



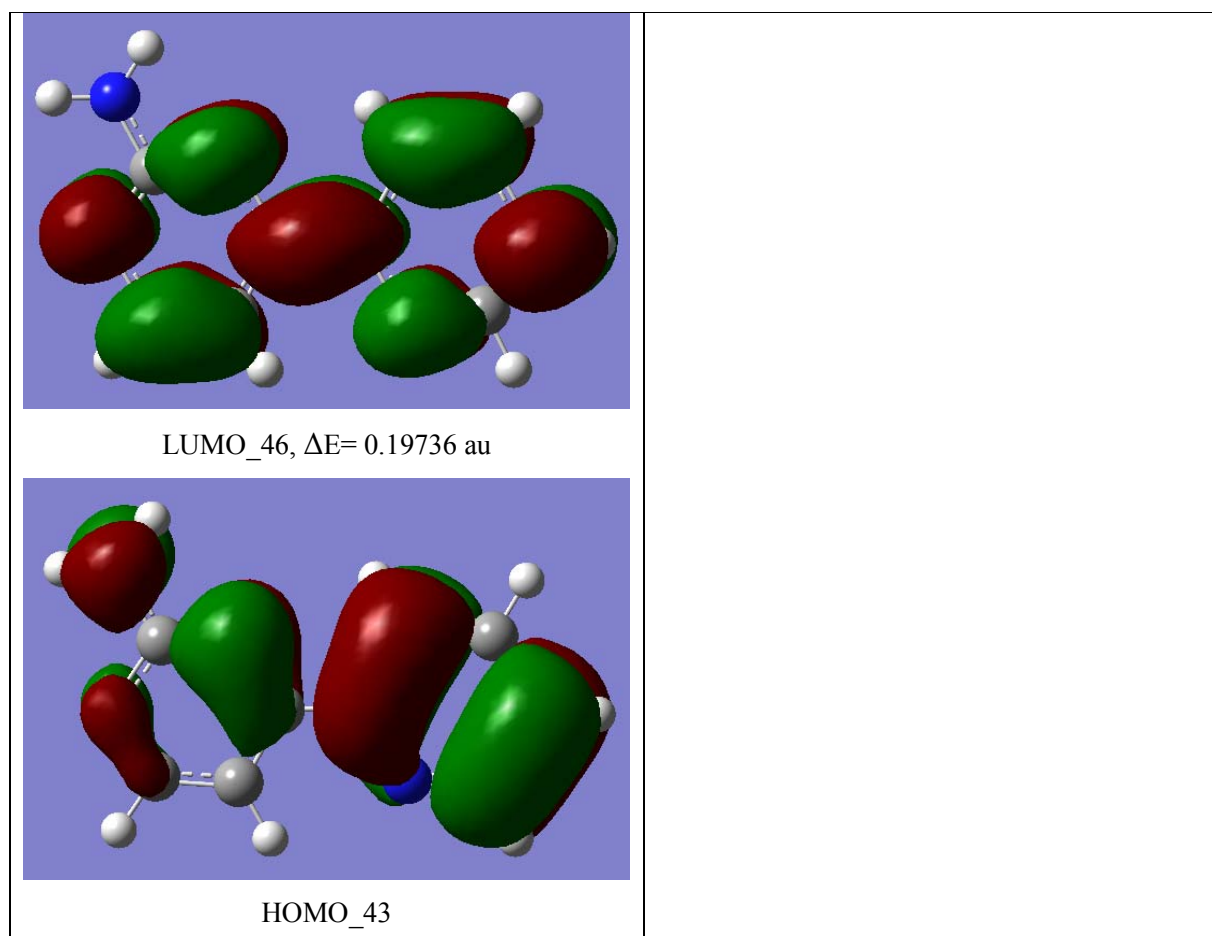
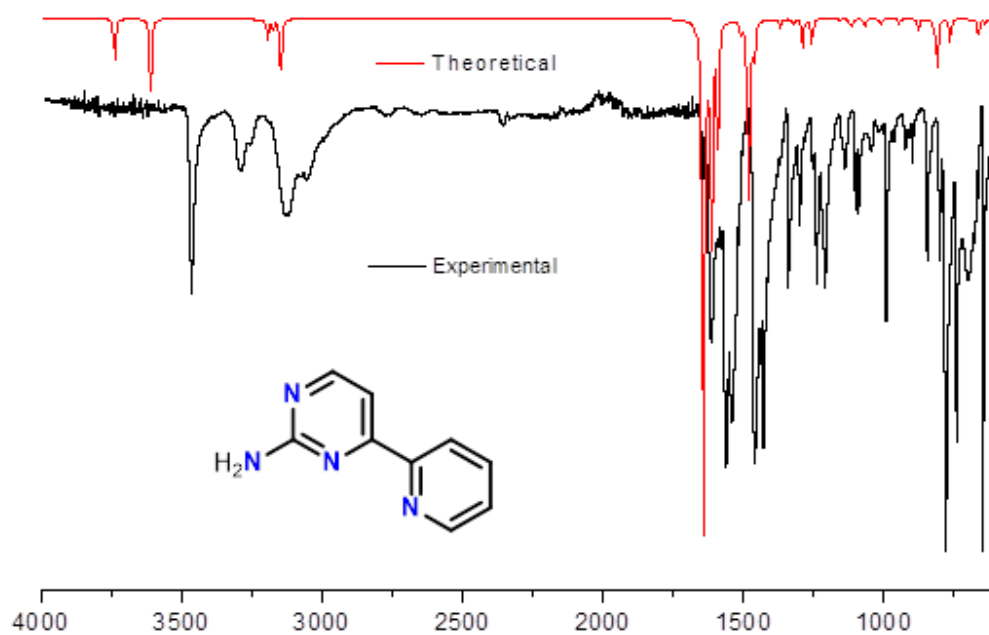
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Supporting information for article:

Synthesis, spectroscopic (FT–IR and UV–Vis), crystallographic and theoretical studies, and molecular docking simulation of an imatinib-like template

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Excitation energies and oscillator strengths of UV spectrum for pyrimidine-piridine compound

Excited State 2: Singlet-A 3.9238 eV 315.98 nm $f=0.0964$ $\langle S^{*2} \rangle=0.000$

44 -> 46 -0.13040

45 -> 46 0.68340

Excited State 6: Singlet-A 4.9640 eV 249.77 nm $f=0.3648$ $\langle S^{*2} \rangle=0.000$

41 -> 46 0.10469

41 -> 47 0.10401

43 -> 46 0.60913

43 -> 47 -0.10229

45 -> 47 -0.28880

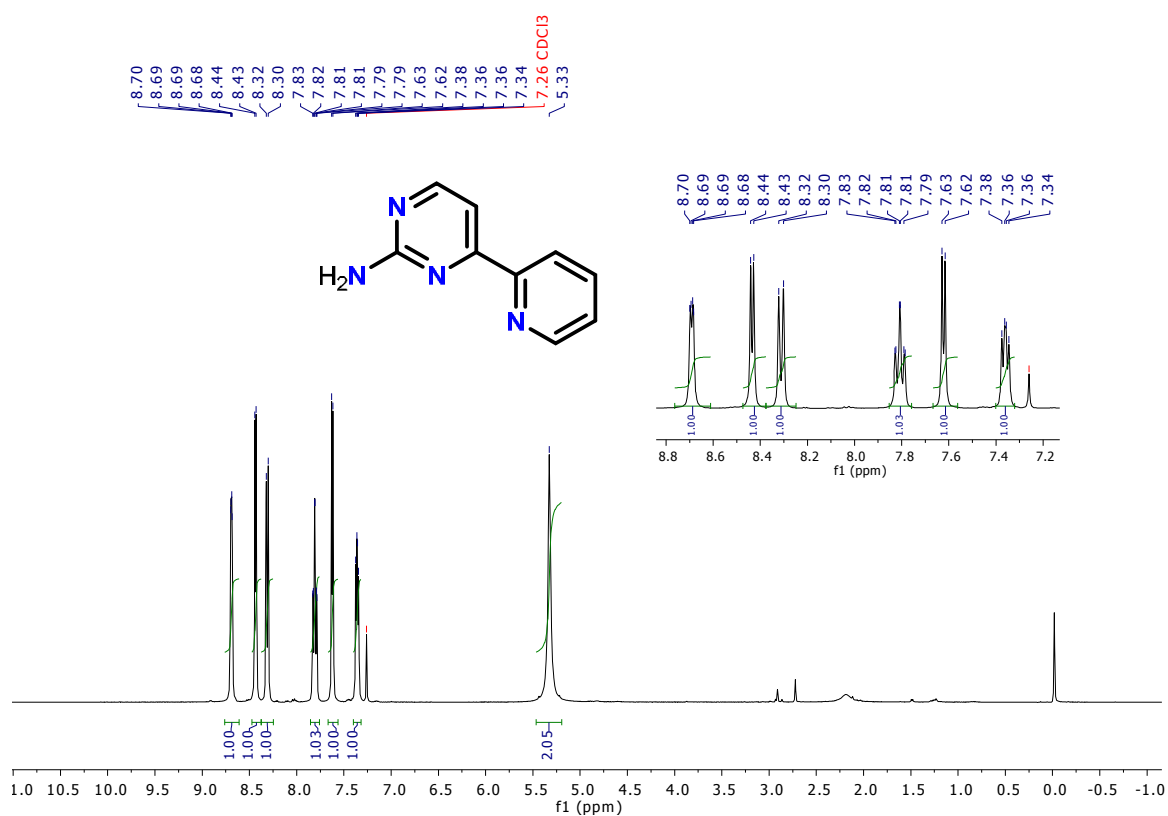
Excited State 8: Singlet-A 5.3490 eV 231.79 nm $f=0.0295$ $\langle S^{*2} \rangle=0.000$

41 -> 46 -0.44300

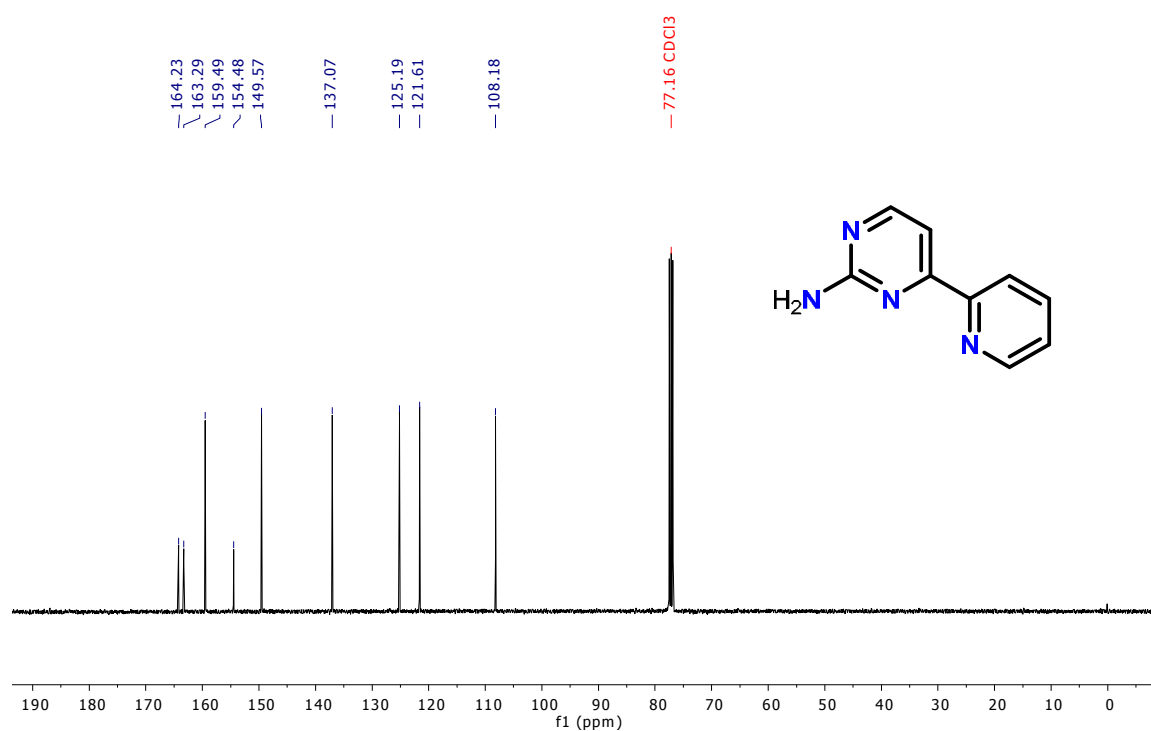
43 -> 46 0.18774

43 -> 47 0.49688

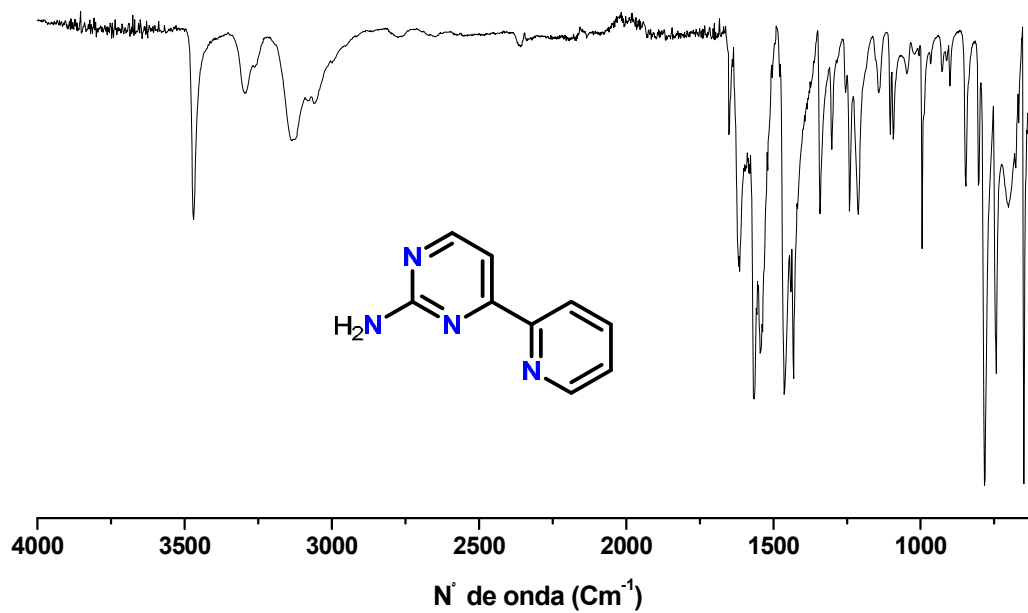
4-(pyridin-2-yl)pyrimidin-2-amine



¹H NMR (400 MHz, Chloroform-*d*), δ (ppm): 8.69 (dd, $J = 4.7, 1.7$ Hz, 1H), 8.43 (d, $J = 5.2$ Hz, 1H), 8.31 (d, $J = 7.9$ Hz, 1H), 7.81 (td, $J = 7.8, 1.8$ Hz, 1H), 7.62 (d, $J = 5.1$ Hz, 1H), 7.36 (dd, $J = 7.5, 4.8$ Hz, 1H), 5.33 (s, 2H, -NH₂).



^{13}C NMR (100 MHz, Chloroform-*d*), δ (ppm): 164.23, 163.29, 159.49, 154.48, 149.57, 137.07, 125.19, 121.61, 108.18.



IR (FT-IR): 3469.94, 3296.35, 3126.61, 1651.07, 1614.42, 1566.20, 1544.98, 1463.97, 1431.18, 1342.46, 1301.95, 1242.16, 1211.30, 1103.28, 1093.64, 846.75, 804.32, 783.10, 742.59, 650.01

