Electronic Supplementary Information

Construction of two Zn(II)/Cd(II) multifunctional coordination polymers with mixed ligands for catalytic and sensing properties

Li-Ping Xue, Zhao-Hao Li, Ting Zhang, Jia-Jia Cui, Yue Gao, Jia-Xin Yao

Table S1 Selected bond distances (Å) and angles (º) for complexes **1**−**2**.

Compound **1**[a]					
Zn(1)−O(1)	1.996(2)	Zn(1)−O(2)	2.105(3)	Zn(1)−O(5)#1	2.022(2)
Zn(1)−N(1)	2.109(3)	Zn(1)−N(4)#2	2.123(3)		
O(1)−Zn(1) −O(2)	88.10(10)	O(1)−Zn(1)−O(5) #1	171.74(11)	O(1)−Zn(1)−N(1)	93.15(11)
O(1)−Zn(1)−N(4)#2	94.07(11)	N(1)−Zn(1)−O(2)	153.52(12)	O(2) −Zn(1)−N(4)#2	106.11(12)
O(5)#1− Zn(1)−O(2)	83.87(11)	O(5)#1− Zn(1)−N(1)	93.16(12)	O(5)#1− Zn(1)−N(4)#2	90.06(12)
N(1)−Zn(1)−N(4)#2	100.18(12)				
[a] Symmetry codes: #1 x+1/2, 1/2-y, z+1/2; #2 1/2-x, y-1/2, 1/2-z.					
Compound **2**[b]					
Cd(1)−O(1)	2.395(8)	Cd(1)−O(2)	2.281(7)	Cd(1)−O(3)#1	2.313(7)
Cd(1)−O(6)	2.391(8)	Cd(1)−N(1)	2.342(9)	Cd(1)−N(3)	2.335(9)
O(1)−Cd(1)−O(2)	78.6(2)	O(2)−Cd(1)−O(3)#1	157.3(3)	O(2) −Cd(1)−O(6)	77.0(3)
O(2)−Cd(1)−N(1)	94.7(3)	O(2) −Cd(1)−N(3)	92.5(3)	O(3)#1−Cd(1)−O(1)	123.9(3)
O(3)#1−Cd(1)−O(6)	80.7(3)	O(3)#1−Cd(1)−N(1)	90.6(3)	O(3) #1−Cd(1)−N(3)	86.4(3)
O(6) −Cd(1)−O(1)	155.5(3)	O(1) −Cd(1)−N(1)	86.3(3)	N(1) −Cd(1)−O(6)	93.7(3)
N(3)−Cd(1)−O(1)	85.6(3)	N(3)−Cd(1)−O(6)	97.4(3)	N(1)−Cd(1)−N(3)	167.9(3)
[b]Symmetry codes: #1 x-1, y, z.					

Table S2 Hydrogen Bond Lengths (Å) and Bond Angles (º) in Compound **2**.

Compound **2**[a]				
D−H···A	d(D−H)	d(H···A)	d(D···A)	<(DHA)
O(6)−H(1W)···O(7)	0.851	1.955	2.762	157.99
O(6)−H(2W)···O(8)[#2]	0.851	2.244	2.854	128.74
O(7)−H(3W)···O(4)[#3]	0.850	2.263	2.933	135.83
O(7)−H(4W)···O(2)	0.850	2.307	2.820	119.08
[a]Symmetry codes: (#2) -x+1/2, y-1/2, -z+3/2; (#3) x-1/2, - y+3/2, z+1/2.				

Fig. S1 PXRD patterns of as-synthesized and simulated **1-2**.

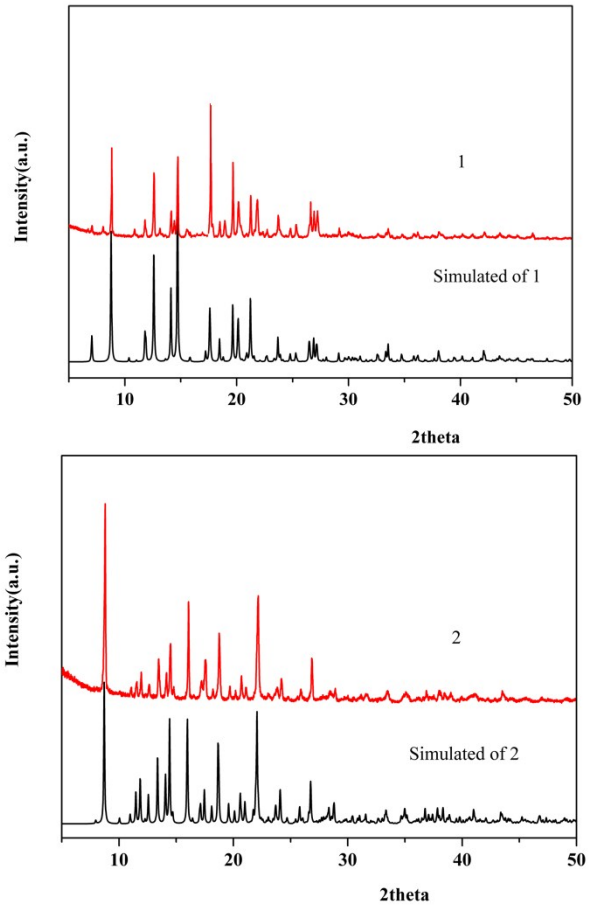


Fig. S2 TG curves of complexes **1-2**.

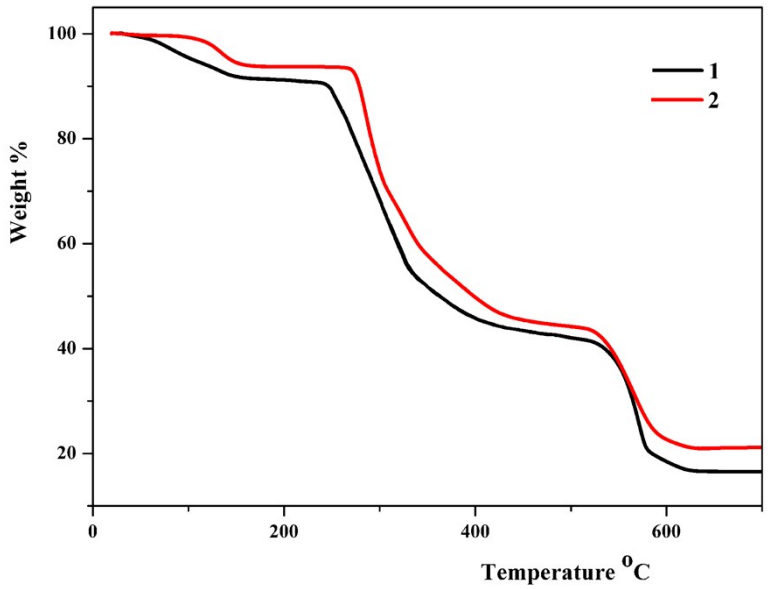


Fig. S3 The reaction time examination and leaching test in the Knoevenagel condensation.

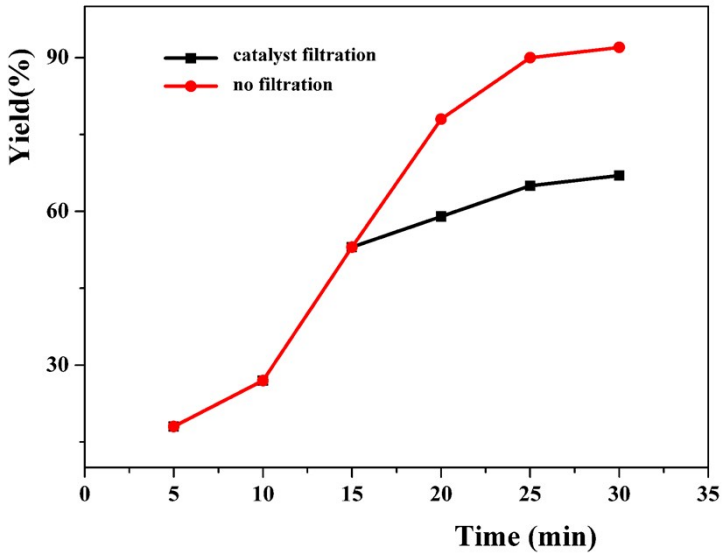


Fig. S4 PXRD patterns for as-synthesized and reused compound **1** in the Knoevenagel condensation.

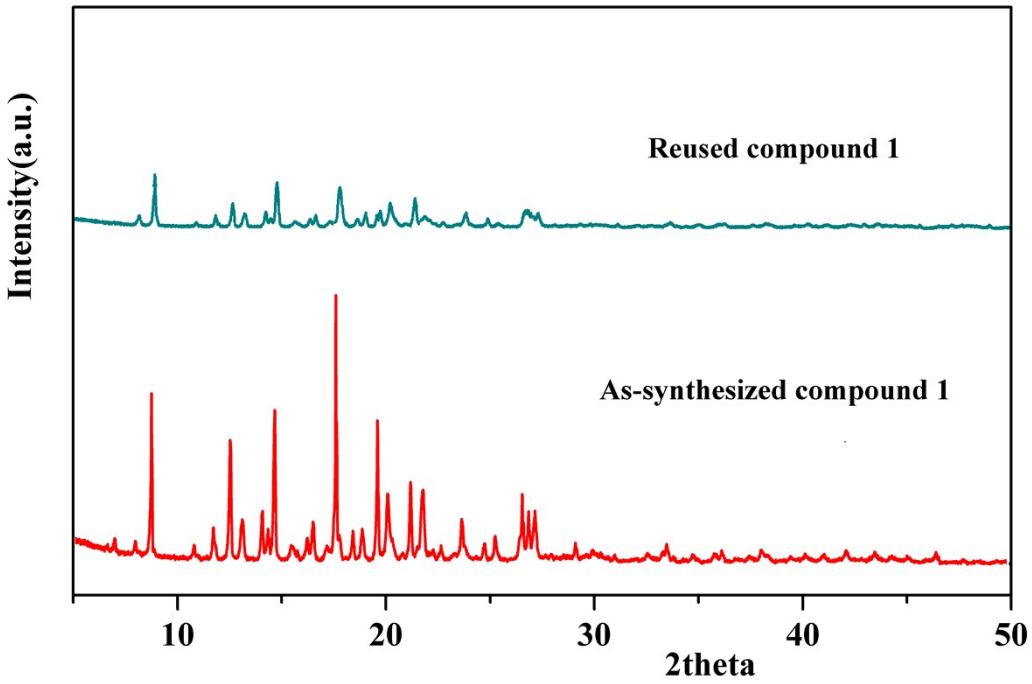


Fig. S5 The luminescent intensities of compound **1** upon the addition of various amino acids when excited at 290 nm at room temperature

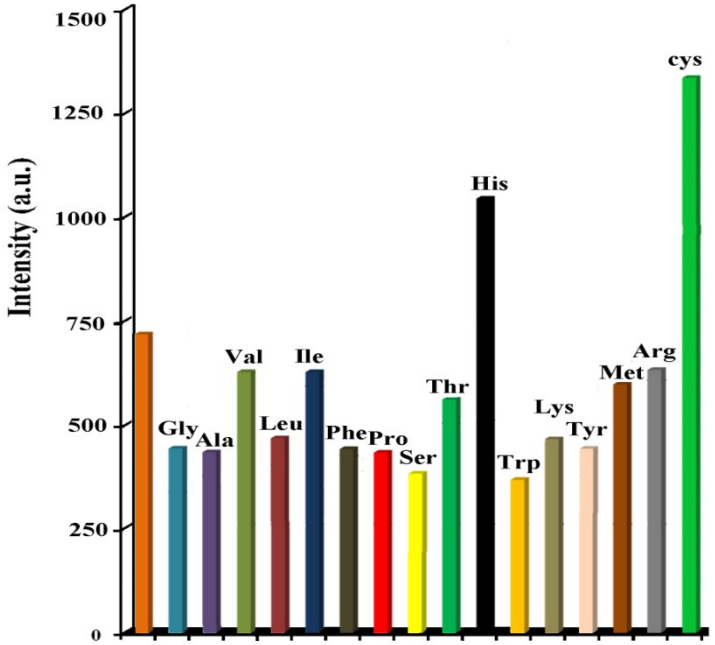


Fig. S6 PXRD patterns for as-synthesized and compound **2** after sensing of Cys.

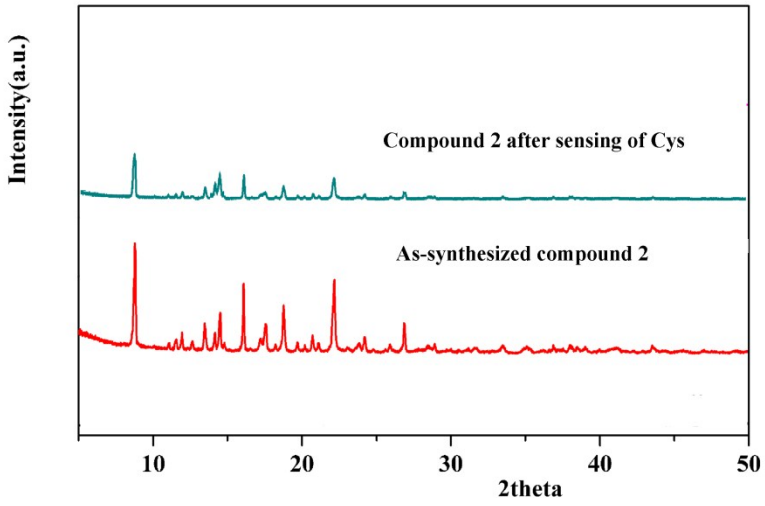
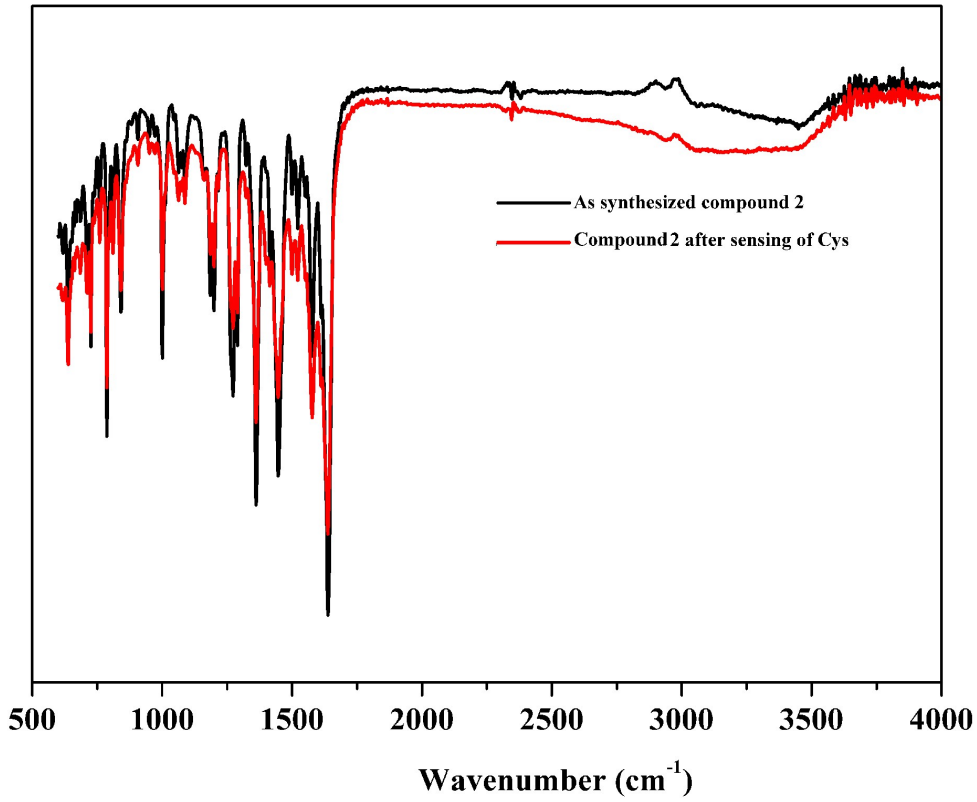
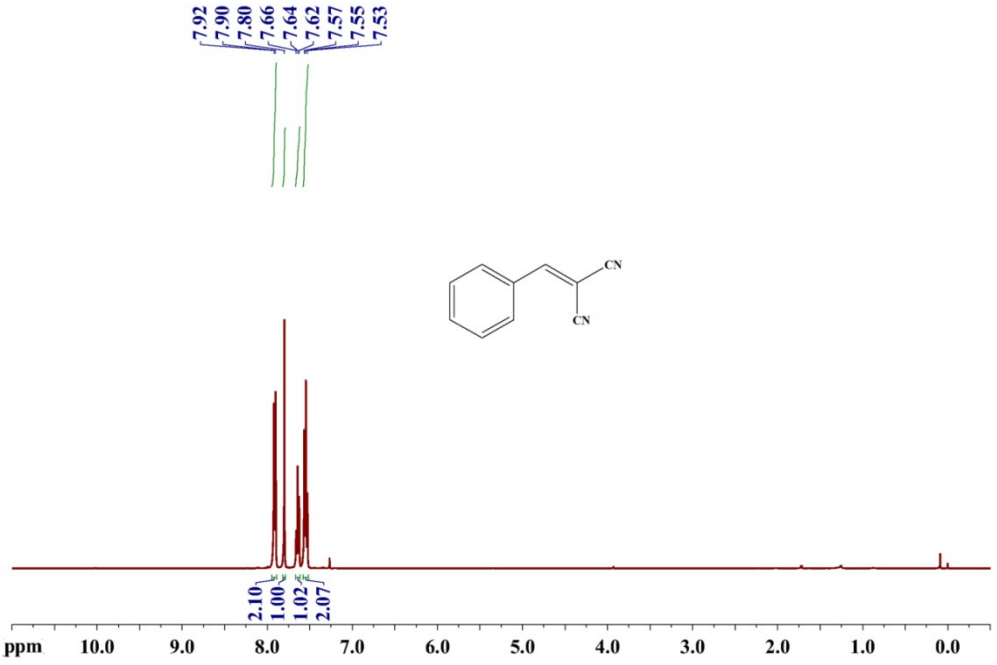


Fig. S7 IR spectra for as-synthesized and compound **2** after sensing of Cys.

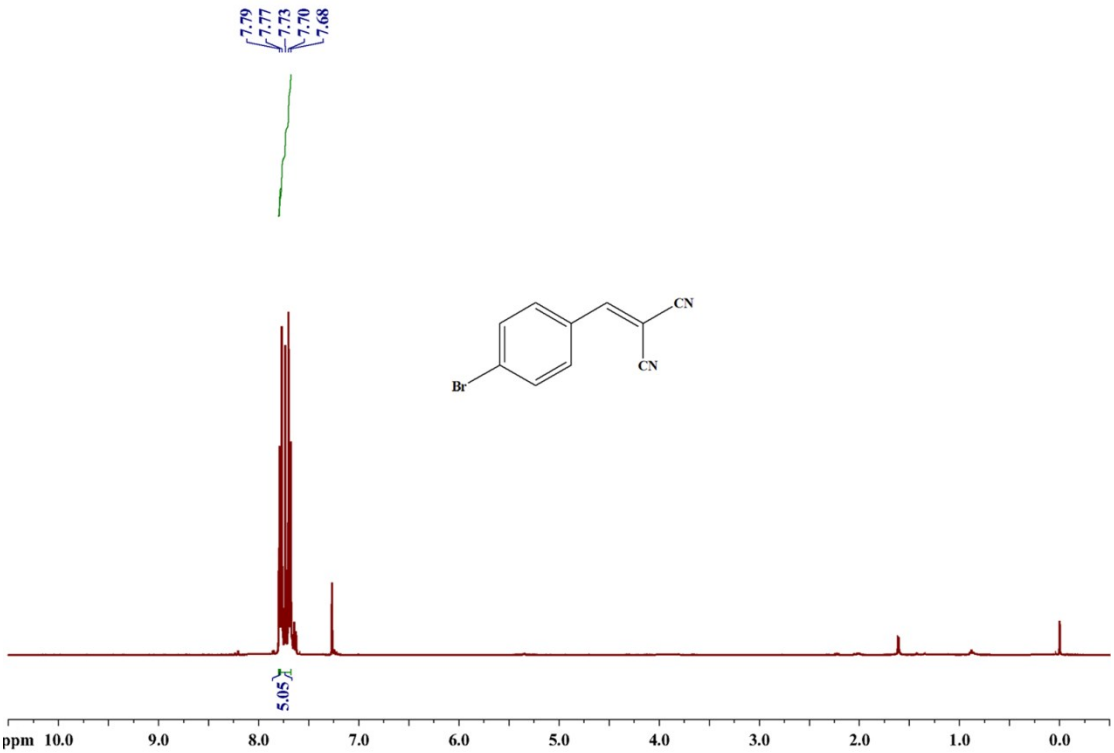


H[1]-NMR Spectra of All Compounds

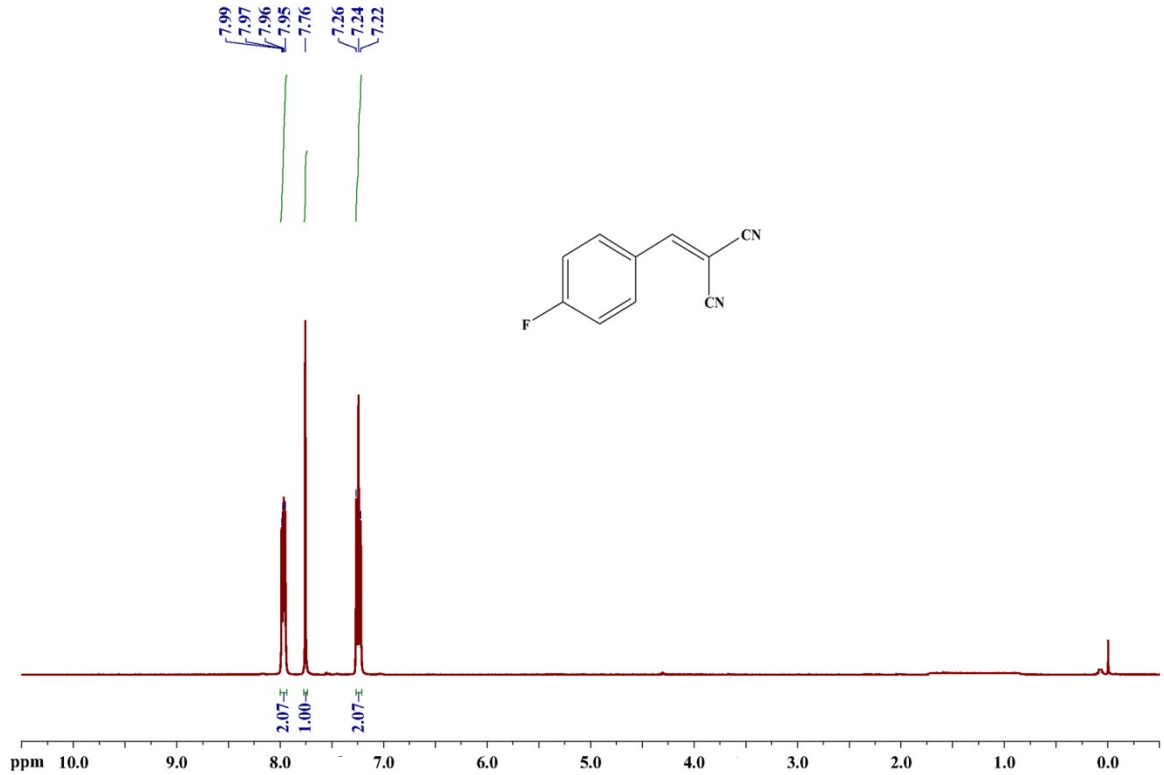
2-(Phenylmethylene)malononitrile. White solid; ^{1}H NMR ($CDCl_3$, 300 MHz): δ(ppm): 7.91 (d, J = 7.6 Hz, 2H), 7.80 (s, 1H), 7. 63 (t, J = 7.4 Hz, 1H), 7.55 (t, J = 7.7 Hz, 2H).



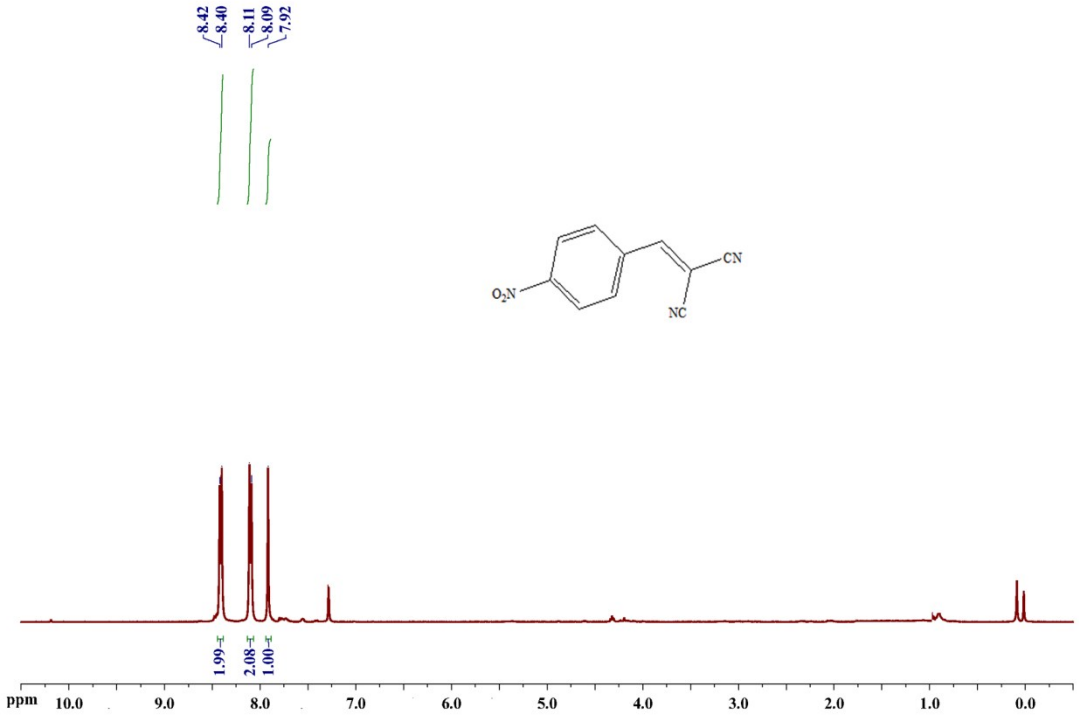
2-(4-Bromophenylmethylene)malononitrile. White solid; ^{1}H NMR ($CDCl_3$, 300 MHz): δ (ppm): 7.79-7.68 (m, 5H).



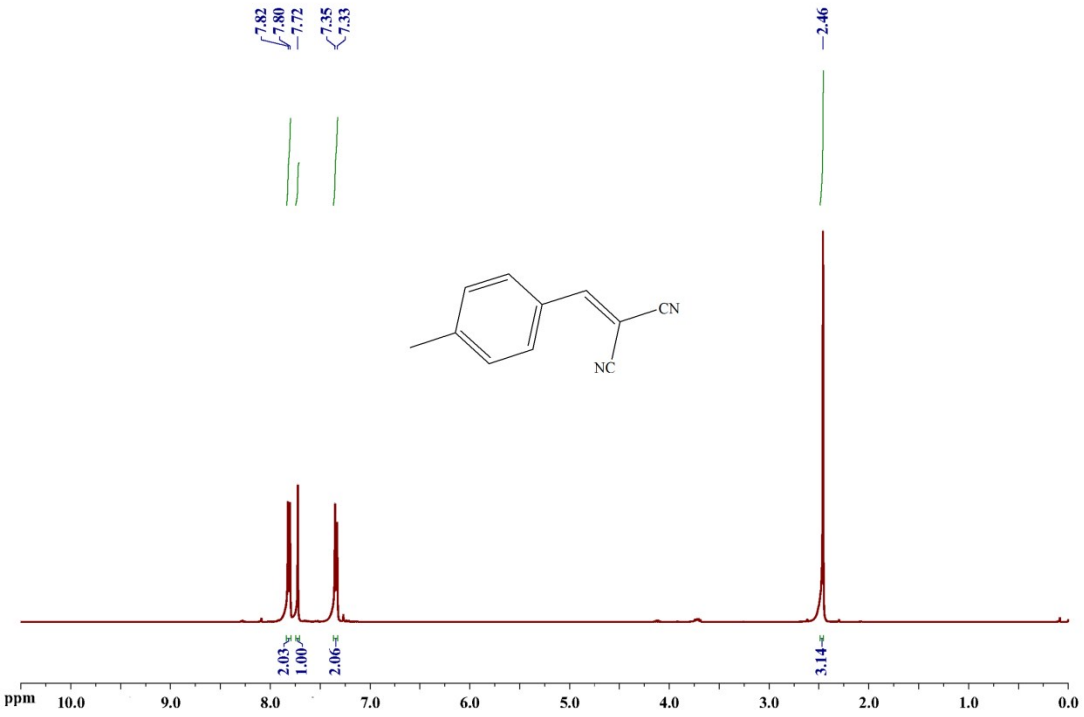
2-(4-Fluorophenylmethylene)malononitrile. White solid; ^{1}H NMR ($CDCl_3$, 500 MHz,): δ(ppm): 7.99-7.95 (m, 2H), 7.76 (s, 1H), 7.26-7.22 (m, 2H).



2-(4-Nitrophenylmethylene)malononitrile. Yellow solid; ^{1}H NMR ($CDCl_3$, 500 MHz): δ(ppm): 8.41 (d, J = 8.6, 2H), 8.10 (d, J = 8.5, 2H), 7.92(s, 1H).

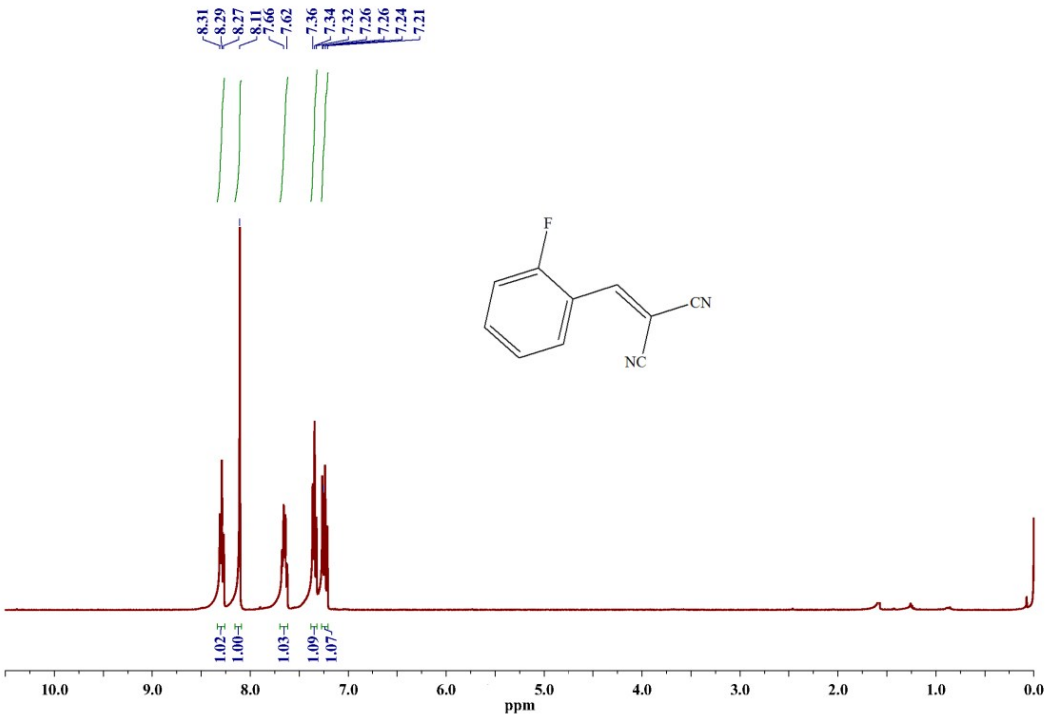


2-(4-Methylphenylmethylene)malononitrile. White solid; ^{1}H NMR ($CDCl_3$, 300 MHz): δ (ppm): 7.81 (d, J = 8.3, 2H), 7.72 (s, 1H), 7.34 (d, J= 8.2, 2H), 2.46 (s, 3H).



2-(2-Fluorophenylmethylene)malononitrile. White solid; ^{1}H NMR ($CDCl_3$, 300 MHz): δ (ppm): 8.27-8.931(m, 1H), 8.11 (s, 1H), 7.62-7.68 (m, 1H), 7.32-7.36(m, 1H), 7.21-

7.36(m, 1H).



2-(3-Fluorophenylmethylene)malononitrile. White solid; ^{1}H NMR ($CDCl_3$, 300 MHz): δ(ppm): 7.76 (s, 1H), 7.62-7,69 (m, 2H), 7.57-7.52 (m, 1H), 7.37-7.32(m, 1H).