Electronic Supplementary Information

Isomers of 2,2′;6′,2″-terpyridine and 2,6-dipyrazin-2-ylpyridine with aliphatic substituents: synthesis, coordination chemistry, catalytic and anticancer activities

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Table S1. X-ray crystallographic data for compounds **3-10**.

	3	**4**	**5**	**6**
lattice	Monoclinic	Monoclinic	Orthohombic	Triclinic
formula	$C_{19}H_{19}N_3$	$C_7H_{17}N_5$	$C_7H_{17}N_{58}$	$C_{19}H_{25}N_3O_2$
formula weight	289.37	291.36	1050.54	327.42
space group	*P2₁*	*P2₁c*	*Pnma*	*P-1*
a/Å	17.3665(12)	13.2742(9)	11.105(2)	5.7724(5)
b/Å	10.9964(8)	11.2472(6)	6.6065(14)	11.3381(11)
c/Å	18.1432(13)	10.3605(6)	20.111(4)	13.8104(13)
α/°	90	90	90	80.530(7)
β/°	116.170(4)	107.302(2)	90	83.942(7)
γ/°	90	90	90	88.685(7)
V/Å³	3109.6(4)	1476.81(15)	1475.4(5)	886.55(14)
Z	8	4	4	2
temperature (K)	130(2)	200(2)	90(2)	130(2)
radiation (λ, Å)	0.71073	0.71073	0.71073	0.71073
ρ (calcd.) g cm^{-3}	1.236	1.310	1.312	1.227
μ (Mo/Cu Kα),	0.074	0.075	0.082	0.081
θ max, deg.	32.325	25.74	27.728	30.660
no. of data coll.	177666	18916	13004	52849
no. of data	21847	4360	1869	5430
no. of parameters	843	202	173	232
R_1 [$I > 2\sigma(I)$]	0.0669	0.0424	0.0382	0.0551
wR_2 [$I > 2\sigma(I)$]	0.1710	0.0978	0.0404	0.1019
R_1 [all data]	0.1101	0.0710	0.1102	0.1309
wR_2 [all data]	0.2017	0.1138	0.1131	0.1293
GOF	1.032	1.015	1.038	1.006
R_{int}	0.0570	0.0619	0.0180	0.1013

	7	**8**	**9**	**10**
lattice	Monoclinic	Orthohombic	Monoclinic	Orthohombic
formula	$C_{17}H_{21}N_5O$	$C_{19}H_{19}I_2N_3Zn$	$C_{42}H_{46}CoN_8O_2S_2$	$C_{24}H_{25}Cl_2CoN_5$
formula weight	311.39	608.59	817.92	513.32
space group	$P2_1/c$	$Pbcn$	$C2/c$	$P2_12_12_1$
a/Å	11.0946(13)	21.6220(17)	31.739(9)	11.817(2)
b/Å	12.8260(15)	14.9251(12)	11.768(3)	12.712(2)
c/Å	11.4322(14)	15.7371(14)	24.007(6)	16.105(3)
α/°	90	90	90	90
β/°	96.419(6)	90	97.035(7)	90
γ/°	90	90	90	90
V/Å^3	1616.6(3)	5078.5(7)	8899(4)	2419.2(7)
Z	4	2	8	4
temperature (K)	130(2)	120.0	130(2)	90(2)
radiation (λ, Å)	0.71073	0.71073	0.71073	0.71073
ρ (calcd.) g cm^{-3}	1.279	1.5918	1.221	1.409
μ (Mo/Cu Kα), mm^{-1}	0.084	3.404	0.522	0.952
θ max, deg.	33.141	25.41	25.027	30.516
no. of data coll.	61895	176564	64477	28401
no. of data	6158	4655	7582	7382
no. of parameters	215	228	486	347
R_1 [$I > 2\sigma(I)$]	0.0446	0.0317	0.0479	0.0236
wR_2 [$I > 2\sigma(I)$]	0.1134	0.0387	0.1230	0.0243
R_1 [all data]	0.0554	0.0732	0.0760	0.0611
wR_2 [all data]	0.1261	0.0797	0.1379	0.0617
GOF	1.083	1.1101	1.027	1.042
R_{int}	0.0443	0.0678	0.0581	0.0209

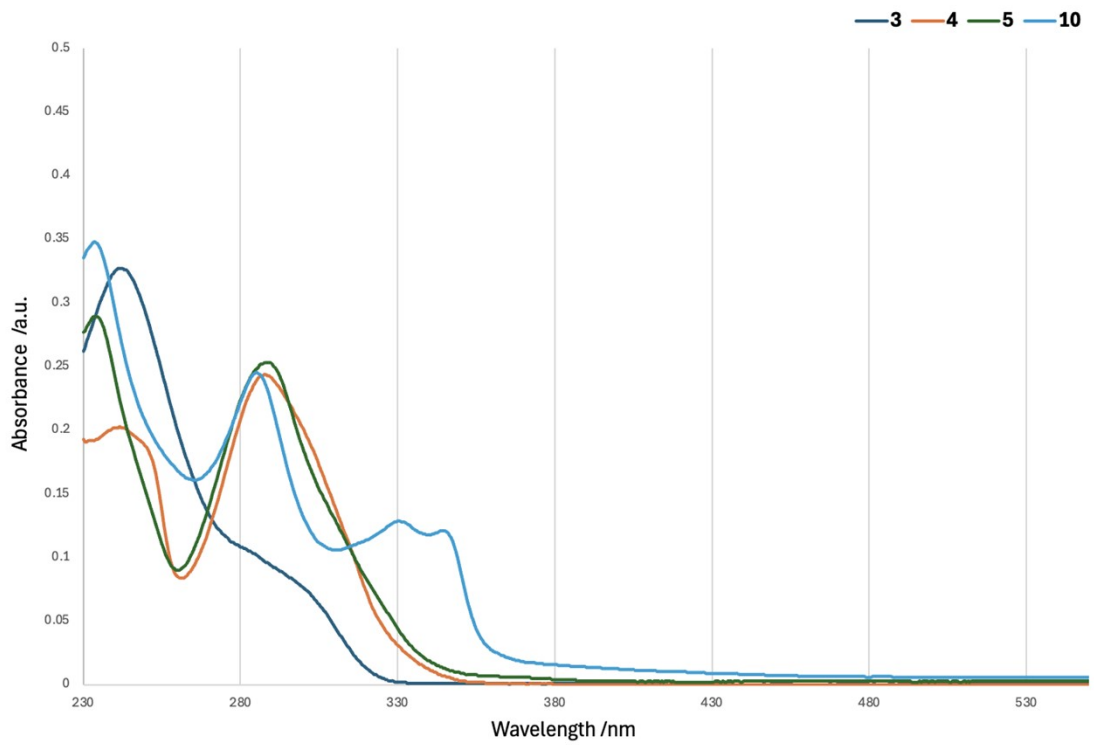


Figure S1. The UV-Vis spectra of compounds **3-5** and **10** in CH_2Cl_2 (concentration = 1×10^{-5} M).

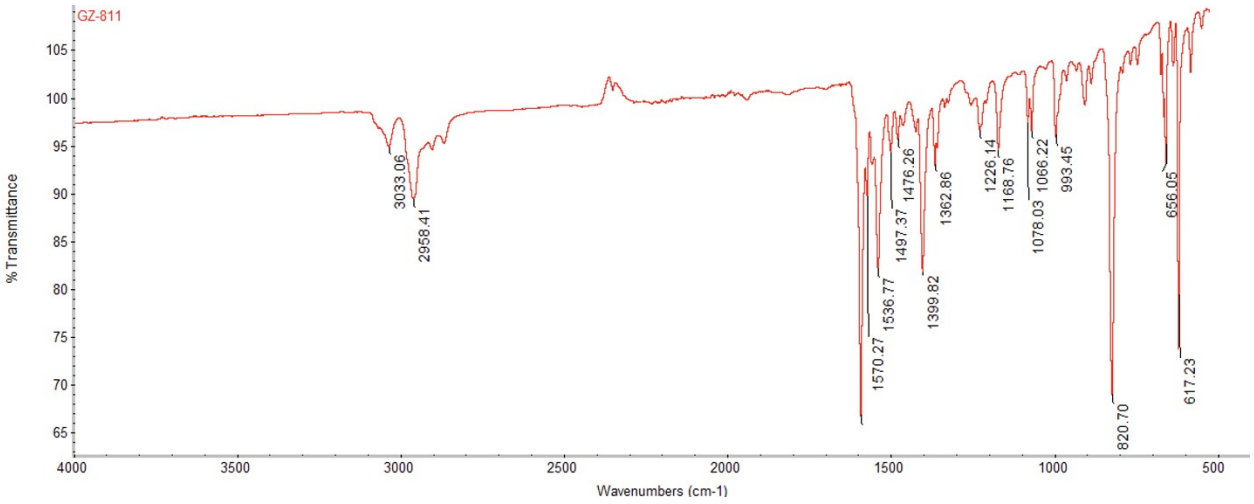


Figure S2. The FT-IR spectrum of **3**.

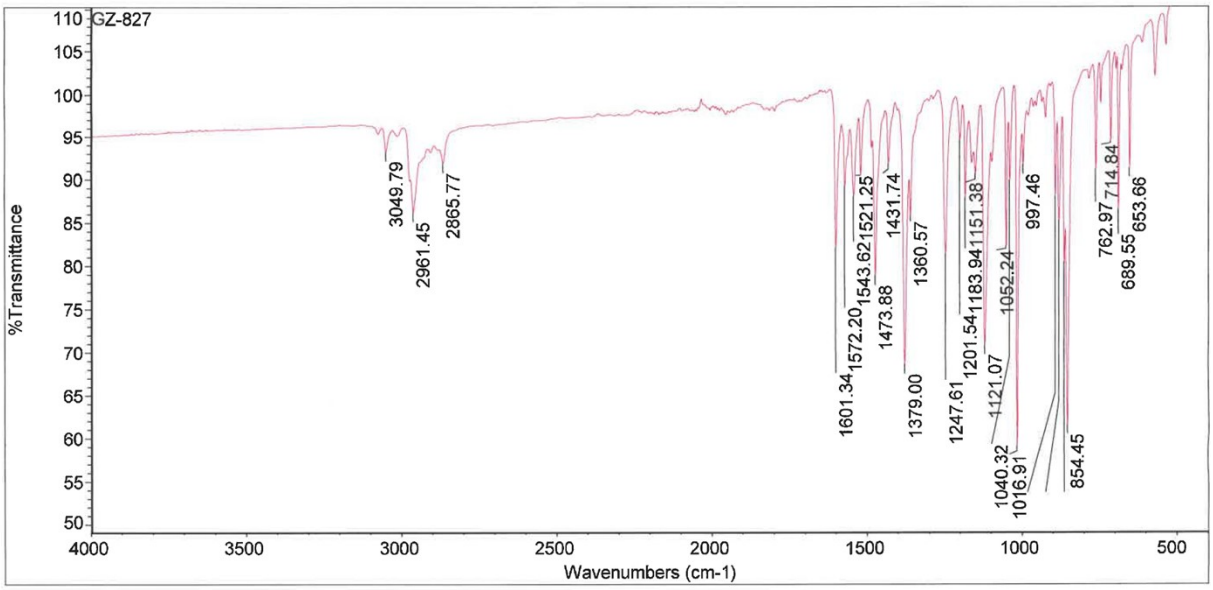


Figure S3. The FT-IR spectrum of **4**.

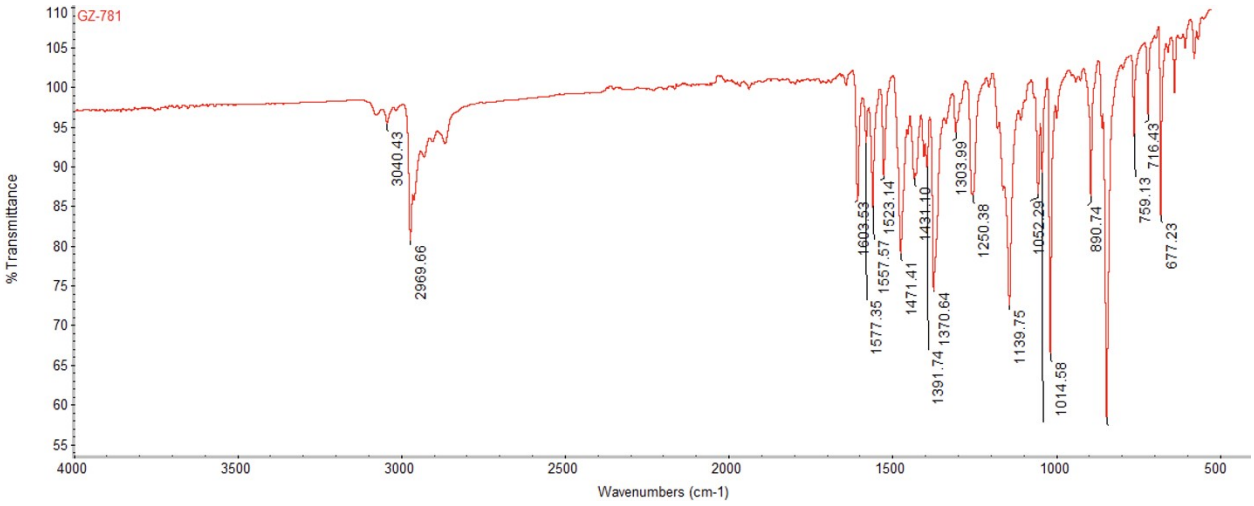


Figure S4. The FT-IR spectrum of **5**.

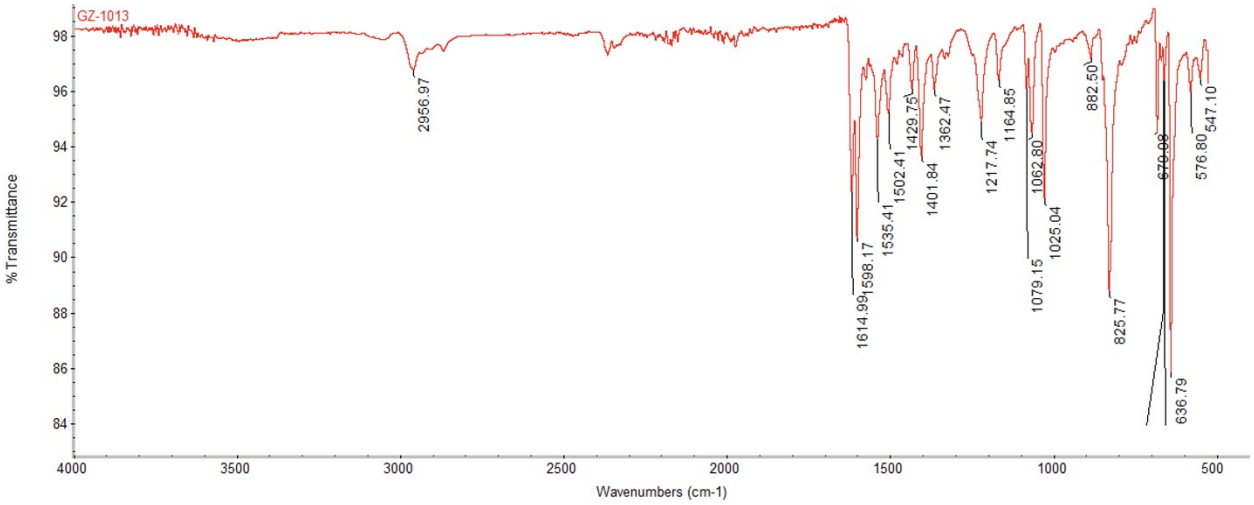


Figure S5. The FT-IR spectrum of **8**.

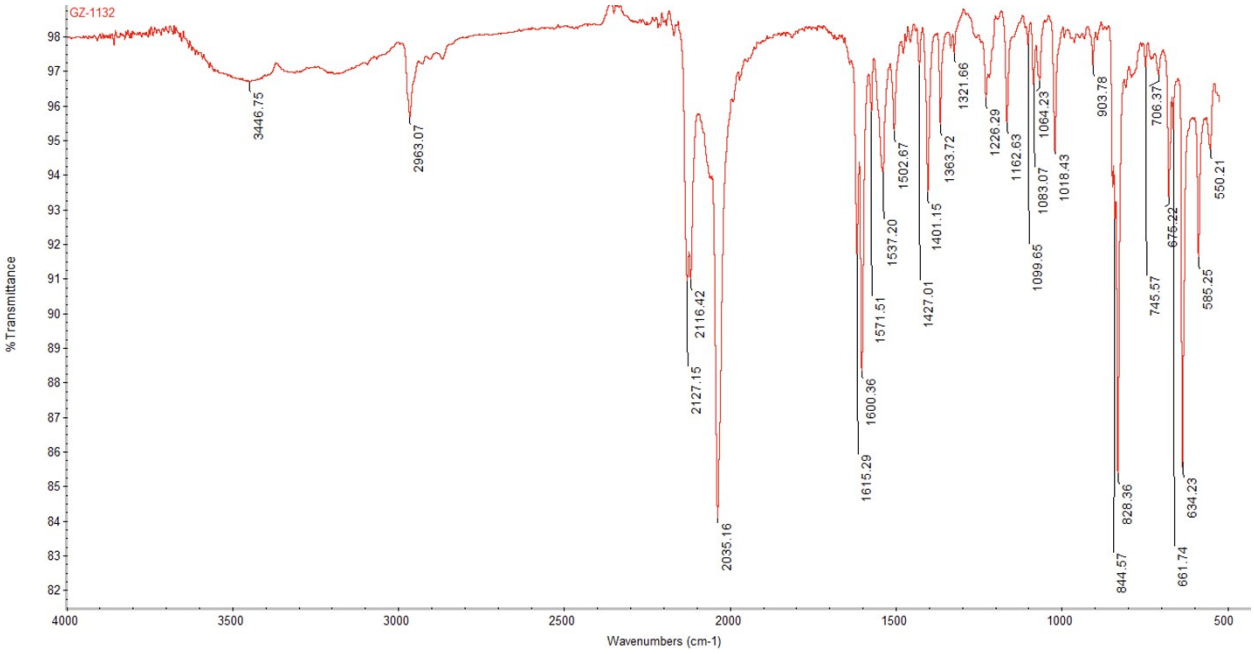


Figure S6. The FT-IR spectrum of **9**.

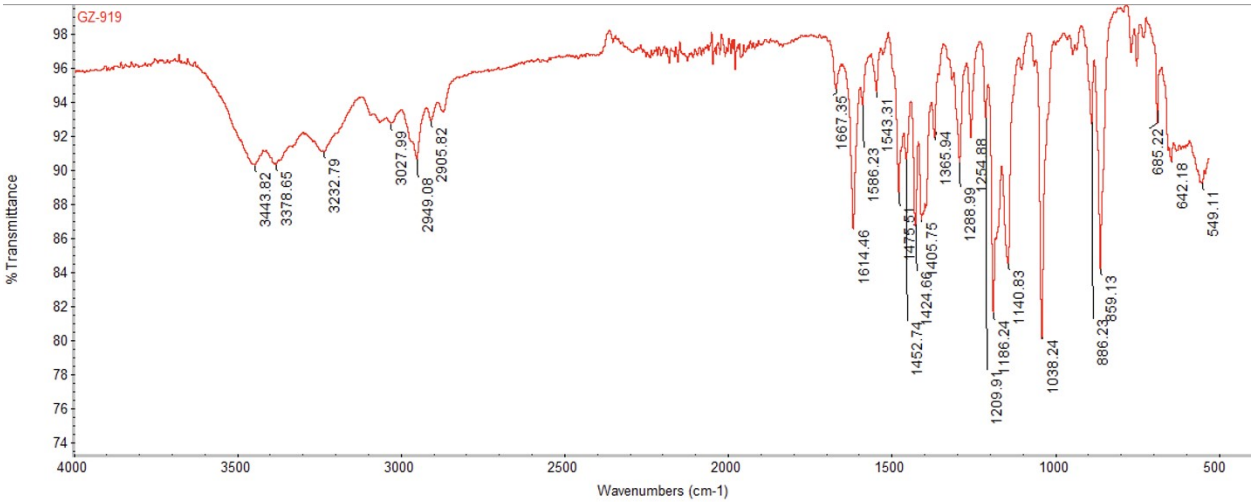
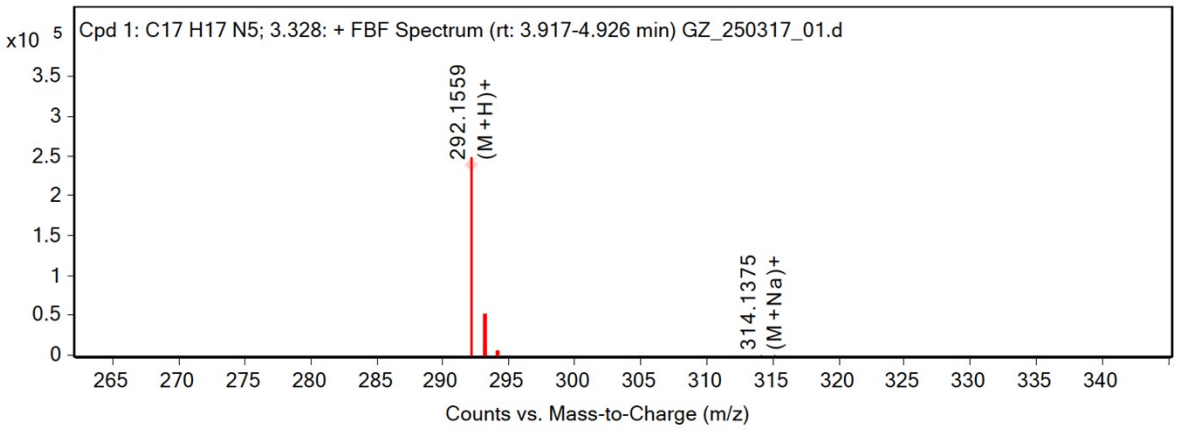


Figure S7. The FT-IR spectrum of **10**.



MS Spectrum Peak List

m/z	z	Abund	Ion
292.1559	1	246873.28	(M+H)+
293.1591	1	45237.37	(M+H)+
294.162	1	4467.33	(M+H)+
314.1375	1	255.19	(M+Na)+
315.1422	1	97.69	(M+Na)+

Figure S8. The HR-MS spectrum of **4**.

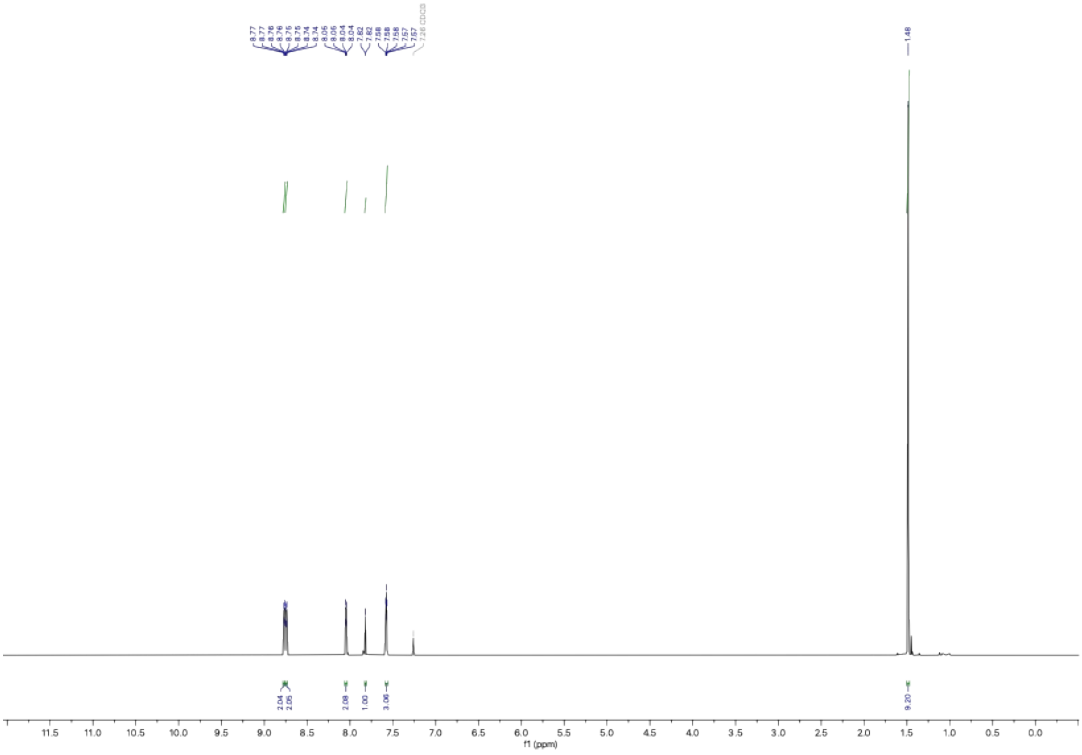


Figure S9. The ^{1}H NMR spectrum of **3** in $CDCl_3$ (500 MHz).

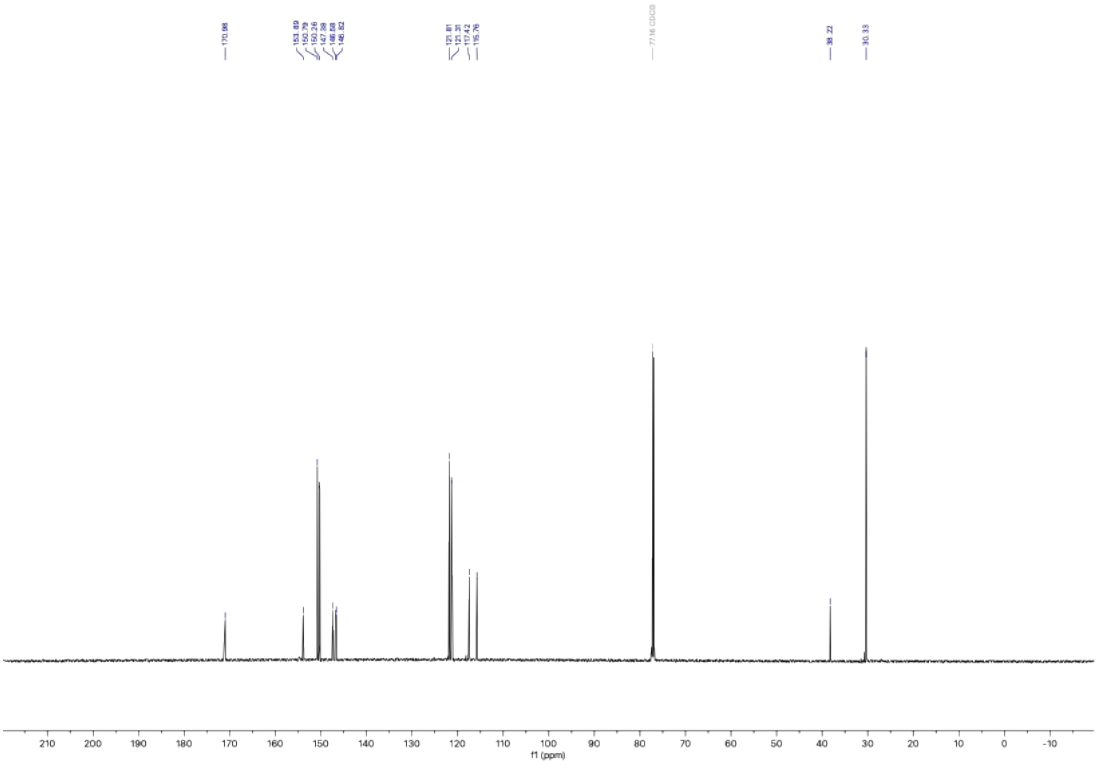


Figure S10. The ^{13}C NMR spectrum of **3** in $CDCl_3$ (126 MHz).

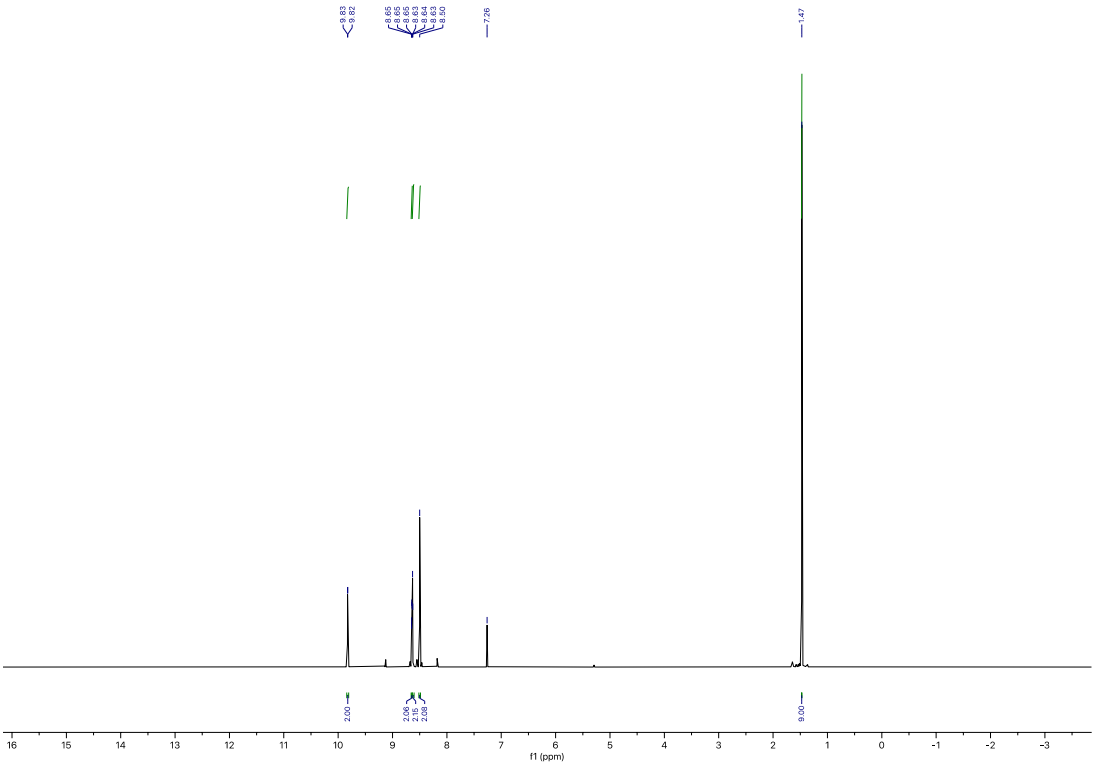


Figure S11. The ^{1}H NMR spectrum of **4** in $CDCl_3$ (500 MHz).

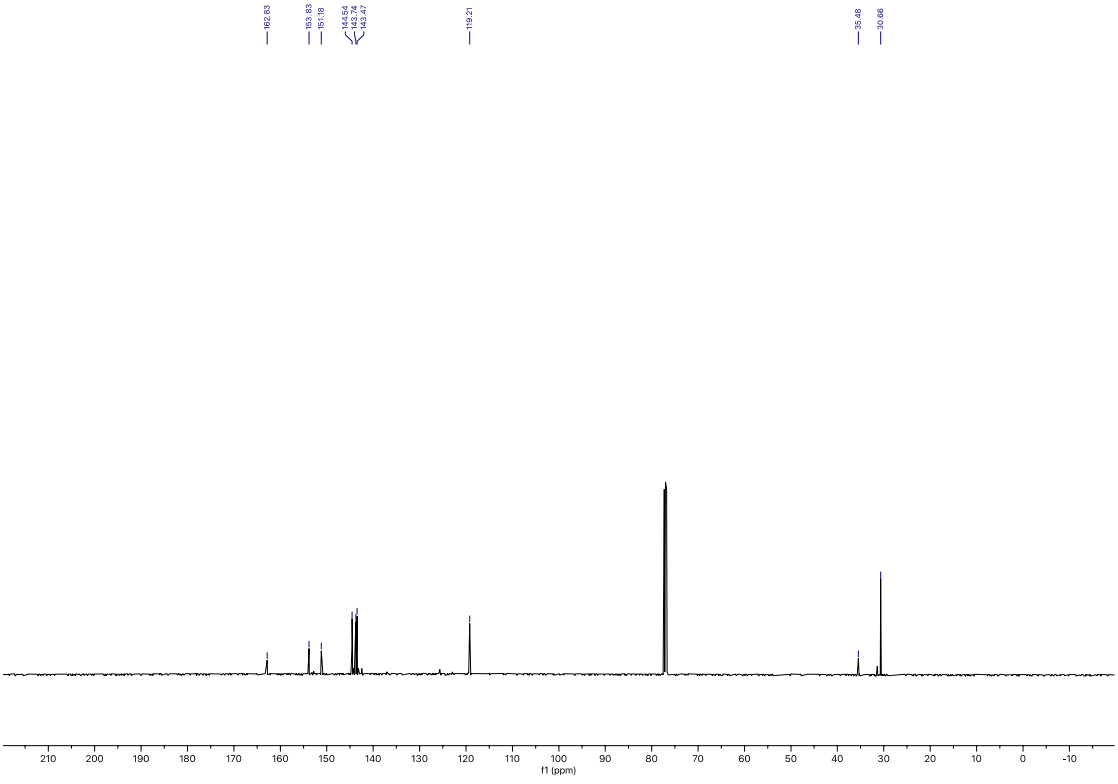


Figure S12. The ^{13}C NMR spectrum of **4** in $CDCl_3$ (126 MHz).

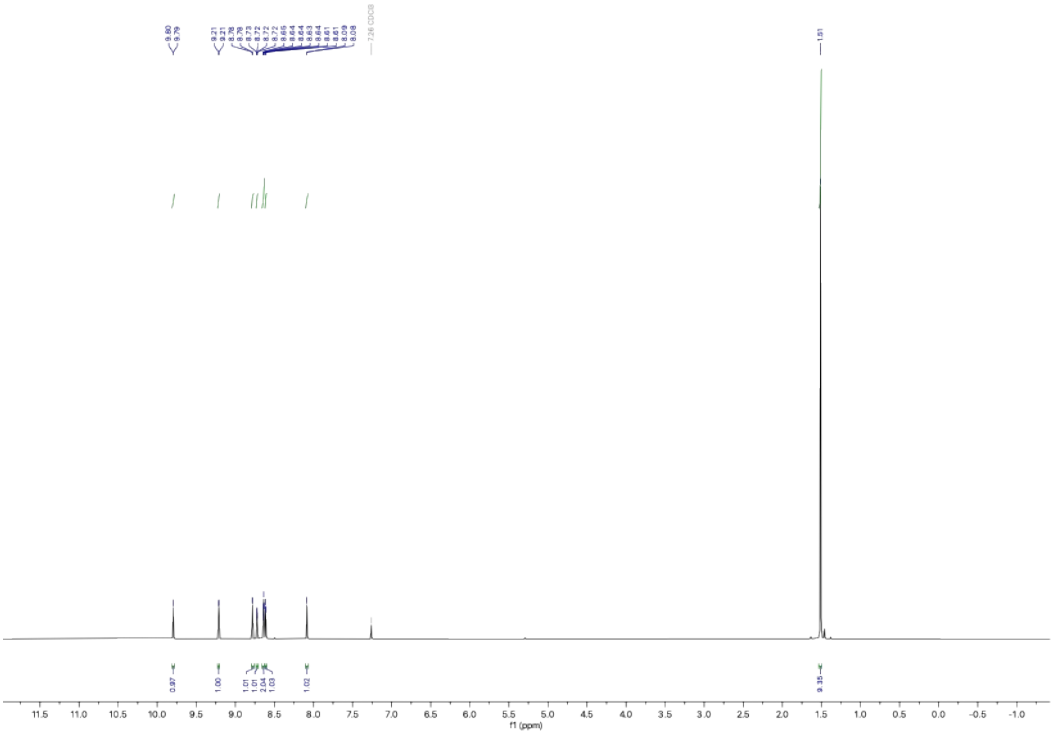


Figure S13. The ^{1}H NMR spectrum of **5** in $CDCl_3$ (500 MHz).

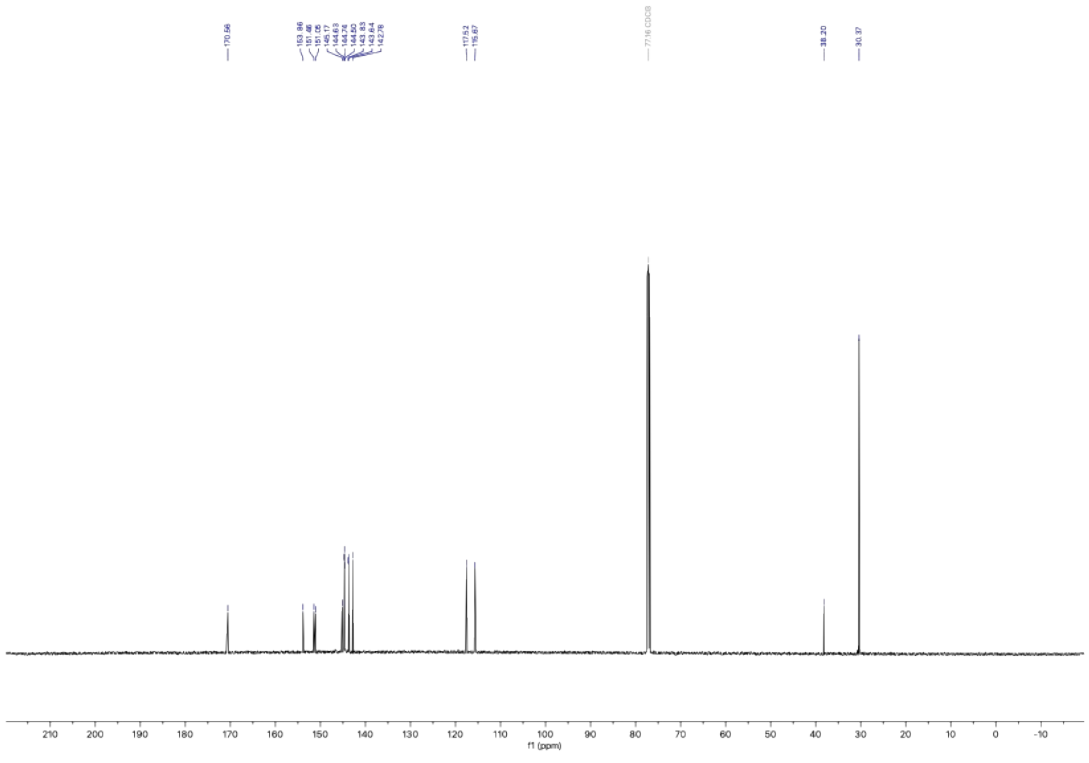


Figure S14. The ^{13}C NMR spectrum of **5** in $CDCl_3$ (126 MHz).

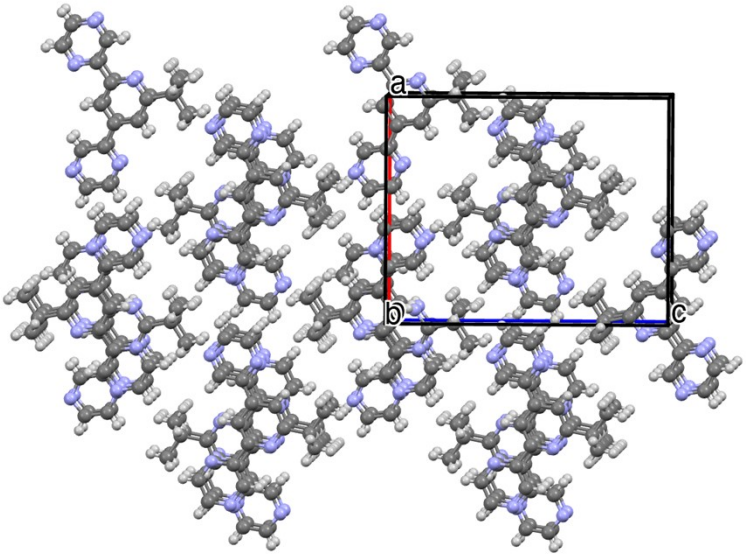


Fig. S15. The columnar packing mode formed in the crystal structure of **5**.

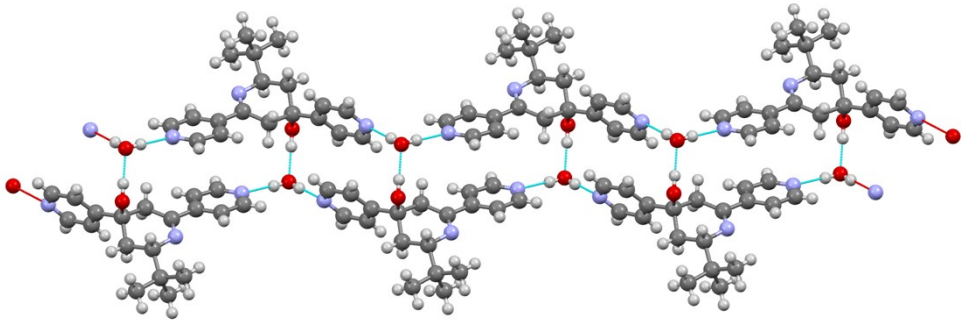


Fig. S16. The one-dimensional double-chained hydrogen-bonded framework formed in **6**. H-bonding parameter for O1-H1···O2: H1···O2 = 1.81(2), O1···O2 = 2.716(2) Å, <O1-H1···O2 = 178(2)°; for O2-H2A···N1^{i}: H2A··· N1^{i} = 1.95(3), O2··· N1^{i} = 2.842(2) Å, < O2-H2A···N1^{i} = 176(2)°; for O2-H2B···N3^{ii}: H2B··· N3^{ii} = 1.97(3), O2··· N3^{ii} = 2.827(2) Å; < O2-H2B···N3^{ii} = 172(3)°. Symmetry code: ^{i}2 - x, 1 - y, -z, ^{ii}2 - x, 1 - y, 1 - z.

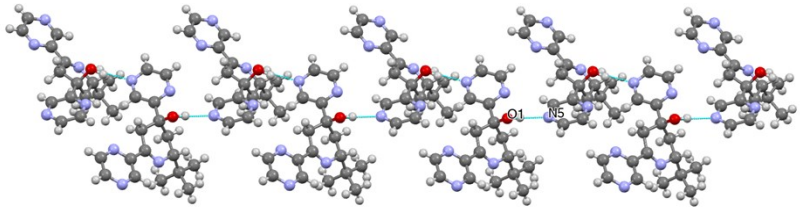


Fig. S17. The one-dimensional hydrogen-bonded chain formed in **7**. H-bonding parameter for O1-H1···N5^{i}: H1···N5^{i} = 1.994(16), O1···N5^{i} = 2.8925(11) Å; <O1-H1···N5^{i} = 168.6(15)°. Symmetry code: ^{i} x, -y + $^{3}/_{2}$, z + $^{1}/_{2}$.

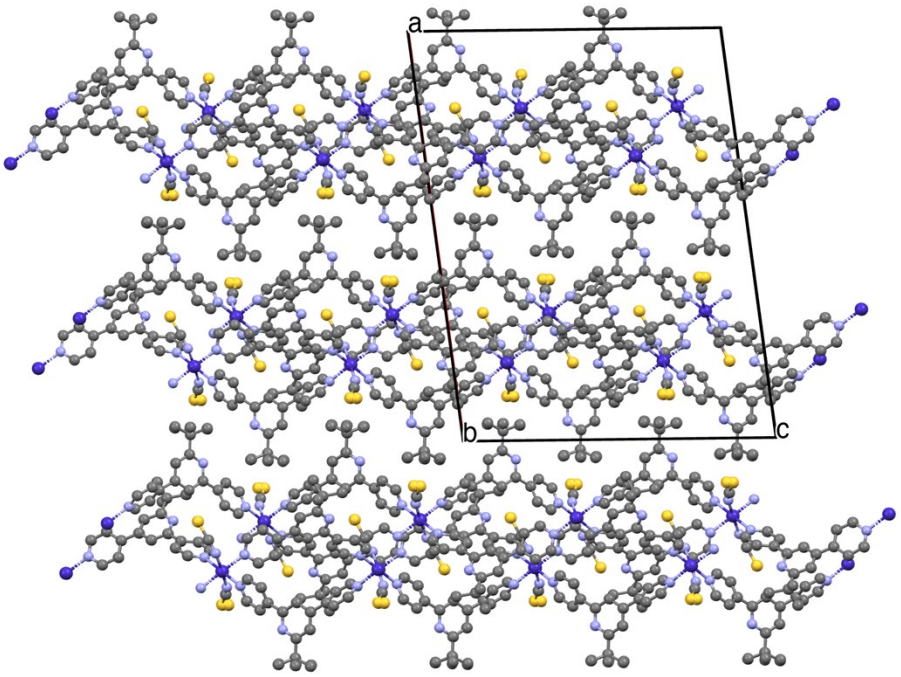


Fig. S18. The three-dimensional packing of 2D grid-like sheets in the crystal structure of **9** viewing down the crystallographic *b* axis.