NaHSO$_3$-Promoted Ring Opening of Aziridines and Epoxides with H$_2$O

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Supporting Information

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1. General Information

$^1$H NMR spectra were taken with a Bruker AVANCE III 600 MHz NMR spectrometers. The chemical shifts are reported in ppm downfield to the CDCl$_3$ resonance ($\delta = 7.27$) and $d_6$-DMSO ($\delta = 2.50$). Spectra are reported as follows: chemical shift ($\delta$ ppm), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet), coupling constants (Hz), integration, and assignment. $^{13}$C NMR data were collected at 150 MHz with complete proton decoupling. The chemical shifts are reported in ppm downfield to the central CDCl$_3$ resonance ($\delta = 77.0$) and $d_6$-DMSO ($\delta = 39.5$). Coupling constants in $^1$H NMR spectra are given in Hz.

High-resolution mass spectra were performed on a micrTOF-Q II instrument with an ESI source. Melting points were measured with a RD-II melting point apparatus and are uncorrected. A variety of aziridines were synthesized from the corresponding alkenes according the literatures$^{[1-2]}$. The commercially available reagents were used without further purification. All solvents were purchased from commercial sources and used without further purification. Deuterated solvents were purchased from aladdin. All reactions were performed under atmosphere using oven-dried glassware. Column chromatography was performed on silica gel (200-300 mesh).

2. General procedure for the ring openings of aziridines

A glass test tube was charged with N-tosylaziridines 1 (0.2 mmol), NaHSO$_3$ (41.9 mg, 2.0 equiv.), acetone (1.5 mL) and H$_2$O (1.5 mL). The reaction mixture was stirred under air atmosphere at the specified temperature for a period of time. After completion of the reaction, as indicated by TLC, the reaction mixture was evaporated under vacuum. Subsequently, the remainder was extracted with CH$_2$Cl$_2$ (2×5 mL) and the NaHSO$_3$ was filtered. The combined organic layers were dried over anhydrous Na$_2$SO$_4$ and concentrated under vacuum. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate to afford 3 or 4.

3. Screening of the reaction condition

Subsequently, the effect of the amount of NaHSO$_3$ was investigated. Trace product was detected in the absence of NaHSO$_3$ (Table 1, entry 1). With the increase of its amount, the yield improved gradually (Table 1, entries 2-4) and the best yield was obtained when 2.0 equiv of NaHSO$_3$ was used (Table 1, entry 4). Screening of the volume of mixture solvent revealed that higher amount led to higher yield (Table 1,
entry 9 vs. 4, 6-8). The best 70% yield was obtained when 3.0 mL of mixture solvent was utilized, which was probably due to the solubility and ionization of NaHSO₃ (Table 1, entry 9). It was also found that the reaction temperature had a significant influence on the reaction rate. The yield rose following the increase of the temperature and the most suitable temperature was 55 °C (Table 1, entry 12). At last, extensive screening showed that the optimal reaction conditions were 0.2 mmol N-tosylcyclohexylaziridine 1a and 2.0 equiv of NaHSO₃ in 3.0 mL of acetone/H₂O (1:1) mixture system under air atmosphere at 55 °C for 24 h, which provided the ring-opening product with the quantitative transformation and 100% regioselectivity (Table 1, entry 12).

**Table 1.** Screening of reaction conditions for ring opening of N-tosylcyclohexylaziridine 1a with H₂O

<table>
<thead>
<tr>
<th>Entry</th>
<th>Solvent</th>
<th>Amount of NaHSO₃ (equiv.)</th>
<th>Solvent dosage (mL)</th>
<th>T (°C)</th>
<th>Yield (%)</th>
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<td>1</td>
<td>Acetone/H₂O=1:1</td>
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<tr>
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<td>35</td>
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<tr>
<td>7</td>
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* Unless otherwise noted, all reactions were carried out with N-tosylcyclohexylaziridine 1a (50 mg, 0.2 mmol) and NaHSO₃ under identified conditions for 24 h. * Isolated yield.

3. Characterization of products

**trans-2-(N-Tosylamino)-1-cyclohexanol 3a**[^3]

White solid; mp 128-130 °C; ¹H NMR (600 MHz, CDCl₃): δ 1.21-1.26 (m, 4H), 1.57-1.59 (m, 1H), 1.64-1.67 (m, 1H), 1.72-1.74 (m, 1H), 1.99-2.02 (m, 1H), 2.43 (s, 3H).
3H), 2.68 (d, J = 3.2 Hz, 1H), 2.84-2.88 (m, 1H), 3.28-3.32 (m, 1H), 5.02 (d, J = 7.1 Hz, 1H), 7.32 (d, J = 8.0 Hz, 2H), 7.80 (d, J = 8.3 Hz, 2H) ppm; IR (neat): 3481, 3273, 2934, 2861, 1519, 1450, 1322, 1283, 1156 cm⁻¹.

2-(N-Tosylamino)-1-phenyl-1-ethanol 3b [4-5]

White solid; mp 109-111 °C; ¹H NMR (600 MHz, CDCl₃): δ 2.41 (s, 3H), 2.69 (br, 1H), 3.01 (dd, J = 12.7, 9.1 Hz, 1H), 3.22 (d, J = 12.0 Hz, 1H), 4.79 (dd, J = 8.8, 3.5 Hz, 1H), 5.32 (brs, 1H), 7.26-7.32 (m, 7H), 7.72 (d, J = 8.3 Hz, 2H) ppm; IR (neat): 3402, 3169, 2921, 2856, 1588, 1486, 1442, 1318, 1151 cm⁻¹.

2-(N-Tosylamino)-1-(2-methylphenyl)-1-ethanol 3c

White solid; mp 116-118 °C; ¹H NMR (600 MHz, CDCl₃): δ 2.20 (s, 3H), 2.38 (s, 3H), 2.88-2.93 (m, 1H), 3.11-3.15 (m, 1H), 3.31 (br, 1H), 4.99 (dd, J = 9.2, 2.8 Hz, 1H), 5.76 (brs, 1H), 7.06 (dd, J = 5.3, 3.6 Hz, 1H), 7.12 (dd, J = 5.6, 3.4 Hz, 1H), 7.24 (d, J = 8.2 Hz, 2H), 7.36 (dd, J = 5.5, 2.7 Hz, 1H), 7.71 (d, J = 8.3 Hz, 2H) ppm; ¹³C NMR (150 MHz, CDCl₃): δ 18.9, 21.5, 49.2, 69.7, 125.4, 126.3, 127.1, 127.8, 129.8, 130.4, 134.6, 136.8, 139.0, 143.5 ppm; MS (ESI): Calcd for C₁₆H₁₉NO₃S [M + Na⁺] 328.0983, Found 328.0980; IR (neat): 3448, 3145, 2929, 2865, 1609, 1493, 1260, 1217 cm⁻¹.

2-(N-Tosylamino)-1-(3-methylphenyl)-1-ethanol 3d

White solid; mp 97-99 °C; ¹H NMR (600 MHz, CDCl₃): δ 2.30 (s, 3H), 2.40 (s, 3H), 2.98-3.02 (m, 1H), 3.12 (br, 1H), 3.17-3.22 (m, 1H), 4.74 (dd, J = 8.8, 3.0 Hz, 1H), 5.45 (br, 1H), 7.04-7.07 (m, 3H), 7.18 (td, J = 7.8, 1.4 Hz, 1H), 7.26 (dd, J = 8.5, 0.6 Hz, 2H), 7.71 (d, J = 8.3 Hz, 2H) ppm; ¹³C NMR (150 MHz, CDCl₃): δ 21.4, 21.5, 50.3, 72.8, 122.9, 126.6, 127.1, 128.5, 128.9, 129.8, 136.8, 138.3, 140.9, 143.5 ppm; MS (ESI): Calcd for C₁₆H₁₉NO₃S [M + Na⁺] 328.0983, Found 328.0981; IR (neat): 3513, 3281, 3032, 2924, 2870, 1601, 1493, 1330, 1158 cm⁻¹.

2-(N-Tosylamino)-1-(4-methylphenyl)-1-ethanol 3e
2-(N-Tosylamino)-1-(2-chlorophenyl)-1-ethanol 3f

White solid; mp 105-107 °C; $^1$H NMR (600 MHz, CDCl$_3$): $\delta$ 2.40 (s, 3H), 2.93-2.98 (m, 1H), 3.25 (d, $J = 4.0$ Hz, 1H), 3.33-3.37 (m, 1H), 5.14-5.17 (m, 1H), 5.44 (dd, $J = 7.6$, 5.0 Hz, 1H), 7.18 (td, $J = 7.6$, 1.7 Hz, 1H), 7.23 (dd, $J = 7.6$, 1.3 Hz, 1H), 7.25-7.27 (m, 3H), 7.52 (dd, $J = 7.6$, 1.7 Hz, 1H), 7.73 (d, $J = 8.3$ Hz, 1H) ppm; $^{13}$C NMR (150 MHz, CDCl$_3$): $\delta$ 21.5, 48.4, 69.5, 127.2, 127.5, 129.1, 129.4, 129.8, 131.6, 136.6, 138.2, 143.6 ppm; MS (ESI): Calcd for C$_{18}$H$_{17}$ClNO$_3$S [M + Na$^+$] 348.0437, Found 348.0433; IR (neat): 3502, 3281, 3064, 2929, 2854, 1601, 1498, 1331, 1158 cm$^{-1}$.

2-(N-Tosylamino)-1-(3-chlorophenyl)-1-ethanol 3g

White solid; mp 126-129 °C; $^1$H NMR (600 MHz, CDCl$_3$): $\delta$ 2.41 (s, 3H), 2.95-2.99 (m, 1H), 3.16-3.20 (m, 1H), 4.79 (dd, $J = 8.6$, 3.4 Hz, 1H), 5.41 (dd, $J = 7.4$, 5.2 Hz, 1H), 7.19 (d, $J = 8.5$ Hz, 2H), 7.25 (dd, $J = 6.5$, 1.8 Hz, 2H), 7.27 (d, $J = 8.6$ Hz, 2H), 7.69 (J = 8.3 Hz, 2H) ppm; IR (neat): 3428, 3314, 2942, 2861, 1598, 1486, 1335, 1156 cm$^{-1}$.

2-(N-Tosylamino)-1-(4-chlorophenyl)-1-ethanol 3h

White solid; mp 135-137 °C; $^1$HNMR (600 MHz, CDCl$_3$): $\delta$ 2.39 (s, 3H), 2.94-2.97 (m, 1H), 3.15-3.18 (m, 1H), 3.34 (br, 1H), 4.76-4.79 (m, 1H), 5.65 (br, 1H), 7.12-7.26 (m, 6H), 7.68 (dd, $J = 8.2$, 6.5 Hz, 2H); IR(neat): 3502, 3286, 3070, 2924, 2854, 1601, 1493, 1325, 1158 cm$^{-1}$.

2-(N-Tosylamino)-1-(2-methoxyphenyl)-1-ethanol 3i
Colorless liquid; $^1$H NMR (600 MHz, CDCl$_3$): $\delta$ 2.41 (s, 3H), 3.02 (br, 1H), 3.04-3.09 (m, 1H), 3.78 (s, 3H), 4.94 (dd, $J = 8.4, 3.5$ Hz, 1H), 5.16 (dd, $J = 8.0, 4.3$ Hz, 1H), 6.82 (d, $J = 7.4$ Hz, 1H), 6.93 (t, $J = 7.4$ Hz, 1H), 7.24 (td, $J = 7.9, 1.7$ Hz, 1H), 7.27 (d, $J = 7.9$ Hz, 3H), 7.72 (d, $J = 8.3$ Hz, 2H) ppm; $^{13}$C NMR (150 MHz, CDCl$_3$): $\delta$ 21.5, 48.4, 55.3, 69.1, 110.4, 120.9, 127.0, 128.6, 129.1, 129.7, 137.0, 143.4, 156.2 ppm; MS (ESI): Calcd for C$_{16}$H$_{19}$NO$_4$S [M + Na$^+$] 344.0932, Found 344.0928; IR (neat): 3502, 3286, 3064, 2924, 2853, 1601, 1493, 1325, 1158 cm$^{-1}$.

2-(N-Tosylamino)-1-(3-methoxyphenyl)-1-ethanol 3j

White solid; mp 125-127 °C; $^1$H NMR (600 MHz, CDCl$_3$): $\delta$ 2.39 (s, 3H), 2.62 (br, 1H), 3.09-3.13 (m, 1H), 3.31-3.35 (m, 1H), 4.96 (dd, $J = 8.4, 3.6$ Hz, 1H), 5.17 (br, 1H), 7.23 (d, $J = 8.0$ Hz, 2H), 7.35 (dd, $J = 8.5, 1.6$ Hz, 1H), 7.46-7.49 (m, 2H), 7.70 (d, $J = 8.3$ Hz, 2H), 7.74 (s, 1H), 7.77-7.81 (m, 3H) ppm; IR (neat): 3465, 3313, 2951, 2839, 1601, 1489, 1331, 1147 cm$^{-1}$.

2-(N-Tosylamino)-1-(Naphthalene-2-yl)-1-ethanol 3k

White solid; mp 160-162 °C; $^1$H NMR (600 MHz, $d_6$-DMSO): $\delta$ 2.31 (s, 3H), 2.86-2.90 (m, 1H), 3.08 (m, 1H), 3.39 (s, 1H), 5.38-5.39 (m, 1H), 5.71 (d, $J = 4.1$ Hz, 1H), 7.31 (d, $J = 8.0$ Hz, 2H), 7.46-7.49 (m, 2H), 7.64 (d, $J = 7.1$ Hz, 1H), 7.68 (d, $J = 8.2$ Hz, 2H), 7.80 (d, $J = 8.1$ Hz, 1H), 7.84 (s, 1H), 7.90 (d, $J = 7.9$ Hz, 1H), 8.01 (d, $J = 8.3$ Hz, 1H); $^{13}$C NMR (150 MHz, DMSO-$d_6$): $\delta$ 21.4, 50.4, 69.3, 123.3, 124.0, 129.3, 131.4, 142.6, 143.6, 147.5, 152.7, 160.5 ppm; MS (ESI): Calcd for C$_{16}$H$_{19}$NO$_4$S [M + Na$^+$] 344.0932, Found 344.0930; IR (neat): 3465, 3313, 2951, 2839, 1601, 1489, 1331, 1147 cm$^{-1}$.

2-(N-Tosylamino)-1-(Naphthalene-1-yl)-1-ethanol 3l

White solid; mp 160-162 °C; $^1$H NMR (600 MHz, $d_6$-DMSO): $\delta$ 2.31 (s, 3H), 2.86-2.90 (m, 1H), 3.08 (m, 1H), 3.39 (s, 1H), 5.38-5.39 (m, 1H), 5.71 (d, $J = 4.1$ Hz, 1H), 7.31 (d, $J = 8.0$ Hz, 2H), 7.46-7.49 (m, 2H), 7.64 (d, $J = 7.1$ Hz, 1H), 7.68 (d, $J = 8.2$ Hz, 2H), 7.80 (d, $J = 8.1$ Hz, 1H), 7.84 (s, 1H), 7.90 (d, $J = 7.9$ Hz, 1H), 8.01 (d, $J = 8.3$ Hz, 1H); $^{13}$C NMR (150 MHz, DMSO-$d_6$): $\delta$ 21.4, 50.4, 69.3, 123.3, 124.0, 129.3, 131.4, 142.6, 143.6, 147.5, 152.7, 160.5 ppm; MS (ESI): Calcd for C$_{16}$H$_{19}$NO$_4$S [M + Na$^+$] 344.0932, Found 344.0930; IR (neat): 3465, 3313, 2951, 2839, 1601, 1489, 1331, 1147 cm$^{-1}$.
125.9, 126.0, 126.5, 127.0, 128.1, 129.2, 130.0, 130.4, 133.7, 138.1, 139.1, 143.0 ppm; MS (ESI): Calcd for C_{19}H_{19}NO_{3}S [M + Na^+] 364.0983, Found 364.0979; IR (neat): 3416, 3183, 3064, 2940, 2919, 2854, 1601, 1493, 1320, 1142 cm⁻¹.

2-(N-Tosylamino)-1-(4-bromophenyl)-1-ethanol 3m

![Image](image_url)

White solid; mp 145-147 °C; \(^1H\) NMR (600 MHz, CDCl₃): \(\delta\) 2.42 (s, 3H), 2.93 (br, 1H), 2.95-3.00 (m, 1H), 3.18-3.22 (m, 1H), 4.78 (dd, \(J = 8.5, 3.4\) Hz, 1H), 5.24 (m, 1H), 7.15 (d, \(J = 8.4\) Hz, 2H), 7.28 (d, \(J = 8.1\) Hz, 2H), 7.42 (d, \(J = 8.4\) Hz, 2H), 7.69 (d, \(J = 8.3\) Hz, 2H) ppm; IR (neat): 3524, 3243, 3048, 2924, 2854, 1601, 1493, 1320, 1158 cm⁻¹.

Trans- 2-(N-Tosylamino)-1-cyclopentanol 3o[^7-8]

![Image](image_url)

White solid; mp 86-88 °C; \(^1H\) NMR (600 MHz, CDCl₃): \(\delta\) 1.28-1.35 (m, 1H), 1.45-1.60 (m, 3H), 1.78-1.84 (m, 1H), 2.40 (s, 3H), 3.06 (br, 1H), 3.22 (dd, \(J = 8.0, 6.2\) Hz, 1H), 4.01 (q, \(J = 6.8\) Hz, 1H), 5.64 (br, 1H), 7.28 (d, \(J = 8.3\) Hz, 2H), 7.77 (d, \(J = 8.3\) Hz, 2H) ppm; IR (neat): 3465, 3186, 3067, 2951, 2843, 2854, 1612, 1599, 1510, 1493, 1261, 1127 cm⁻¹.

2-(N-Tosylamino)octan-1-ol 3p

![Image](image_url)

Colorless liquid; \(^1H\) NMR (600 MHz, CDCl₃): \(\delta\) 0.82-0.88 (m, 3H), 1.08-1.09 (m, 3H), 1.16-1.19 (m, 1H), 1.24-1.27 (m, 2H), 1.32-1.34 (m, 1H), 1.39-1.43 (m, 1H), 1.77 (s, 2H), 2.43 (s, 3H), 3.22 (br, 1H), 3.47-3.50 (m, 1H), 3.56-3.58 (m, 1H), 4.69 (d, \(J = 7.6\) Hz, 1H), 5.30 (s, 1H), 7.31 (d, \(J = 8.2\) Hz, 2H), 7.77 (d, \(J = 8.2\) Hz, 2H) ppm; IR (neat): 3507, 3286, 2950, 2919, 2854, 1601, 1514, 1330, 1158 cm⁻¹.

2-(N-Tosylamino) hexadecan-1-ol 3q

![Image](image_url)

White solid; mp 43-45 °C; \(^1H\) NMR (600 MHz, CDCl₃): \(\delta\) 0.86-0.90 (m, 3H), 1.16-1.28 (m, 24H), 1.38-1.45 (m, 3H), 1.66 (s, 1H), 2.43 (s, 3H), 2.86 (d, \(J = 6.4\) Hz, 2H), 4.91 (t, \(J = 6.4\) Hz, 1H), 7.31 (d, \(J = 8.0\) Hz, 2H), 7.75 (d, \(J = 8.3\) Hz, 2H) ppm; \(^13C\) NMR (150 MHz, CDCl₃): \(\delta\) 14.0, 14.1, 21.5, 23.1, 23.3, 25.5, 29.3, 29.5, 29.7, 30.1, 31.7, 31.9, 36.5, 36.8, 50.3, 73.9, 73.9, 73.9, 73.9, 73.9, 73.9.
137.1, 129.7, 136.8, 143.3 ppm; MS (ESI): Calcd for C12H30NO3S [M + Na+] 434.2705, Found 434.2703; IR (neat): 3443, 3145, 2962, 2929, 2865, 1601, 1493, 1320, 1153 cm⁻¹.

**trans-1,2-Cyclohexanediol 3r**

White solid; mp 103-104 °C; ¹H NMR (600 MHz, CDCl₃): δ 1.25-1.27 (m, 4H), 1.17 (s, 2H), 1.97-1.98 (m, 2H), 2.21 (br, 2H), 3.36 (s, 2H) ppm; IR (neat): 3369, 3271, 2933, 2869, 2627, 1606, 1468, 1364 cm⁻¹.

**octane-1,2-diol**

¹H NMR (600 MHz, CDCl₃): δ 0.87-0.90 (t, 3H), 1.28-1.44 (m, 10H), 2.82 (s, 2H), 3.41-3.44 (m, 1H), 3.63-3.70 (m, 2H) ppm.

**hexane-1,2-diol**

¹H NMR (600 MHz, CDCl₃): δ 0.89-0.93 (t, 3H), 1.31-1.44 (m, 6H), 2.97 (s, 2H), 3.40-3.45 (m, 1H), 3.63-3.70 (m, 2H) ppm.

**(R)-3-(benzyloxy)propane-1,2-diol**

¹H NMR (600 MHz, CDCl₃): δ 2.34 (s, 1H), 2.81 (s, 1H), 3.52-3.59 (m, 2H), 3.61-3.72 (m, 2H), 3.88-3.92 (m, 1H), 4.55 (s, 2H), 7.30-7.36 (m, 5H) ppm.

**1-Phenyl-1, 2-ethanediol 3s**

White solid; mp 66-67 °C; ¹H NMR (600 MHz, CDCl₃): δ 3.01 (brs, 2H), 3.62-3.65 (m, 1H), 3.73 (s, 1H), 4.79 (s, 1H), 7.27-7.36 (m, 5H) ppm; IR (neat): 3316, 3204, 3085, 3062, 2966, 1636, 1490 cm⁻¹.

**ethyl 2,3-dihydroxy-3-phenylpropanoate**

¹H NMR (600 MHz, CDCl₃): δ 1.14-1.16 (t, 3H), 2.95-2.97 (d, 1H), 3.26-3.27 (d, 1H), 4.11-4.12 (d, 1H), 4.24-4.25 (d, 2H), 4.90-5.10 (d, 1H), 7.29-7.40 (m, 5H) ppm.
4. Reference


5. NMR spectrum of products
Display Report

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<td>Set End Plate Offset</td>
<td>-500 V</td>
<td>Set Dry Gas</td>
<td>6.0 l/min</td>
</tr>
<tr>
<td>Scan End</td>
<td>700 m/z</td>
<td>Set Collision Cell RF</td>
<td>150.0 Vpp</td>
<td>Set Dilute Valve</td>
<td>Source</td>
</tr>
</tbody>
</table>

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**Diagram:**

![Chemical Structure](image)

**Chemical Structure:**
- MeO
- OH
- NHTs
Display Report

Analysis Info
Analysis Name: D:\Date\Chang-Hong\long20110815-4.d
Method: tune_low.m
Sample Name: 
Comment: 

Acquisition Parameter
Source Type: ESI
Focus: Not active
Scan Begin: 50 m/z
Scan End: 700 m/z

Ionization: Positive
Set Capillary: 4000 V
Set End Plate Offset: -500 V
Set Collision Cell RF: 150.0 Vpp
Set Nebulizer: 0.8 L/min
Set Dry Heater: 180 °C
Set Dry Gas: 5.0 L/min
Set Divert Valve: Source

Intens. x10^5

364.0679

OH  NHTs

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