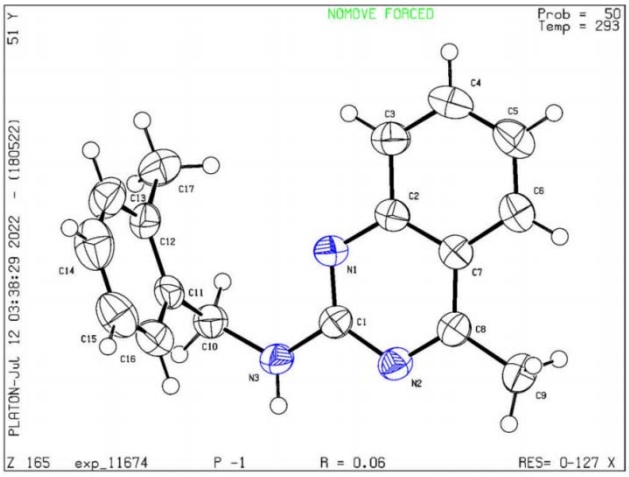
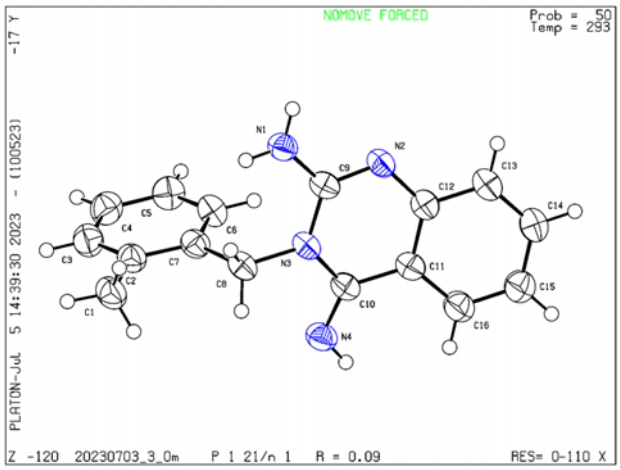
The Crystallographic Data



The purified compound **3aa** is dissolved in a mixed solvent of acetonitrile, $CHCl_3$, EtOAc and EtOH, placed in a dark cabinet to slowly evaporate. After several days, a white bulk crystal is obtained. The X-ray crystal-structure determinations were obtained on a Bruker APEX DUO CCD system.

Table S1. The crystallographic data of **3aa** (CCDC: 2294005).

Identification code	exp_11674
Empirical formula	$C_{17}H_{17}N_3$
Formula weight	263.33
Temperature	293(2)
Crystal system	triclinic
Space group	P-1
Unit cell dimensions	a = 7.6755(14) Å α = 88.372(14)°. b = 8.2355(15) Å β = 72.051(16)°. c = 11.482(2) Å γ = 85.342(15)°.
Volume	688.2(2) $Å^3$
Z	2
ρ_{calc} g/cm^3	1.271
μ /mm-1	0.077
F (000)	280.0
Crystal size	0.2 x 0.12 x 0.09 mm^3
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.962 to 54
Index ranges	-9 ⩽h ⩽9, -10⩽k⩽10, -14⩽l⩽14
Reflections collected	5825
Independent reflections	2941[R_{int} = 0.0370, R_{sigma} = 0.0657]
Data / restraints / parameters	2941/0/183
Goodness-of-fit on F^2	1.029
Final R indices [I>2sigma(I)]	R_1 = 0.0598, wR_2 = 0.1290
R indices (all data)	R_1 = 0.1004, wR_2 = 0.1571
Largest diff. peak and hole	0.15 and -0.24 e.$Å^{-3}$



The purified compound 5**ab** is dissolved in a mixed solvent of acetonitrile, $CHCl_3$, EtOAc and EtOH, placed in a dark cabinet to slowly evaporate. After several days, a white bulk crystal is obtained. The X-ray crystal-structure determinations were obtained on a Bruker APEX DUO CCD system.

Table S2. The crystallographic data of **5ab** (CCDC: 2294029).

Identification code	20230703_3_0m
Empirical formula	$C_{16}H_{16}N_4$
Formula weight	264.33
Temperature	293.30
Crystal system	monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 11.3243(5) Å α = 90°. b = 9.3817(4) Å β = 108.821(2)°. c = 13.5342(6) Å γ = 90°.
Volume	1361.01(10) $Å^3$
Z	4
ρ_{calc} g/cm^3	1.290
μ /mm-1	0.080
F (000)	560.0
Crystal size	0.2 x 0.14 x 0.12 mm^3
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	5.382 to 52.718
Index ranges	-14 ⩽h⩽13, 0⩽k⩽11, 0⩽l⩽16
Reflections collected	2729
Independent reflections	2729[R_{int} = ?, R_{sigma} = 0.0559]
Data / restraints / parameters	2729/0/183
Goodness-of-fit on F^2	1.080
Final R indices [I>2sigma(I)]	R_1 = 0.0942, wR_2 = 0.2251
R indices (all data)	R_1 = 0.1218, wR_2 = 0.2544
Largest diff. peak and hole	0.34 and -0.42 e.$Å^{-3}$