



SUPPLEMENTARY MATERIAL TO

Synthesis, structural characterization and antimicrobial evaluation of some novel piperidin-4-one oxime esters

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ANALYTICAL AND SPECTRAL DATA OF THE SYNTHESIZED COMPOUNDS

(E)-3-Methyl-2,6-diphenylpiperidin-4-one O-benzoyloxime (**8**). Colorless solid; m.p.: 116–118 °C; FTIR (KBr, cm^{-1}): 3446 (N–H stretching), 2786–3064 (C–H stretching), 1745 (C=O stretching), 1629 (C=N stretching), 1456 (C=C stretching), 735 (N–O stretching); $^1\text{H-NMR}$ (400 MHz, CDCl_3 , δ / ppm): 8.03 (2H, *d*, $J = 7.2$ Hz, Ar), 7.29–7.57 (13H, *m*, Ar), 3.95 (2H, *d*, $J = 11.6$ Hz, 1H, H6), 3.66 (2H, *d*, $J = 10$ Hz, 1H, H2), 3.56 (2H, *d*, $J = 13.6$ Hz, 1H, H5_{eq}), 2.67 (2H, *m*, 1H, H3), 2.30 (2H, *t*, $J = 12.6$ Hz, 1H, H5_{ax}), 2.00 (1H, *br s*, N–H), 1.07 (3H, *d*, $J = 6.4$ Hz, CH₃ at C3); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3 , δ / ppm): 69.02 (C2), 44.36 (C3), 164.22 (C4), 36.48 (C5), 60.94 (C6), 11.84 (CH₃ at C3), 169.51 (–O–C=O), 143.03, 141.98, 133.25, 129.63, 129.41, 128.77, 128.62, 128.15, 128.06, 127.98, 126.89 (aryl carbons); ESI-HRMS (m/z): Calcd. for $\text{C}_{25}\text{H}_{24}\text{N}_2\text{O}_2$: 384.1838. Found: 385.1916 (M+1).

(E)-3-Methyl-2,6-diphenylpiperidin-4-one O-nicotinoyloxime (**9**). Colorless solid; m.p.: 130–132 °C; FTIR (KBr, cm^{-1}): 3318 (N–H stretching), 2832–3036 (C–H stretching), 1746 (C=O stretching), 1631 (C=N stretching), 1453 (C=C, stretching), 755 (N–O stretching); $^1\text{H-NMR}$ (400 MHz, CDCl_3 , δ / ppm): 9.22 (1H *s*), 8.77 (1H, *d*, $J = 2.8$ Hz), 8.30 (1H, *d*, $J = 8.0$ Hz), 7.25–7.48 (11H, *m*, Ar), 3.97 (1H, *d*, $J = 11.2$ Hz, H6), 3.67 (1H, *d*, $J = 10$ Hz, H2), 3.54 (1H, *d*, $J = 13.6$ Hz, H5_{eq}), 2.71 (1H, *m*, H3), 2.32 (1H, *t*, $J = 12.6$ Hz, H5_{ax}), 2.08 (1H, *s*, N–H), 1.07 (3H, *d*, $J = 6.4$ Hz, CH₃ at C3); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3 , δ / ppm): 68.99 (C2), 44.37 (C3), 162.89 (C4), 36.59 (C5), 60.90 (C6), 11.75 (CH₃ at C3), 170.16 (–O–C=O), 153.67, 150.64, 142.78, 141.81, 137.17, 128.79, 128.61, 128.41, 128.17, 128.11, 127.94, 127.05, 126.78, 125.51, 123.57 (aryl carbons); GC–MS (m/z): Calcd. for $\text{C}_{24}\text{H}_{23}\text{N}_3\text{O}_2$: 385.18. Found: 386.13 (M+1).

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(E)-3-Methyl-2,6-diphenylpiperidin-4-one O-(4-chlorobenzoyl)oxime (**10**). Colorless solid; m.p.: 126–130 °C; FTIR (KBr, cm^{-1}): 3312 (N–H stretching), 2831–3084 (C–H stretching), 1746 (C=O stretching), 1641 (C=N stretching), 1447 (C=C stretching), 753 (N–O stretching); $^1\text{H-NMR}$ (400 MHz, CDCl_3 , δ / ppm): 7.95 (2H, *d*, $J = 7.6$ Hz, Ar), 7.29–7.47 (12H, *m*, Ar), 3.94 (1H, *d*, $J = 11.6$ Hz, H₆), 3.64 (1H, *d*, $J = 10$ Hz, H₂), 3.52 (1H, *d*, $J = 13.6$ Hz, H_{5eq}), 2.67 (1H, *m*, H₃), 2.30 (1H, *t*, $J = 12.6$ Hz, H_{5ax}), 2.03 (1H, *s*, N–H), 1.06 (3H, *d*, $J = 6.4$ Hz, CH₃ at C3); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3 , δ / ppm): 68.99 (C₂), 44.37 (C₃), 163.36 (C₄), 36.51 (C₅), 60.93 (C₆), 11.82 (CH₃ at C₃), 169.73 (–O–C=O), 142.96, 141.91, 139.70, 131.01, 130.73, 128.99, 128.80, 128.62, 128.17, 128.11, 127.97, 127.83, 127.15, 126.88 (aryl carbons); GC–MS (*m/z*): Calcd. for $\text{C}_{25}\text{H}_{23}\text{ClN}_2\text{O}_2$: 418.14. Found: 419.07 (M+1).

(E)-3-Methyl-2,6-diphenylpiperidin-4-one O-(4-nitrobenzoyl)oxime (**11**). Pale yellow solid; m.p.: 138–142 °C; FTIR (KBr, cm^{-1}): 3309 (N–H stretching), 2830–3106 (C–H stretching), 1745 (C=O stretching), 1607 (C=N stretching), 1453 (C=C stretching), 755 (N–O stretching); $^1\text{H-NMR}$ (400 MHz, CDCl_3 , δ / ppm): 8.28 (2H, *d*, $J = 7.2$ Hz), 8.19 (2H, *d*, $J = 7.2$ Hz), 7.31–7.48 (10H, *m*, Ar), 3.98 (1H, *d*, $J = 11.2$ Hz, H₆), 3.67 (1H, *d*, $J = 9.6$ Hz, H₂), 3.52 (1H, *d*, $J = 13.6$ Hz, H_{5eq}), 2.74 (1H, *m*, H₃), 2.35 (1H, *t*, $J = 12.6$ Hz, H_{5ax}), 1.97 (1H, *s*, N–H), 1.07 (3H, *d*, $J = 5.6$ Hz, CH₃ at C₃); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3 , δ / ppm): 68.97 (C₂), 44.40 (C₃), 162.38 (C₄), 36.57 (C₅), 60.92 (C₆), 11.73 (CH₃ at C₃), 170.47 (–O–C=O), 150.64, 149.74, 142.75, 141.71, 134.84, 130.72, 128.82, 128.63, 128.23, 128.20, 127.92, 126.83, 123.78 (aryl carbons); GC–MS (*m/z*): Calcd. for $\text{C}_{25}\text{H}_{23}\text{N}_3\text{O}_4$: 429.16. Found: 430.13 (M+1).

(E)-3-Methyl-2,6-diphenylpiperidin-4-one O-(3-methylbenzoyl)oxime (**12**). Colorless solid; m.p.: 122–124 °C; FTIR (KBr, cm^{-1}): 3320 (N–H stretching), 2790–3064 (C–H stretching), 1746 (C=O stretching), 1628 (C=N stretching), 1454 (C=C stretching), 758 (N–O stretching); $^1\text{H-NMR}$ (400 MHz, CDCl_3 , δ / ppm): 7.86 (1H, *s*, Ar), 7.82 (1H, *d*, $J = 7.6$ Hz, Ar), 7.24–7.47 (12H, *m*, Ar), 3.97 (1H, *d*, $J = 11.2$ Hz, H₆), 3.67 (1H, *d*, $J = 10$ Hz, H₂), 3.57 (1H, *d*, $J = 13.6$ Hz, H_{5eq}), 2.70 (1H, *m*, H₃), 2.39 (3H, *s*, *m*-CH₃), 2.30 (1H, *t*, $J = 12.8$ Hz, H_{5ax}), 2.05 (1H, *br s*, N–H), 1.07 (3H, *d*, $J = 6.4$ Hz, CH₃ at C₃); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3 , δ / ppm): 69.01 (C₂), 44.36 (C₃), 164.43 (C₄), 36.50 (C₅), 60.93 (C₆), 21.38 (*m*-CH₃), 11.82 (CH₃ at C₃), 169.51 (–O–C=O), 143.07, 141.99, 138.43, 134.02, 130.18, 129.32, 128.74, 128.59, 128.45, 128.12, 128.02, 127.96, 126.86, 126.68 (aryl carbons); GC–MS (*m/z*): Calcd. for $\text{C}_{26}\text{H}_{26}\text{N}_2\text{O}_2$: 398.19. Found: 399.13 (M+1).

(E)-3-Ethyl-2,6-diphenylpiperidin-4-one O-benzoyloxime (**13**). Colorless solid; m.p.: 130–134 °C; FTIR (KBr, cm^{-1}): 3311 (N–H stretching), 2866–3068 (C–H stretching), 1739 (C=O stretching), 1631 (C=N stretching), 1450 (C=C stretching), 750 (N–O stretching); $^1\text{H-NMR}$ (400 MHz, CDCl_3 , δ / ppm): 8.03

(2H, *d*, *J* = 7.6 Hz), 7.26–7.57 (13H, *m*), 3.96 (1H, *d*, *J* = 11.2 Hz, H6), 3.79 (1H, *d*, *J* = 10 Hz, H2), 3.54 (1H, *d*, *J* = 13.6 Hz, H5_{eq}), 2.59 (1H, *m*, H3), 2.29 (1H, *t*, *J* = 12.6 Hz, H5_{ax}), 1.95 (1H, *br s*, N–H), 1.74 (1H, *m*, CH₂CH₃ at C3), 1.39 (1H, *q*, CH₂CH₃ at C3), 0.95 (3H, *t*, *J* = 7.2 Hz, CH₂CH₃ at C3); ¹³C-NMR (100 MHz, CDCl₃, δ / ppm): 67.40 (C2), 51.16 (C3), 164.22 (C4), 36.81 (C5), 61.00 (C6), 19.14 (CH₂CH₃ at C3), 12.06 (CH₂CH₃ at C3), 168.15 (–O–C=O), 143.08, 142.04, 133.22, 129.62, 129.45, 128.76, 128.64, 128.61, 128.12, 128.09, 128.03, 126.87 (aryl carbons); ESI-HRMS (*m/z*): Calcd. for C₂₆H₂₆N₂O₂: 398.1994. Found: 399.2076 (M+1).

(E)-3-Ethyl-2,6-diphenylpiperidin-4-one O-nicotinoyloxime (**14**). Colorless solid; m.p.: 126–128 °C; FTIR (KBr, cm⁻¹): 3275 (N–H stretching), 2813–3034 (C–H stretching), 1751 (C=O stretching), 1629 (C=N stretching), 1456 (C=C stretching), 761 (N–O stretching); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 9.22 (1H, *s*), 8.77 (1H, *d*, *J* = 4 Hz), 8.30 (1H, *d*, *J* = 8 Hz), 7.29–7.48 (11H, *m*, Ar), 3.97 (1H, *d*, *J* = 11.2 Hz, H6), 3.80 (1H, *d*, *J* = 10 Hz, H2), 3.52 (1H, *d*, *J* = 13.2 Hz, H5_{eq}), 2.60 (1H, *m*, H3), 2.31 (1H, *t*, *J* = 12.6 Hz, H5_{ax}), 2.02 (1H, *s*, N–H), 1.74 (1H, *m*, CH₂CH₃ at C3), 1.39 (1H, *q*, CH₂CH₃ at C3), 0.95 (3H, *t*, *J* = 7.2 Hz, CH₂CH₃ at C3); ¹³C-NMR (100 MHz, CDCl₃, δ / ppm): 67.38 (C2), 51.19 (C3), 162.88 (C4), 36.90 (C5), 60.95 (C6), 19.08 (CH₂CH₃ at C3), 11.97 (CH₂CH₃ at C3), 168.81 (–O–C=O), 153.63, 150.64, 142.83, 141.88, 137.15, 128.77, 128.63, 128.14, 128.08, 128.04, 126.75, 125.55, 123.56 (aryl carbons); GC-MS (*m/z*): Calcd. for C₂₅H₂₅N₃O₂: 399.1. Found: 399.6 (M+).

(E)-3-Ethyl-2,6-diphenylpiperidin-4-one O-(4-chlorobenzoyl)oxime (**15**). Colorless solid; m.p.: 130–132 °C; FTIR (KBr, cm⁻¹): 3294 (N–H stretching), 2874–3064 (C–H stretching), 1741 (C=O stretching), 1638 (C=N stretching), 1454 (C=C stretching), 747 (N–O stretching); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 7.96 (2H, *d*, *J* = 8 Hz, Ar), 7.28–7.47 (12H, *m*, Ar), 3.95 (1H, *d*, *J* = 11.2 Hz, H6), 3.79 (1H, *d*, *J* = 10 Hz, H2), 3.49 (1H, *d*, *J* = 13.6 Hz, H5_{eq}), 2.59 (1H, *m*, H3), 2.29 (1H, *t*, *J* = 12.2 Hz, H5_{ax}), 1.96 (1H, *br s*, N–H), 1.74 (1H, *m*, CH₂CH₃ at C3), 1.38 (1H, *t*, CH₂CH₃ at C3), 0.94 (3H, *t*, *J* = 7.2 Hz, CH₂CH₃ at C3); ¹³C-NMR (100 MHz, CDCl₃, δ / ppm): 67.36 (C2), 51.15 (C3), 163.36 (C4), 36.80 (C5), 60.97 (C6), 19.11 (CH₂CH₃ at C3), 12.00 (CH₂CH₃ at C3), 168.38 (–O–C=O), 142.98, 141.94, 139.66, 130.98, 128.97, 128.77, 128.64, 128.14, 128.06, 127.87, 126.83 (aryl carbons); GC-MS (*m/z*): Calcd. for C₂₆H₂₅ClN₂O₂: 432.16. Found: 433.07 (M+1).

(E)-3-Ethyl-2,6-diphenylpiperidin-4-one O-(4-nitrobenzoyl)oxime (**16**). Pale yellow solid; m.p.: 124–128 °C; FTIR (KBr, cm⁻¹): 3295 (N–H stretching), 2816–3065 (C–H stretching), 1743 (C=O stretching), 1640 (C=N stretching), 1454 (C=C stretching), 755 (N–O stretching); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 8.26 (2H, *d*, *J* = 8.4 Hz), 8.18 (2H, *d*, *J* = 8.4 Hz), 7.28–7.47 (10H, *m*, Ar), 3.97 (1H, *d*, *J* = 10.8 Hz, H6), 3.80 (1H, *d*, *J* = 10 Hz, H2), 3.50 (1H, *d*, *J* =

= 13.2 Hz, H5_{eq}), 2.61 (1H, *m*, H3), 2.34 (1H, *t*, *J* = 12.6 Hz, H5_{ax}), 1.99 (1H, *s*, N–H), 1.73 (1H, *m*, CH₂CH₃ at C3), 1.38 (1H, *q*, CH₂CH₃ at C3), 0.95 (3H, *t*, *J* = 7.2 Hz, CH₂CH₃ at C3); ¹³C-NMR (100 MHz, CDCl₃, δ / ppm): 67.32 (C2), 51.19 (C3), 162.36 (C4), 36.86 (C5), 60.96 (C6), 19.11 (CH₂CH₃ at C3), 11.98 (CH₂CH₃ at C3), 169.11 (–O–C=O), 150.62, 142.85, 141.83, 134.92, 130.72, 128.82, 128.68, 128.20, 128.16, 128.06, 126.83, 123.78 (aryl carbons); GC–MS (*m/z*): Calcd. for C₂₆H₂₅N₃O₄: 443.1. Found: 444.6 (M+1).

(*E*)-3-Ethyl-2,6-diphenylpiperidin-4-one O-(3-methylbenzoyl)oxime (**17**). Colorless solid; m.p.: 114–116 °C; FTIR (KBr, cm⁻¹): 3323 (N–H stretching), 2802–3029 (C–H stretching), 1748 (C=O stretching), 1625 (C=N stretching), 1454 (C=C stretching), 741 (N–O stretching); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 7.86 (1H, *s*, Ar), 7.82 (1H, *d*, *J* = 7.2 Hz, Ar), 7.26–7.45 (12H, *m*, Ar), 3.95 (1H, *d*, *J* = 11.2 Hz, H6), 3.79 (1H, *d*, *J* = 10 Hz, H2), 3.53 (1H, *d*, *J* = 13.2 Hz, H5_{eq}), 2.58 (1H, *m*, H3), 2.37 (3H, *s*, *m*-CH₃), 2.28 (1H, *t*, *J* = 12.6 Hz, H5_{ax}), 1.98 (1H, *br s*, N–H), 1.76 (1H, *m*, CH₂CH₃ at C3), 1.39 (1H, CH₂CH₃ at C3), 0.95 (3H, *t*, *J* = 7 Hz, CH₂CH₃ at C3); ¹³C-NMR (100 MHz, CDCl₃, δ / ppm): 67.42 (C2), 51.18 (C3), 164.42 (C4), 36.83 (C5), 61.00 (C6), 21.42 (*m*-CH₃), 19.15 (CH₂CH₃ at C3), 12.08 (CH₂CH₃ at C3), 168.17 (–O–C=O), 143.12, 142.07, 138.43, 134.02, 130.19, 129.40, 128.76, 128.64, 128.50, 128.11, 128.02, 126.87, 126.72 (aryl carbons); ESI-HRMS (*m/z*): Calcd. for C₂₇H₂₈N₂O₂: 412.2151. Found: 413.2225 (M+1).

(*E*)-3-Isopropyl-2,6-diphenylpiperidin-4-one O-benzoyloxime (**18**). Colorless solid; m.p.: 124–126 °C; FTIR (KBr, cm⁻¹): 3321 (N–H stretching), 2822–3087 (C–H stretching), 1747 (C=O stretching), 1635 (C=N stretching), 1456 (C=C stretching), 759 (N–O stretching); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 8.00 (2H, *d*, *J* = 7.6 Hz, Ar), 7.26–7.54 (13H, *m*, Ar), 4.03 (2H, *t*, *J* = 7.2 Hz), 3.33 (1H, *d*, *J* = 14.8 Hz, H5_{eq}), 2.76 (1H, *t*, *J* = 3.4 Hz, H3), 2.55 (1H, *t*, *J* = 12.6 Hz, H5_{ax}), 1.90 (1H, *t*, *J* = 6.4 Hz, CH(CH₃)₂ at C3), 1.86 (1H, *br s*, N–H), 1.17 (3H, *d*, *J* = 6.8 Hz, CH–(Me)CH₃), 1.02 (3H, *d*, *J* = 6.4 Hz, CH–(Me)CH₃); ¹³C-NMR (100 MHz, CDCl₃, δ / ppm): 64.95 (C2), 54.16 (C3), 164.05 (C4), 36.16 (C5), 59.64 (C6), 28.48 (CH(CH₃)₂ at C3), 21.08, 18.75 (CH(CH₃)₂ at C3 carbon), 167.51 (–O–C=O), 143.45, 143.03, 133.16, 129.63, 129.45, 128.76, 128.64, 128.57, 128.01, 127.96, 126.82 (aryl carbons); ESI-HRMS (*m/z*): Calcd. for C₂₇H₂₈N₂O₂: 412.1151. Found: 413.1329 (M+1).

(*E*)-3-Isopropyl-2,6-diphenylpiperidin-4-one O-nicotinoyloxime (**19**). Colorless solid; m.p.: 128–132 °C; FTIR (KBr, cm⁻¹): 3272 (N–H stretching), 2819–3035 (C–H stretching), 1752 (C=O stretching), 1628 (C=N stretching), 1456 (C=C stretching), 761 (N–O stretching); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 9.18 (1H, *s*), 8.72 (1H, *d*, *J* = 2 Hz), 8.25 (1H, *d*, *J* = 7.6 Hz), 7.26–7.50 (11H, *m*, Ar), 4.05 (2H, *d*, *J* = 8.8 Hz), 3.31 (1H, *d*, *J* = 14.4 Hz, H5_{eq}), 2.77 (1H, *m*, H3), 2.56 (1H, *t*, *J* = 12.6 Hz, H5_{ax}), 1.91 (2H, *br s*, CH(CH₃)₂ at C3 merged with

N–H), 1.16 (3H, *d*, *J* = 6.4 Hz, CH–(Me)CH₃), 1.02 (3H, *d*, *J* = 6.4 Hz, CH–Me)CH₃); ¹³C-NMR (100 MHz, CDCl₃, δ / ppm): 64.89 (C2), 54.25 (C3), 162.69 (C4), 36.25 (C5), 59.54 (C6), 28.42 (CH(CH₃)₂ at C3), 21.11, 18.69 (CH(CH₃)₂ at C3 carbon), 168.20 (–O–C=O), 153.59, 150.66, 143.26, 142.90, 137.12, 128.79, 128.64, 128.02, 127.97, 126.72, 125.53, 123.54 (aryl carbons); ESI-HRMS (*m/z*): Calcd. for C₂₆H₂₇N₃O₂: 413.2103. Found: 414.2180 (M+1).

(*E*)-3-Isopropyl-2,6-diphenylpiperidin-4-one O-(4-chlorobenzoyl)oxime (**20**). Colorless solid; m.p.: 134–136 °C; FTIR (KBr, cm⁻¹): 3315 (N–H stretching), 2803–3073 (C–H stretching), 1745 (C=O stretching), 1631 (C=N stretching), 1454 (C=C stretching), 753 (N–O stretching); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 7.91 (*d*, *J* = 8 Hz), 7.25–7.48 (12H, *m*, Ar), 4.03 (2H, *d*, *J* = 7.6 Hz), 3.29 (1H, *d*, *J* = 14.8 Hz, H5_{eq}), 2.75 (1H, *m*, H3), 2.54 (1H, *t*, *J* = 12.6 Hz, H5_{ax}), 1.89 (1H, *t*, *J* = 6 Hz, CH(CH₃)₂ at C3), 1.85 (1H, *br s*, N–H), 1.16 (3H, *d*, *J* = 6.4 Hz, CH–(Me)CH₃), 1.02 (3H, *d*, *J* = 6.8 Hz, CH–(Me)CH₃); ¹³C-NMR (100 MHz, CDCl₃, δ / ppm): 64.96 (C2), 54.29 (C3), 163.17 (C4), 36.20 (C5), 59.64 (C6), 28.46 (CH(CH₃)₂ at C3), 21.16, 18.78 (CH(CH₃)₂ at C3 carbon), 167.79 (–O–C=O), 143.46, 143.00, 139.57, 131.03, 128.96, 128.82, 128.69, 128.04, 127.97, 127.83 (aryl carbons); GC–MS (*m/z*): Calcd. for C₂₇H₂₇ClN₂O₂: 446.1. Found: 446.0 (M+).

(*E*)-3-Isopropyl-2,6-diphenylpiperidin-4-one O-(4-nitrobenzoyl)oxime (**21**). Pale yellow solid; m.p.: 140–142 °C; FTIR (KBr, cm⁻¹): 3318 (N–H stretching), 2816–3087 (C–H stretching), 1752 (C=O stretching), 1635 (C=N stretching), 1456 (C=C stretching), 777 (N–O stretching); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 8.23 (2H, *d*, *J* = 8 Hz), 8.14 (2H, *d*, *J* = 8 Hz), 7.27–7.50 (10H, *m*, Ar), 4.07 (2H, *d*, *J* = 8 Hz), 3.31 (1H, *d*, *J* = 14.4 Hz, H5_{eq}), 2.79 (1H, *m*, H3), 2.59 (1H, *t*, *J* = 12.4 Hz, H5_{ax}), 1.92 (2H, *br s*, CH(CH₃)₂ at C3 merged with N–H), 1.16 (3H, *d*, *J* = 6 Hz, CH–(Me)CH₃), 1.02 (3H, *d*, *J* = 6 Hz, CH–(Me)CH₃); ¹³C-NMR (100 MHz, CDCl₃, δ / ppm): 64.89 (C2), 54.32 (C3), 162.20 (C4), 36.21 (C5), 59.55 (C6), 28.44 (CH(CH₃)₂ at C3), 21.11, 18.67 (CH(CH₃)₂ at C3 carbon), 168.55 (–O–C=O), 150.57, 143.28, 142.81, 134.93, 130.72, 128.82, 128.68, 128.08, 127.96, 126.76, 123.73 (aryl carbons); GC–MS (*m/z*): Calcd. for C₂₇H₂₇N₃O₄: 457.2. Found: 458.9 (M+1).

(*E*)-3-Isopropyl-2,6-diphenylpiperidin-4-one O-(3-methylbenzoyl)oxime (**22**). Colorless solid; m.p.: 136–138 °C; FTIR (KBr, cm⁻¹): 3313 (N–H stretching), 2797–3030 (C–H stretching), 1749 (C=O stretching), 1632 (C=N stretching), 1455 (C=C stretching), 757 (N–O stretching); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 7.83 (1H, *s*, Ar), 7.79 (1H, *d*, *J* = 7.6 Hz, Ar), 7.26–7.50 (12H, *m*, Ar), 4.05 (2H, *d*, *J* = 8 Hz), 3.32 (1H, *dd*, *J* = 14.4 Hz, H5_{eq}), 2.77 (1H, *m*, H3), 2.56 (1H, *q*, *J* = 11.2 Hz, H5_{ax}), 2.37 (3H, *s*, *m*-CH₃), 1.91 (1H, *t*, *J* = 5.8 Hz, CH(CH₃)₂ at C3), 1.83 (1H, *br s*, N–H), 1.16 (3H, *d*, *J* = 6.8 Hz, CH–(Me)CH₃), 1.01 (3H, *d*, *J* = 6.8 Hz, CH–(Me)CH₃); ¹³C-NMR (100 MHz,

CDCl₃, δ / ppm): 64.94 (C2), 54.18 (C3), 164.27 (C4), 36.10 (C5), 59.63 (C6), 28.49 (CH(CH₃)₂ at C3), 21.39 (*m*-CH₃), 21.05, 18.78 (CH(CH₃)₂ at C3 carbon), 167.54 (–O–C=O), 143.49, 143.05, 138.35, 133.93, 130.18, 129.38, 128.74, 128.62, 128.42, 128.01, 127.97, 127.93, 126.81, 126.72 (aryl carbons); GC–MS (*m/z*): Calcd. for C₂₈H₃₀N₂O₂: 426.2. Found: 426.9 (M⁺).

TABLE S-I. Crystal data and structural refinement for compounds **12** and **20**

Parameter	Compound	
	(<i>E</i>)-3-Methyl-2,6-diphenyl-piperidin-4-one <i>O</i> -(3-methylbenzoyl)oxime (12)	(<i>E</i>)-3-Isopropyl-2,6-diphenyl-piperidin-4-one <i>O</i> -(4-chlorobenzoyl)oxime (20)
CCDC No.	CCDC 1005453	CCDC 951598
Empirical formula	C ₂₆ H ₂₆ N ₂ O ₂	C ₂₇ H ₂₇ N ₂ O ₂ Cl
Formula weight	398.49	446.96
Color/Shape	Colorless	Colorless
Crystal dimensions, mm	0.20×0.25×0.30	0.20×0.25×0.30
Temperature, K	293(2)	293(2)
Wavelength, Å	0.71073	0.71073
Crystal system, space group	Monoclinic; <i>P</i> 2 ₁ / <i>n</i>	Monoclinic; <i>P</i> 2 ₁ / <i>n</i>
Unit cell dimensions	$a = 10.6265(6) \text{ \AA}$ $\alpha = 90.00^\circ$ $b = 12.7146(7) \text{ \AA}$ $\beta = 99.52(2)^\circ$ $c = 16.4031(8) \text{ \AA}$ $\gamma = 90.00^\circ$	$a = 11.2010(3) \text{ \AA}$ $\alpha = 90.00^\circ$ $b = 13.3924(4) \text{ \AA}$ $\beta = 100.87(2)^\circ$ $c = 16.3108(5) \text{ \AA}$ $\gamma = 90.00^\circ$
<i>Z</i> , volume, Å ³	4, 2185.7(2)	4, 2402.8(12)
Calculated density, g cm ⁻¹	1.21	1.24
Absorption coefficient	0.077	0.185
<i>F</i> (000)	848	944
Reflections Collected	5367 (3097 unique reflections)	22941 (5982 unique reflections)
θ range	2.04 – 28.26	1.98 – 28.40
Index ranges	$h = -14 - 14$; $k = -16 - 16$; $l = -21 - 19$	$h = -14 - 14$; $k = -15 - 17$; $l = -21 - 20$
Final <i>R</i> , <i>R</i> _w (obs., data)	<i>R</i> 2 = 0.057; w <i>R</i> 2 = 0.151	<i>R</i> 2 = 0.052; w <i>R</i> 2 = 0.137
Final <i>R</i> , <i>R</i> _w (all data)	<i>R</i> 2 = 0.112; w <i>R</i> 2 = 0.195	<i>R</i> 2 = 0.087; w <i>R</i> 2 = 0.159
Goodness of fit	1.045	1.022