

X-ray Crystal Data for Compound 4b. X-ray diffraction analysis was carried out on a Bruker SMART APEX II CCD area detector system equipped with a graphite monochromator and a Mo K α fine-focus sealed tube ($\lambda=0.71073$ Å), at 100K. The structure was solved by direct methods (SHELXS-97) and refined with full-matrix least-squares on F^2 (SHELXL-97). All non-hydrogen atoms were refined anisotropically, and all hydrogen atoms were placed in idealized positions and refined as riding atoms with the relative isotropic parameters.

Crystallographic data of **Compound 4b**: Colorless block crystals from EtOH, C₃₆H₃₆N₂O₆.H₂O, $M_r = 610.68$, monoclinic, space group $P2_1/c$, $a = 16.4733(3)$ Å, $b = 18.0651(3)$ Å, $c = 31.8360(6)$ Å, $\alpha = \gamma = 90^\circ$, $\beta = 91.2600(10)^\circ$, $V = 9471.8(3)$ Å³, $T = 100$ K, $Z = 12$, $D_{\text{calcd}} = 1.285$ gcm⁻³, crystal size 0.20 x 0.35 x 0.49 mm³, $F(000) = 3888$. The final R_1 value is 0.0534 ($wR_2 = 0.1141$) for 21783 reflections [$I > 2\sigma(I)$].

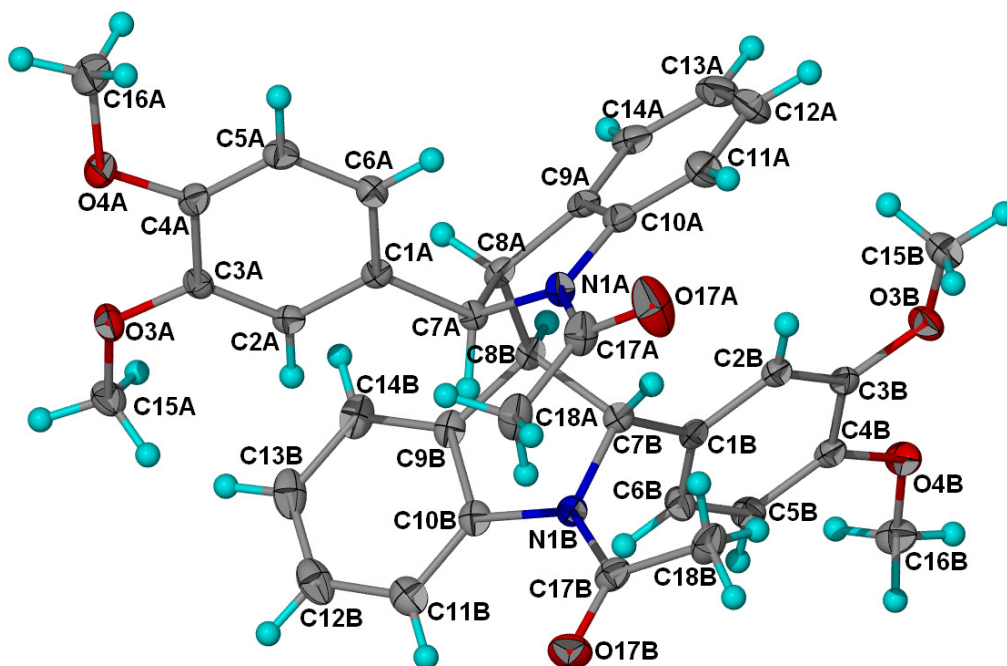


Figure 1. X-ray crystal structure of **Compound 4b**. Thermal ellipsoids are shown at the 50% probability level.

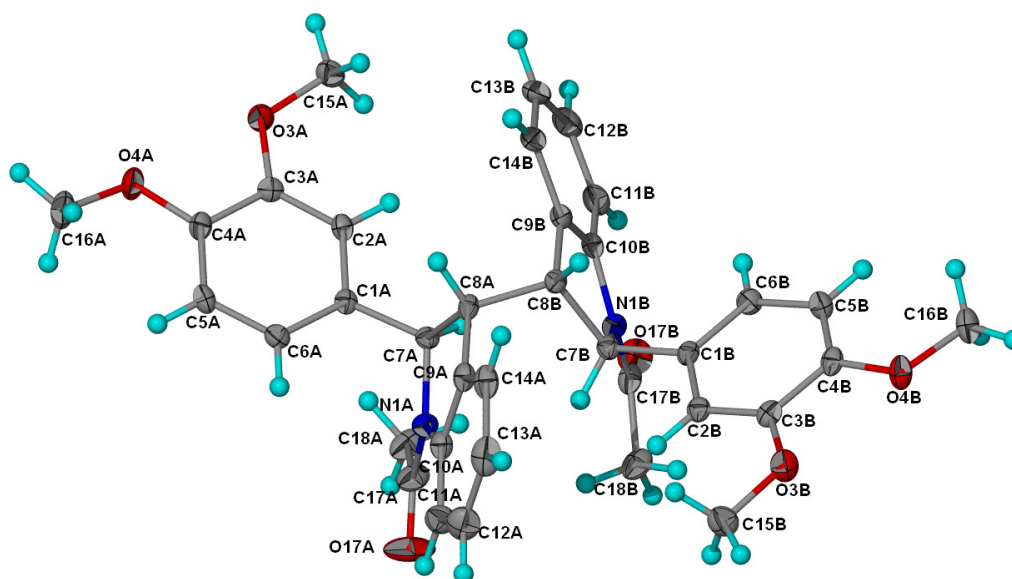


Figure 2. X-ray crystal structure of **Compound 4b**. Thermal ellipsoids are shown at the 50% probability level.