ELECTRONIC SUPPLEMENTARY INFORMATION

Protic onium salts-catalyzed synthesis of 5-aryl-2-oxazolidinones from aziridines and CO\textsubscript{2} under mild conditions

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1. General experimental methods

Caution

Experiments using compressed gases CO\(_2\) are potentially hazardous and must only be carried out by using the appropriate equipment and under rigorous safety precautions.

Materials

Aziridines and ionic liquids were synthesized according to the published procedures.\(^1\) CO\(_2\) with a purity of 99.99% was commercially available. The other organic and inorganic compounds from Tianjin Guangfu Fine Chemical Research Institute were used without further purification except for the solvents, which were distilled by the known method prior to use.

Experimental methods

\(^1\)H NMR spectra was recorded at Bruck 300 or 400 spectrometer in CDCl\(_3\) and CDCl\(_3\) (7.26 ppm) was used as internal reference. \(^{13}\)C NMR was recorded at 75 or 100.6 MHz in CDCl\(_3\) and CDCl\(_3\) (77.0 ppm) was used as internal reference. ESI-MS were recorded on a Thermo Finnigan LCQ Advantage spectrometer in ESI mode with a spray voltage of 4.8 kV. GC analyses were performed on Shimadzu GC-2014, equipped with a capillary column (RTX-5, 30 m × 0.25 μm) using a flame ionization detector. Melting points were measured on an X4 apparatus and uncorrected.

2. General procedures for the preparation of protic onium salts

Protic onium salts

To a 50 mL three-necked flask was added the base (10 mmol). A solution of the corresponding acid (10 mmol) was then added dropwise at the temperature of < 5 °C cooled by ice bath. After addition, the ice bath was removed and the reaction mixture was stirred for a further 10 h and then the solvent was evaporated. The remaining solid was dried under vacuum at 60 °C for 24 h after washing by ethyl ether for three times to afford the protic onium salts.

\(\text{CDABCOCl}\)

A solution of freshly sublimed DABCO (0.5609 g, 5 mmol) in MeCN (5 mL) was prepared at r.t. under Ar in a flame dried round-bottomed flask equipped with a reflux condenser. The resulting clear, colorless solution was treated with 1-chlorobutane (2.5 mmol), added dropwise via syringe, and the reaction mixture was heated to 80 °C (oil bath temperature) and stirred for 22 h. After being cooled to r.t., the reaction mixture was transferred via cannula into 20 mL of Et\(_2\)O, yielding a white slurry which eventually separated into two layers. The whole was transferred to a separatory funnel, and the bottom layer was collected, washed repeatedly with Et\(_2\)O and dried under high vacuum at 60 °C for 16 h to yield 1-buty1-4-aza-1-azaniabicyclo[2.2.2]octane chloride as a white solid.

3. General procedure for the preparation of aziridines

Typical procedure was described as below. The bromine (32.0 g, 0.2 mol) in dry CH\(_2\)Cl\(_2\) (40 mL) was added dropwise over 30 min to ice-cooled 40 mL CH\(_2\)Cl\(_2\) solution of dimethyl sulfonium bromide began to separate. After addition of bromine, the orange crystals S1 were collected by filtration and then washed with dry diethyl ether and dried under vacuum. Yield: 80%, Mp 80 °C (dec).

Olefin (160 mmol) was added dropwise to the 160 mL CH\(_2\)CN solution of S1 (35.56 g, 160 mmol) in ice-water bath. During the addition, the white solid began to separate. The solution was further stirred for 10 min. The crystals S2 was collected by filtration, dried under vacuum. Yield: 32-38.6 %.

A solution of amine (20-50 mmol) in water was added dropwise to a stirred solution of compound S2 (10 mmol) in 20 mL of H\(_2\)O at r.t., and the resulting mixture was stirred overnight. The mixture was added into 20 mL of saturated brine, extracted with diethyl ether (3×20 mL), dried with anhydrous MgSO\(_4\) overnight and evaporated under reduced pressure. Aziridine was obtained by distillation under reduced pressure. Yield: 85-100 %.

4. General Procedure for Carboxylation of Aziridine with CO\(_2\)

In a typical reaction, the carboxylation of aziridines with CO\(_2\) was carried out in a 25 mL stainless steel
autoclave. Aziridine (1 mmol) and the catalyst were charged into the reactor at room temperature. CO₂ was introduced into the autoclave and then the mixture was stirred at predetermined temperature for 5 min to reach the equilibration. The pressure was then adjusted to the desired pressure and the mixture was stirred continuously. When the reaction finished, the reactor was cooled in ice-water and CO₂ was ejected slowly. An aliquot of sample was taken from the resultant mixture and dissolved in dry CH₂Cl₂ for GC analysis using a flame ionization detector. The residue was purified by column chromatography on silica gel (eluting with 8:1 to 1:1 petroleum ether/ethyl acetate) to afford the product. The products were further identified by ¹H NMR, ¹³C NMR and MS which are consistent with those reported in the literature¹ and in good agreement with the assigned structures. For the catalyst recycling process, firstly, a very small part of the resultant mixture was taken and analyzed by GC and then, substrate (1a, 1 mmol) for the next run was added to the residual reaction mixture. Finally, the reaction was carried out under identical reaction conditions.

5. Characterization of protic onium salts

HPyI
Light yellow solid; Mp 172-173 °C; ¹H NMR (400 MHz, D₂O) δ 8.78 (d, ¹J = 6 Hz, 2 H), 8.63 (t, ¹J = 8 Hz, 1 H), 8.08 (t, ¹J = 6.8 Hz, 2 H); ¹³C [¹H] NMR (100.6 MHz, D₂O) δ 147.1, 141.1, 127.4; Elemental analysis calcd. (%): for C₇H₈NI: C 29.01, H 2.92, N 6.77, I 61.30, found: C 29.02, H 3.01, N 6.45.

HPyBr
Light yellow solid; Mp 146-149 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.99 (d, ¹J = 4 Hz, 2 H), 8.55 (t, ¹J = 7.6 Hz, 1 H), 8.08 (t, ¹J = 6.8 Hz, 2 H); ¹³C [¹H] NMR (100.6 MHz, D₂O) δ 146.2, 140.9, 127.3; ESI-MS (4.8 kV): m/z (%) = 80.13 (100) [M-Br]+.

HPyCl
White solid; Mp 118-120 °C; ¹H NMR (400 MHz, D₂O) δ 8.78 (d, ¹J = 5.6 Hz, 2 H), 8.62 (t, ¹J = 7.6 Hz, 1 H), 8.07 (t, ¹J = 6.8 Hz, 2 H); ¹³C [¹H] NMR (100.6 MHz, D₂O) δ 147.2, 141.0, 127.4; ESI-MS (4.8 kV): m/z (%) = 80.11 (100) [M-Cl]+.

HPyNO₃
White solid; Mp 110-113 °C; ¹H NMR (400 MHz, D₂O) δ 8.80 (d, ¹J = 5.6 Hz, 2 H), 8.64 (t, ¹J = 8 Hz, 1 H), 8.10 (t, ¹J = 7.2 Hz, 2 H); ¹³C [¹H] NMR (100.6 MHz, D₂O) δ 147.1, 141.1, 127.4.

HPyHSO₄:
White solid; Mp 93-95 °C; ¹H NMR (400 MHz, D₂O) δ 8.79 (d, ¹J = 5.6 Hz, 2 H), 8.64 (t, ¹J = 8 Hz, 1 H), 8.09 (t, ¹J = 6.8 Hz, 2 H); ¹³C [¹H] NMR (100.6 MHz, D₂O) δ 147.2, 141.1, 127.4.

HMImCl
White solid; Mp 78-79 °C; ¹H NMR (400 MHz, D₂O) δ 8.70 (s, 1 H), 7.47 (s, 2 H), 3.95 (s, 3 H); ¹³C [¹H] NMR (100.6 MHz, D₂O) δ 135.0, 123.0, 119.5, 35.5; ESI-MS (4.8 kV): m/z (%) = 83.16 (100) [M-Cl]+.

HDABCOCI
White solid; Mp 207-208 °C; ¹H NMR (400 MHz, D₂O) δ 3.22 (s, 12 H); ¹³C [¹H] NMR (100.6 MHz, D₂O) δ 43.9; ESI-MS (4.8 kV): m/z (%) = 113.20 (100) [M-CI]+.

C₃DABCOCI
White solid; Mp 36-37 °C; ¹H NMR (400 MHz, CDCl₃) δ 3.67 (t, ¹J = 7.2 Hz, 6 H), 3.54 (t, ¹J = 8.4 Hz, 2 H), 3.25 (t, ¹J = 7.2 Hz, 6 H), 1.69-1.77 (m, 2 H), 1.36-1.45 (m, 2 H), 0.97 (t, ¹J = 7.2 Hz, 3 H); ¹³C [¹H] NMR (100.6 MHz, CDCl₃) δ 64.3, 52.4, 45.4, 23.9, 19.7, 13.7; ESI-MS calcd for C₃D₄H₇N₂Cl 204.74, found 169.44 [M-CI]+.
White solid; Mp 65-66 °C; 1H NMR (400 MHz, D$_2$O) δ 3.57-3.60 (m, 2 H), 3.54 (t, $^3$J = 6 Hz, 2 H), 3.33 (t, $^3$J = 5.6 Hz, 2 H); 2.63-2.65 (m, 2 H); 2.02 (quintet, $^3$J = 5.6 Hz, 2 H); 1.69-1.74 (m, 6 H); 13C [1H] NMR (100.6 MHz, CDCl$_3$) δ 165.9, 54.2, 48.5, 37.7, 31.9, 28.7, 26.5, 23.7, 19.2; HR-MS (ESI): m/z = 135.1386, calcd. for C$_3$H$_7$N$_2$ (M-Cl$^-$): 153.1383.

HTBDCI

White solid; Mp 179-180 °C; 1H NMR (400 MHz, D$_2$O) δ 3.36 (t, $^3$J = 6 Hz, 4 H), 3.28 (t, $^3$J = 5.6 Hz, 4 H); 2.02 (quintet, $^3$J = 6 Hz, 4 H); 13C [1H] NMR (100.6 MHz, D$_2$O) δ 151.0, 46.5, 37.8, 20.2; HR-MS (ESI): m/z = 140.1182, calcd. for C$_3$H$_7$N$_2$ (M-Cl$^-$): 140.1177.

HHMTACI

White solid; Mp 139-141 °C; 1H NMR (400 MHz, D$_2$O) δ 4.75 (s, 6 H), 4.74 (s, 6 H); 13C [1H] NMR (100.6 MHz, D$_2$O) δ 71.7; HR-MS (ESI): m/z = 141.1135, calcd. for C$_9$H$_{18}$N$_4$(M-Cl$^-$): 141.1131, 317.1963, calcd. for C$_{12}$H$_{26}$N$_4$Cl (2 M-Cl$^-$): 317.1971.

6. Characterization of aziridines

1-Ethyl-2-phenylaziridine

1H NMR (400 MHz, CDCl$_3$) δ 1.17 (t, $^3$J = 9.6 Hz, 3H), 1.65 (d, $^3$J = 8.8 Hz, 1H), 1.89 (d, $^3$J = 4.4 Hz, 1H), 2.30 (dd, $^3$J = 4.4 Hz, $^3$J = 4.8 Hz, 1H), 2.44 (q, $^3$J = 9.6 Hz, 2H), 7.18-7.31 (m, 5H); ESI-MS calcd for C$_{10}$H$_{13}$N 147.10, found 148.31 [M + H]$^+$.  

2-(4-Chlorophenyl)-1-ethylaziridine

1H NMR (400 MHz, CDCl$_3$) δ 1.18 (t, $^3$J = 6.9 Hz, 3H), 1.65 (d, $^3$J = 6.6 Hz, 1H), 1.83 (d, $^3$J = 3.3 Hz, 1H), 2.25-2.46 (m, 3H), 7.15-7.23 (m, 4H); ESI-MS calcd for C$_9$H$_{11}$ClN 178.16, found 178.18 [M + H]$^+$.  

1-Ethyl-2-p-tolylaziridine

1H NMR (400 MHz, CDCl$_3$) δ 1.19 (t, $^3$J = 7.2 Hz, 3H), 1.62 (d, $^3$J = 6.4 Hz, 1H), 1.86 (d, $^3$J = 3.2 Hz, 1H), 2.26 (dd, $^3$J = 3.6 Hz, $^3$J = 3.2 Hz, 1H), 2.31 (s, 3H), 2.37-2.48 (m, 2H), 7.09-7.15 (m, 4H); ESI-MS calcd for C$_{11}$H$_{12}$N 161.24, found 162.20 [M + H]$^+$.  

1-Propyl-2-phenylaziridine

1H NMR (400 MHz, CDCl$_3$) δ 0.95 (t, $^3$J = 10.0 Hz, 3H), 1.60-1.67 (m, 3H), 1.89 (d, $^3$J = 4.0 Hz, 1H), 2.24-2.33 (m, 2H), 2.43-2.51 (m, 1H), 7.18-7.31 (m, 5H); ESI-MS calcd for C$_{11}$H$_{15}$N 161.12, found 162.28 [M + H]$^+$.  

1-Isopropyl-2-phenylaziridine

1H NMR (400 MHz, CDCl$_3$) δ 1.17 (d, $^3$J = 0.9 Hz, 3H), 1.19 (d, $^3$J = 0.9 Hz, 3H), 1.57-1.66 (m, 2H), 1.89 (d, $^3$J = 3.3 Hz, 1H), 2.34 (dd, $^3$J = 3.3 Hz, $^3$J = 3.3 Hz, 1H), 7.17-7.31 (m, 5H); ESI-MS calcd for C$_{11}$H$_{15}$N 161.12, found 162.32 [M + H]$^+$.  

1-Butyl-2-phenylaziridine

1H NMR (300 MHz, CDCl$_3$) δ 0.91 (t, $^3$J = 7.2 Hz, 3H), 1.33-1.45 (m, 2H), 1.55-1.67 (m, 3H), 1.88 (d, $^3$J = 3.3 Hz, 1H), 2.27-2.36 (m, 2H), 2.45-2.54 (m, 1H), 7.17-7.31 (m, 5H); ESI-MS calcd for C$_{13}$H$_{17}$N 175.14, found 176.38 [M + H]$^+$.  

1-Isobutyl-2-phenylaziridine

1H NMR (300 MHz, CDCl$_3$) δ 0.95 (d, $^3$J = 6.6 Hz, 3H), 0.98 (d, $^3$J = 6.6 Hz, 3H), 1.65 (d, $^3$J = 6.3 Hz, 1H), 1.85-1.94 (m, 2H), 2.08 (dd, $^3$J = 6.3 Hz, $^3$J = 6.6 Hz, 1H), 2.28 (q, $^3$J = 3.3 Hz, 1H), 2.44 (dd, $^3$J = 7.2 Hz, $^3$J = 11.4 Hz, 1H), 7.17-7.31 (m, 5H); ESI-MS calcd for C$_{13}$H$_{17}$N 175.14, found 176.36 [M + H]$^+$.  

1-Benzyl-2-phenylaziridine

1H NMR (300 MHz, CDCl$_3$) δ 1.84 (d, $^3$J = 6.3 Hz, 1H), 1.98 (d, $^3$J = 3.3 Hz, 1H), 2.50 (q, $^3$J = 3.3 Hz, 1H), 3.65 (ABq, $^3$J$_{AB}$ = 13.8 Hz, $^3$J$_{AB}$ = 18.8 Hz, 2H), 7.18-7.38 (m, 10H); ESI-MS calcd for C$_{13}$H$_{20}$N 209.29, found 210.13 [M + H]$^+$.  

1-Cyclohexyl-2-phenylaziridine

1H NMR (300 MHz, CDCl$_3$) δ 1.19-1.87 (m, 13H), 2.34 (dd, $^3$J = 3.3 Hz, $^3$J = 3.0 Hz, 1H), 7.17-7.27 (m, 5H);
ESI-MS calcd for C_{13}H_{19}N 201.15, found 202.37 [M + H]^+.

1-Cyclohexyl-2-p-tolyaziridine

^1^H NMR (300 MHz, CDCl₃) δ 1.19-1.85 (m, 13 H), 2.29-2.32 (m, 4 H), 7.07-7.16 (m, 4 H).

2-(4-Chlorophenyl)-1-cyclohexylaziridine

^1^H NMR (300 MHz, CDCl₃) δ 1.16-1.82 (m, 13 H), 2.31 (dd, J=3.3 Hz, J=3.0 Hz, 1 H), 7.17-7.26 (m, 4 H).

7. Characterization of oxazolidinones and piperazines

3-Ethyl-5-phenoxazolidin-2-one

Colorless liquid; ^1^H NMR (300 MHz, CDCl₃) δ 1.17 (t, J=7.2 Hz, 3H), 3.29-3.45 (m, 3H), 3.92 (t, J=8.7 Hz, 1H), 5.48 (t, J=7.8 Hz, 1H), 7.34-7.42 (m, 5H); ^13^C NMR (75 MHz, CDCl₃) δ 12.4, 38.8, 51.5, 74.2, 125.4, 128.6, 128.8, 138.8, 157.5; ESI-MS calcd for C_{11}H_{15}NO_{2} 191.09, found 192.29 (M + H)^+, 214.38 (M + Na)^+.

4. 1,4-Diethyl-2, 5-diphenyl-piperazine

White crystals; Mp 116-119 °C; ^1^H NMR (400 MHz, CDCl₃) δ 0.91 (t, J=7.2 Hz, 6H), 1.99-2.05 (m, 2H), 2.30 (t, J=10.8 Hz, 2H), 2.54-2.62 (m, 2H), 3.08 (dd, J=11.6 Hz, J=2.4 Hz, 2H), 3.45 (dd, J=2.0 Hz, J=12.0 Hz, 2H), 7.29-7.43 (m, 10H), LC-MS, calcd for C_{20}H_{22}N_{2} 294.21, found 295.35 (M + H)^+.

5. 1,4-Diethyl-2, 5-diphenyl-piperazine

Colorless liquid; ^1^H NMR (300 MHz, CDCl₃) δ 1.05 (t, J=7.2 Hz, 3H), 2.79-2.88 (m, 1H), 3.48-3.57 (m, 1H), 4.10 (t, J=8.0 Hz, 1H), 4.62 (t, J=8.8 Hz, 1H), 4.81 (t, J=7.2 Hz, 1H), 7.30-7.44 (m, 5H); ^13^C NMR (75 MHz, CDCl₃) δ 12.1, 36.9, 59.3, 69.7, 126.9, 129.0, 129.7, 138.8, 158.1; ESI-MS calcd for C_{11}H_{15}NO_{2} 191.09, found 192.29 (M + H)^+, 214.38 (M + Na)^+.

3-Ethyl-4-(chlorophenyl)oxazolidin-2-one

White solid; ^1^H NMR (400 MHz, CDCl₃) δ 1.17 (t, J=7.3 Hz, 3H), 3.30-3.43 (m, 2H), 3.69-3.76 (m, 1H), 3.92 (t, J=8.7 Hz, 1H), 5.44 (t, J=8.0 Hz, 1H), 7.27-7.38 (m, 4H); ^13^C NMR (100 MHz, CDCl₃) δ 12.6, 38.9, 51.5, 73.6, 126.9, 129.1, 134.7, 157.4; ESI-MS calcd for C_{11}H_{13}CINO_{2} 225.67, found 451.64 (2M + H)^+.

3-Ethyl-5-p-tolyazolidin-2-one

White solid; ^1^H NMR (400 MHz, CDCl₃) δ 1.18 (t, J=7.3 Hz, 3H), 1.62 (d, J=6.4 Hz, 1H), 1.87 (d, J=3.2 Hz, 1H), 2.27 (dd, J=6.6 Hz, J=3.2 Hz, 1H), 2.31 (s, 3H), 2.36-2.48 (m, 2H), 7.09-7.15 (m, 4H); ^13^C NMR (100 MHz, CDCl₃) δ 12.6, 21.2, 38.9, 51.6, 74.3, 125.6, 129.5, 135.8, 138.7, 157.7; ESI-MS calcd for C_{11}H_{12}NO_{2} 205.25, found 206.45 (M + H)^+, 411.15 (2M + H)^+.

3-Propyl-5-phenoxazolidin-2-one

Colorless liquid; ^1^H NMR (300 MHz, CDCl₃) δ 0.91 (t, J=7.2 Hz, 3H), 1.52-1.61 (m, 2H), 3.18-3.31 (m, 2H), 3.40 (t, J=8.0 Hz, 1H), 3.90 (t, J=8.0 Hz, 1H), 5.46 (t, J=8.0 Hz, 1H), 7.31-7.37 (m, 5H); ^13^C NMR (75 MHz, CDCl₃) δ 10.7, 20.3, 45.5, 51.8, 74.0, 125.2, 128.4, 128.5, 138.7, 157.6; ESI-MS calcd for C_{13}H_{15}NO_{2} 205.11, found 206.30 (M + H)^+, 228.30 (M + Na)^+, 433.04 (2M + Na)^+.

3-Isopropyl-5-phenoxazolidin-2-one

Colorless liquid; ^1^H NMR (300 MHz, CDCl₃) δ 1.16 (d, J=6.8 Hz, 3H), 1.22 (d, J=6.8 Hz, 3H), 3.37 (t, J=8.0 Hz, 1H), 3.87 (t, J=8.8 Hz, 1H), 4.13-4.23 (m, 1H), 5.48 (t, J=8.0 Hz, 1H), 7.34-7.42 (m, 5H); ^13^C NMR (75 MHz, CDCl₃) δ 19.1, 19.6, 44.5, 47.0, 74.2, 125.1, 128.3, 128.5, 138.5, 156.7; ESI-MS calcd for C_{13}H_{15}NO_{2} 205.11, found 206.29 (M + H)^+, 433.08 (2M + Na)^+.

3-Butyl-5-phenoxazolidin-2-one

Colorless liquid; ^1^H NMR (300 MHz, CDCl₃) δ 0.94 (t, J=7.2 Hz, 3H), 1.31-1.40 (m, 2H), 1.51-1.58 (m, 2H), 3.23-3.38 (m, 2H), 3.43 (t, J=8.0 Hz, 1H), 3.92 (t, J=8.8 Hz, 1H), 5.49 (t, J=8.0 Hz, 1H), 7.28-7.42 (m, 5H); ^13^C NMR (75 MHz, CDCl₃) δ 13.4, 19.5, 29.1, 43.6, 51.8, 74.1, 125.2, 128.4, 128.5, 138.7, 157.7; ESI-MS calcd for C_{13}H_{15}NO_{2} 219.13, found 220.34 (M + H)^+, 259.48 (M + K)^+, 461.05 (2M + Na)^+.

3-Isobutyl-5-phenoxazolidin-2-one

Electronic Supplementary Material (ESI) for Green Chemistry
White crystals; Mp 38-42 °C; 1H NMR (300 MHz, CDCl3) δ 0.91 (d, 3J=4.8 Hz, 3H), 0.93 (d, 3J=4.8 Hz, 3H), 1.81-1.95 (m, 1H), 3.02-3.16 (m, 2H), 3.42 (dd, 3J=8.7 Hz, 3J=7.5 Hz, 1H), 3.91 (t, 3J=8.7 Hz, 1H), 5.48 (t, 3J=8.4 Hz, 1H), 7.32-7.41 (m, 5H); 13C NMR (75 MHz, CDCl3) δ 19.7, 19.8, 26.7, 51.6, 52.6, 74.1, 125.3, 128.5, 128.7, 138.8, 158.0; ESI-MS calcd for C11H17NO2 219.13, found 246.22 (M + Na)+, 679.70 (3M + Na)+.

3-Benzyl-5-phenyloxazolidin-2-one

White crystals; Mp 60-64 °C; 1H NMR (300 MHz, CDCl3) δ 3.28 (t, 3J=8.4 Hz, 1H), 3.75 (t, 3J=8.7 Hz, 1H), 4.45 (ABq, JAB=15.0 Hz, ΔνAB =36.0 Hz, 2H), 5.43 (t, 3J=8.1 Hz, 1H), 7.27-7.35 (m, 10H); 13C NMR (75 MHz, CDCl3) δ 48.1, 51.3, 74.3, 125.3, 127.8, 127.9, 128.6, 128.7, 135.5, 138.5, 157.8; ESI-MS calcd for C16H15NO2 253.11, found 276.44(M + Na)+, 781.66 (3M + Na)+.

3-Cyclohexyl-5-phenyloxazolidin-2-one

White crystals; Mp 92-93 °C; 1H NMR (300 MHz, CDCl3) δ 1.0-1.8 (m, 10H), 3.38 (t, 3J=8.4 Hz, 1H), 3.70-3.73 (m, 1H), 3.88 (t, 3J=8.7 Hz, 1H), 5.45 (t, 3J=8.4 Hz, 1H), 7.35-7.38 (m, 5H); 13C NMR (75 MHz, CDCl3) δ 25.1, 25.2, 29.9, 30.3, 48.1, 52.4, 74.4, 125.3, 128.5, 128.7, 138.9, 157.0; ESI-MS calcd for C14H19NO2 245.14, found 246.27 (M + H)+, 757.70 (3M + Na)+.

3-Cyclohexyl-5-p-tolyloxazolidin-2-one

White crystals; Mp 89-91 °C; 1H NMR (300 MHz, CDCl3) δ 1.03-1.86 (m, 10 H), 2.36 (s, 3 H), 3.38 (t, 3J = 8.0 Hz, 1H), 3.71-3.75 (m, 1 H), 3.85 (t, 3J = 8.7 Hz, 1 H), 5.43 (t, 3J = 8.0 Hz, 1 H), 7.17-7.26 (m, 4 H); 13C NMR (75 MHz, CDCl3) δ 21.1, 25.2, 25.3, 25.4, 30.1, 30.5, 48.3, 52.5, 74.5, 125.5, 129.5, 136.0, 138.6, 157.3; ESI-MS calcd for C13H19NO2 259.16, found 260.02 (M + H)+, 799.55 (3M + Na)+; HRMS: calcd for C14H20NO2 (M + H) + 260.1645, found 260.1652.

5-(4-Chlorophenyl)-3-cyclohexyloxazolidin-2-one

White crystals; Mp 94-96 °C; 1H NMR (300 MHz, CDCl3) δ 1.05 - 1.83 (m, 10 H), 3.34 (t, 3J = 8.0 Hz, 1 H), 3.69-3.76 (m, 1 H), 3.89 (t, 3J = 8.7 Hz, 1 H), 5.44 (t, 3J = 8.0 Hz, 1 H), 7.27-7.38 (m, 4 H); 13C NMR (75 MHz, CDCl3) δ 25.2, 25.3, 30.0, 30.4, 48.2, 52.6, 73.8, 126.8, 129.0, 134.5, 137.6, 156.8; APCI-MS calcd for C18H16ClNO2 279.10, found 839.62 (3M+H)+, 859.60 (3M+Na)+; HRMS: calcd for C19H16ClNO2 (M + H)+ 280.1099, found 280.1101.

8. References :
9. The $^1$H NMR and $^{13}$C NMR Charts for protic onium salts

HPyl: pyridin-1-ium iodide

$^1$H NMR (400 MHz, D$_2$O)

$^{13}$C NMR (100.6 MHz, D$_2$O)
HPyBr: pyridin-1-ium bromide

\[
\text{Br}^- \\
\text{H}
\]

1H NMR (CDCl₃, 400 MHz)

13C NMR (CDCl₃, 100.6 MHz)

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HPyCl: pyridin-1-i um chloride

1H NMR (400MHz, D2O)

13C NMR (100.6MHz, D2O)
HPyNO$_3$: pyridin-1-ium nitrate

1H NMR (D$_2$O, 400 MHz)

13C NMR (D$_2$O, 100.6 MHz)
HPyHSO₄⁻: pyridin-1-ium bisulfate

1H NMR (D₂O, 400 MHz)

13C NMR (D₂O, 100.6 MHz)
HPyH₂PO₄: pyridin-1-ium dihydrogen phosphate

1H NMR (D₂O, 400 MHz)

13C NMR (D₂O, 100.6 MHz)
HMImCl: 1-hydro-3-methylimidazolium chloride

1H NMR (400MHz, D2O)

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**HDABCOCl: 1-hydro-4-aza-1-azaniabicyclo-[2.2.2]octane chloride**

**$^1$H NMR (400 MHz, D$_2$O)**

**$^{13}$C NMR (100.6 MHz, D$_2$O)**
[C₄DABCO]Cl: 1-butyl-4-aza-1-azaniabicyclo[2.2.2]octane chloride

1H NMR (400MHz,CDCl₃)

13C NMR (100.6MHz,CDCl₃)
HDBUCI: 1,8-diazabicyclo[5.4.0]undec-7-enium chloride

1H NMR (400MHz,D2O)

13C NMR (100.6MHz, CDCl3)
HTBDCl: 1,5,7-triazabicyclo[4.4.0]dec-5-enium chloride

\[
\text{1H NMR (400MHz,D2O)}
\]

\[
\text{13C NMR (100.6MHz,D2O)}
\]
HHMTACl: 1,3,5,7-tetraazatricyclo[1.1.1.1.1]dec-1-anium chloride

1H NMR (400MHz,D2O)

13C NMR (100.6MHz,D2O)
10. The $^1$H NMR charts for aziridines
1H NMR (300MHz, CDCl3)
1H NMR (300MHz, CDCl3)
11. The $^1$H NMR and $^{13}$C NMR Charts for oxazolidinones
$^{13}$C NMR (75MHz, CDCl₃)

$^1$H NMR (400 MHz, CDCl₃)
13C NMR (75MHz, CDCl3)

1H NMR (400 MHz, CDCl3)

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13C NMR (75MHz, CDCl3)

1H NMR (400 MHz, CDCl3)

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This journal is © The Royal Society of Chemistry 2011
13C NMR (100.6MHz, CDCl3)

1H NMR (400 MHz, CDCl3)
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13C NMR (75MHz, CDCl₃)
12. The $^1$H NMR charts of dimer of 1a