

SUPPLEMENTARY MATERIAL TO
**Synthesis of some 3,5-diarylisoaxazoline derivatives
in ionic liquids media**

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J. Serb. Chem. Soc. 77 (6) (2012) 733–739

SPECTRAL DATA FOR THE COMPOUNDS

3,5-Diphenyl-2-isoaxazoline (3a). White crystals; FTIR (KBr, cm^{-1}): 1640 (C=N), 1580, 1472, 1434 (C=C); $^1\text{H-NMR}$ (400 MHz, CDCl_3 , δ /ppm): 2.7 (1H, *dd*, $^2J_{\text{gem}} = 14.5$ Hz, $^3J_{\text{trans}} = 6.6$ Hz, CHHCH), 3.1 (1H, *dd*, $^2J_{\text{gem}} = 14.5$ Hz, $^3J_{\text{cis}} = 8.7$ Hz, CHHCH), 5.2 (1H, *dd*, $^3J_{\text{cis}} = 8.6$ Hz, $^3J_{\text{trans}} = 6.5$ Hz, CHHCH), 6.9–7.8 (10H, *m*, Ar–H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3 , δ /ppm): 38.5, 75.2, 121.3, 125.2, 128.1, 130.0, 133.2, 137.2, 140.1, 142.5, 148.3.

3-Phenyl-5-p-tolyl-2-isoaxazoline (3b). Yellow crystals; FTIR (KBr, cm^{-1}): 1642 (C=N), 1595, 1475, 1430 (C=C); $^1\text{H-NMR}$ (400 MHz, CDCl_3 , δ /ppm): 2.1 (3H, *s*, CH_3), 2.8 (1H, *dd*, $^2J_{\text{gem}} = 14.4$ Hz, $^3J_{\text{trans}} = 6.6$ Hz, CHHCH), 3.1 (1H, *dd*, $^2J_{\text{gem}} = 14.4$ Hz, $^3J_{\text{cis}} = 8.7$ Hz, CHHCH), 5.4 (1H, *dd*, $^3J_{\text{cis}} = 8.7$ Hz, $^3J_{\text{trans}} = 6.5$ Hz, CHHCH), 6.88–7.75 (9H, *m*, Ar–H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3 , δ /ppm): 21.5, 38.2, 75.5, 121.1, 125.7, 127.2, 132.2, 134.6, 137.5, 138.2, 142.2, 147.1.

5-(4-Chlorophenyl)-3-phenyl-2-isoaxazoline (3c). White crystals; FTIR (KBr, cm^{-1}): 1645 (C=N), 1602, 1467, 1441 (C=C); $^1\text{H-NMR}$ (400 MHz, CDCl_3 , δ /ppm): 2.8 (1H, *dd*, $^2J_{\text{gem}} = 14.6$ Hz, $^3J_{\text{trans}} = 6.6$ Hz, CHHCH), 3.2 (1H, *dd*, $^2J_{\text{gem}} = 14.6$ Hz, $^3J_{\text{cis}} = 8.5$ Hz, CHHCH), 5.3 (1H, *dd*, $^3J_{\text{cis}} = 8.5$ Hz, $^3J_{\text{trans}} = 6.6$ Hz, CHHCH), 6.92–7.81 (9H, *m*, Ar–H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3 , δ /ppm): 37.7, 76.2, 120.3, 123.6, 127.2, 130.6, 133.4, 137.8, 143.2, 148.5, 155.8.

5-(4-Methoxyphenyl)-3-phenyl-2-isoaxazoline (3d). White crystals; FTIR (KBr, cm^{-1}): 1640 (C=N), 1590, 1485, 1442 (C=C); $^1\text{H-NMR}$ (400 MHz, CDCl_3 , δ /ppm): 2.9 (1H, *dd*, $^2J_{\text{gem}} = 14.5$ Hz, $^3J_{\text{trans}} = 6.4$ Hz, CHHCH), 3.3 (1H, *dd*, $^2J_{\text{gem}} = 14.5$ Hz, $^3J_{\text{cis}} = 8.8$ Hz, CHHCH), 3.6 (3H, *s*, OCH_3), 5.2 (1H, *dd*, $^3J_{\text{cis}} = 8.7$ Hz, $^3J_{\text{trans}} = 6.5$ Hz, CHHCH), 6.78–7.68 (9H, *m*, Ar–H); $^{13}\text{C-NMR}$

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-NMR (100 MHz, CDCl₃, δ / ppm): 38.4, 51.5, 75.7, 122.8, 124.6, 126.9, 130.1, 132.5, 136.8, 137.9, 139.2, 144.1.

3-(4-Bromophenyl)-5-(4-nitrophenyl)-2-isoxazoline (3e). Yellow crystals; FTIR (KBr, cm⁻¹): 1642 (C=N), 1590, 1477, 1445 (C=C); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 2.8 (1H, *dd*, ²J_{gem} = 14.8 Hz, ³J_{trans} = 6.5 Hz, CHHCH), 3.3 (1H, *dd*, ²J_{gem} = 14.8 Hz, ³J_{cis} = 8.3 Hz, CHHCH), 5.4 (1H, *dd*, ³J_{cis} = 8.4 Hz, ³J_{trans} = 6.5 Hz, CHHCH), 7.12–7.97 (8H, *m*, Ar-H); ¹³C-NMR (100 MHz, CDCl₃, δ / ppm): 38.3, 76.3, 123.2, 125.1, 127.8, 129.5, 133.8, 139.5, 145.4, 149.2, 154.7.

5-(4-Hydroxyphenyl)-3-phenyl-2-isoxazoline (3f). White crystals; Anal. Calcd. for C₁₅H₁₃NO₂: C, 75.30; H, 5.48; N, 5.85 %. Found: C, 75.25; H, 5.51; N, 5.89 %; FTIR (KBr, cm⁻¹): 1640 (C=N), 1595, 1472, 1440 (C=C); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 3.0 (1H, *dd*, ²J_{gem} = 14.7 Hz, ³J_{trans} = 6.3 Hz, CHHCH), 3.3 (1H, *dd*, ²J_{gem} = 14.7 Hz, ³J_{cis} = 8.5 Hz, CHHCH), 5.1 (1H, *bs*, OH), 5.6 (1H, *dd*, ³J_{cis} = 8.6 Hz, ³J_{trans} = 6.3 Hz, CHHCH), 6.75–7.57 (9H, *m*, Ar-H); ¹³C-NMR (100 MHz, CDCl₃, δ / ppm): 38.2, 76.1, 122.5, 124.8, 127.3, 128.8, 131.5, 134.4, 137.8, 139.9, 144.3; MS-EI (*m/z*): 239 (M⁺).

5-(4-Hydroxyphenyl)-3-p-tolyl-2-isoxazoline (3g). White crystals; Anal. Calcd. for C₁₆H₁₅NO₂: C, 75.87; H, 5.97; N, 5.53 %. Found: C, 75.91; H, 5.99; N, 5.85 %; FTIR (KBr, cm⁻¹): 1645 (C=N), 1585, 1483, 1440 (C=C); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 2.1 (3H, *s*, CH₃), 2.9 (1H, *dd*, ²J_{gem} = 14.6 Hz, ³J_{trans} = 6.4 Hz, CHHCH), 3.4 (1H, *dd*, ²J_{gem} = 14.6 Hz, ³J_{cis} = 8.2 Hz, CHHCH), 5.1 (1H, *bs*, OH), 5.5 (1H, *dd*, ³J_{cis} = 8.3 Hz, ³J_{trans} = 6.5 Hz, CHHCH), 6.88–7.67 (8H, *m*, Ar-H); ¹³C-NMR (100 MHz, CDCl₃, δ / ppm): 21.3, 37.9, 75.8, 122.2, 124.4, 125.8, 127.3, 134.6, 138.3, 141.1, 143.5, 148.5; MS-EI (*m/z*): 253 (M⁺).

5-(4-Nitrophenyl)-3-p-tolyl-2-isoxazoline (3h). Yellow crystals; FTIR (KBr, cm⁻¹): 1645 (C=N), 1595, 1480, 1442 (C=C); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 2.2 (3H, *s*, CH₃), 2.8 (1H, *dd*, ²J_{gem} = 14.8 Hz, ³J_{trans} = 6.6 Hz, CHHCH), 3.2 (1H, *dd*, ²J_{gem} = 14.8 Hz, ³J_{cis} = 8.1 Hz, CHHCH), 5.3 (1H, *dd*, ³J_{cis} = 8.1 Hz, ³J_{trans} = 6.5 Hz, CHHCH), 6.95–7.81 (8H, *m*, Ar-H); ¹³C-NMR (100 MHz, CDCl₃, δ / ppm): 21.2, 38.2, 76.5, 123.7, 124.1, 126.9, 129.2, 134.5, 140.3, 145.7, 150.2, 154.6.

5-(4-Bromophenyl)-3-p-tolyl-2-isoxazoline (3i). White crystals; FTIR (KBr, cm⁻¹): 1644 (C=N), 1588, 1472, 1448 (C=C); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 2.1 (3H, *s*, CH₃), 3.0 (1H, *dd*, ²J_{gem} = 14.5 Hz, ³J_{trans} = 6.7 Hz, CHHCH), 3.4 (1H, *dd*, ²J_{gem} = 14.5 Hz, ³J_{cis} = 8.1 Hz, CHHCH), 5.3 (1H, *dd*, ³J_{cis} = 8.1 Hz, ³J_{trans} = 6.6 Hz, CHHCH), 6.92–7.75 (8H, *m*, Ar-H); ¹³C-NMR (100 MHz, CDCl₃, δ / ppm): 21.2, 38.1, 75.6, 120.1, 123.2, 126.7, 129.3, 133.8, 136.3, 139.5, 142.4, 148.1.

3-(4-Bromophenyl)-5-(4-methoxyphenyl)-2-isoxazoline (3j). White crystals; Anal. Calcd. for $C_{16}H_{14}BrNO_2$: C, 57.85; H, 4.25; N, 4.22 %. Found: C, 57.94; H, 4.21; N, 4.16 %; FTIR (KBr, cm^{-1}): 1642 (C=N), 1592, 1475, 1440 (C=C); 1H -NMR (400 MHz, $CDCl_3$, δ / ppm): 2.8 (1H, *dd*, $^2J_{gem} = 14.7$ Hz, $^3J_{trans} = 6.6$ Hz, **CHHCH**), 3.3 (1H, *dd*, $^2J_{gem} = 14.7$ Hz, $^3J_{cis} = 8.5$ Hz, **CHHCH**), 3.6 (3H, *s*, OCH_3), 5.4 (1H, *dd*, $^3J_{cis} = 8.6$ Hz, $^3J_{trans} = 6.6$ Hz, **CHHCH**), 6.85–7.71 (8H, *m*, Ar-H); ^{13}C -NMR (100 MHz, $CDCl_3$, δ / ppm): 38.2, 52.4, 75.9, 121.5, 123.4, 125.9, 132.3, 134.5, 137.6, 140.2, 144.1, 149.3; MS-EI (*m/z*): 333 ($M+2$)⁺.