

Supplementary Material:

One-pot solvent-participated synthesis of 5-O-substituted 5H-chromeno[2,3-b]pyridines

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1. The copies of ^1H NMR and ^{13}C NMR spectra for compounds 4a-i

Figure S1. ^1H NMR spectrum of 2,4-diamino-5-methoxy-5*H*-chromeno[2,3-*b*]pyridine-3-carbonitrile **4a** in $\text{DMSO-}d_6$.

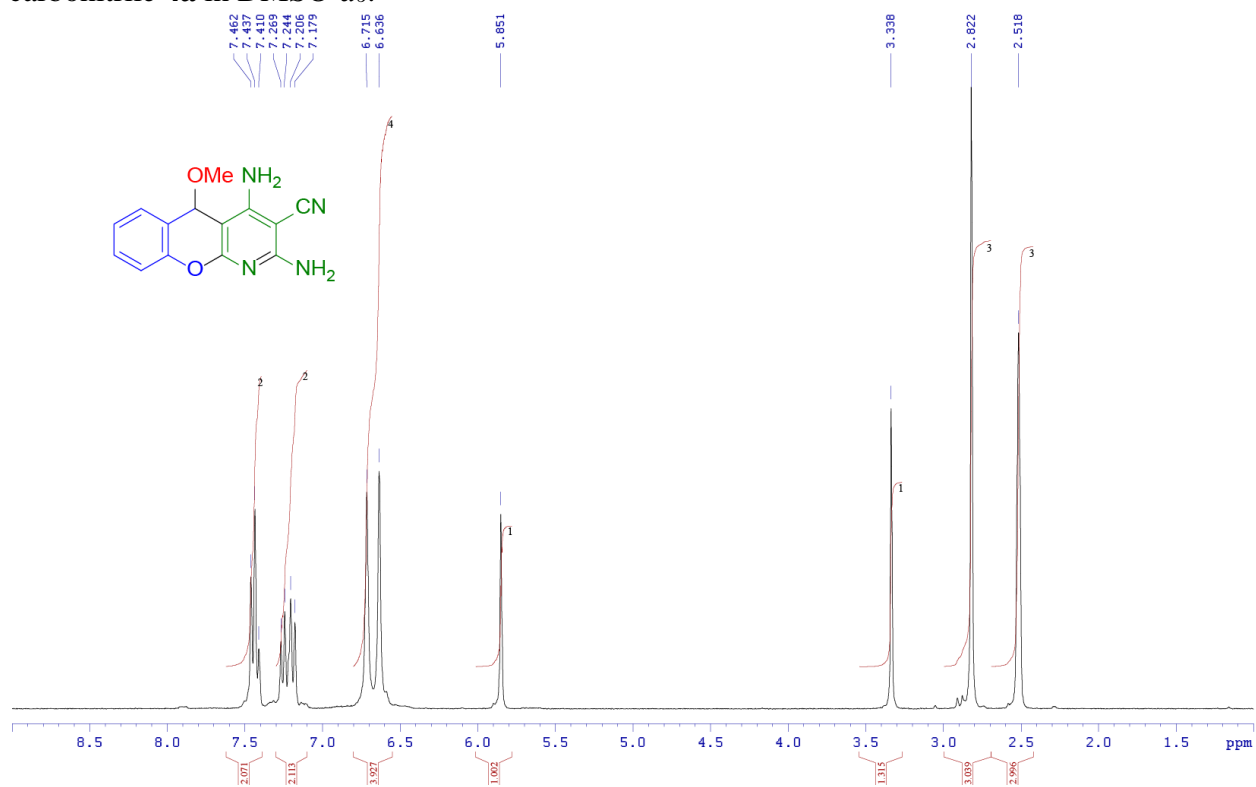


Figure S2. ^{13}C NMR spectrum of 2,4-diamino-5-methoxy-5*H*-chromeno[2,3-*b*]pyridine-3-carbonitrile **4a** in $\text{DMSO-}d_6$.

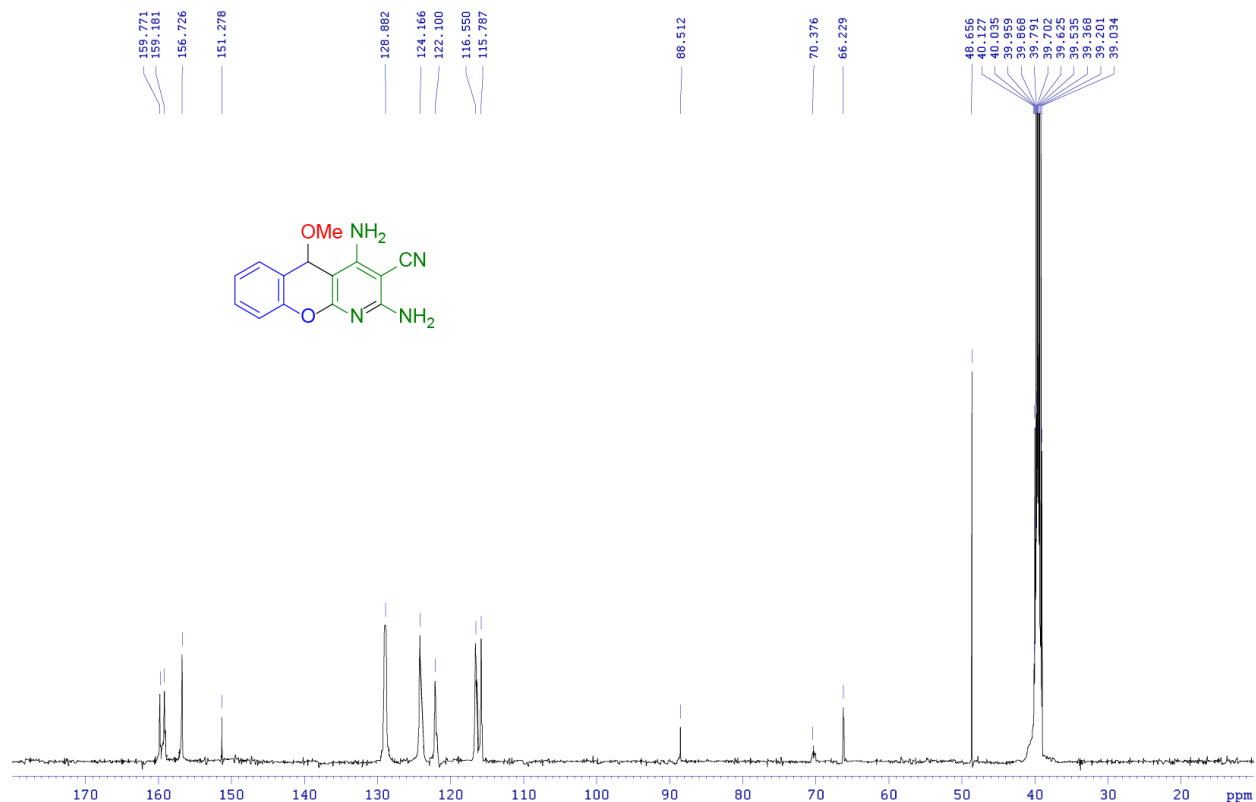


Figure S3. ^1H NMR spectrum of 2,4-diamino-5-ethoxy-5*H*-chromeno[2,3-*b*]pyridine-3-carbonitrile **4b** in $\text{DMSO-}d_6$.

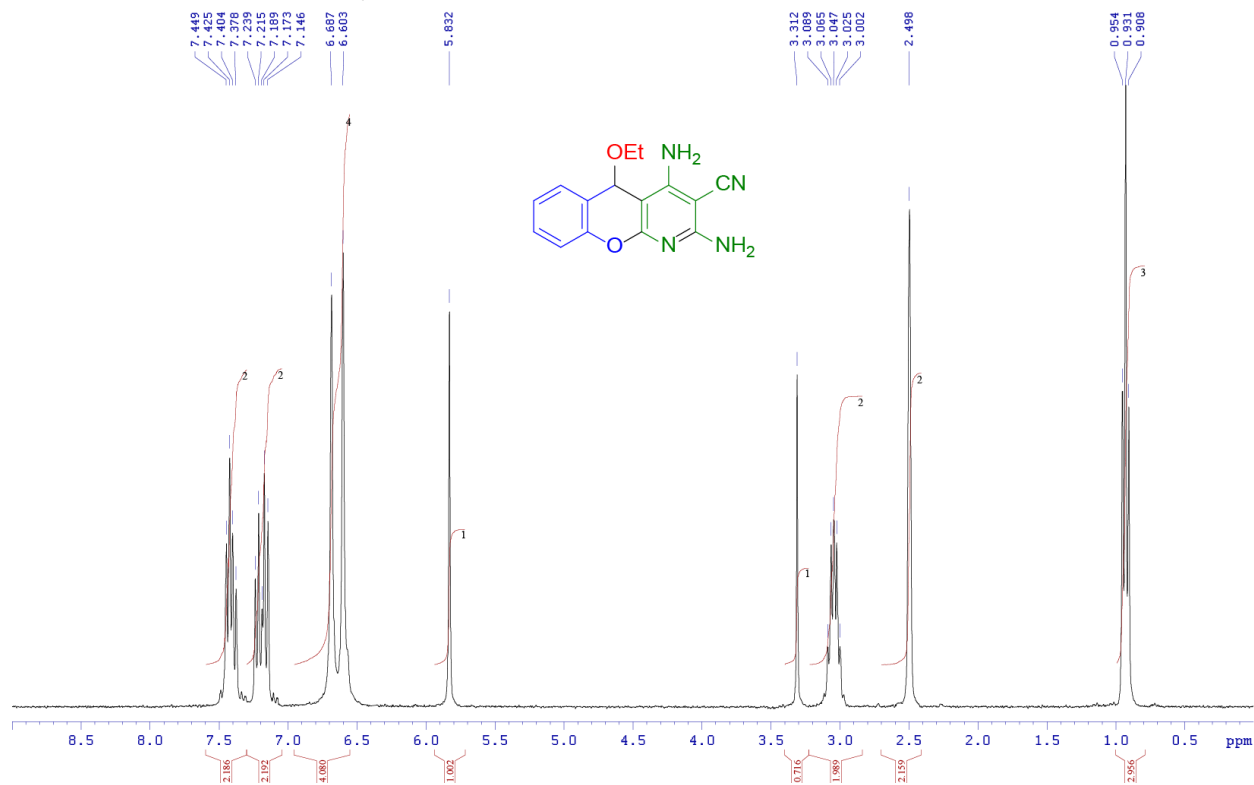


Figure S4. ^{13}C NMR spectrum of 2,4-diamino-5-ethoxy-5*H*-chromeno[2,3-*b*]pyridine-3-carbonitrile **4b** in $\text{DMSO-}d_6$.

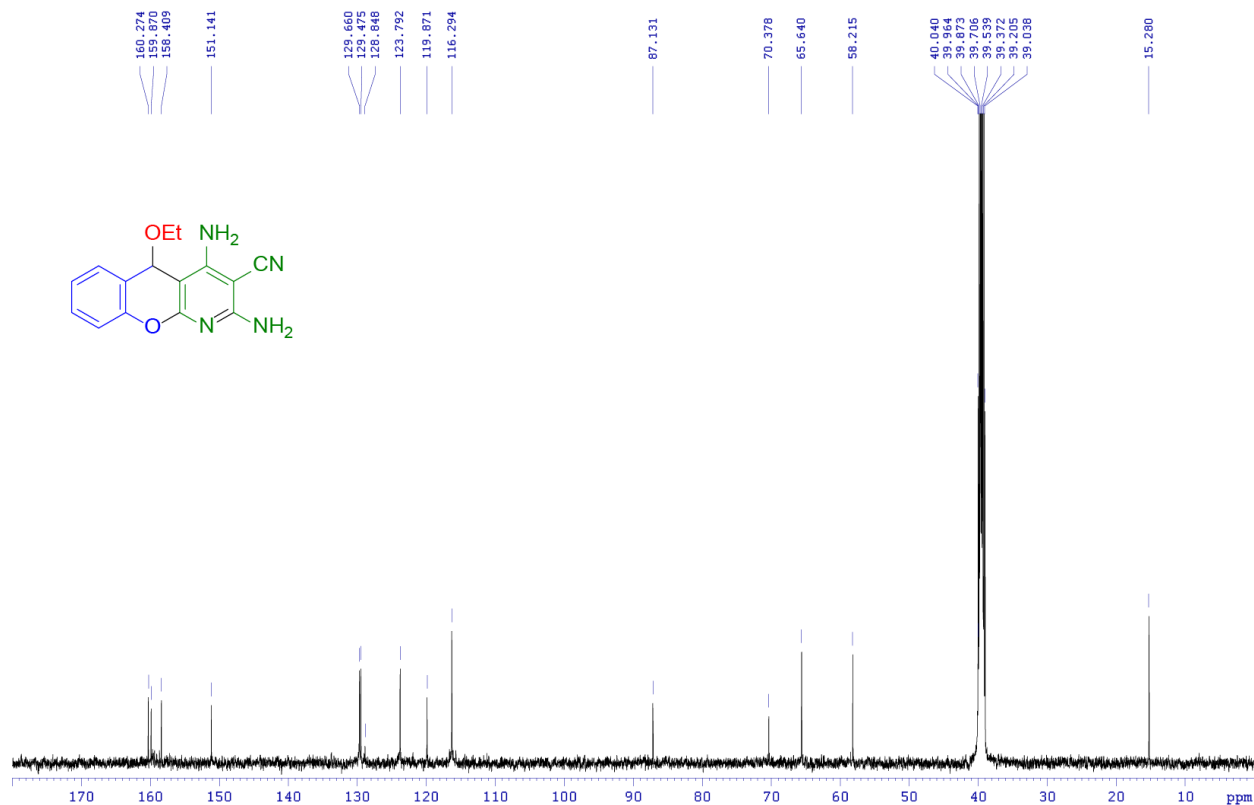


Figure S5. ^1H NMR spectrum of 2,4-diamino-5-propoxy-5*H*-chromeno[2,3-*b*]pyridine-3-carbonitrile **4c** in $\text{DMSO-}d_6$.

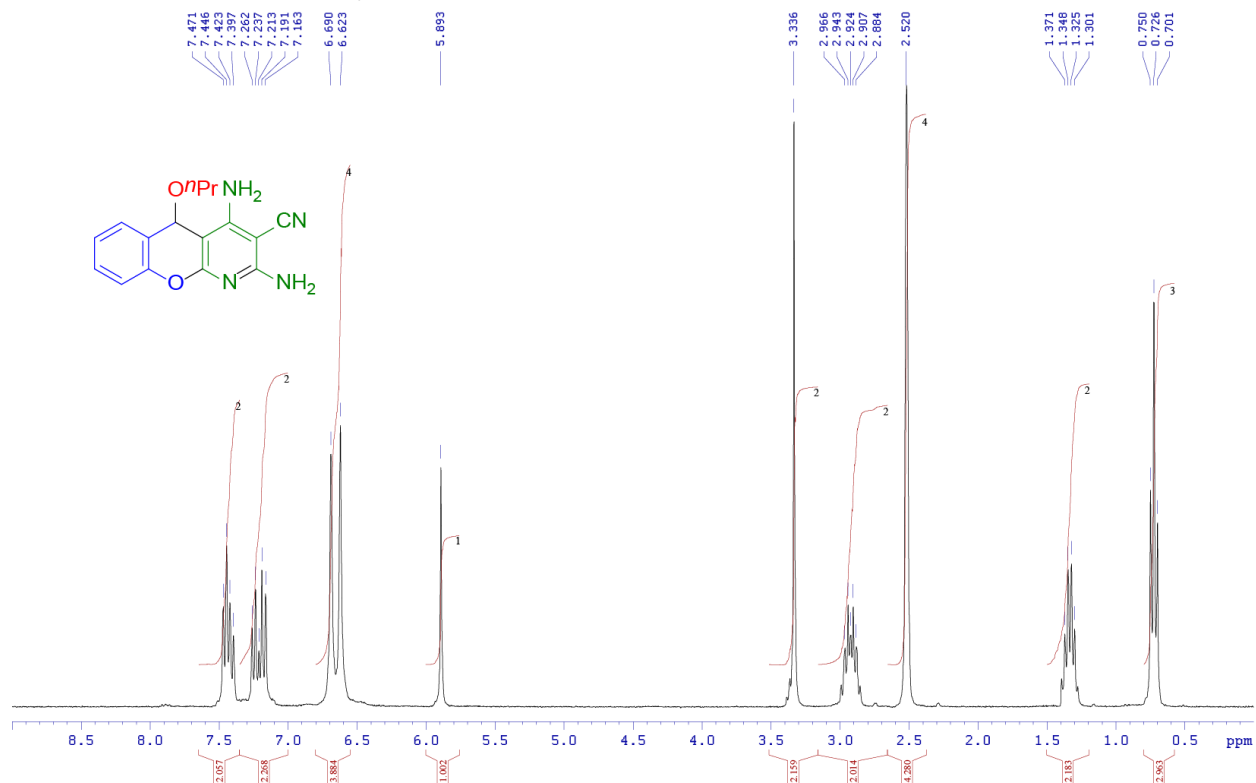


Figure S6. ^{13}C NMR spectrum of 2,4-diamino-5-propoxy-5*H*-chromeno[2,3-*b*]pyridine-3-carbonitrile **4c** in $\text{DMSO-}d_6$.

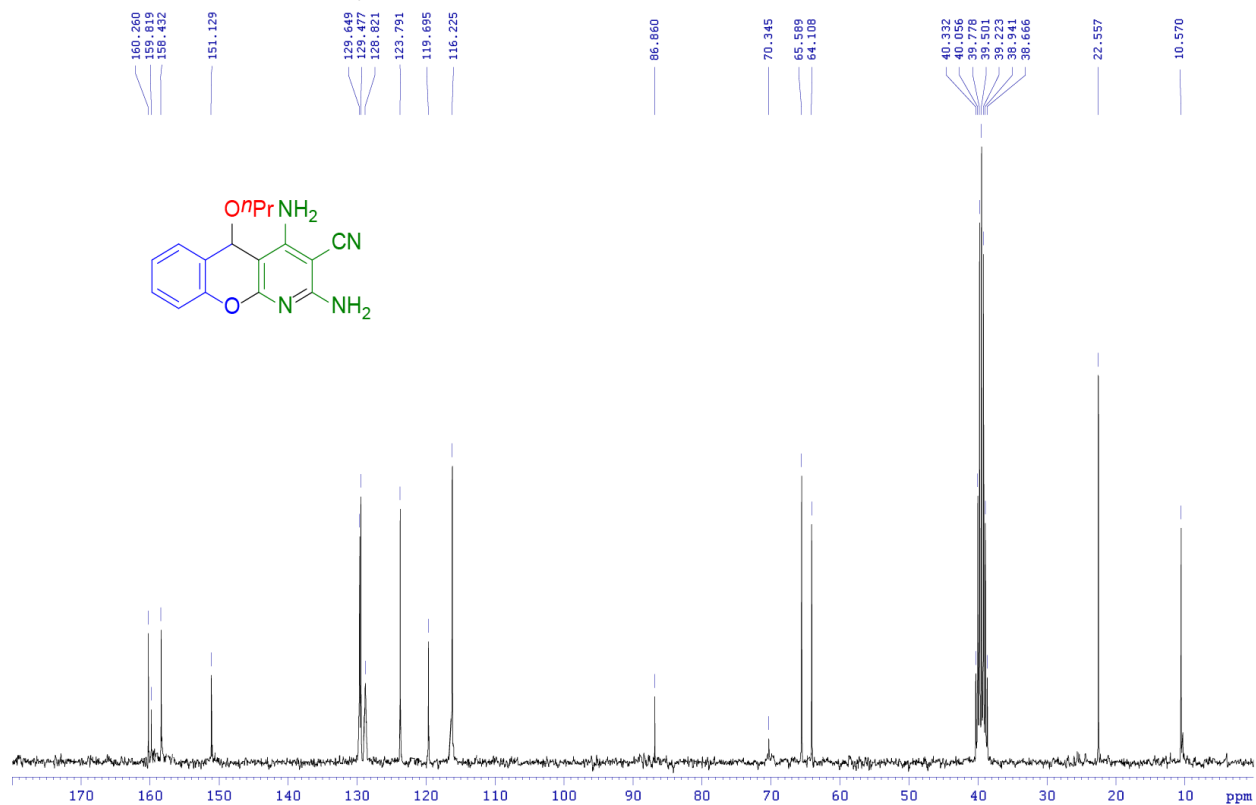


Figure S7. ^1H NMR spectrum of 2,4-diamino-5,8-dimethoxy-5*H*-chromeno[2,3-*b*]pyridine-3-carbonitrile **4d** in $\text{DMSO-}d_6$.

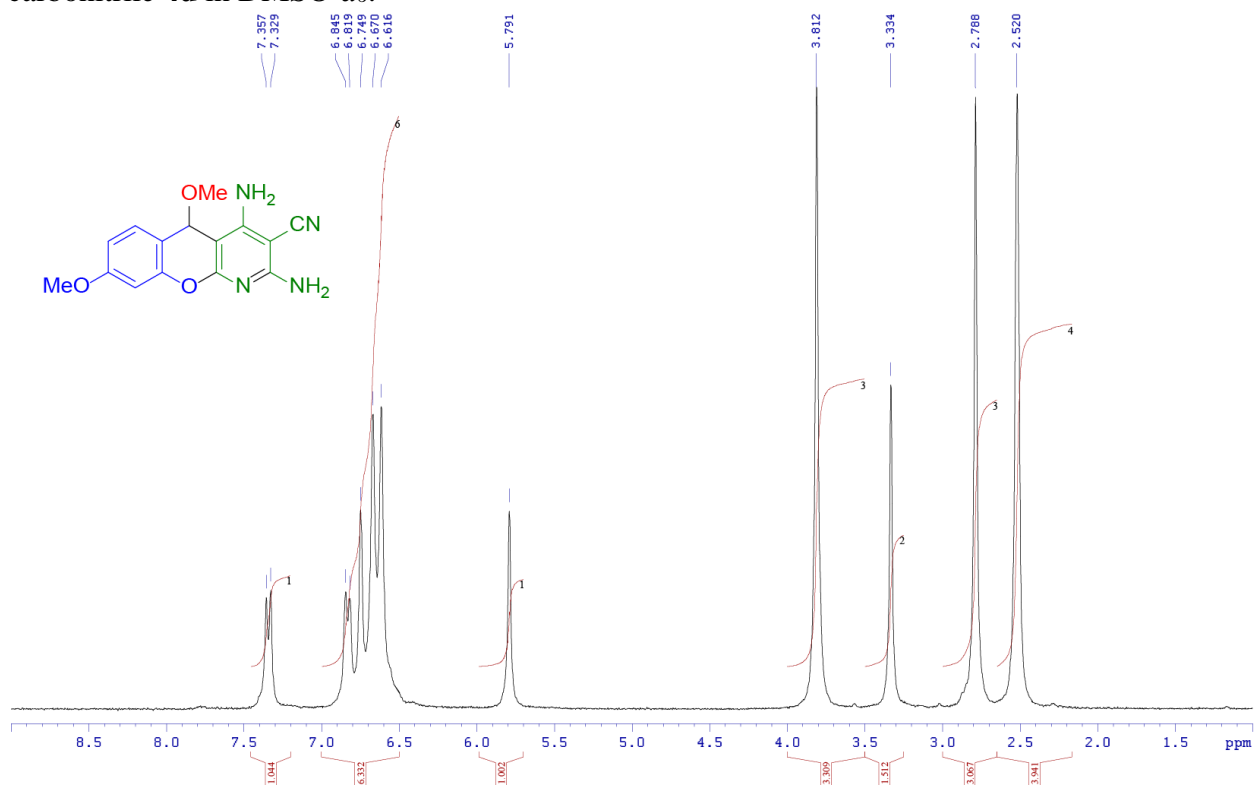
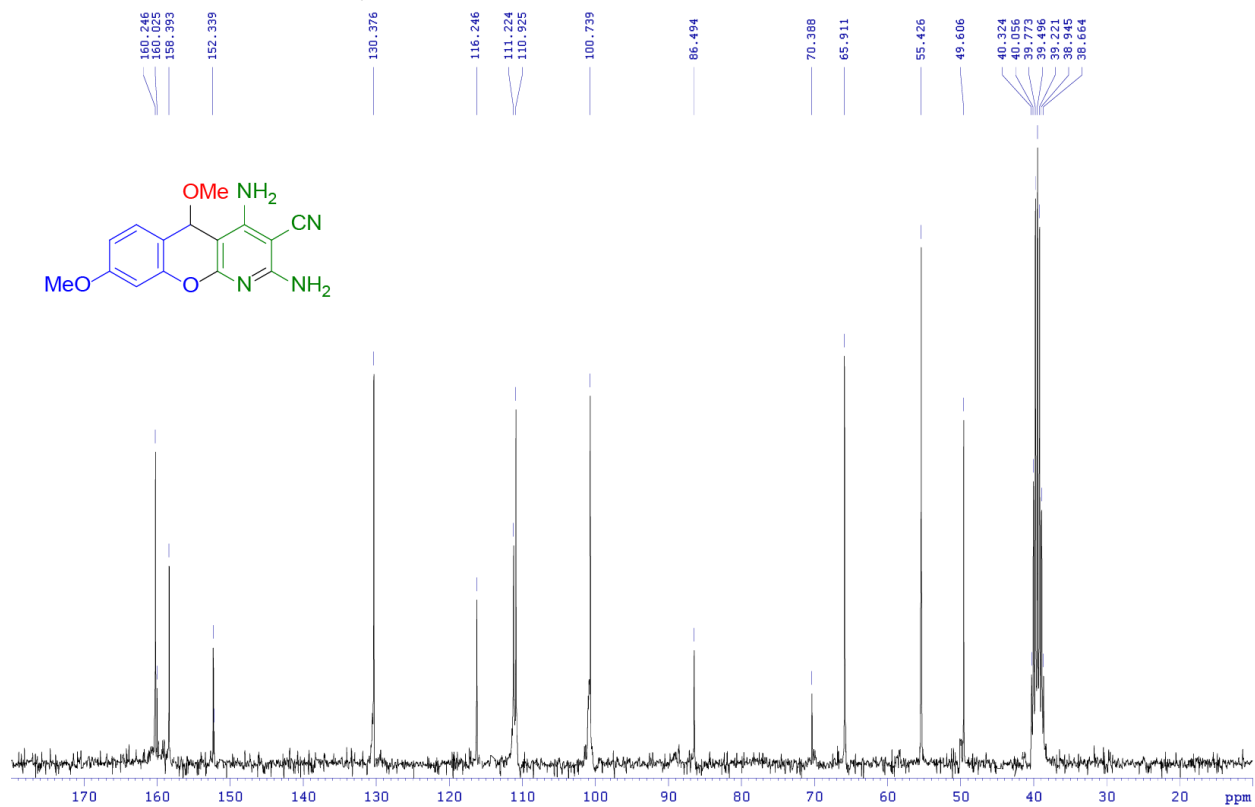


Figure S8. ^{13}C NMR spectrum of 2,4-diamino-5,8-dimethoxy-5*H*-chromeno[2,3-*b*]pyridine-3-carbonitrile **4d** in $\text{DMSO-}d_6$.



Chemical structure: CCOC1=CC=C2C(=C1)N=CN(C=C2)C#N

¹H NMR spectrum (CDCl₃) showing peaks labeled 1, 2, 3, 4, and 6. The x-axis is chemical shift in ppm (0.5 to 8.5). Integration values are shown below the baseline.

Peak Label	Chemical Shift (ppm)	Integration
1	~7.4	1.000
2	~3.1	1.999
3	~3.8	2.004
4	~2.5	4.384
6	~6.7	6.170

Chemical structure of the compound is shown above the spectrum. The structure is a benzimidazole derivative with a 4-methoxyphenyl group, an ethoxy group, and a 2,6-diaminophenyl group.

COc1ccc2c(c1)oc3c(nc(N)c(N)c3c2)OCC

The spectrum shows peaks corresponding to the chemical structure, with the following chemical shifts (ppm) labeled above the peaks:

- 160.159, 159.622, 158.347, 152.106, 152.007, 130.255, 116.259, 111.982, 110.842, 100.776, 87.209, 70.370, 65.326, 57.714, 55.406, 40.319, 40.053, 39.773, 39.486, 38.218, 38.040, 38.663, 15.264.

The spectrum is a ¹³C NMR spectrum, showing peaks in the aromatic region (100-160 ppm) and aliphatic region (15-60 ppm).

Figure S11. ^1H NMR spectrum of 2,4-diamino-8-methoxy-5-propoxy-5*H*-chromeno[2,3-*b*]-pyridine-3-carbonitrile **4f** in $\text{DMSO-}d_6$.

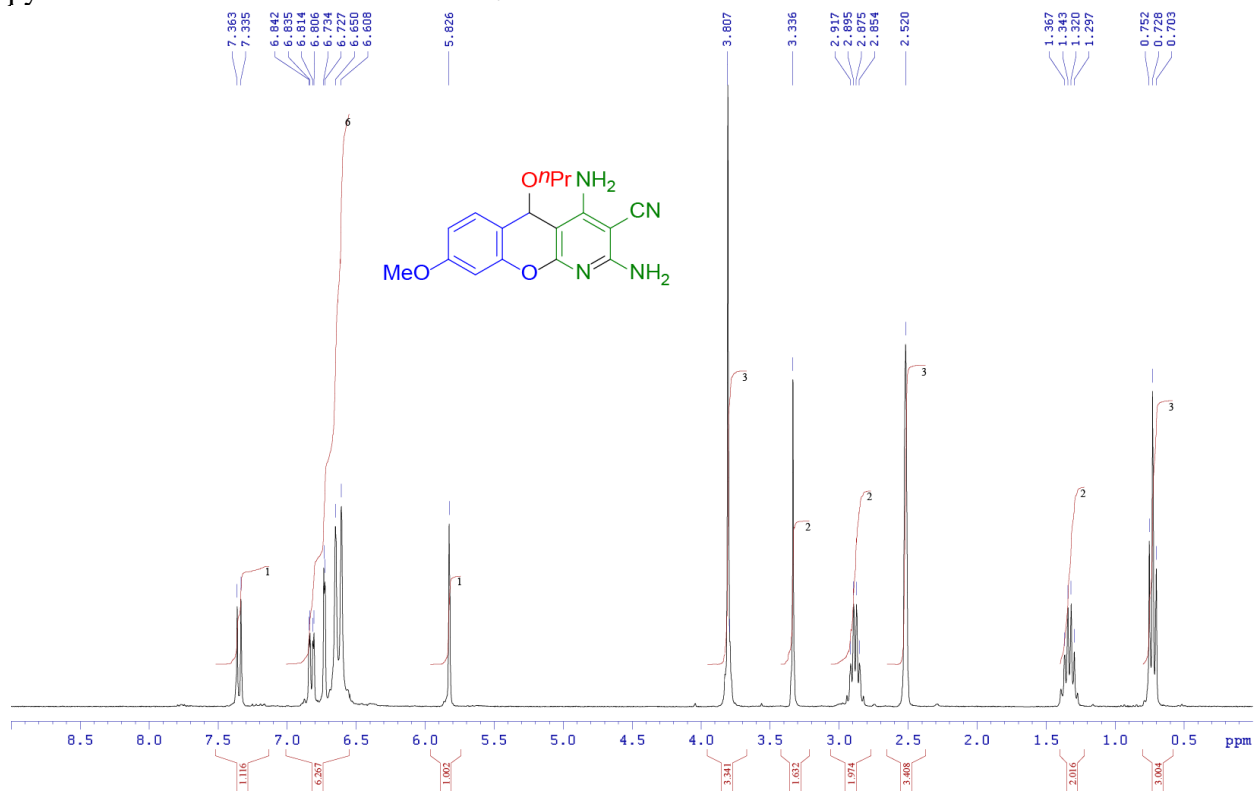


Figure S12. ^{13}C NMR spectrum of 2,4-diamino-8-methoxy-5-propoxy-5*H*-chromeno[2,3-*b*]-pyridine-3-carbonitrile **4f** in $\text{DMSO-}d_6$.

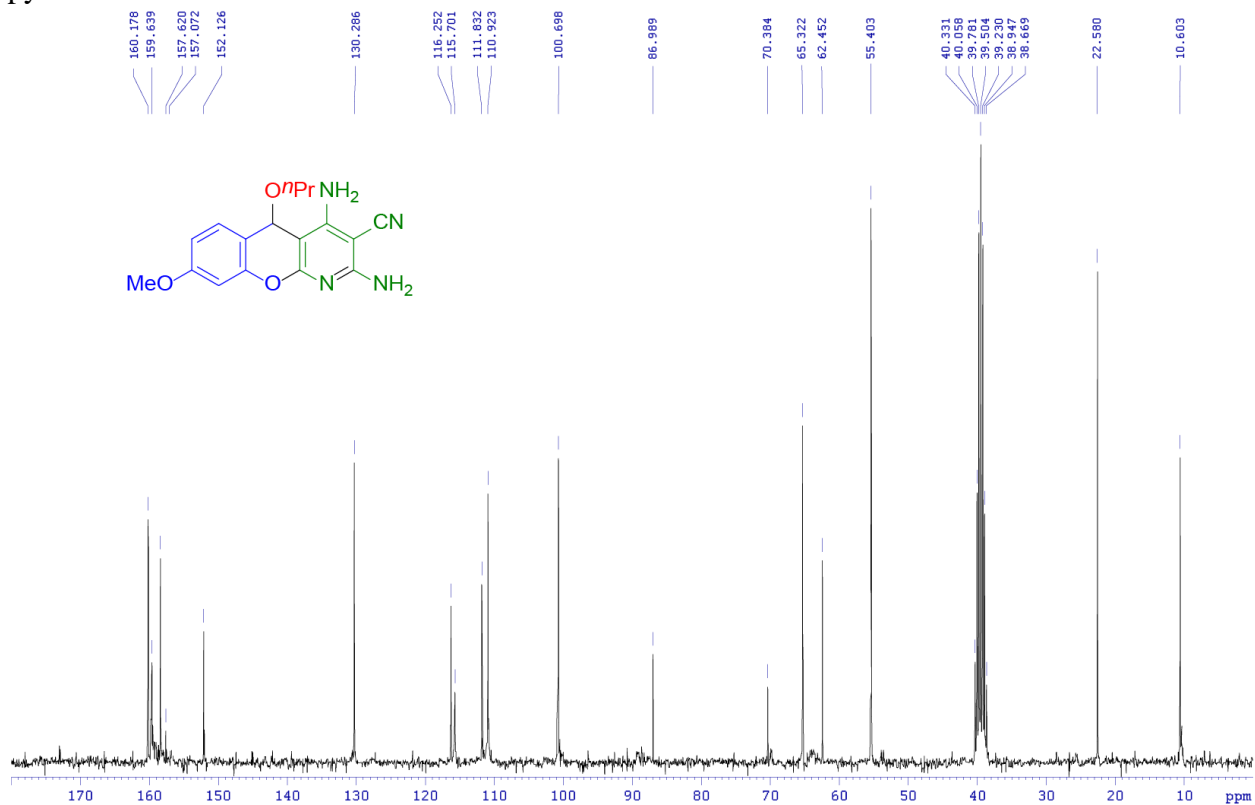


Figure S13. ^1H NMR spectrum of 2,4-diamino-7-chloro-5-methoxy-5*H*-chromeno[2,3-*b*]-pyridine-3-carbonitrile **4g** in $\text{DMSO-}d_6$.

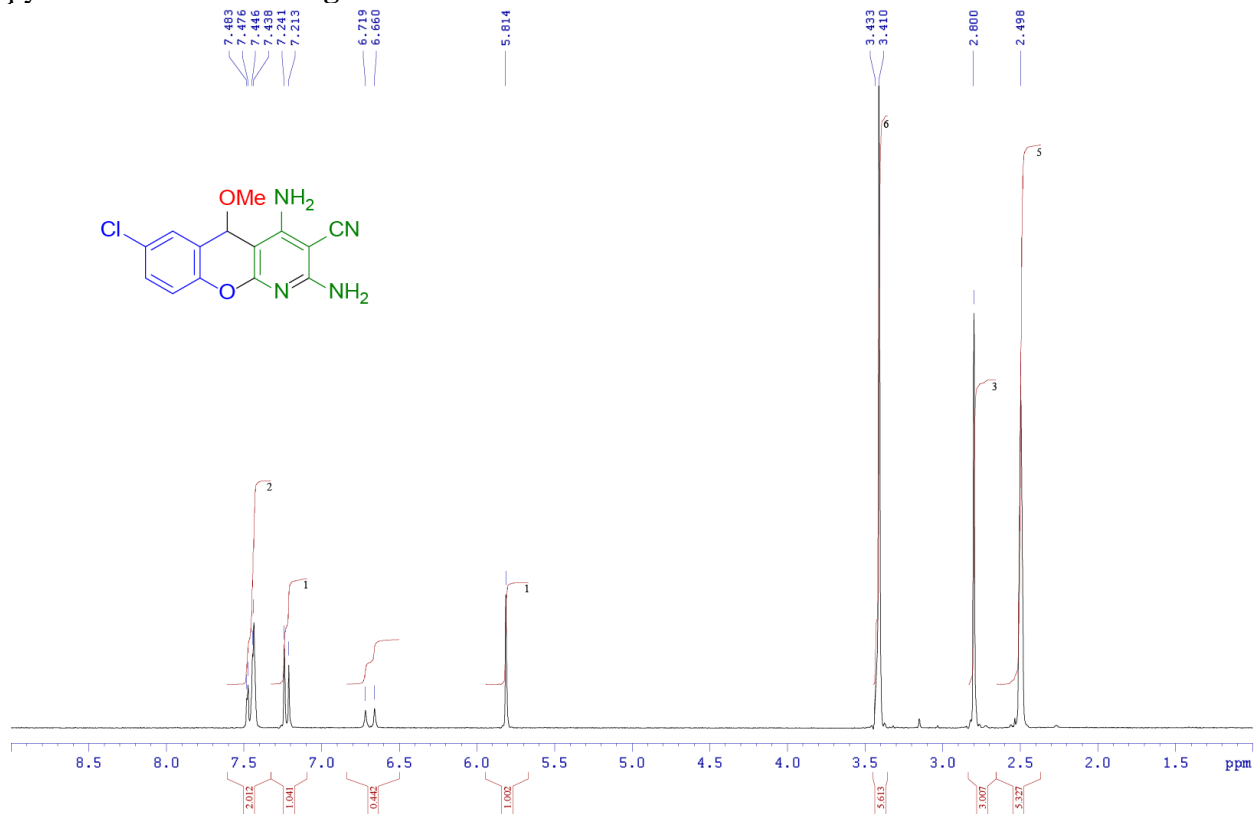


Figure S14. ^{13}C NMR spectrum of 2,4-diamino-7-chloro-5-methoxy-5*H*-chromeno[2,3-*b*]pyridine-3-carbonitrile **4g** in $\text{DMSO-}d_6$.

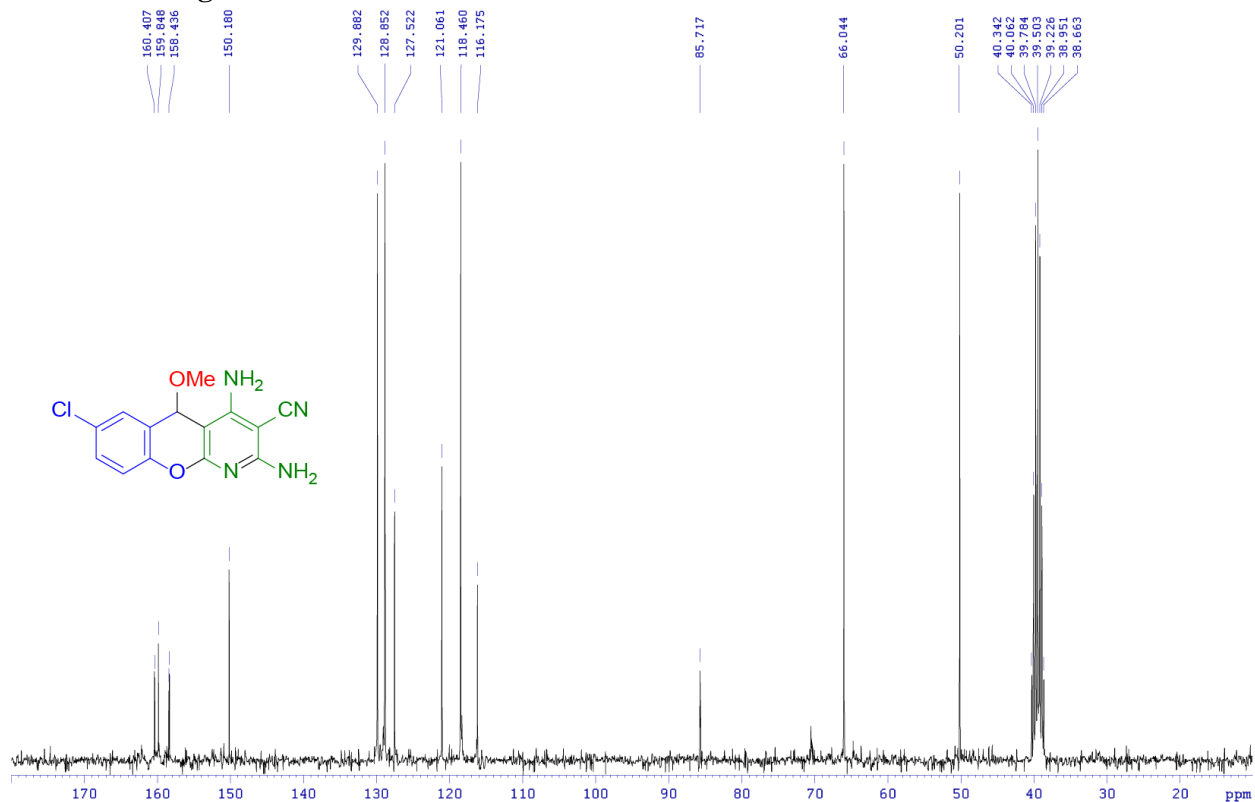


Figure S15. ^1H NMR spectrum of 2,4-diamino-7-chloro-5-ethoxy-5*H*-chromeno[2,3-*b*]pyridine-3-carbonitrile **4h** in $\text{DMSO}-d_6$.

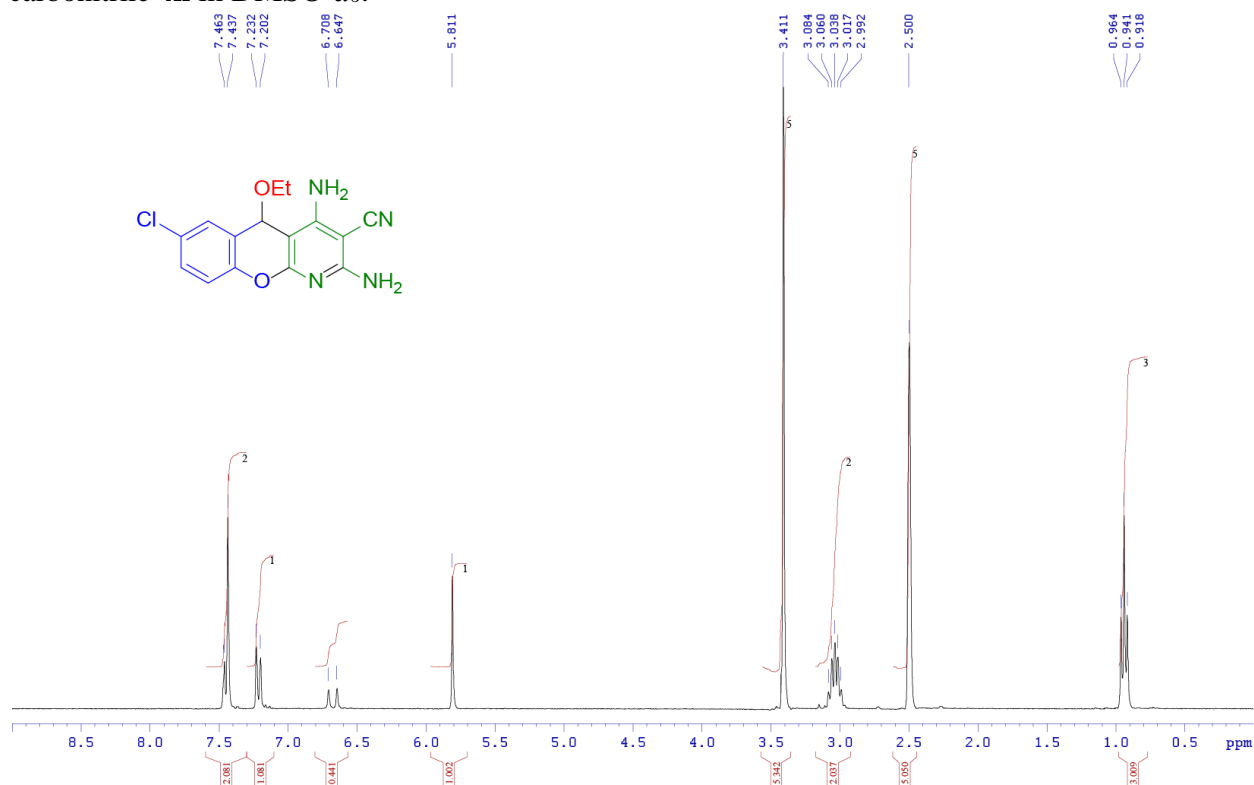


Figure S16. ^{13}C NMR spectrum of 2,4-diamino-7-chloro-5-ethoxy-5*H*-chromeno[2,3-*b*]pyridine-3-carbonitrile **4h** in $\text{DMSO}-d_6$.

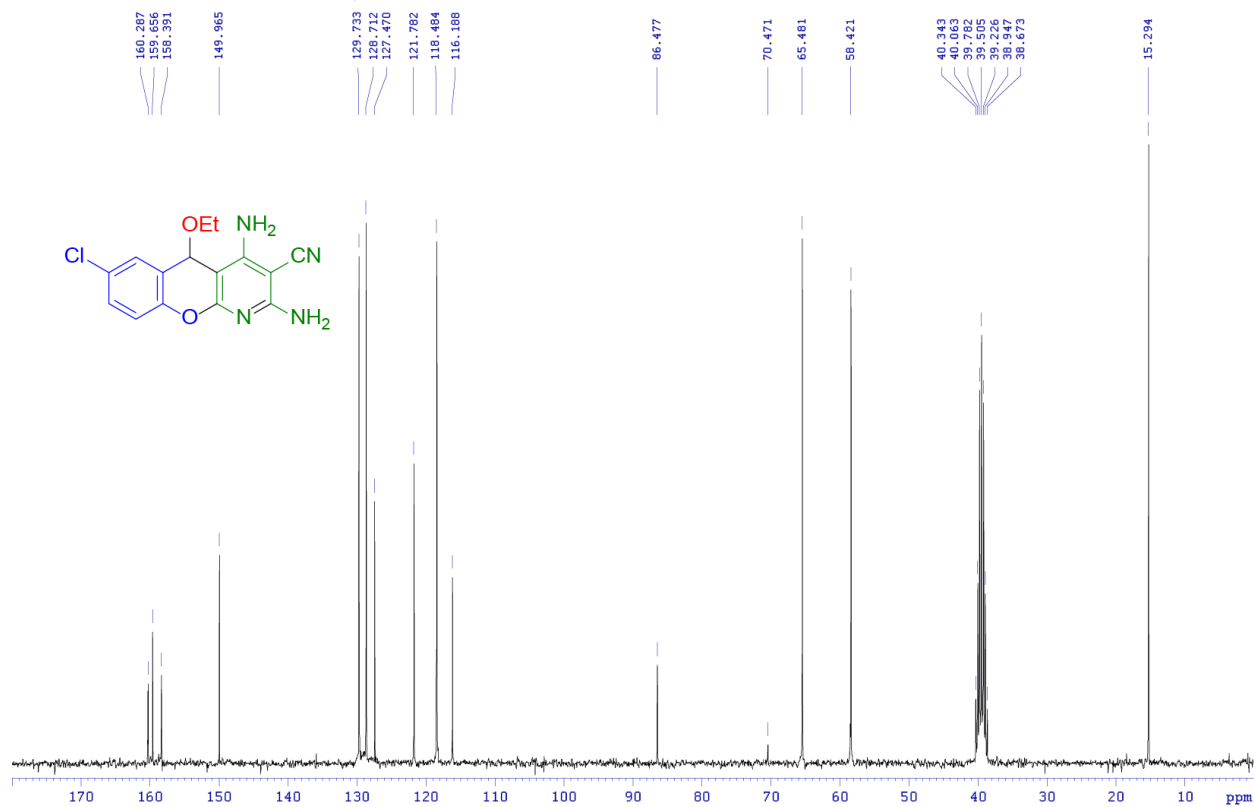


Figure S17. ^1H NMR spectrum of 2,4-diamino-7-chloro-5-ethoxy-5*H*-chromeno[2,3-*b*]pyridine-3-carbonitrile **4i** in $\text{DMSO-}d_6$.

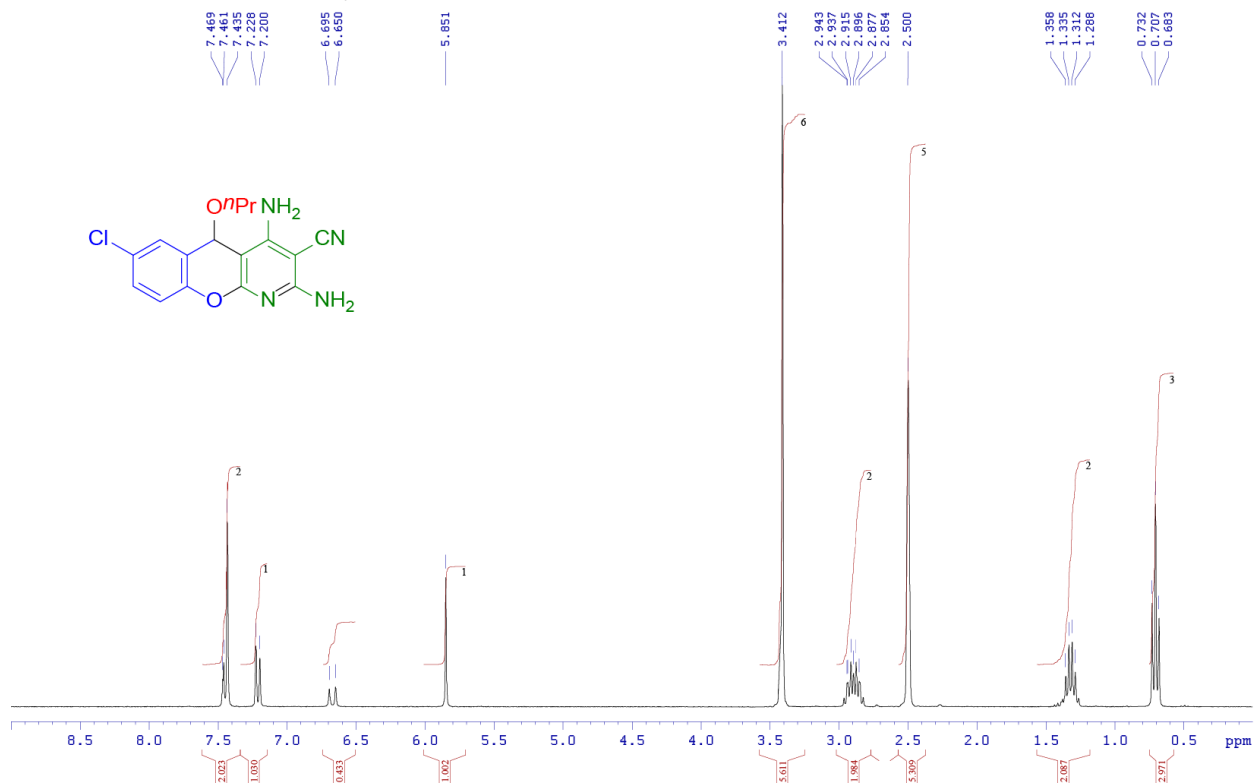
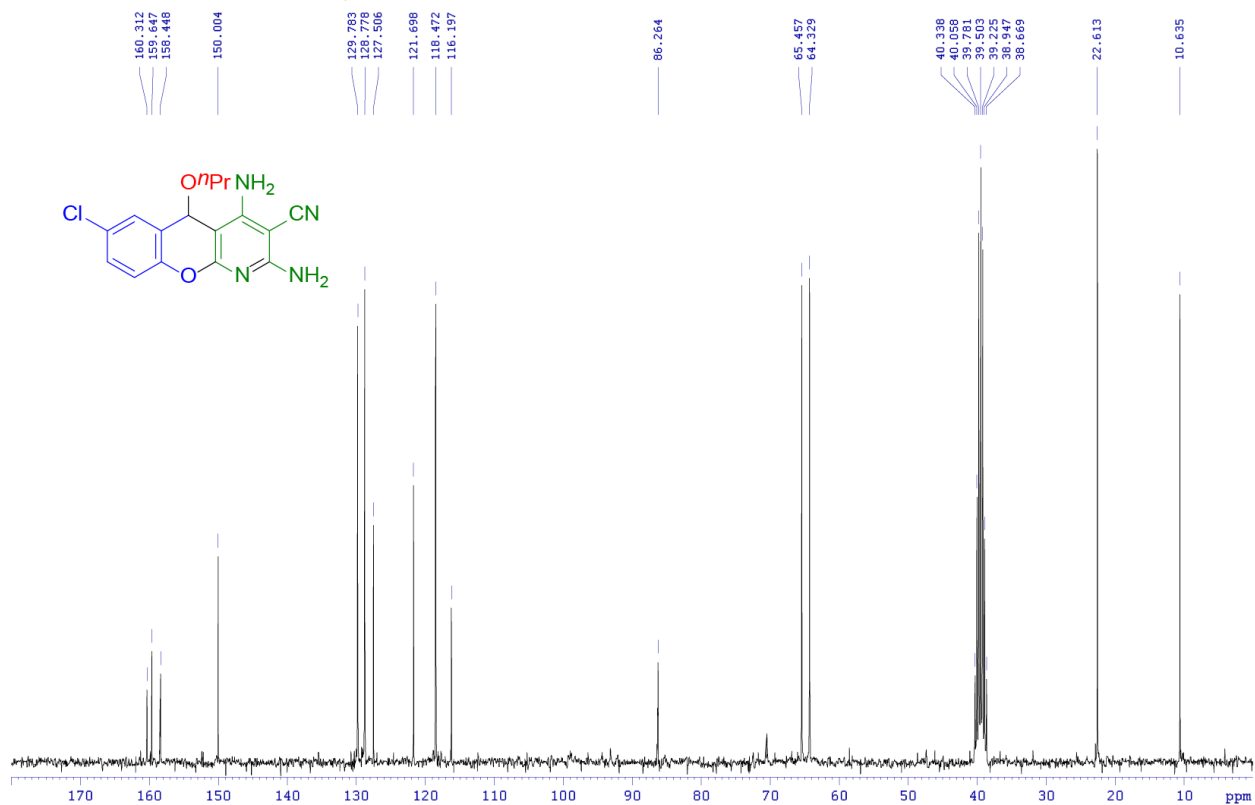


Figure S18. ^{13}C NMR spectrum of 2,4-diamino-7-chloro-5-ethoxy-5*H*-chromeno[2,3-*b*]pyridine-3-carbonitrile **4i** in $\text{DMSO-}d_6$.



2. Detailed 1D ^1H and ^{13}C NMR spectra for compound **4d**

Figure S19. Detailed ^1H NMR spectrum of 2,4-diamino-5,8-dimethoxy-5*H*-chromeno[2,3-*b*]-pyridine-3-carbonitrile **4d** in DMSO- d_6 (500 MHz, 298 K).

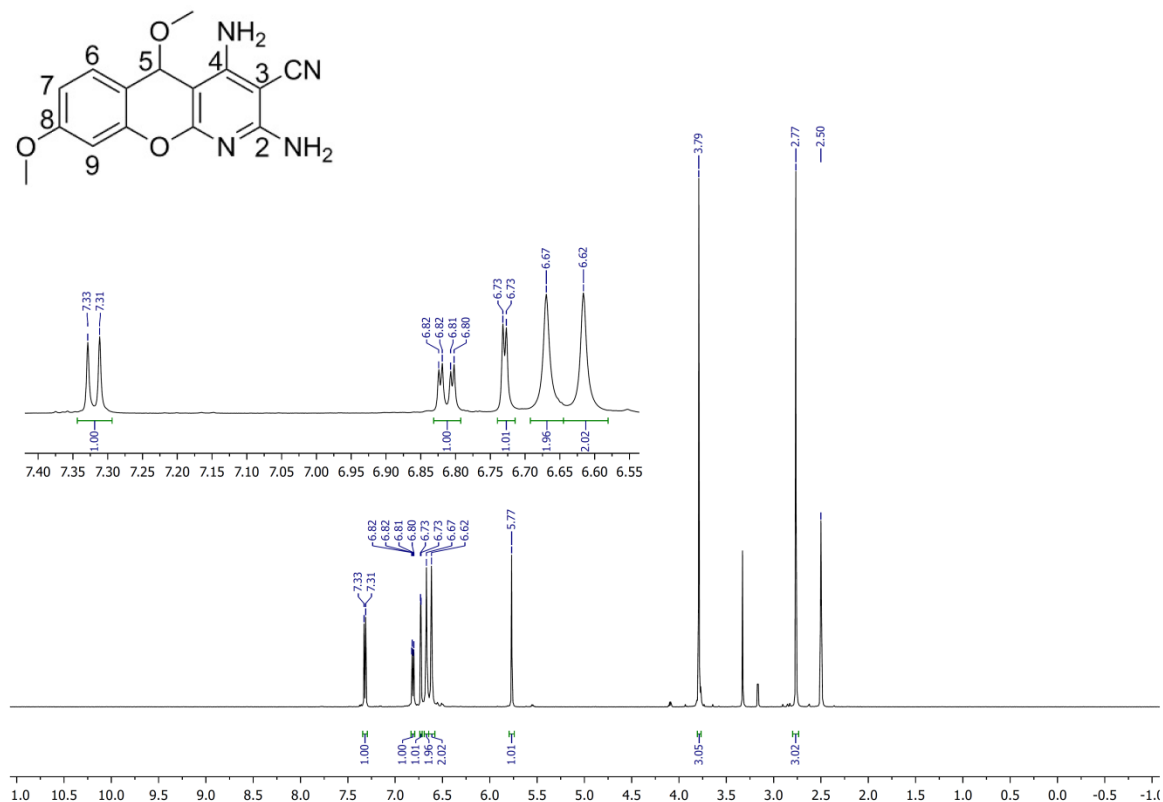
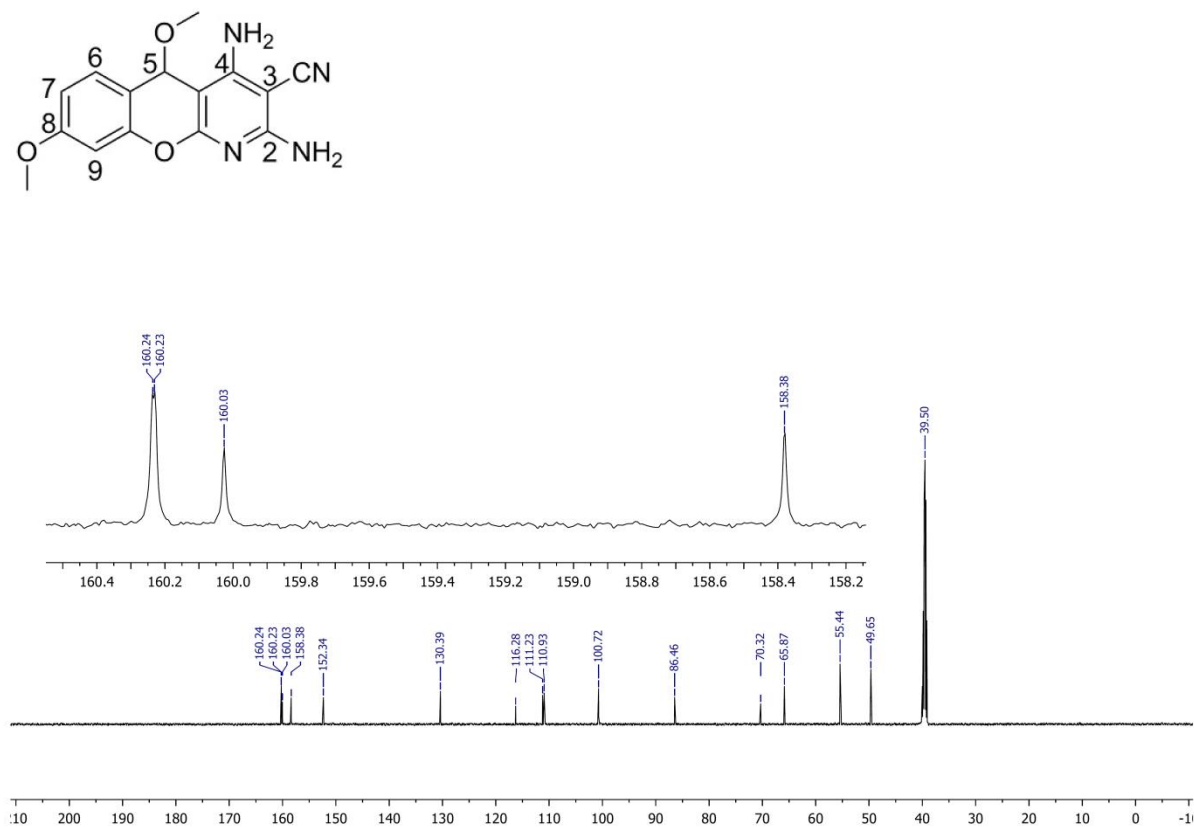


Figure S20. Detailed ^{13}C NMR spectrum of 2,4-diamino-5,8-dimethoxy-5*H*-chromeno[2,3-*b*]-pyridine-3-carbonitrile **4d** in DMSO- d_6 (126 MHz, 298 K).



3. 2D NMR data for compound **4d**

Figure S21. ^1H - ^{13}C HMBC NMR spectrum of 2,4-diamino-5,8-dimethoxy-5*H*-chromeno[2,3-*b*]pyridine-3-carbonitrile **4d** in DMSO- d_6 (400 MHz, 298 K).

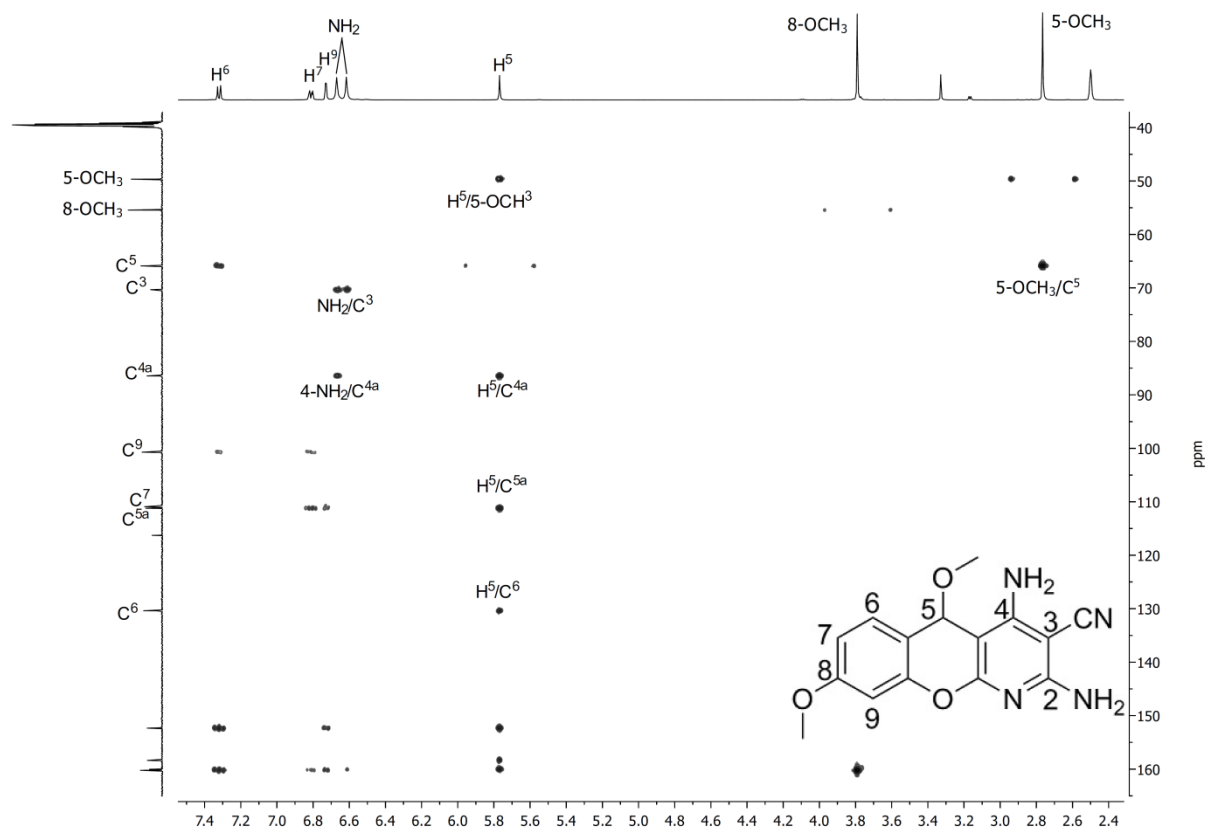


Figure S22. ^1H - ^{13}C HSQC NMR spectrum of 2,4-diamino-5,8-dimethoxy-5*H*-chromeno[2,3-*b*]pyridine-3-carbonitrile **4d** in DMSO- d_6 (400 MHz, 298 K).

