

Summary of the Crystallographic Information

Crystal data for **2a**: $C_{18}H_{15}N_3O$, $M = 289.33$, monoclinic, $a = 13.7985(9)$, $b = 5.5755(4)$, $c = 19.3734(13)$ Å, $\alpha = 90.00$, $\beta = 90.922(1)$, $\gamma = 90.00^\circ$, $V = 1490.27(18)$ Å³, $T = 293(2)$ K, space group $P2_1/c$, $Z = 4$, 9358 reflections was measured, 3281 unique ($R_{\text{int}} = 0.0364$) which were used in all calculations. $R_1 = 0.0498$, $wR_2 = 0.1448$ for 200 parameters and 2698 contributing reflections ($|F_o| > 4\sigma(F_o)$). CCDC 682967.

Crystal data for **7d**: $C_{17}H_{14}ClN_3O$, $M = 311.76$, triclinic, $a = 8.1063(6)$, $b = 9.5886(6)$, $c = 11.0798(8)$ Å, $V = 769.42(9)$ Å³, $\alpha = 75.304(1)$, $\beta = 78.028(1)$, $\gamma = 68.630(1)^\circ$, $T = 293(2)$ K, space group $P\bar{1}$, $Z = 2$, 5072 reflections was measured, 3282 unique ($R_{\text{int}} = 0.0327$) which were used in all calculations. $R_1 = 0.0565$, $wR_2 = 0.1634$ for 227 parameters and 2762 contributing reflections ($|F_o| > 4\sigma(F_o)$). CCDC 682968.

Crystal data for **N-1-3a**: $C_{23}H_{19}N_3$, $M = 337.41$, triclinic, $a = 9.6394(9)$, $b = 10.7499(10)$, $c = 10.9959(9)$ Å, $\alpha = 62.390(1)$, $\beta = 68.503(2)$, $\gamma = 68.570(2)^\circ$, $V = 912.63(14)$ Å³, $T = 293(2)$ K, space group $P\bar{1}$, $Z = 2$, 6310 reflections was measured, 4000 unique ($R_{\text{int}} = 0.0327$) which were used in all calculations. $R_1 = 0.0560$, $wR_2 = 0.1543$ for 235 parameters and 2986 contributing reflections ($|F_o| > 4\sigma(F_o)$). CCDC 682966.

Crystal data for **N-1-5a**: $C_{22}H_{19}N_3O$, $M = 341.40$, monoclinic, $a = 18.7577(12)$, $b = 10.4782(6)$, $c = 19.7381(12)$ Å, $\alpha = 90.00$, $\beta = 110.054(1)$, $\gamma = 90.00^\circ$, $V = 3644.2(4)$ Å³, $T = 293(2)$ K, space group $P2_1/n$, $Z = 8$, 24801 reflections was measured, 8190 unique ($R_{\text{int}} = 0.0392$) which were used in all calculations. $R_1 = 0.0498$, $wR_2 = 0.1313$ for 471 parameters and 5540 contributing reflections ($|F_o| > 4\sigma(F_o)$). CCDC 682970.

Crystal data for **N-2-4a (7a)**: $C_{22}H_{17}N_3O$, $M = 339.39$, orthorhombic, $a = 8.4845(8)$, $b = 20.369(2)$, $c = 20.976(2)$ Å, $\alpha = 90.00$, $\beta = 90.00$, $\gamma = 90.00^\circ$, $V = 3625.1(6)$ Å³, $T = 293(2)$ K, space group $P2_12_12_1$, $Z = 8$, 25799 reflections was measured, 8259 unique ($R_{\text{int}} = 0.0501$) which were used in all calculations. $R_1 = 0.0509$, $wR_2 = 0.1250$ for 469 parameters and 5061 contributing reflections ($|F_o| > 4\sigma(F_o)$). CCDC 682969.