	-1.495358	3.904582	1.270463
8	1	0	-2.765974	2.789790	0.824754
9	6	0	-0.807540	1.929865	1.259504
10	1	0	-0.977934	1.843773	2.334484
11	1	0	0.245329	2.193906	1.115105
12	7	0	-0.960179	0.549653	0.704611
13	6	0	-1.860166	0.223061	-0.162115
14	16	0	0.268528	-0.681891	1.520331
15	8	0	0.433583	-0.066339	2.825490
16	8	0	-0.344591	-1.984138	1.320190
17	6	0	1.719752	-0.482595	0.538427
18	6	0	1.900974	-1.288708	-0.593519
19	6	0	2.680971	0.454532	0.939546
20	6	0	3.064396	-1.133801	-1.336774
21	1	0	1.165155	-2.036818	-0.867992
22	6	0	3.835525	0.587534	0.175118
23	1	0	2.541019	1.039891	1.841979
24	6	0	4.048131	-0.197711	-0.969817
25	1	0	3.221011	-1.758635	-2.211449
26	1	0	4.591989	1.304624	0.480372
27	6	0	5.318062	-0.070464	-1.769345
28	1	0	6.029766	-0.854787	-1.480533
29	1	0	5.129401	-0.184035	-2.841458
30	1	0	5.805639	0.893825	-1.602528
31	6	0	-2.175928	-1.089400	-0.798108
32	1	0	-1.371664	-1.807637	-0.645060
33	1	0	-2.500317	1.044876	-0.481542
34	6	0	-3.450606	-1.644658	-0.080931
35	1	0	-3.237408	-1.716344	0.991271
36	1	0	-4.276332	-0.930854	-0.201764
37	6	0	-2.391752	-0.849421	-2.307647
38	1	0	-2.594278	-1.800597	-2.805329
39	1	0	-3.242402	-0.183294	-2.491906
40	1	0	-1.505433	-0.410834	-2.777878
41	6	0	-3.870533	-3.022991	-0.603560
42	1	0	-4.717602	-3.392124	-0.017154
43	1	0	-4.184879	-2.992591	-1.650924
44	1	0	-3.056145	-3.749233	-0.506462

Entry 5: R=CH₂Ph E-iminium

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.161164	2.951988	-2.232903
2	6	0	1.555749	3.431240	-1.144744

3	6	0	0.062183	3.498252	-0.969101
4	6	0	-0.468159	2.797590	0.296752
5	7	0	-0.219988	1.331637	0.296341
6	6	0	-0.878871	0.459695	-0.383256
7	16	0	1.074201	0.707866	1.577199
8	8	0	1.923717	1.878800	1.715328
9	8	0	0.226209	0.196541	2.641472
10	6	0	1.888629	-0.603584	0.726349
11	6	0	1.563170	-1.924732	1.063120
12	6	0	2.882602	-0.298866	-0.214328
13	6	0	2.251950	-2.955472	0.431392
14	6	0	3.549483	-1.350727	-0.829608
15	6	0	3.252710	-2.690352	-0.517792
16	6	0	-2.067288	0.691267	-1.260233
17	6	0	4.017939	-3.813800	-1.166277
18	6	0	-4.552494	-2.201856	-0.985209
19	6	0	-5.230957	-1.874001	0.190806
20	6	0	-4.890079	-0.716806	0.893888
21	6	0	-3.870938	0.110673	0.422988
22	6	0	-3.191465	-0.211091	-0.760359
23	6	0	-3.531942	-1.376661	-1.457410
24	1	0	1.600947	2.557601	-3.078750
25	1	0	3.242515	2.971209	-2.336282
26	1	0	2.152416	3.835859	-0.328389
27	1	0	-0.444053	3.104101	-1.858312
28	1	0	-0.251034	4.547569	-0.871048
29	1	0	0.024586	3.195519	1.185304
30	1	0	-1.544840	2.950206	0.411527
31	1	0	-0.561200	-0.577253	-0.269864
32	1	0	0.809195	-2.133180	1.814804
33	1	0	3.123896	0.731091	-0.453063
34	1	0	2.016422	-3.983993	0.688833
35	1	0	4.324296	-1.131417	-1.558729
36	1	0	-1.785595	0.404517	-2.282402
37	1	0	-2.361778	1.742948	-1.281046
38	1	0	4.272529	-3.579164	-2.204407
39	1	0	4.961168	-3.988537	-0.632397
40	1	0	3.453099	-4.749940	-1.149118
41	1	0	-4.822261	-3.095763	-1.539529
42	1	0	-6.026940	-2.516141	0.555594
43	1	0	-5.417986	-0.456071	1.806137
44	1	0	-3.617849	1.014992	0.972310
45	1	0	-3.014565	-1.630736	-2.379600

Entry 5: CH₂Ph Z-iminium

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.099656	-2.517097	0.357315
2	6	0	3.569355	-2.523214	-0.869742
3	6	0	2.236831	-3.127045	-1.215354
4	6	0	1.161121	-2.072455	-1.566208
5	7	0	0.836291	-1.210831	-0.397559
6	6	0	1.601324	-0.209861	-0.097457

7	16	0	-0.540421	-1.872662	0.745122
8	8	0	-0.695574	-3.218811	0.219955
9	8	0	-0.049062	-1.579913	2.081618
10	6	0	-1.936200	-0.874137	0.332197
11	6	0	-2.311668	0.167446	1.189941
12	6	0	-2.675648	-1.187350	-0.816179
13	6	0	-3.440827	0.914613	0.870369
14	6	0	-3.795944	-0.420392	-1.112773
15	6	0	-4.198502	0.638663	-0.280442
16	6	0	-5.439789	1.432187	-0.593271
17	6	0	1.508982	0.767083	1.028423
18	6	0	1.637349	2.173301	0.454950
19	6	0	2.847217	2.872283	0.539263
20	6	0	2.958244	4.152078	-0.005143
21	6	0	1.863972	4.738782	-0.644394
22	6	0	0.655915	4.044672	-0.735256
23	6	0	0.543207	2.765036	-0.191159
24	1	0	3.594427	-2.981418	1.202045
25	1	0	5.076864	-2.084880	0.553917
26	1	0	4.123285	-2.069946	-1.693567
27	1	0	1.865768	-3.757047	-0.401234
28	1	0	2.327848	-3.768995	-2.101296
29	1	0	1.495699	-1.408354	-2.368714
30	1	0	0.241460	-2.562259	-1.884100
31	1	0	2.407418	-0.019983	-0.805543
32	1	0	-1.754735	0.365669	2.099250
33	1	0	-2.397454	-2.024203	-1.447707
34	1	0	-3.747713	1.717529	1.534423
35	1	0	-4.378089	-0.655524	-1.999102
36	1	0	-5.632024	1.470644	-1.669399
37	1	0	-6.315757	0.968520	-0.121026
38	1	0	-5.369704	2.456070	-0.214798
39	1	0	2.355683	0.551495	1.695559
40	1	0	0.604783	0.636168	1.620517
41	1	0	3.699640	2.424975	1.045153
42	1	0	3.896520	4.692563	0.076302
43	1	0	1.951068	5.735939	-1.065334
44	1	0	-0.198825	4.500375	-1.226462
45	1	0	-0.403932	2.233327	-0.250986

Table 2: Optimized structures (B3LYP/6-31G(d)) corresponding to trans- and cis-2-Alkyl-4-choro-1-tosylpiperidines

Entry 1: R=Me Trans

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.771847	0.252160	-1.261261
2	6	0	-1.960445	-1.046170	-1.131077
3	6	0	-1.209505	-0.407917	1.176944
4	6	0	-2.025655	0.900294	1.062474
5	6	0	-3.215666	0.736279	0.116966
6	7	0	-0.846416	-0.823465	-0.197343
7	6	0	-1.916860	-1.499442	1.997913

8	17	0	-4.114265	2.326170	-0.029972
9	16	0	0.574099	-1.712726	-0.400074
10	8	0	0.752194	-2.682087	0.690834
11	8	0	0.575680	-2.159017	-1.797555
12	6	0	1.838826	-0.454970	-0.189280
13	6	0	2.713639	-0.532834	0.891843
14	6	0	1.960063	0.564917	-1.138718
15	6	0	3.713041	0.433254	1.029067
16	6	0	2.961266	1.516776	-0.987139
17	6	0	3.852578	1.468824	0.098992
18	6	0	4.934446	2.511936	0.245825
19	1	0	-3.641510	0.080873	-1.904696
20	1	0	-2.150525	1.022246	-1.732317
21	1	0	-2.607548	-1.870497	-0.795578
22	1	0	-1.542284	-1.332359	-2.096448
23	1	0	-0.271123	-0.157348	1.683838
24	1	0	-2.370831	1.205738	2.055778
25	1	0	-1.375216	1.692409	0.675610
26	1	0	-3.954272	0.049996	0.538914
27	1	0	-2.116341	-1.130330	3.010539
28	1	0	-1.283455	-2.386282	2.068509
29	1	0	-2.875670	-1.795786	1.560017
30	1	0	2.612562	-1.343161	1.605708
31	1	0	1.282488	0.604046	-1.985528
32	1	0	4.396200	0.375483	1.872626
33	1	0	3.058322	2.310313	-1.724382
34	1	0	4.508135	3.520656	0.307473
35	1	0	5.533090	2.344641	1.146066
36	1	0	5.613529	2.502521	-0.615544

Entry 1: R=Me Cis

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.018791	0.121265	-1.236611
2	6	0	1.950009	1.183389	-0.967865
3	6	0	1.361028	0.174371	1.215162
4	6	0	2.466839	-0.880290	0.988864
5	6	0	3.582948	-0.367926	0.088672
6	7	0	0.866024	0.619029	-0.123883
7	17	0	4.829771	-1.680983	-0.180722
8	16	0	-0.537969	1.613080	-0.140656
9	8	0	-0.632229	2.415619	1.088734
10	8	0	-0.541305	2.282542	-1.447024
11	6	0	-1.881301	0.424045	-0.132949
12	6	0	-2.951343	0.628329	0.735273
13	6	0	-1.898802	-0.621165	-1.061003
14	6	0	-4.044931	-0.237421	0.681504
15	6	0	-2.994702	-1.476302	-1.097255
16	6	0	-4.085291	-1.299327	-0.229111
17	6	0	-5.268025	-2.236280	-0.286849
18	1	0	3.808751	0.552493	-1.860765
19	1	0	2.577355	-0.719275	-1.783810
20	1	0	2.407606	2.060147	-0.480781

21	1	0	1.510332	1.521510	-1.904967
22	1	0	2.872513	-1.173589	1.962832
23	1	0	2.017462	-1.771566	0.534834
24	1	0	4.133770	0.437128	0.584355
25	1	0	-2.921069	1.448923	1.444205
26	1	0	-1.059484	-0.767253	-1.732482
27	1	0	-4.879589	-0.082436	1.360465
28	1	0	-3.007383	-2.295362	-1.812518
29	1	0	-4.961389	-3.275096	-0.114089
30	1	0	-6.020453	-1.978765	0.464322
31	1	0	-5.751412	-2.203508	-1.270965
32	6	0	0.282244	-0.437849	2.114109
33	1	0	-0.470688	0.293287	2.409604
34	1	0	-0.210843	-1.282310	1.622378
35	1	0	0.762051	-0.808004	3.026626
36	1	0	1.795200	1.043575	1.735384

Entry 2: R=Et Trans

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.497008	0.774598	-1.505797
2	6	0	-1.777316	-0.577983	-1.618348
3	6	0	-1.210924	-0.544648	0.829415
4	6	0	-1.933078	0.818092	0.955620
5	6	0	-3.036992	0.965143	-0.090961
6	7	0	-0.747769	-0.663159	-0.572430
7	6	0	-2.039404	-1.758220	1.309241
8	17	0	-3.825068	2.612298	0.067373
9	16	0	0.661468	-1.537415	-0.873916
10	8	0	0.739361	-2.719327	-0.003308
11	8	0	0.747822	-1.677266	-2.331838
12	6	0	1.945519	-0.406916	-0.327232
13	6	0	2.693216	-0.708133	0.808886
14	6	0	2.205154	0.749065	-1.070739
15	6	0	3.702572	0.169237	1.211673
16	6	0	3.214968	1.609461	-0.656692
17	6	0	3.978414	1.336462	0.491687
18	6	0	5.072093	2.283153	0.924819
19	1	0	-3.311730	0.822118	-2.236403
20	1	0	-1.791379	1.581367	-1.734235
21	1	0	-2.499225	-1.404206	-1.535829
22	1	0	-1.286287	-0.670429	-2.587273
23	1	0	-0.310883	-0.490939	1.453322
24	1	0	-2.348381	0.932288	1.961137
25	1	0	-1.199429	1.618258	0.808473
26	1	0	-3.850391	0.260768	0.101138
27	1	0	-1.479591	-2.659267	1.042111
28	1	0	-2.993859	-1.807756	0.770124
29	1	0	2.491064	-1.621466	1.357922
30	1	0	1.629589	0.961230	-1.965979
31	1	0	4.287106	-0.063736	2.098123
32	1	0	3.420065	2.507566	-1.234624
33	1	0	4.675465	3.287649	1.116517

34	1	0	5.563760	1.936185	1.838392
35	1	0	5.839751	2.384044	0.147818
36	6	0	-2.306248	-1.755469	2.819434
37	1	0	-2.939249	-0.917619	3.133090
38	1	0	-2.814150	-2.678100	3.119935
39	1	0	-1.368464	-1.696588	3.385688

Entry 2: R=Et cis

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.929548	0.659802	-1.352057
2	6	0	1.872561	1.562520	-0.712014
3	6	0	1.354004	-0.111677	1.043450
4	6	0	2.452728	-1.018124	0.443645
5	6	0	3.535875	-0.227646	-0.277985
6	7	0	0.816691	0.741169	-0.065774
7	17	0	4.772169	-1.370715	-0.998934
8	16	0	-0.600172	1.663494	0.249594
9	8	0	-0.690590	2.035124	1.670469
10	8	0	-0.633370	2.714559	-0.774864
11	6	0	-1.928682	0.512646	-0.111535
12	6	0	-3.015515	0.455716	0.758308
13	6	0	-1.922199	-0.221208	-1.300899
14	6	0	-4.101765	-0.359485	0.436493
15	6	0	-3.011424	-1.031478	-1.602957
16	6	0	-4.118532	-1.114149	-0.741951
17	6	0	-5.291799	-1.999679	-1.087632
18	1	0	3.697375	1.280185	-1.826544
19	1	0	2.467767	0.040012	-2.128743
20	1	0	2.347975	2.232402	0.023158
21	1	0	1.402040	2.187702	-1.468982
22	1	0	2.906294	-1.607566	1.244293
23	1	0	1.985984	-1.716986	-0.261070
24	1	0	4.104571	0.377455	0.434358
25	1	0	-3.003368	1.036244	1.674669
26	1	0	-1.069108	-0.167314	-1.968625
27	1	0	-4.949516	-0.407643	1.115199
28	1	0	-3.004908	-1.609920	-2.523862
29	1	0	-4.987647	-3.050998	-1.162902
30	1	0	-6.080699	-1.932631	-0.332685
31	1	0	-5.727126	-1.721291	-2.054968
32	6	0	0.285362	-0.977408	1.739005
33	1	0	-0.503157	-0.329567	2.125144
34	1	0	-0.174504	-1.645307	1.000128
35	1	0	1.806764	0.547730	1.802769
36	6	0	0.833656	-1.795403	2.916901
37	1	0	0.007585	-2.276667	3.450987
38	1	0	1.521209	-2.586804	2.601985
39	1	0	1.360275	-1.154975	3.635019

Entry 3: R=iPr trans

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.159264	1.488403	-1.579399
2	6	0	-1.235575	-0.021620	-1.843999
3	6	0	-1.486910	-0.491203	0.660545
4	6	0	-1.580658	1.046946	0.862093
5	6	0	-2.031664	1.819677	-0.376600
6	7	0	-0.887836	-0.814458	-0.657308
7	6	0	-2.772867	-1.320539	0.947434
8	6	0	-4.016798	-0.951180	0.125783
9	6	0	-3.103993	-1.303313	2.449720
10	17	0	-1.973843	3.619429	-0.022390
11	16	0	0.460387	-1.815035	-0.696088
12	8	0	0.254167	-2.828684	0.342725
13	8	0	0.669767	-2.171968	-2.102384
14	6	0	1.873536	-0.827832	-0.181014
15	6	0	2.272074	-0.833231	1.156756
16	6	0	2.554756	-0.050948	-1.123123
17	6	0	3.346277	-0.035973	1.552144
18	6	0	3.624627	0.738344	-0.710304
19	6	0	4.033063	0.766570	0.632245
20	6	0	5.179102	1.646637	1.070311
21	1	0	-1.499128	2.035649	-2.465354
22	1	0	-0.123786	1.785686	-1.375819
23	1	0	-2.249552	-0.288975	-2.167070
24	1	0	-0.567312	-0.314650	-2.654539
25	1	0	-0.769869	-0.841522	1.407859
26	1	0	-2.244889	1.267207	1.703058
27	1	0	-0.585847	1.416521	1.136684
28	1	0	-3.080947	1.626987	-0.608343
29	1	0	-2.490124	-2.347406	0.686049
30	1	0	-3.840364	-1.017165	-0.952059
31	1	0	-4.834869	-1.642113	0.360600
32	1	0	-4.376015	0.059321	0.357705
33	1	0	-3.430491	-0.312539	2.789798
34	1	0	-2.240439	-1.601529	3.056003
35	1	0	1.766231	-1.478087	1.867320
36	1	0	2.267816	-0.091235	-2.168767
37	1	0	3.662309	-0.047660	2.592354
38	1	0	4.160776	1.334343	-1.445002
39	1	0	5.981717	1.659346	0.325046
40	1	0	4.848054	2.684519	1.207425
41	1	0	5.603097	1.309272	2.021137
42	1	0	-3.918088	-2.003713	2.666816

Entry 3 R=iPr cis

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.905378	-1.441560	-0.758416
2	6	0	1.546573	-1.246539	-1.453274
3	6	0	1.297368	1.018475	-0.537536

4	6	0	2.624191	0.876976	0.246470
5	6	0	3.552417	-0.085574	-0.497212
6	7	0	0.653224	-0.323954	-0.715867
7	17	0	5.119745	-0.297209	0.431205
8	16	0	-0.176691	-1.046842	0.596397
9	8	0	-0.053065	-2.498042	0.407841
10	8	0	0.218201	-0.429041	1.871174
11	6	0	-1.898547	-0.624856	0.311146
12	6	0	-2.537220	-1.075545	-0.848530
13	6	0	-2.602448	0.073687	1.288354
14	6	0	-3.886810	-0.797799	-1.031294
15	6	0	-3.958727	0.341354	1.089328
16	6	0	-4.619916	-0.084055	-0.067497
17	6	0	-6.085937	0.206144	-0.283358
18	1	0	3.558358	-2.062033	-1.382716
19	1	0	2.751974	-1.972183	0.187324
20	1	0	1.680064	-0.806438	-2.449901
21	1	0	1.045410	-2.205863	-1.575797
22	1	0	3.121095	1.846900	0.330857
23	1	0	2.423094	0.509467	1.256883
24	1	0	3.863876	0.365480	-1.445281
25	1	0	-1.983648	-1.635003	-1.595697
26	1	0	-2.093875	0.396064	2.190434
27	1	0	-4.384655	-1.143432	-1.934233
28	1	0	-4.509791	0.887339	1.850836
29	1	0	-6.512424	0.762846	0.556301
30	1	0	-6.243985	0.797329	-1.193734
31	1	0	-6.660908	-0.720797	-0.398418
32	6	0	0.323960	2.122887	-0.053937
33	1	0	-0.157108	1.785725	0.869345
34	6	0	1.060971	3.433616	0.269837
35	1	0	1.720429	3.340095	1.137618
36	1	0	1.662276	3.778244	-0.581999
37	6	0	-0.754191	2.389450	-1.118451
38	1	0	-1.263159	1.473734	-1.428369
39	1	0	-1.509489	3.084547	-0.734822
40	1	0	-0.306956	2.846247	-2.011472
41	1	0	1.562553	1.297699	-1.569300
42	1	0	0.332233	4.220435	0.494463

Entry 4 R=s-Bu trans

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.530448	1.940038	-1.520514
2	6	0	-0.794565	0.516767	-2.031352
3	6	0	-1.386263	-0.267200	0.334848
4	6	0	-1.271603	1.220770	0.769771
5	6	0	-1.473002	2.227966	-0.360620
6	7	0	-0.707324	-0.492439	-0.965443
7	6	0	-2.800632	-0.916899	0.389322
8	6	0	-3.847484	-0.314890	-0.559597
9	6	0	-3.314664	-0.962836	1.846904

10	6	0	-4.454634	-1.962950	2.077662
11	17	0	-1.194748	3.924404	0.282314
12	16	0	0.503206	-1.656763	-1.033051
13	8	0	0.053542	-2.770184	-0.192174
14	8	0	0.827122	-1.833572	-2.451710
15	6	0	1.960500	-0.962714	-0.237921
16	6	0	2.189608	-1.196108	1.119357
17	6	0	2.846889	-0.180813	-0.984635
18	6	0	3.302154	-0.619959	1.732430
19	6	0	3.953325	0.384499	-0.356323
20	6	0	4.194873	0.183663	1.011518
21	6	0	5.383149	0.825665	1.686549
22	1	0	-0.686643	2.656966	-2.333892
23	1	0	0.507726	2.035993	-1.181502
24	1	0	-1.792497	0.468679	-2.483955
25	1	0	-0.087747	0.242123	-2.815256
26	1	0	-0.809577	-0.829264	1.074302
27	1	0	-1.975539	1.420398	1.582580
28	1	0	-0.264496	1.379814	1.172921
29	1	0	-2.507955	2.240936	-0.708401
30	1	0	-2.623729	-1.953627	0.073990
31	1	0	-3.515142	-0.338961	-1.601352
32	1	0	-4.779904	-0.886929	-0.513321
33	1	0	-4.093755	0.721593	-0.296578
34	1	0	-3.646183	0.037511	2.159735
35	1	0	-2.480363	-1.230066	2.510806
36	1	0	-4.739909	-1.988529	3.135351
37	1	0	-4.152348	-2.976592	1.788631
38	1	0	-5.351919	-1.705618	1.504330
39	1	0	1.522875	-1.846432	1.675402
40	1	0	2.685105	-0.045984	-2.049013
41	1	0	3.485158	-0.808916	2.787377
42	1	0	4.648465	0.983383	-0.939860
43	1	0	6.260206	0.833977	1.030572
44	1	0	5.167793	1.868919	1.952865
45	1	0	5.652536	0.301114	2.608540

Entry 4 R=s-Bu cis

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.157024	2.041704	-1.685250
2	6	0	-0.707913	0.933821	-2.314380
3	6	0	-1.830307	0.457954	-0.179828
4	6	0	-0.939744	1.498782	0.544541
5	6	0	-0.531916	2.593571	-0.442829
6	7	0	-1.089011	-0.116225	-1.348806
7	17	0	0.547545	3.823350	0.388122
8	16	0	-0.095017	-1.493725	-1.302464
9	8	0	-0.840154	-2.552339	-0.619242
10	8	0	0.371764	-1.666053	-2.682054
11	6	0	1.375837	-1.187066	-0.303799
12	6	0	1.360179	-1.461600	1.065463
13	6	0	2.534161	-0.704373	-0.917634

14	6	0	2.503960	-1.217976	1.823816
15	6	0	3.668960	-0.467969	-0.144519
16	6	0	3.670915	-0.708539	1.236826
17	6	0	4.894204	-0.415775	2.071502
18	1	0	0.324953	2.841678	-2.415127
19	1	0	1.136701	1.638772	-1.408553
20	1	0	-1.645570	1.358347	-2.697641
21	1	0	-0.199188	0.466008	-3.156543
22	1	0	-1.485139	1.963311	1.368888
23	1	0	-0.049384	1.019728	0.965087
24	1	0	-1.417296	3.168624	-0.732127
25	1	0	0.474526	-1.888421	1.523903
26	1	0	2.550462	-0.546520	-1.990754
27	1	0	2.493007	-1.438360	2.888460
28	1	0	4.572257	-0.099632	-0.624522
29	1	0	5.813948	-0.531070	1.488984
30	1	0	4.873419	0.615678	2.447528
31	1	0	4.955282	-1.078305	2.940934
32	6	0	-2.568810	-0.574710	0.714095
33	1	0	-1.849980	-1.312145	1.083367
34	6	0	-3.207924	0.109927	1.943880
35	1	0	-2.423129	0.556984	2.565043
36	1	0	-3.850077	0.939889	1.610894
37	6	0	-3.626802	-1.312947	-0.125273
38	1	0	-3.199006	-1.694850	-1.052801
39	1	0	-4.037335	-2.166860	0.420926
40	1	0	-4.459138	-0.639913	-0.373867
41	6	0	-4.027286	-0.835797	2.831564
42	1	0	-4.358034	-0.317525	3.738582
43	1	0	-4.919944	-1.211420	2.322293
44	1	0	-3.431099	-1.702668	3.142712
45	1	0	-2.635259	1.027994	-0.671361

Entry 5 R=CH₂Ph trans

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.188215	-1.557977	-1.258032
2	6	0	1.740819	-1.036649	-1.307139
3	6	0	2.201700	0.626175	0.498847
4	6	0	3.671540	0.137915	0.544907
5	6	0	4.118751	-0.439828	-0.797151
6	7	0	1.306048	-0.419573	-0.042800
7	6	0	2.031173	1.952648	-0.283310
8	17	0	5.839473	-1.058006	-0.667647
9	16	0	0.558394	-1.466350	1.067337
10	8	0	1.174243	-2.801796	1.019301
11	8	0	0.487126	-0.732413	2.336332
12	6	0	-1.092095	-1.623673	0.382735
13	6	0	-1.547493	-2.880053	-0.011825
14	6	0	-1.916966	-0.497227	0.298798
15	6	0	-2.846256	-3.006120	-0.508587
16	6	0	-3.206741	-0.644019	-0.198498
17	6	0	-3.692994	-1.896913	-0.609613

18	6	0	-5.100807	-2.034330	-1.138495
19	6	0	0.628086	2.520056	-0.238326
20	6	0	0.086811	2.998055	0.964452
21	6	0	-1.207097	3.517016	1.012020
22	6	0	-1.984375	3.573103	-0.148192
23	6	0	-1.456331	3.105419	-1.352098
24	6	0	-0.161761	2.583059	-1.392441
25	1	0	3.485894	-1.919285	-2.248782
26	1	0	3.244385	-2.398163	-0.559031
27	1	0	1.631339	-0.280926	-2.095230
28	1	0	1.053077	-1.848283	-1.557231
29	1	0	1.875698	0.803119	1.525095
30	1	0	4.329155	0.962314	0.841912
31	1	0	3.757802	-0.641732	1.310264
32	1	0	4.177448	0.344045	-1.557500
33	1	0	2.339404	1.828379	-1.327922
34	1	0	2.736135	2.670491	0.157236
35	1	0	-0.892408	-3.740140	0.074850
36	1	0	-1.554028	0.475320	0.613353
37	1	0	-3.204791	-3.984363	-0.818838
38	1	0	-3.848651	0.230679	-0.270452
39	1	0	-5.281590	-1.346886	-1.973546
40	1	0	-5.300385	-3.051112	-1.489748
41	1	0	-5.839473	-1.797856	-0.362419
42	1	0	0.682615	2.964443	1.873841
43	1	0	-1.606457	3.883106	1.954150
44	1	0	-2.989752	3.984363	-0.113404
45	1	0	-2.049304	3.148145	-2.262060
46	1	0	0.242079	2.223315	-2.336332

Entry 5 R=CH₂Ph cis

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.545079	-3.214738	0.242042
2	6	0	0.581239	-2.756438	-0.854146
3	6	0	1.047199	-0.367287	-0.398533
4	6	0	2.058604	-0.808504	0.681706
5	6	0	2.649939	-2.182203	0.397845
6	7	0	-0.000248	-1.430644	-0.513295
7	17	0	3.799390	-2.663031	1.739402
8	16	0	-1.370405	-1.076220	-1.493070
9	8	0	-1.027747	-0.113964	-2.553333
10	8	0	-1.957907	-2.371410	-1.855982
11	6	0	-2.492648	-0.268528	-0.348931
12	6	0	-3.179063	0.869039	-0.777951
13	6	0	-2.752976	-0.834705	0.899129
14	6	0	-4.124513	1.448782	0.064526
15	6	0	-3.699660	-0.238394	1.729997
16	6	0	-4.399554	0.908134	1.329189
17	6	0	-5.424472	1.552232	2.232059
18	6	0	0.487294	1.028512	-0.028627
19	6	0	3.052176	3.674625	1.020540

20	6	0	2.078608	2.675496	1.085673
21	6	0	1.547146	2.111985	-0.081238
22	6	0	2.010118	2.580571	-1.320133
23	6	0	2.984050	3.576429	-1.389162
24	6	0	3.509685	4.126318	-0.217630
25	1	0	1.957536	-4.193208	-0.026298
26	1	0	1.005820	-3.324047	1.189743
27	1	0	1.109272	-2.711932	-1.820752
28	1	0	-0.235728	-3.468332	-0.959921
29	1	0	1.565814	-0.280335	-1.366272
30	1	0	2.852549	-0.059850	0.744607
31	1	0	1.547695	-0.834236	1.652013
32	1	0	3.272781	-2.153612	-0.501231
33	1	0	-2.963958	1.291619	-1.753683
34	1	0	-2.212230	-1.718256	1.220880
35	1	0	-4.657156	2.337353	-0.265912
36	1	0	-3.898739	-0.672073	2.706719
37	1	0	-5.527996	1.007048	3.174855
38	1	0	-6.410293	1.584551	1.752571
39	1	0	-5.149135	2.586790	2.470789
40	1	0	-0.304489	1.298768	-0.728581
41	1	0	0.040402	0.979944	0.970830
42	1	0	3.450563	4.099894	1.938018
43	1	0	1.724043	2.331469	2.054827
44	1	0	1.592881	2.166578	-2.235678
45	1	0	3.328116	3.928172	-2.358327
46	1	0	4.266549	4.904299	-0.270443