Supporting information

A dual-functional Cd(II)-organic-framework demonstrating selective sensing of Zn^{2+} and Fe^{3+} ions exclusively and size-selective catalysis towards cyanosilylation

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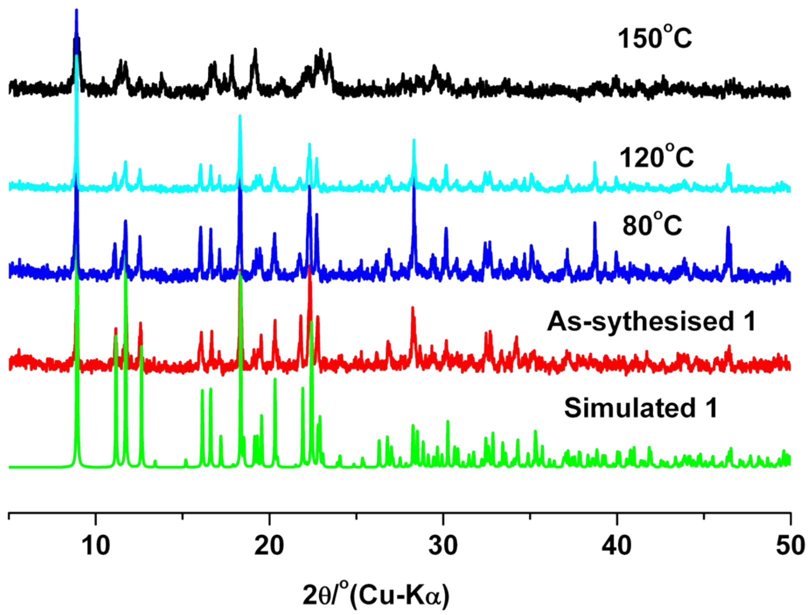
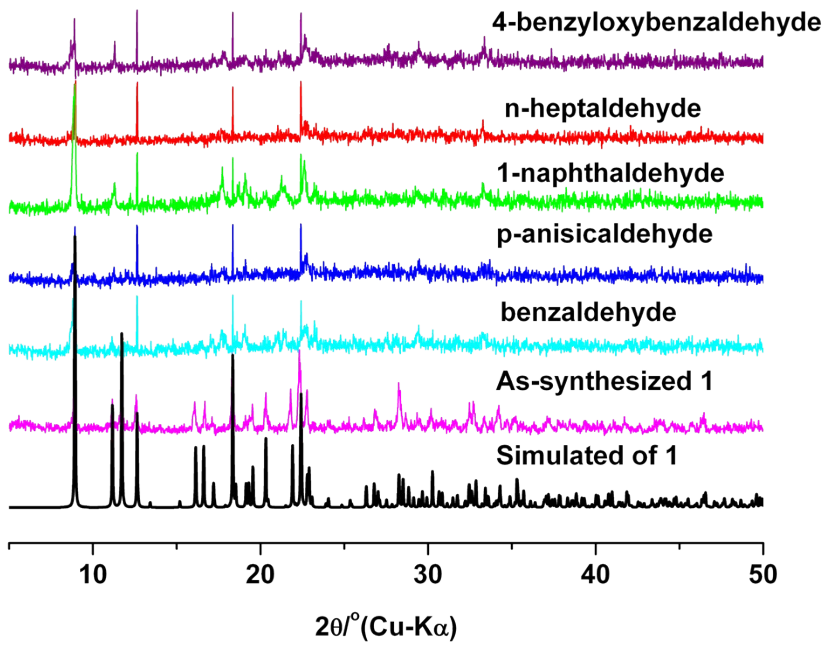


(a)



(b)

Fig. S1. (a) The PXRD patterns of simulated and complex **1** (a) at varied temperature and (b) after cyanosilylation of aldehydes

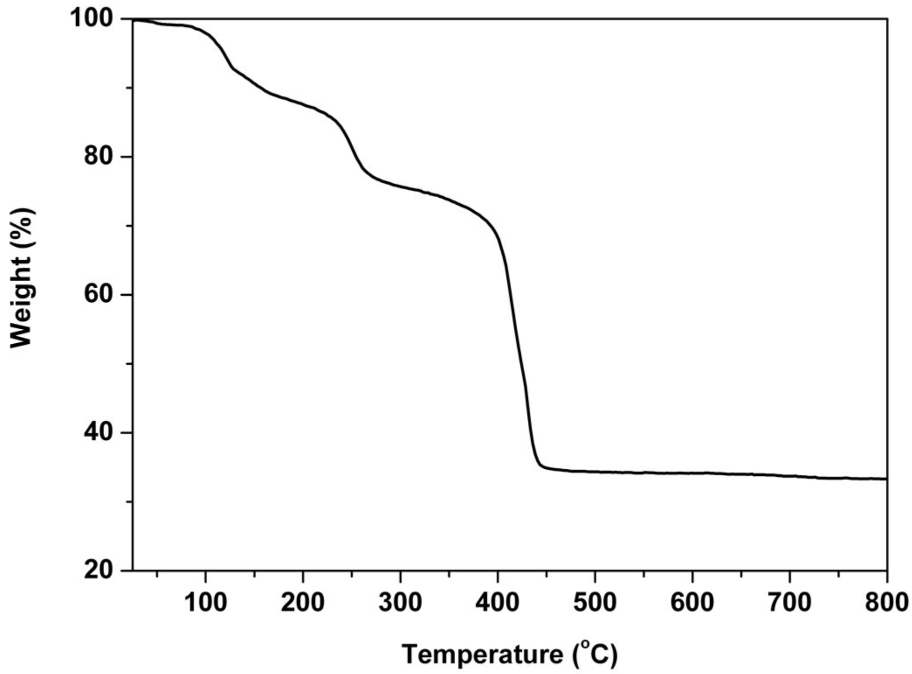
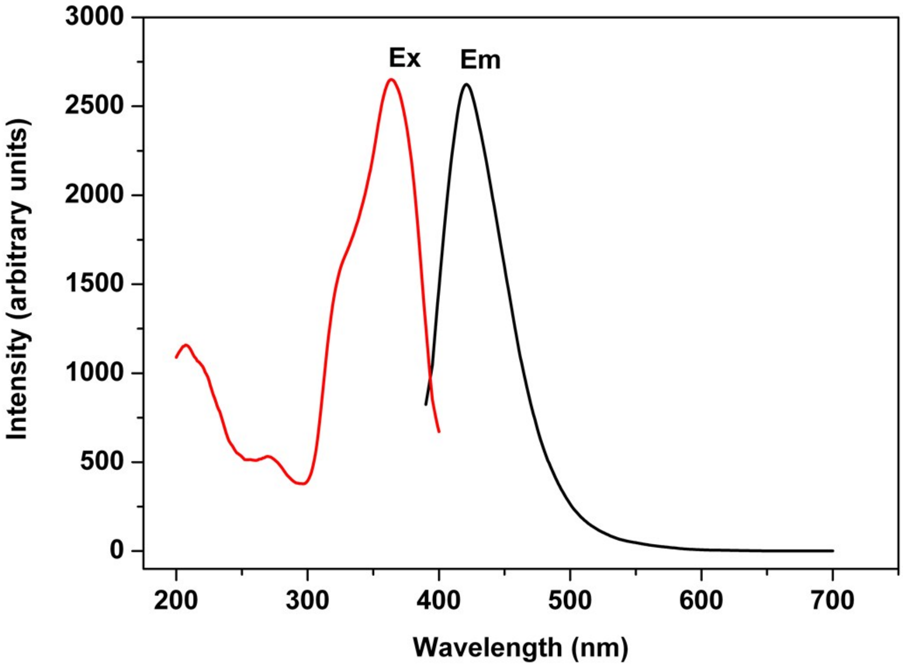
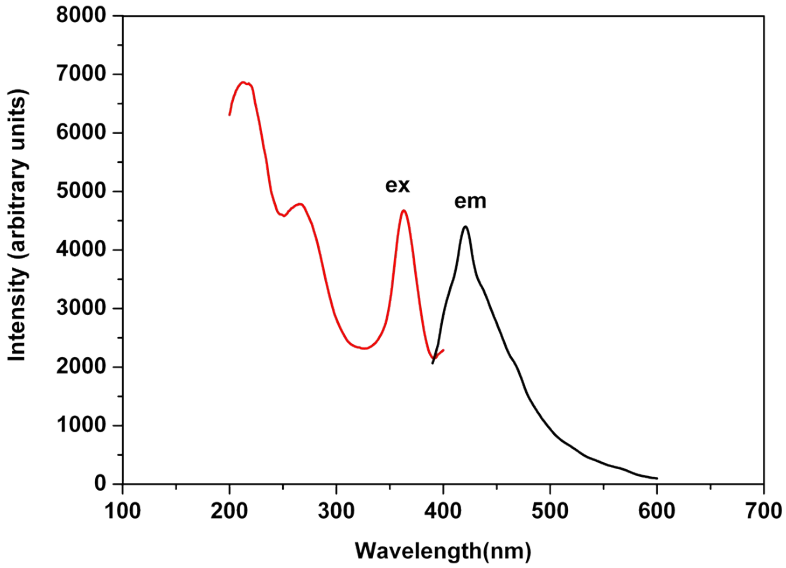


Fig. S2. TGA curve of **1**.

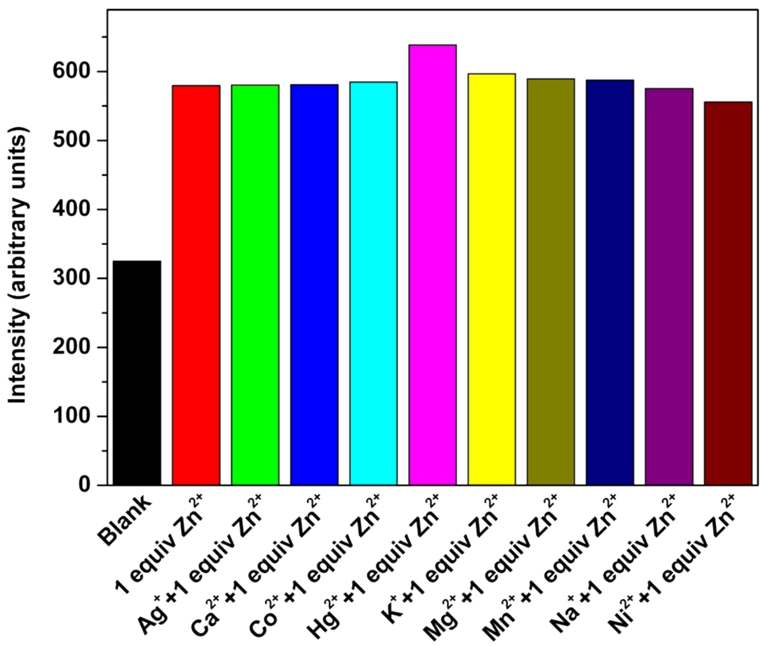


(a)

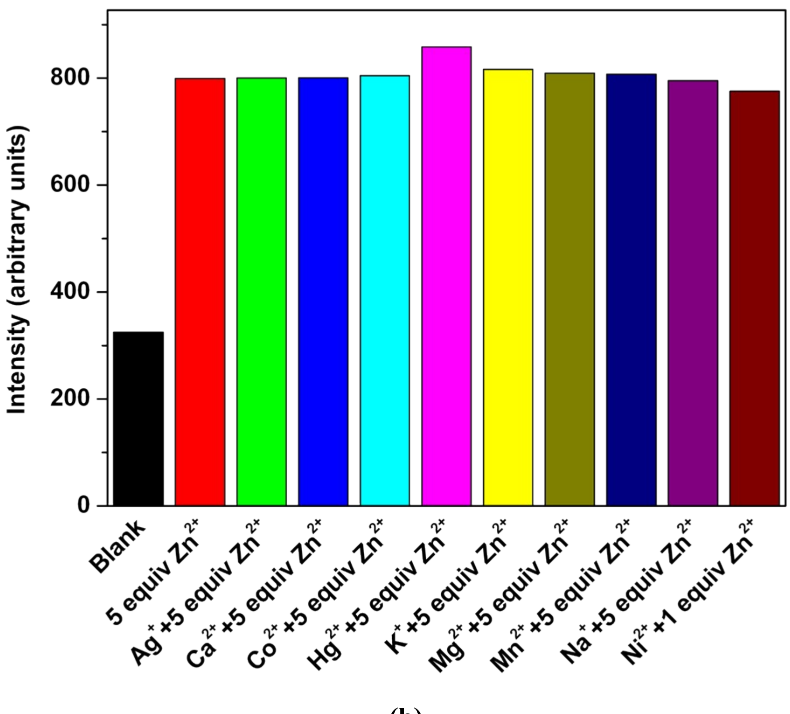


(b)

Fig. S3. (a) Luminescence excitation (at 363 nm) and emission (at 420 nm) spectra of H_4L ligand in the solid state at room temperature. (b) Luminescence excitation (at 368 nm) and emission (at 420 nm) spectra of **1** in the solid state at room temperature.

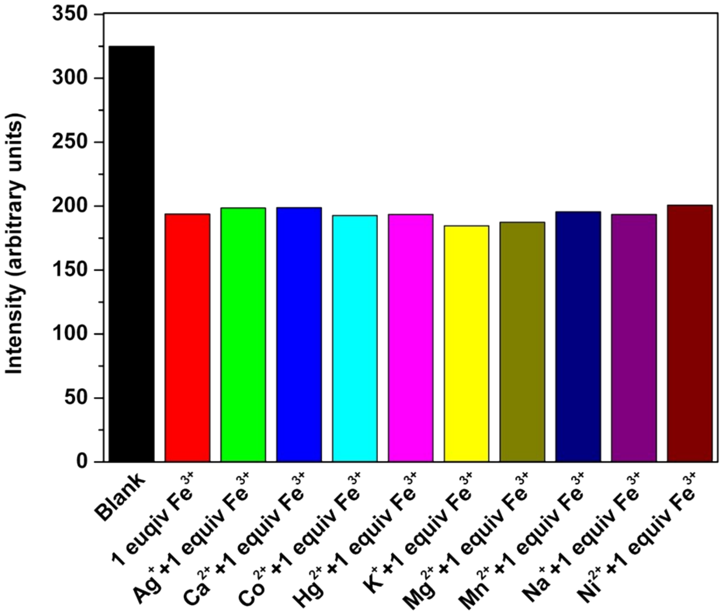


(a)

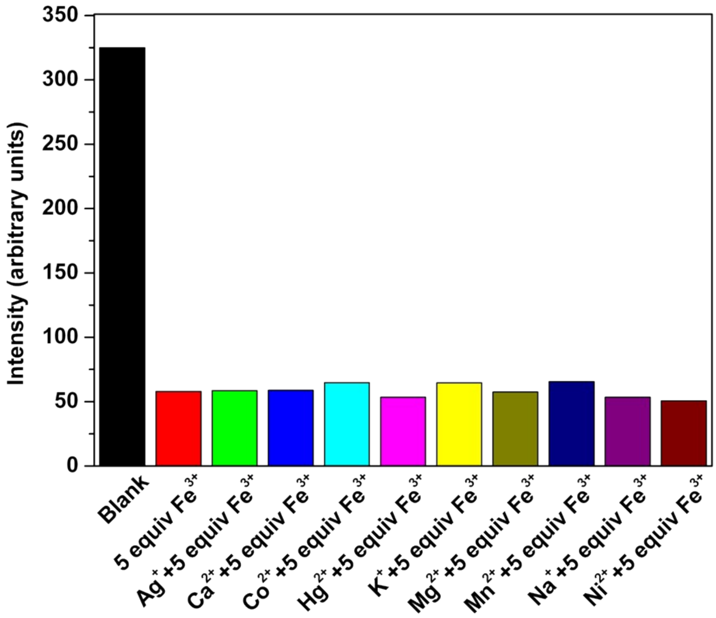


(b)

Fig. S4. Room-temperature luminescent intensities of **1** upon addition of 1 equiv of Zn^{2+} and 1 equiv of various metal ions (a) and with adding 5 equiv of Zn^{2+} and 1 equiv of other metal ions (b) in methanol (excited at 250 nm).



(a)



(b)

Fig. S5. Room-temperature luminescent intensity of **1** upon addition of 1 equiv of Fe^{3+} and 1 equiv of various metal ions (a) and with adding 5 equiv of Fe^{3+} and 1 equiv of other metal ions (b) in methanol (excited at 250 nm).

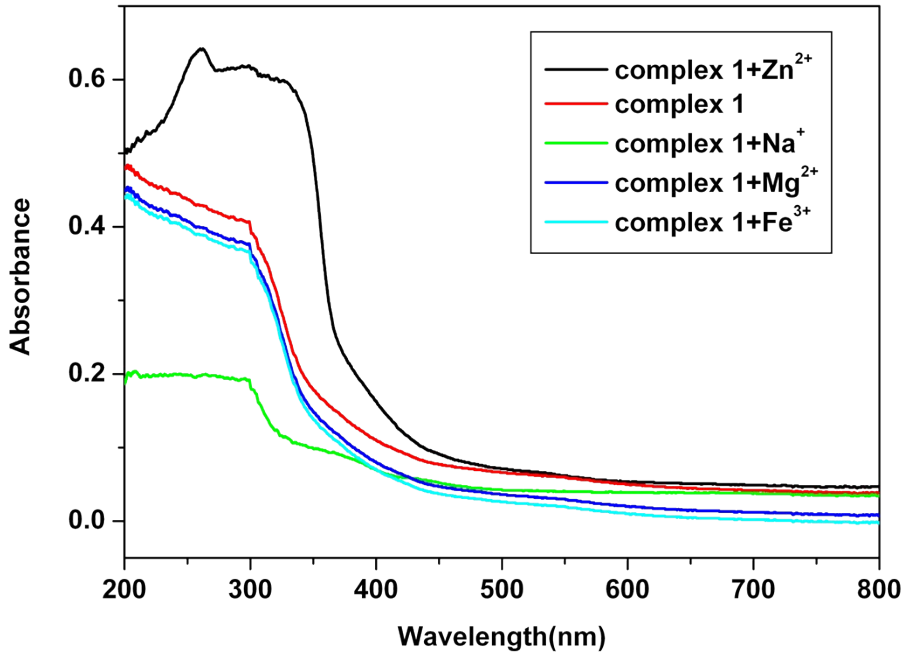
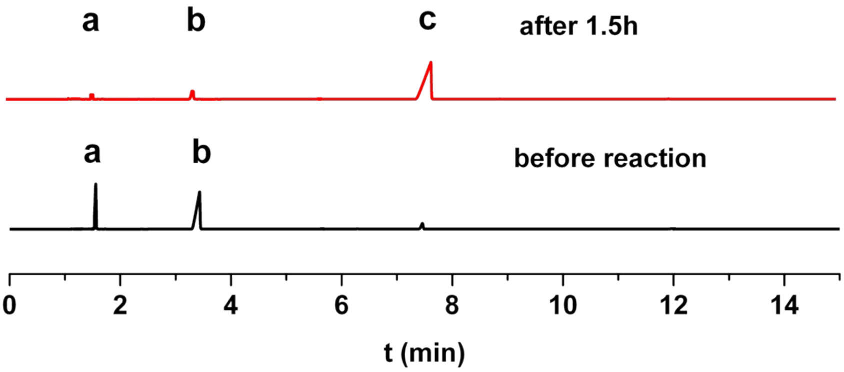
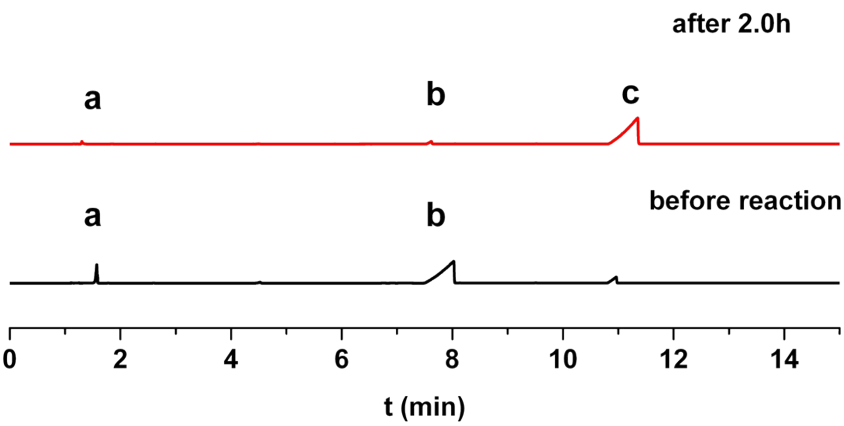


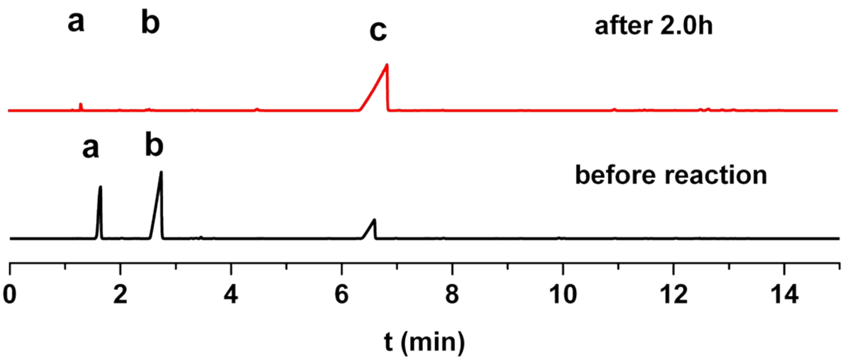
Fig. S6. UV studies for complex **1** in methanol suspension with the introduction of Zn^{2+}, Na^{+}, Mg^{2+}, Fe^{3+}.



(a)



(b)



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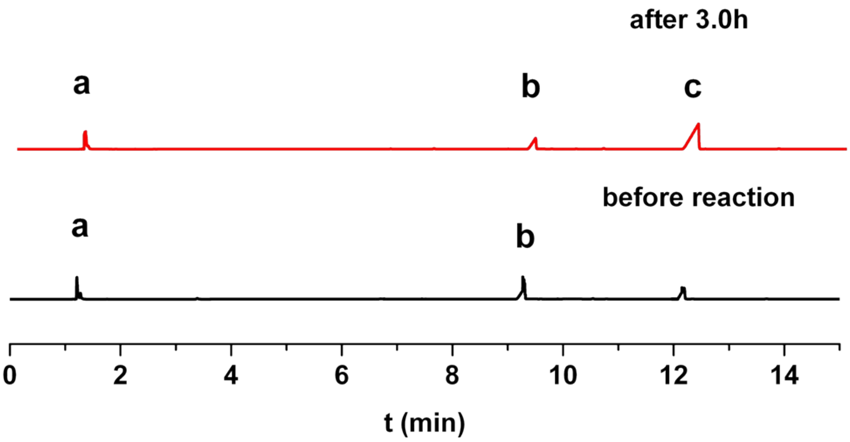
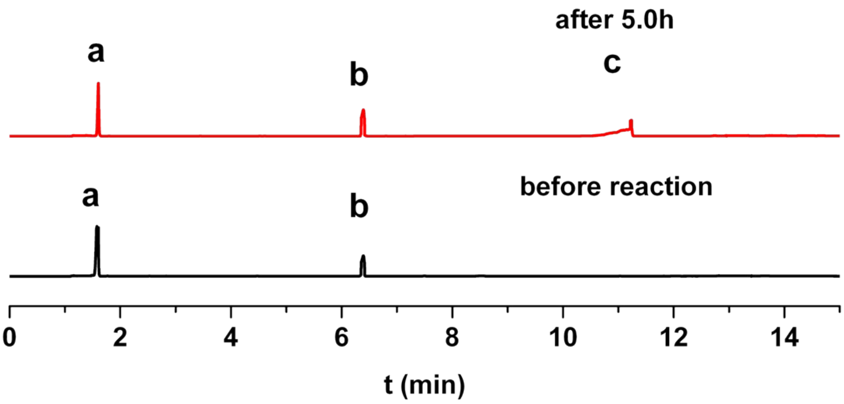


(d)



(e)

Fig. S7. The GC of the reactions of **(a)** Benzaldehyde and Cyanotrimethylsilane, **(b)** p-Anisic aldehyde and Cyanotrimethylsilane, **(c)** 1-Naphthaldehyde and Cyanotrimethylsilane, **(d)** n-Heptaldehyde and Cyanotrimethylsilane, **(e)** 4-Benzyloxybenzaldehyde and Cyanotrimethylsilane catalyzed by **1**.

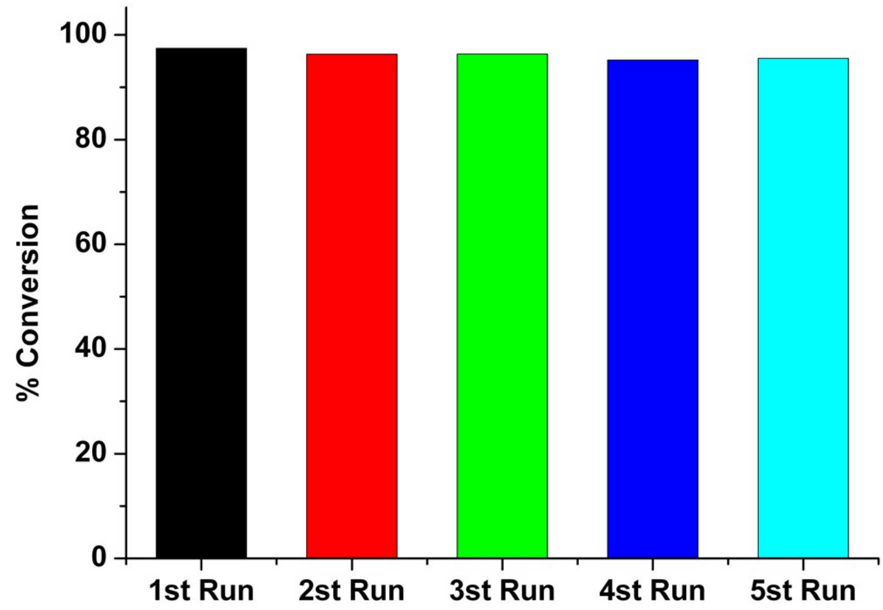


Fig. S8. The comparison of 5 cycles of cyanosilylation reaction (benzaldehyde and TMSCN) with activated **1** as catalyst after 1.5h (The catalyst was isolated from the reaction solution at the end of the catalytic reaction such as the benzaldehyde and TMSCN, dried at 423 K, and then reused in the second run of the reaction.).

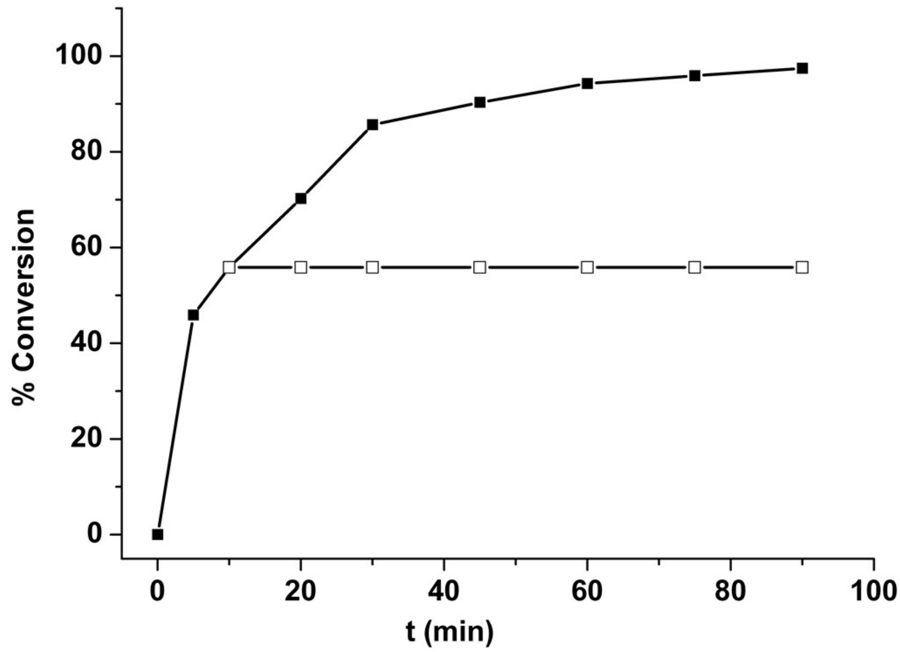


Fig. S9. The conversion (%) versus time (min) for cyanosilylation reaction: **1**-catalyzed reactions with and without filtering off the catalyst.

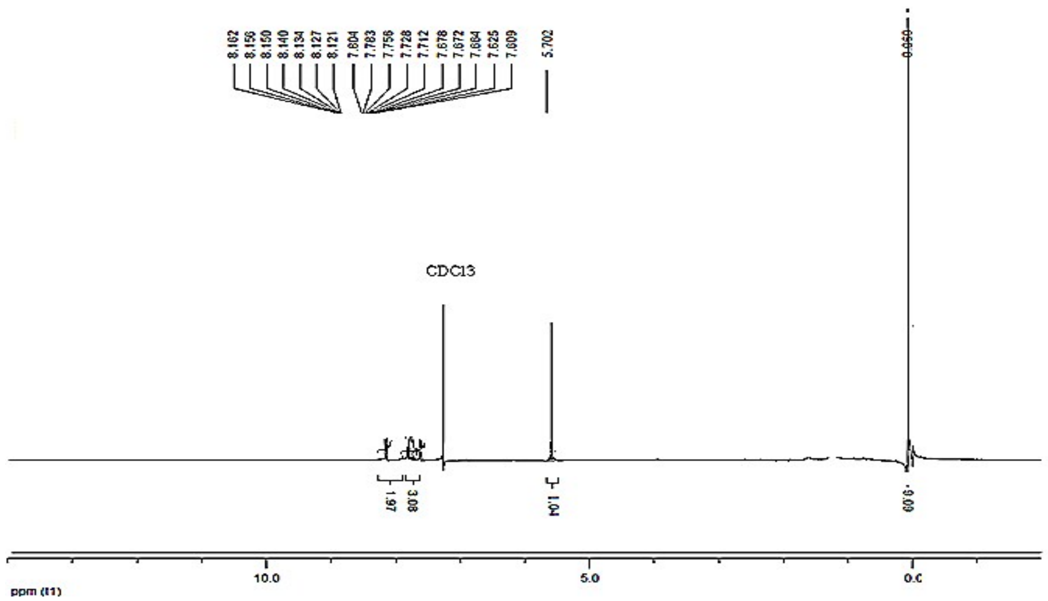
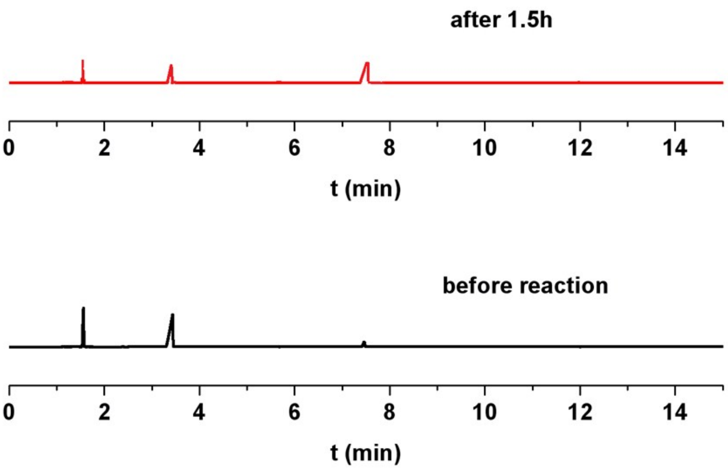
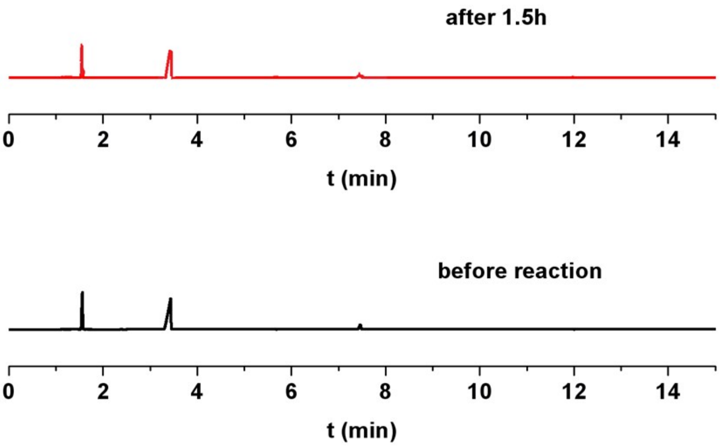


Fig. S10. ^{1}H-NMR ($CDCl_3$): 7.61-8.16 (m, 5H), 5.70 (s, 1H), 0.69 (s, 9H) of cyanosilylation (benzaldehyde and TMSCN) reaction's product. And the crude product was purified by column chromatography to give the pure product.





(b)

Fig. S11. The GC of the reactions of benzaldehyde (4 mmol) and cyanotrimethylsilane (4mmol) catalyzed by **(a)** $Cd(NO_3)_2\cdot 4H_2O$ (0.04 mmol) and **(b)** H_4L (0.04 mmol).

Table S1. Cyanosilylation of benzaldehyde (comparison of yields)

Catalyst	Solvent	Temp.K	Time/h	Conversion %
MIL-101 (0.5% mol)[26a]	heptane	313K	3	98.5
$Mn_3[(Mn_4Cl)_3(BTT)_8(CH_3OH)_{10}]_2$ (11 mol%)[16c]	CH_2Cl_2	298K	9	98
$Cu_3(BTC)_2$ (5 mol%)[18c]	CH_2Cl_2	313 K	48	50
(O_2H_3)Sc-MOF (5 mol%)[26b]	ethanol	313K	8	84
(μ-OH)6Sc-MOF (5 mol%)[26b]	ethanol	313K	8.5	77.3
(Phen)Sc-MOF (5 mol%)[26b]	ethanol	313K	7	55
$[\{Et_4N[Co(L^{p\text{-}COOH})_2]_2Zn_6(OH)_2(H_2O)_{10}\}\cdot 14H_2O]_n$ (5 mol %)[26c]	Solvent-Free	298K	4	90
$[\{Et_4N[Co(L^{m\text{-}COOH})_2]Zn_3(OH)(H_2O)_6\}\cdot 11H_2O]_n$ (5 mol %)[26c]	Solvent-Free	298K	4	94
$[\{Et_4N[Co(L^{p\text{-}COOH})_2]_2Cd_{2.5}(H_2O)_{10}\}\cdot 24H_2O]_n$ (5 mol %)[26c]	Solvent-Free	298K	4	86
$[\{Et_4N[Co(L^{m\text{-}COOH})_2Cd_{2.5}(H_2O)_{15}\}\cdot 9H_2O]_n$ (5 mol %)[26c]	Solvent-Free	298K	4	92
$\{[Zn_3(4,4'\text{-bpy})_{3.5}(\mu\text{-}O_2CH)_4(H_2O)_2](ClO_4)_2(H_2O)_2\}_n$ (5 mol %)[26d]	CH_2Cl_2	298K	24	22
$[Cu_2(bpy)(H_2O)_{5.5}]_2[H_2W_{11}O_{38}]\cdot 3H_2O\cdot 0.5CH_3CN$ (2 mol %)[26e]	CH_2Cl_2	313K	24	98.1
DUT-4 (4% mol)[26f]	N-heptane	313K	12h	~100
Complex **1** (1% mol)	CH_2Cl_2	313K	1.5h	97.44