

Electronic Supplementary Material (ESI) for RSC Advances.  
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## **Supporting Information**

### **For**

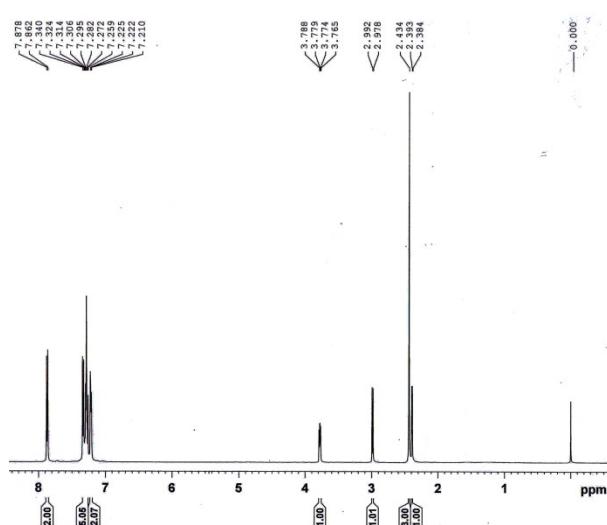
# **First graphene oxide promoted metal-free nitrene insertion to olefins in water towards facile synthesis of activated aziridines†**

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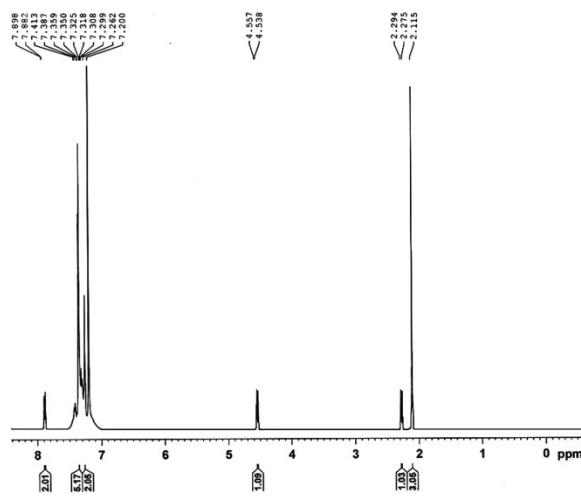
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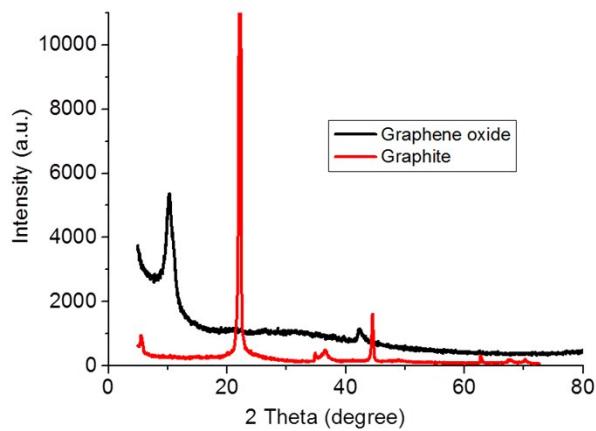
**Fig. S1.**  $^1\text{H}$  NMR spectra of aziridines 3a.



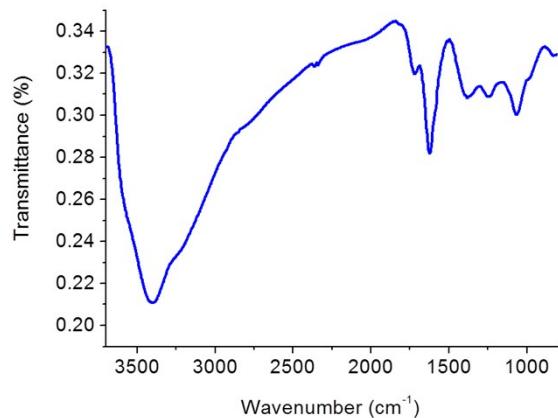
**Fig. S2.**  $^1\text{H}$  NMR spectra of nitroaziridine 5a.



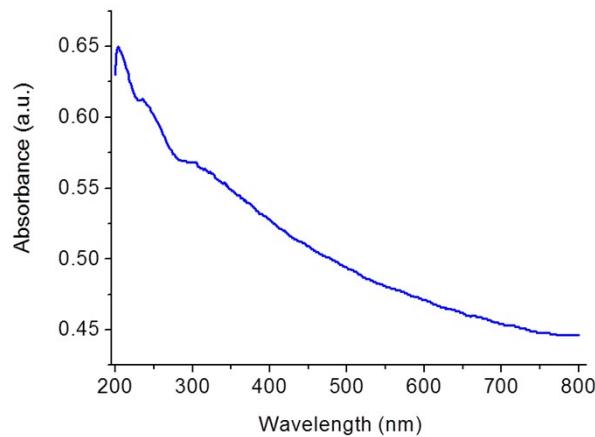
**Fig. S3: XRD pattern of Graphene oxide nanosheets.**



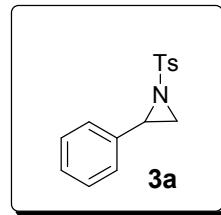
**Fig. S4: FTIR Spectrum of graphene oxide nanosheets.**



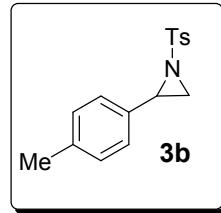
**Fig. S5: UV-Vis Spectrum of graphene oxide nanosheets.**



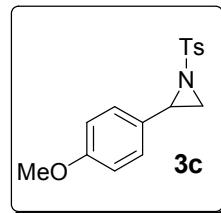
**Characterization data of the synthesized pure compounds:**



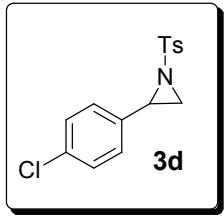
**3a:** IR (KBr)  $\nu_{\max}$  = 3051, 2838, 1603, 1582, 1455 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  = 2.39 (d, 1H, *J* = 4.5 Hz, 3-H<sub>a</sub>), 2.43 (s, 3H, TsCH<sub>3</sub>), 2.99 (d, 1H, *J* = 7.0 Hz, 3-H<sub>b</sub>), 3.78 (dd, 1H, *J* = 4.5, 7.0 Hz, 2-H), 7.21-7.34 (m, 7H<sub>arom</sub>), 7.87 (d, *J* = 8.0 Hz, 2H<sub>arom</sub>) ppm. <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  = 23.7, 34.7, 43.8, 125.1, 126.3, 127.5, 128.3, 129.6, 134.1, 136.5, 142.8 ppm. EIMS: *m/z* = 273 [M<sup>+15H<sub>15</sub>NO<sub>2</sub>S: calcd. C 65.91, H 5.53, N 5.12; found C 65.73, H 5.16, N 5.41.</sup>



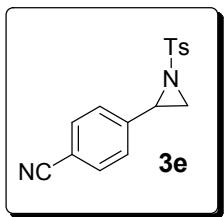
**3b:** IR (KBr)  $\nu_{\max}$  = 3049, 2835, 1601, 1581, 1451 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  = 2.41 (d, 1H, *J* = 4.7 Hz, 3-H<sub>a</sub>), 2.47 (s, 3H, Me), 2.96 (d, 1H, *J* = 7.0 Hz, 3-H<sub>b</sub>), 2.39 (s, 3H, TsCH<sub>3</sub>), 3.77 (dd, 1H, *J* = 4.7, 7.0 Hz, 2-H), 7.28-7.40 (m, 6H<sub>arom</sub>), 7.88 (d, *J* = 8.1 Hz, 2H<sub>arom</sub>) ppm. <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  = 23.2, 23.9, 34.5, 43.7, 124.8, 125.7, 127.8, 128.7, 130.5, 131.2, 135.9, 143.1 ppm. EIMS: *m/z* = 287 [M<sup>+16H<sub>17</sub>NO<sub>2</sub>S: calcd. C 66.87, H 5.96, N 4.87; found C 66.61, H 6.13, N 4.93.</sup>



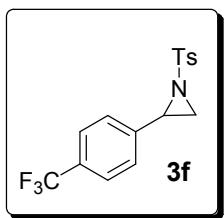
**3c:** IR (KBr)  $\nu_{\max}$  = 3047, 2838, 1606, 1585, 1454 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  = 2.38 (d, 1H, *J* = 4.8 Hz, 3-H<sub>a</sub>), 2.42 (s, 3H, TsCH<sub>3</sub>), 2.98 (d, 1H, *J* = 7.3 Hz, 3-H<sub>b</sub>), 3.67 (s, 3H, OMe), 3.79 (dd, 1H, *J* = 4.8, 7.3 Hz, 2-H), 7.23-7.48 (m, 6H<sub>arom</sub>), 7.85 (d, *J* = 8.3 Hz, 2H<sub>arom</sub>) ppm. <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  = 23.8, 34.2, 43.1, 54.2, 125.6, 126.8, 127.5, 128.3, 128.9, 130.7, 134.8, 143.8 ppm. EIMS: *m/z* = 303 [M<sup>+16H<sub>17</sub>NO<sub>3</sub>S: calcd. C 63.34, H 5.65, N 4.62; found C 63.09, H 6.02, N 4.49.</sup>



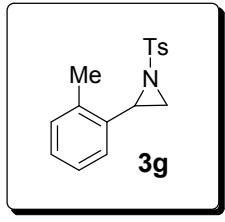
**3d:** IR (KBr)  $\nu_{\max}$  = 3052, 2839, 1599, 1578, 1449 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  = 2.36 (d, 1H, *J* = 4.6 Hz, 3-H<sub>a</sub>), 2.45 (s, 3H, TsCH<sub>3</sub>), 3.01 (d, 1H, *J* = 7.2 Hz, 3-H<sub>b</sub>), 3.76 (dd, 1H, *J* = 4.6, 7.2 Hz, 2-H), 7.21-7.39 (m, 6H<sub>arom</sub>), 7.81 (d, *J* = 8.2 Hz, 2H<sub>arom</sub>) ppm. <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  = 23.7, 34.7, 43.3, 125.5, 126.2, 126.9, 127.8, 128.7, 129.9, 131.5, 139.8 ppm. EIMS: *m/z* = 307, 309 [M<sup>+</sup>, M<sup>+</sup> + 2]. C<sub>15</sub>H<sub>14</sub>ClNO<sub>2</sub>S: calcd. C 58.53, H 4.58, N 4.55; found C 58.63, H 4.71, N 4.22.



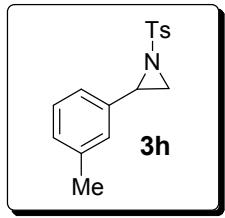
**3e:** IR (KBr)  $\nu_{\max}$  = 3051, 2837, 1603, 1581, 1450 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  = 2.35 (d, 1H, *J* = 4.3 Hz, 3-H<sub>a</sub>), 2.42 (s, 3H, TsCH<sub>3</sub>), 3.07 (d, 1H, *J* = 7.1 Hz, 3-H<sub>b</sub>), 3.75 (dd, 1H, *J* = 4.3, 7.1 Hz, 2-H), 7.29-7.43 (m, 6H<sub>arom</sub>), 7.88 (d, *J* = 8.1 Hz, 2H<sub>arom</sub>) ppm. <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  = 23.9, 34.6, 43.7, 112.1, 124.2, 125.1, 125.7, 126.7, 128.8, 129.5, 131.9, 142.3 ppm. EIMS: *m/z* = 298 [M<sup>+</sup>]. C<sub>16</sub>H<sub>14</sub>N<sub>2</sub>O<sub>2</sub>S: calcd. C 64.41, H 4.73, N 9.39; found C 64.69, H 4.47, N 9.51.



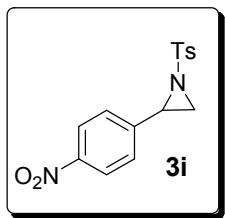
**3f:** IR (KBr)  $\nu_{\max}$  = 3048, 2836, 1597, 1579, 1453 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  = 2.38 (d, 1H, *J* = 4.4 Hz, 3-H<sub>a</sub>), 3.02 (d, 1H, *J* = 7.3 Hz, 3-H<sub>b</sub>), 2.47 (s, 3H, TsCH<sub>3</sub>), 3.79 (dd, 1H, *J* = 4.4, 7.3 Hz, 2-H), 7.25-7.38 (m, 6H<sub>arom</sub>), 7.85 (d, *J* = 8.0 Hz, 2H<sub>arom</sub>) ppm. <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  = 23.8, 34.9, 43.9, 123.2, 124.5, 125.6, 126.7, 127.5, 128.3, 128.9, 130.7, 143.2 ppm. EIMS: *m/z* = 341 [M<sup>+</sup>]. C<sub>16</sub>H<sub>14</sub>F<sub>3</sub>NO<sub>2</sub>S: calcd. C 56.30, H 4.13, N 4.10; found C 56.44, H 4.50, N 4.17.



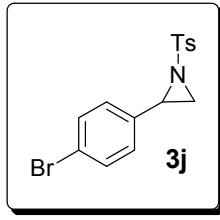
**3g:** IR (KBr)  $\nu_{\max}$  = 3049, 2838, 1596, 1582, 1451 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  = 2.39 (d, 1H, *J* = 4.1 Hz, 3-H<sub>a</sub>), 2.45 (s, 3H, TsCH<sub>3</sub>), 2.48 (s, 3H, Me), 2.99 (d, 1H, *J* = 7.6 Hz, 3-H<sub>b</sub>), 3.78 (dd, 1H, *J* = 4.1, 7.6 Hz, 2-H), 7.21-7.37 (m, 6H<sub>arom</sub>), 7.89 (d, *J* = 8.3 Hz, 2H<sub>arom</sub>) ppm. <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  = 23.4, 24.3, 34.3, 43.8, 124.5, 125.2, 126.1, 127.9, 128.6, 129.3, 130.1, 133.9, 139.5, 141.8 ppm. EIMS: *m/z* = 287 [M<sup>+16H<sub>17</sub>NO<sub>2</sub>S: calcd. C 66.87, H 5.96, N 4.87; found C 66.99, H 5.73, N 4.92.</sup>



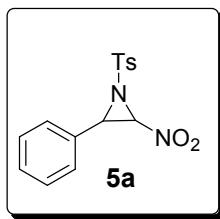
**3h:** IR (KBr)  $\nu_{\max}$  = 3052, 2835, 1602, 1579, 1455 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  = 2.34 (d, 1H, *J* = 4.2 Hz, 3-H<sub>a</sub>), 2.41 (s, 3H, TsCH<sub>3</sub>), 2.47 (s, 3H, Me), 3.03 (d, 1H, *J* = 7.5 Hz, 3-H<sub>b</sub>), 3.75 (dd, 1H, *J* = 4.2, 7.5 Hz, 2-H), 7.22-7.35 (m, 6H<sub>arom</sub>), 7.88 (d, *J* = 8.1 Hz, 2H<sub>arom</sub>) ppm. <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  = 23.1, 23.8, 34.2, 43.5, 125.3, 125.9, 126.7, 127.5, 129.2, 131.7, 132.3, 135.6, 136.3, 142.5 ppm. EIMS: *m/z* = 287 [M<sup>+</sup>]. C<sub>16</sub>H<sub>17</sub>NO<sub>2</sub>S: calcd. C 66.87, H 5.96, N 4.87; found C 66.58, H 6.11, N 5.23.



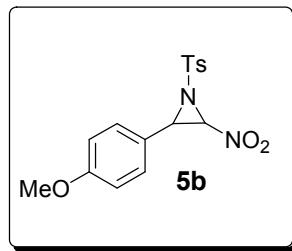
**3i:** IR (KBr)  $\nu_{\max}$  = 3051, 2839, 1598, 1583, 1448 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  = 2.39 (d, 1H, *J* = 4.5 Hz, 3-H<sub>a</sub>), 2.44 (s, 3H, TsCH<sub>3</sub>), 3.02 (d, 1H, *J* = 7.2 Hz, 3-H<sub>b</sub>), 3.75 (dd, 1H, *J* = 4.5, 7.2 Hz, 2-H), 7.29-7.43 (m, 6H<sub>arom</sub>), 7.89 (d, *J* = 8.3 Hz, 2H<sub>arom</sub>) ppm. <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  = 23.5, 34.5, 43.4, 125.5, 126.2, 126.9, 127.5, 128.9, 130.2, 130.8, 142.8 ppm. EIMS: *m/z* = 318 [M<sup>+</sup>]. C<sub>15</sub>H<sub>14</sub>N<sub>2</sub>O<sub>4</sub>S: calcd. C 56.59, H 4.43, N 8.80; found C 56.96, H 4.51, N 8.43.



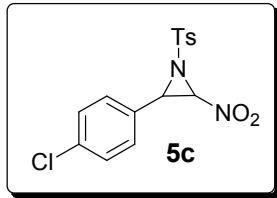
**3j:** IR (KBr)  $\nu_{\max}$  = 3050, 2836, 1604, 1581, 1453 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  = 2.35 (d, 1H, *J* = 4.8 Hz, 3-H<sub>a</sub>), 2.41 (s, 3H, TsCH<sub>3</sub>), 2.98 (d, 1H, *J* = 7.1 Hz, 3-H<sub>b</sub>), 3.78 (dd, 1H, *J* = 4.8, 7.1 Hz, 2-H), 7.21-7.33 (m, 6H<sub>arom</sub>), 7.85 (d, *J* = 8.0 Hz, 2H<sub>arom</sub>) ppm. <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  = 24.2, 34.8, 43.9, 126.7, 128.2, 128.8, 130.2, 130.9, 131.7, 135.2, 143.7 ppm. EIMS: *m/z* = 352 [M<sup>+</sup>]. C<sub>15</sub>H<sub>14</sub>BrNO<sub>2</sub>S: calcd. C 51.15, H 4.01, N 3.98; found C 51.03, H 4.36, N 3.79.



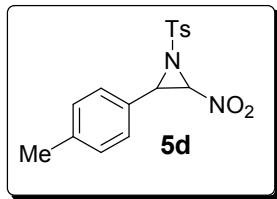
**5a:** IR (KBr)  $\nu_{\max}$  = 3049, 2835, 1607, 1579, 1509, 1459, 1324 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  = 2.12 (s, 3H, TsCH<sub>3</sub>), 2.28 (d, 1H, *J* = 9.5 Hz, 3-H), 4.54 (d, 1H, *J* = 9.5 Hz, 2-H), 7.20-7.41 (m, 7H<sub>arom</sub>), 7.89 (d, *J* = 8.0 Hz, 2H<sub>arom</sub>) ppm. <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  = 23.9, 42.9, 78.1, 125.9, 126.6, 127.5, 128.4, 129.3, 131.5, 137.9, 143.9 ppm. EIMS: *m/z* = 318 [M<sup>+</sup>]. C<sub>15</sub>H<sub>14</sub>N<sub>2</sub>O<sub>4</sub>S: calcd. C 56.59, H 4.43, N 8.80; found: C 56.88, H 4.26, N 8.47.



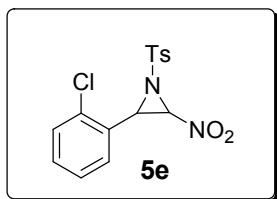
**5b:** IR (KBr)  $\nu_{\max}$  = 3048, 2839, 1605, 1578, 1508, 1455, 1321 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  = 2.15 (s, 3H, TsCH<sub>3</sub>), 2.29 (d, 1H, *J* = 9.2 Hz, 3-H), 4.51 (d, 1H, *J* = 9.2 Hz, 2-H), 7.23-7.45 (m, 6H<sub>arom</sub>), 7.88 (d, *J* = 8.1 Hz, 2H<sub>arom</sub>) ppm. <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  = 23.7, 42.6, 55.1, 78.8, 125.2, 125.9, 126.7, 127.5, 128.2, 129.7, 130.8, 136.8 ppm. EIMS: *m/z* = 348 [M<sup>+</sup>]. C<sub>16</sub>H<sub>16</sub>N<sub>2</sub>O<sub>5</sub>S: calcd. C 55.16, H 4.63, N 8.04; found: C 55.03, H 4.18, N 8.19.



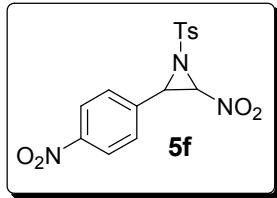
**5c:** IR (KBr)  $\nu_{\max}$  = 3051, 2836, 1602, 1585, 1510, 1451, 1325 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  = 2.17 (s, 3H, TsCH<sub>3</sub>), 2.27 (d, 1H,  $J$  = 9.1 Hz, 3-H), 4.56 (d, 1H,  $J$  = 9.1 Hz, 2-H), 7.19-7.42 (m, 6H<sub>arom</sub>), 7.85 (d,  $J$  = 8.1 Hz, 2H<sub>arom</sub>) ppm. <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  = 23.8, 43.1, 78.6, 126.1, 127.2, 128.5, 129.7, 130.1, 130.9, 135.8, 142.1 ppm. EIMS: *m/z* = 352, 354 [M<sup>+</sup>, M<sup>+</sup>+2]. C<sub>15</sub>H<sub>13</sub>ClN<sub>2</sub>O<sub>4</sub>S: calcd. C 51.07, H. 3.71, N 7.94; found: C 51.29. H 3.44, N 8.27.



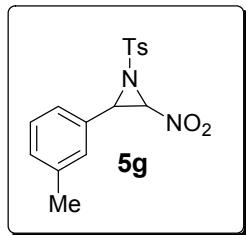
**5d:** IR (KBr)  $\nu_{\max}$  = 3052, 2835, 1601, 1582, 1508, 1452, 1320 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  = 2.13 (s, 3H, TsCH<sub>3</sub>), 2.29 (d, 1H,  $J$  = 9.3 Hz, 3-H), 2.41 (s, 3H, Me), 4.55 (d, 1H,  $J$  = 9.3 Hz, 2-H), 7.21-7.48 (m, 6H<sub>arom</sub>), 7.81 (d,  $J$  = 8.2 Hz, 2H<sub>arom</sub>) ppm. <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  = 23.9, 23.8, 42.8, 78.9, 125.5, 126.3, 127.2, 128.8, 129.2, 130.5, 136.1, 143.5 ppm. EIMS: *m/z* = 332 [M<sup>+</sup>]. C<sub>16</sub>H<sub>16</sub>N<sub>2</sub>O<sub>4</sub>S: calcd. C 57.82, H. 4.85, N 8.43; found: C 57.63. H 4.47, N 8.58.



**5e:** IR (KBr)  $\nu_{\max}$  = 3050, 2838, 1606, 1581, 1509, 1456, 1325 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  = 2.18 (s, 3H, TsCH<sub>3</sub>), 2.31 (d, 1H,  $J$  = 9.5 Hz, 3-H), 4.52 (d, 1H,  $J$  = 9.5 Hz, 2-H), 7.20-7.45 (m, 6H<sub>arom</sub>), 7.88 (d,  $J$  = 8.0 Hz, 2H<sub>arom</sub>) ppm. <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  = 23.5, 43.5, 78.2, 125.1, 125.8, 126.6, 127.5, 128.8, 129.5, 130.2, 131.3, 136.5, 143.5 ppm. EIMS: *m/z* = 352, 354 [M<sup>+</sup>, M<sup>+</sup>+2]. C<sub>15</sub>H<sub>13</sub>ClN<sub>2</sub>O<sub>4</sub>S: calcd. C 51.07, H. 3.71, N 7.94; found: C 51.44. H 3.83, N 7.69.



**5f:** IR (KBr)  $\nu_{\max}$  = 3048, 2837, 1603, 1584, 1512, 1453, 1321 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  = 2.16 (s, 3H, TsCH<sub>3</sub>), 2.30 (d, 1H,  $J$  = 9.2 Hz, 3-H), 4.57 (d, 1H,  $J$  = 9.2 Hz, 2-H), 7.29-7.47 (m, 6H<sub>arom</sub>), 7.82 (d,  $J$  = 8.1 Hz, 2H<sub>arom</sub>) ppm. <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  = 23.6, 42.9, 78.5, 125.2, 127.2, 128.3, 129.2, 130.3, 136.7, 139.2, 142.9 ppm. EIMS: *m/z* = 363 [M<sup>+</sup>]. C<sub>15</sub>H<sub>13</sub>N<sub>3</sub>O<sub>6</sub>S: calcd. C 49.58, H. 3.61, N 11.56; found: C 49.51. H 3.89, N 11.72.



**5g:** IR (KBr)  $\nu_{\max}$  = 3049, 2836, 1605, 1580, 1511, 1455, 1320 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  = 2.19 (s, 3H, TsCH<sub>3</sub>), 2.28 (d, 1H,  $J$  = 9.1 Hz, 3-H), 2.40 (s, 3H, Me), 4.51 (d, 1H,  $J$  = 9.1 Hz, 2-H), 7.23-7.44 (m, 6H<sub>arom</sub>), 7.85 (d,  $J$  = 8.5 Hz, 2H<sub>arom</sub>) ppm. <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  = 23.6, 24.3, 42.6, 78.8, 126.5, 127.4, 128.3, 128.9, 129.7, 130.4, 131.3, 132.7, 135.1, 142.7 ppm. EIMS: *m/z* = 332 [M<sup>+</sup>]. C<sub>16</sub>H<sub>16</sub>N<sub>2</sub>O<sub>4</sub>S: calcd. C 57.82, H. 4.85, N 8.43; found: C 57.99. H 5.13, N 8.21.