Electronic supplementary information for

Molecular recognition of catechol on crystal-like surface of periodic mesoporous organosilica containing pyridinylethynylpyridine

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General:

All reagents and solvents were commercially available and used without further purification. ^{1}H and ^{13}C NMR spectra were obtained using a Jeol ECX-400 spectrometer operating at 400 and 100 MHz, respectively. ^{29}Si dipolar decoupling (DD) and ^{13}C cross polarization (CP) magic-angle-spinning (MAS) NMR measurements were respectively performed at 79.49 and 100.6 MHz at a sample spinning frequency of 4 kHz using a Bruker AVANCE 400 spectrometer with a 7 mm zirconia rotor. For the ^{29}Si DD MAS NMR measurements, the repetition delay was 80 s, and the pulse width was 4.5 μs. For the ^{13}C CP MAS NMR measurements, the repetition delay was 5 s, the contact time was 1.75 ms, and the pulse width was 4.5 μs (^{1}H 90° pulse). Chemical shifts were referenced to tetramethylsilane and glycine for ^{29}Si and ^{13}C NMR, respectively. XRD profiles were recorded on a Rigaku RINT-TTR diffractometer using Cu Kα radiation (50 kV, 300 mA). Nitrogen adsorption and desorption isotherms were measured using a Yuasa Nova3000e sorptometer. Brunauer-Emmett-Teller (BET) surface areas were calculated from the linear sections of BET plots (P/P_0 = 0.1–0.2). Pore size distributions were calculated using the DFT method (DFT kernel: N_2 at 77 K on silica, cylindrical pores, non-local density functional theory (NLDFT) equilibrium model). Pore volumes were estimated by the t-plot method. Transmission electron microscopy (TEM) observations were performed using a Jeol JEM-EX2000 operating at 200 kV. IR spectra were collected on a Thermo Fisher Scientific Nicolet Avatar-360 FT-IR spectrometer using an attenuated total reflection (ATR) attachment. UV/vis absorption spectra were obtained using a Jasco V-670.

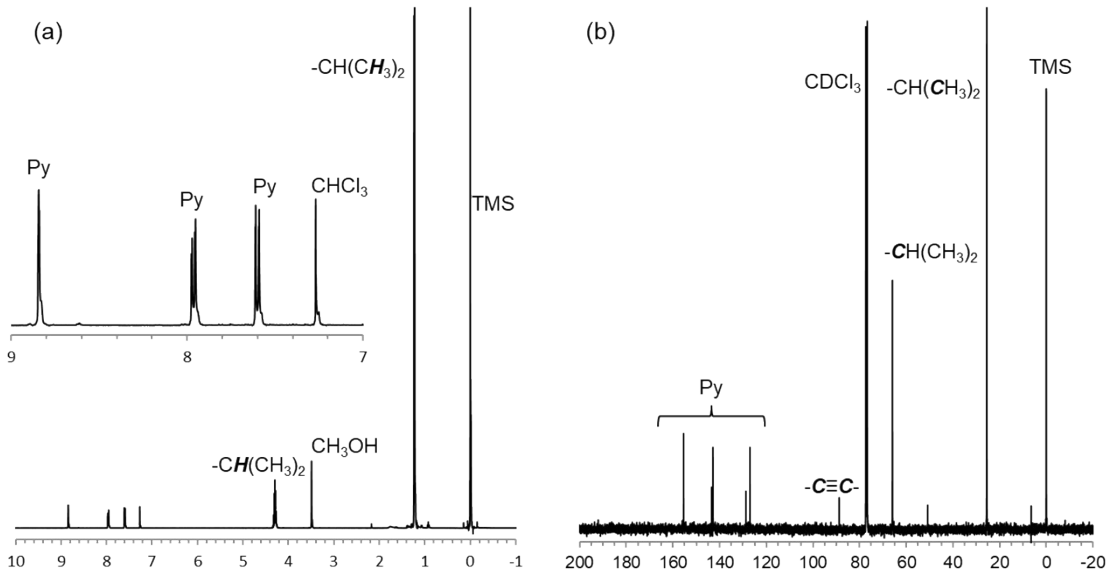

Fig. S1 (a) ^{1}H and (b) ^{13}C NMR spectra of **PEPy-Si** monomer.

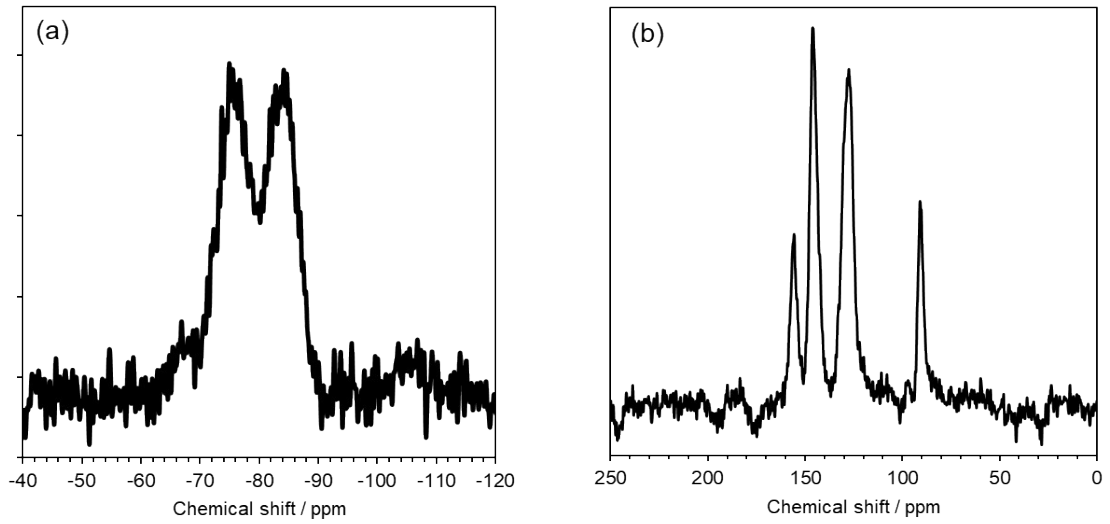

Fig. S2 (a) ^{29}Si DD MAS and (b) ^{13}C CP-MAS NMR spectra of PEPy-PMO.

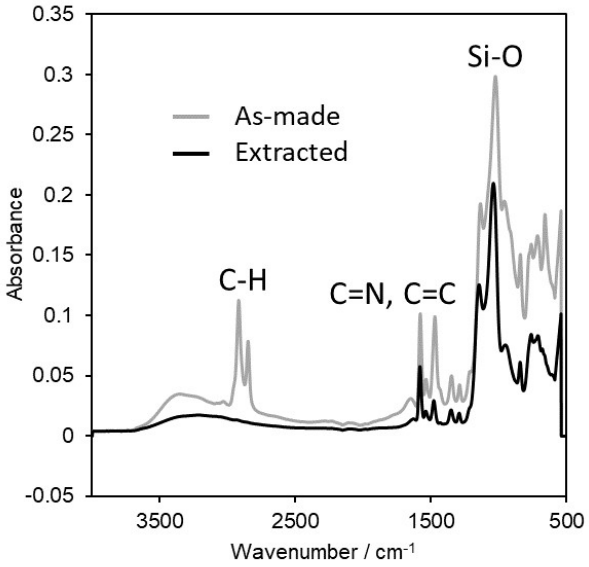

Fig. S3 IR spectra of PEPy-PMO.

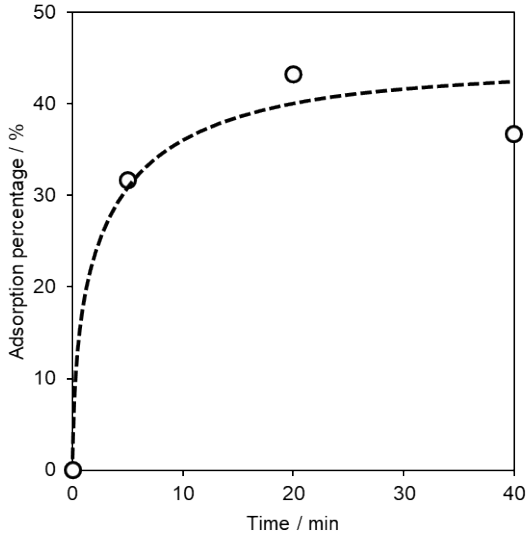

Fig. S4 Adsorption profile of catechol **1** by adding PEPy-PMO in a mixture of Et_2O and hexane.

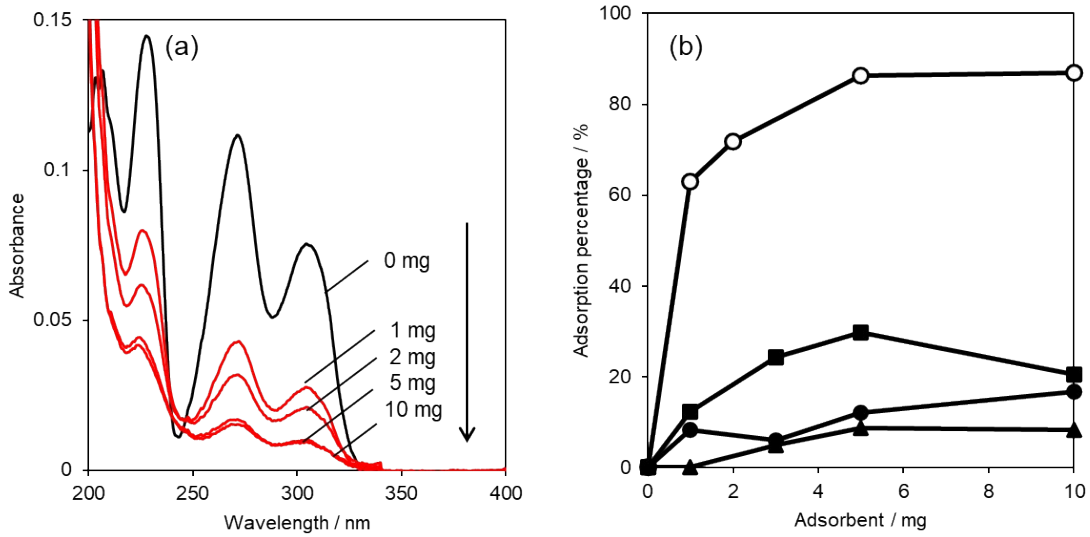

Fig. S5 (a) Changes in the UV/vis spectra of catechol **2** (1×10^{-4} M) in a mixture of Et_2O/hexane by adding PEPy-PMO. (b) Adsorption percentage of catechol **2** by adding PEPy-PMO (○), BPy-PMO (■), Bp-PMO (●), and FSM-16 (▲) using 0-10 mg of adsorbent.

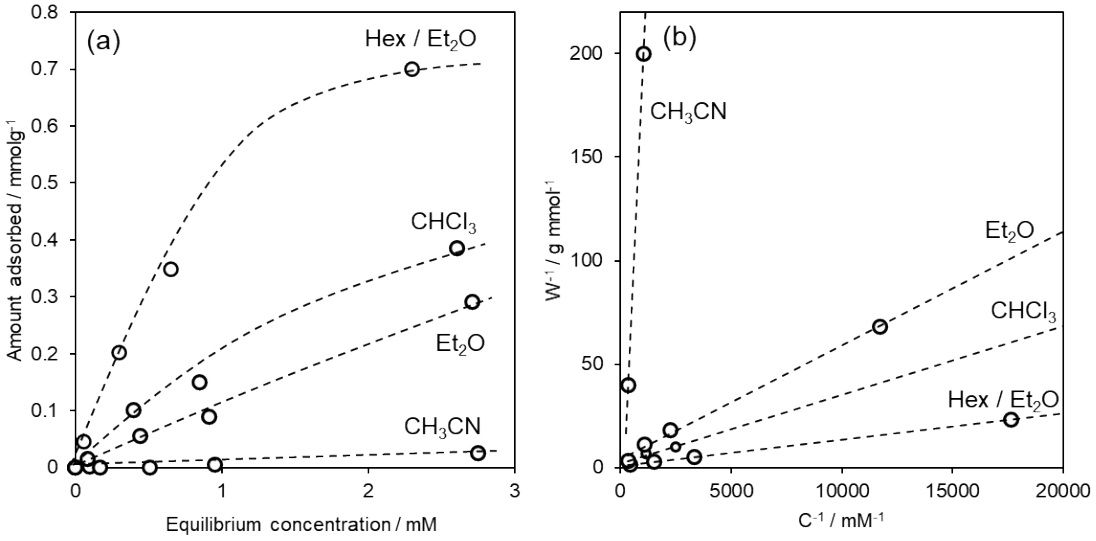

Fig. S6 (a) Langmuir non-linear and (b) linear plots obtained from the adsorption of catechol **1** with PEPy-PMO in various organic solvents. The dashed lines indicate the theoretical profiles.

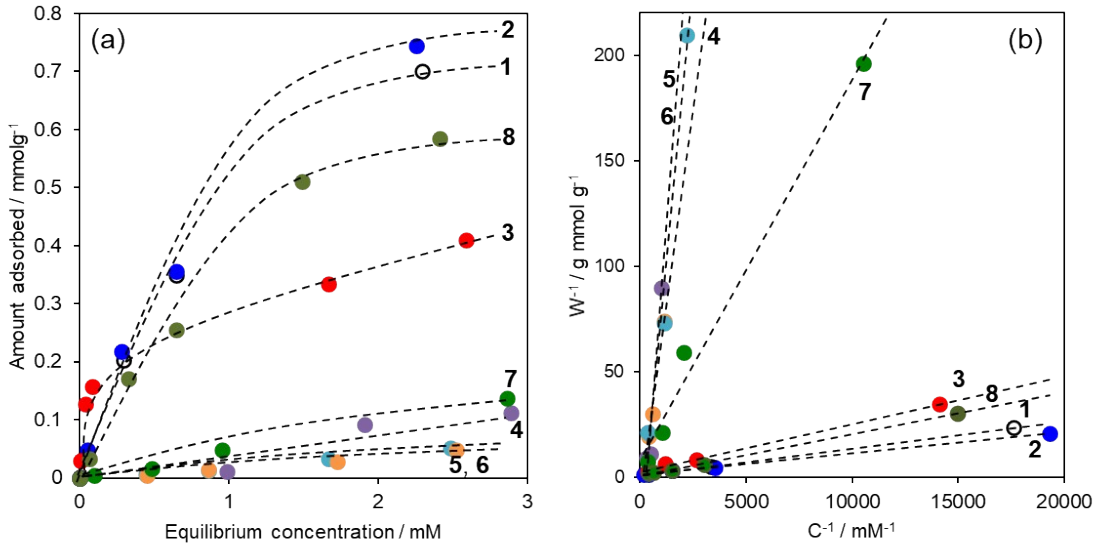

Fig. S7 (a) Langmuir non-linear and (b) linear plots obtained from the adsorption of catechols and its derivatives **1-8** with PEPy-PMO in a mixture of Et_2O/hexane. The dashed lines indicate the theoretical profiles.

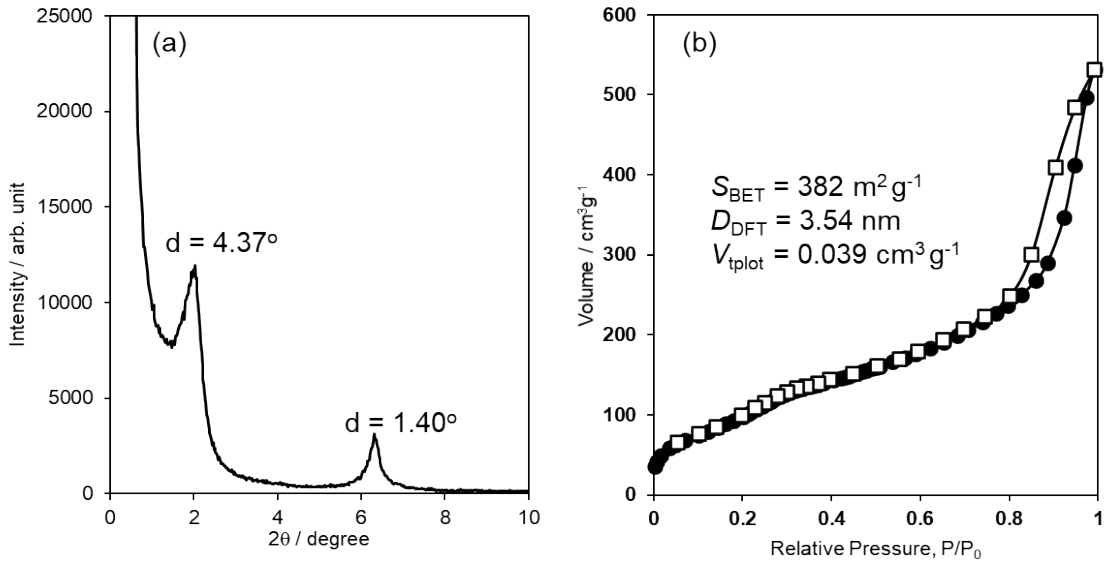

Fig. S8 XRD pattern and N_2 adsorption-desorption isotherms of Cate@PMO.

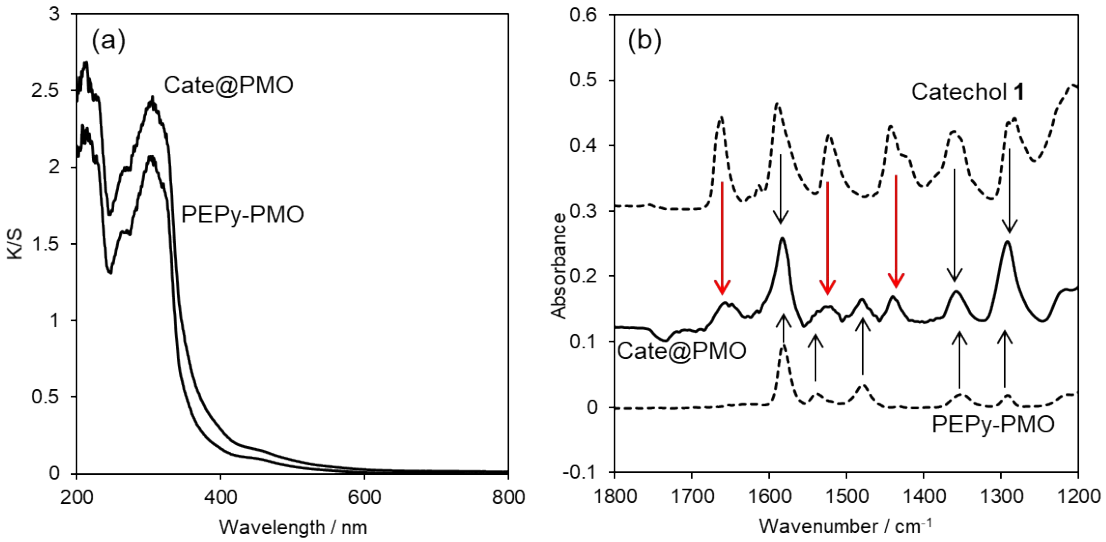

Fig. S9 (a) UV/vis diffuse reflectance and (b) FT-IR spectra of Cate@PMO. Red arrows indicated the C=C stretching vibration peaks of catechol adsorbed in Cate@PMO.

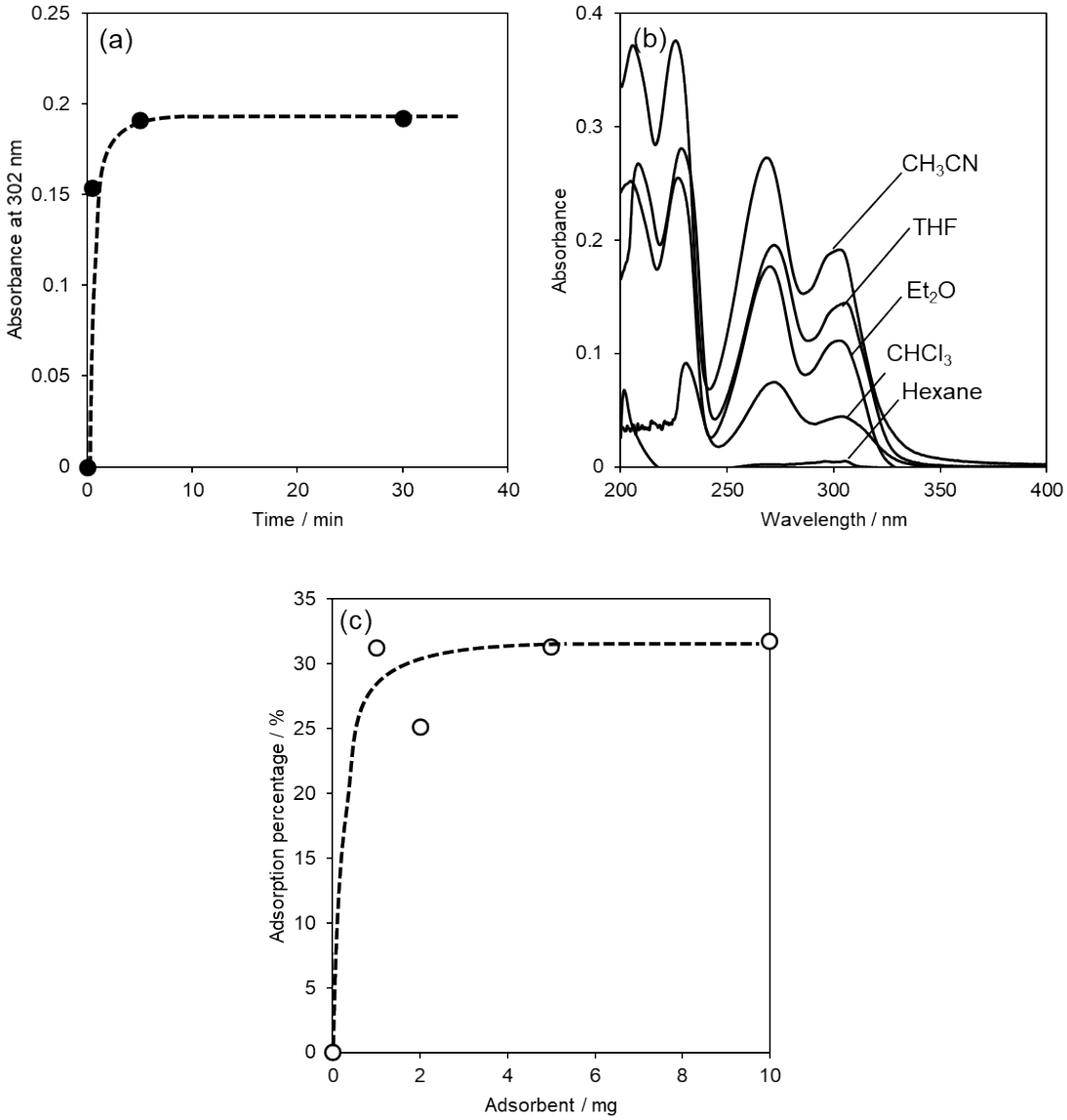

Fig. S10 (a) Release profile of catechol **1** by immersing Cate@PMO (1 mg) in CH_3CN (1 mL). (b) UV/vis absorption spectra of released catechol **1** from Cate@PMO (1 mg) in various organic solvents (1 mL). (c) Adsorption percentages for catechol **1** (1×10^{-4} M) in a mixture of Et_2O/hexane by adding recovered PEPy-PMO (1 – 10 mg).

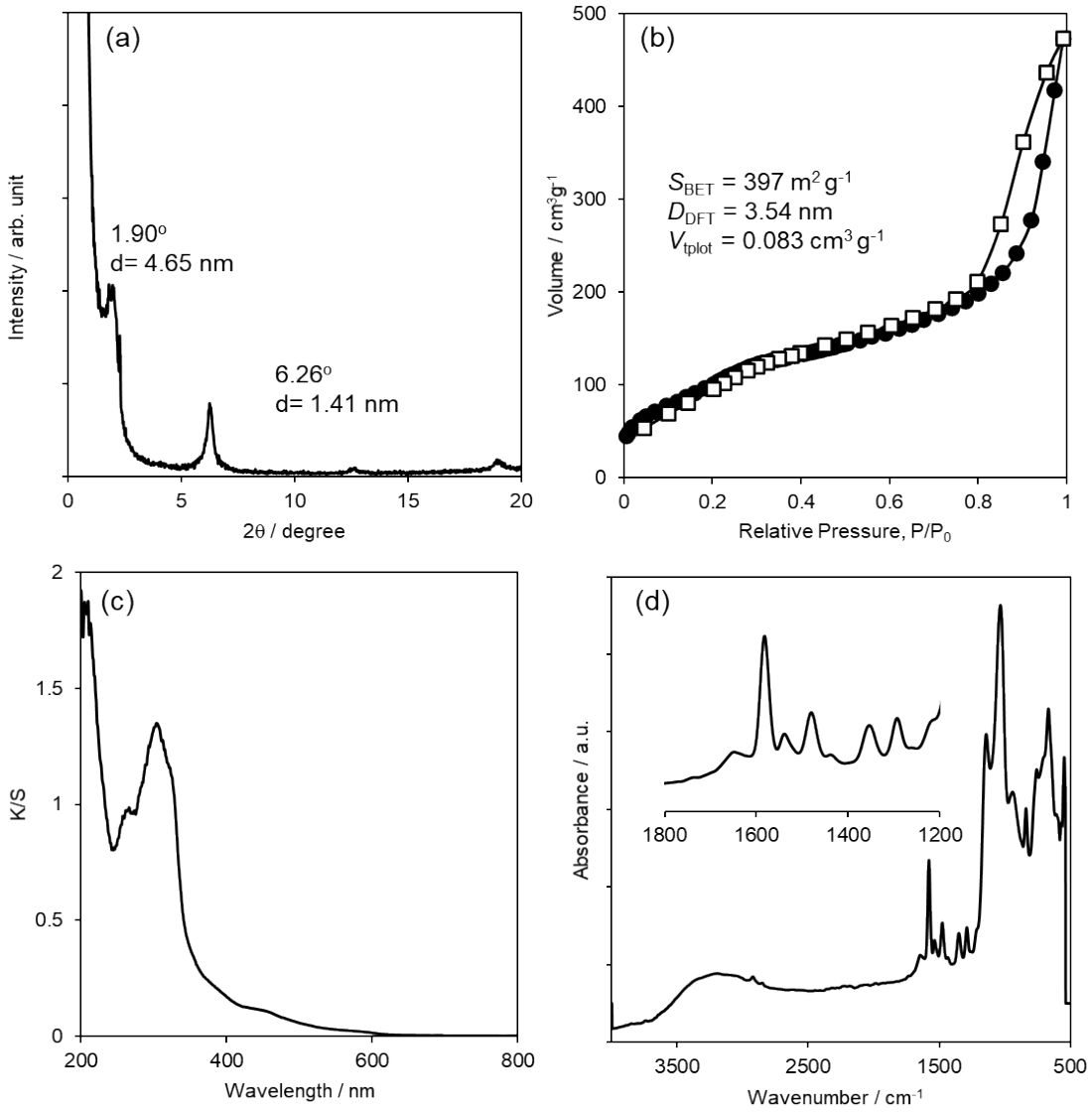

Fig. S11 (a) XRD pattern, (b) N_2 adsorption-desorption isotherms, (c) UV/vis diffuse reflectance spectrum, and (d) FT-IR spectrum of PEPy-PMO after releasing catechol.

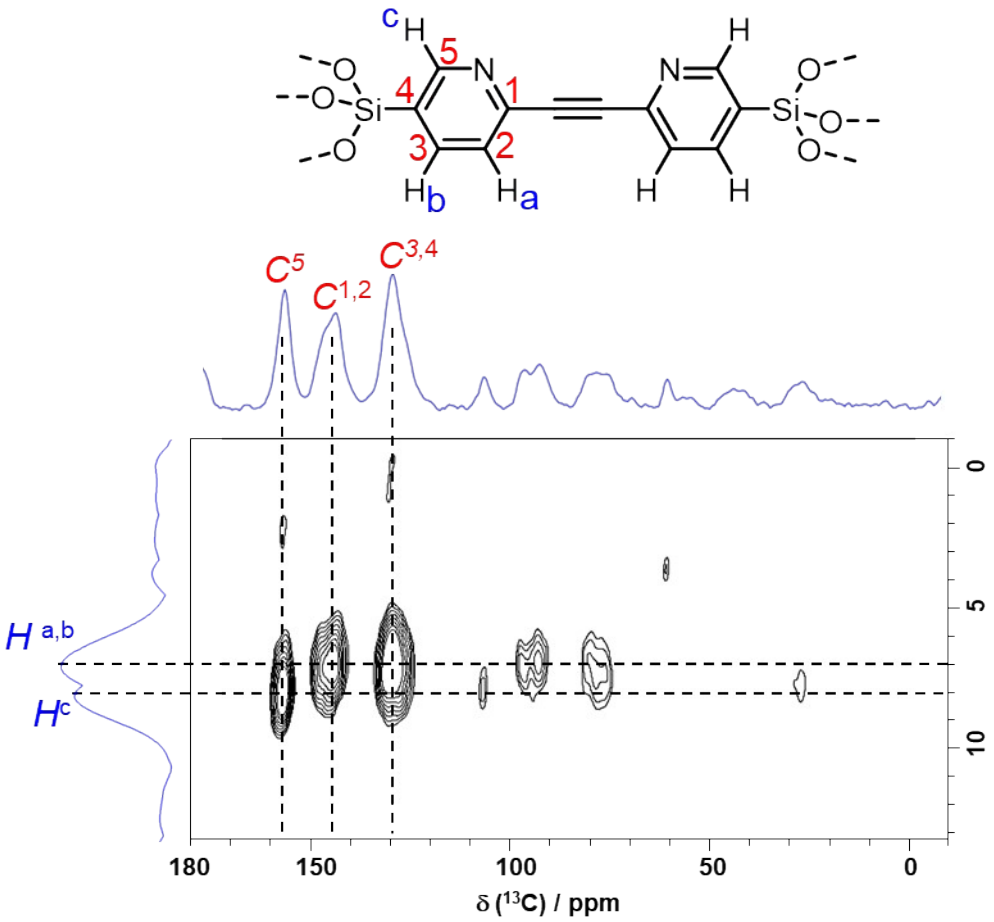

Fig. S12 ^{1}H-^{13}C HETCOR MAS NMR spectrum of PEPy-PMO.

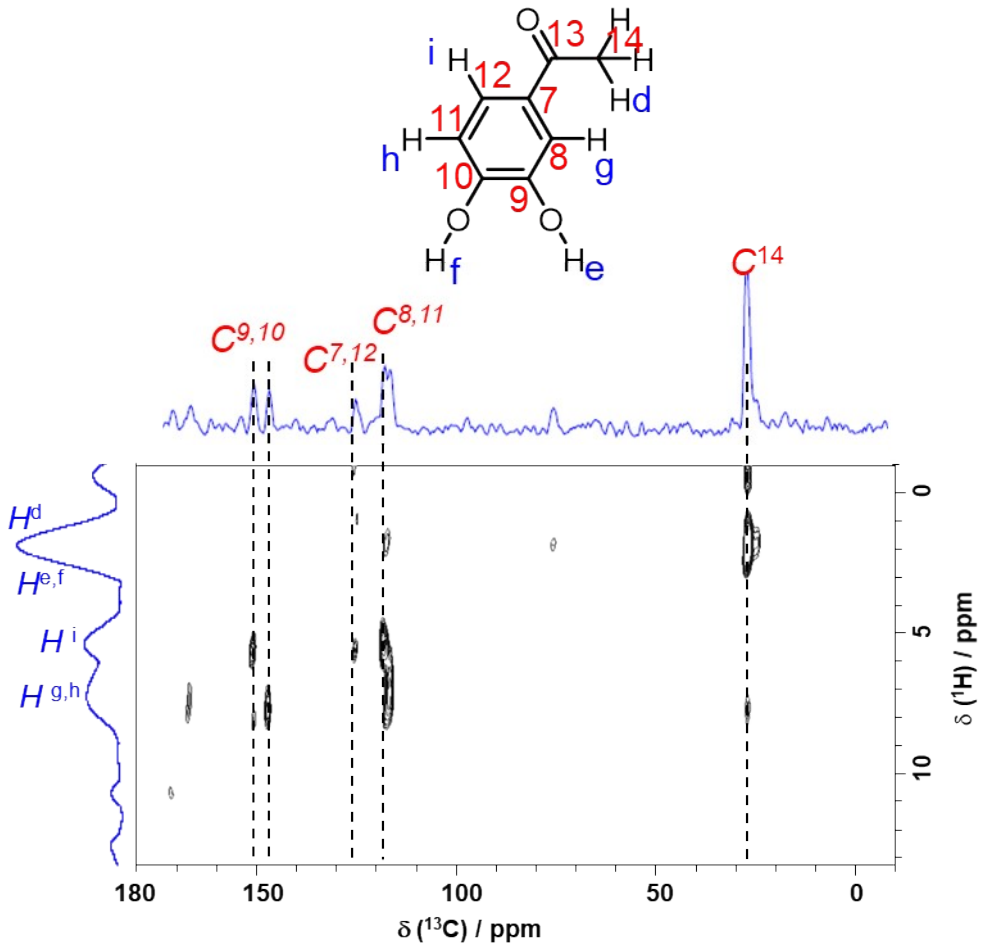

Fig. S13 ^{1}H-^{13}C HETCOR MAS NMR spectrum of catechol **1**.

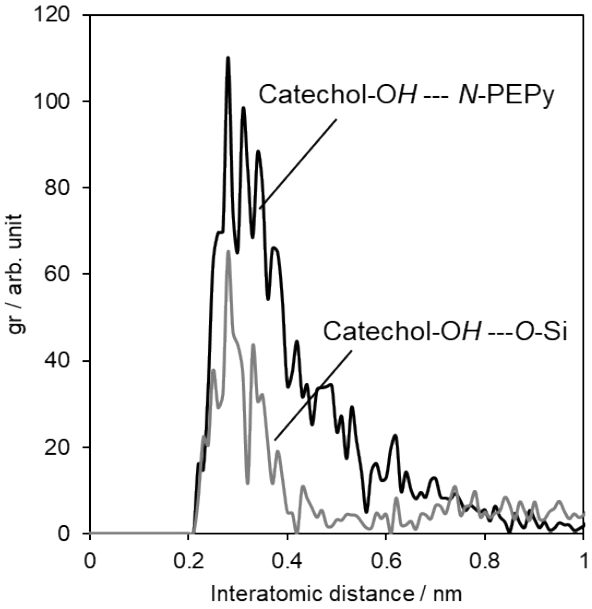

Fig. S14 Radial distribution function (gr) of the interatomic distance between the O*H* of catechol **1** and the *N* atom of PEPy (black) or *O*H of silanol (gray).

Table S1 Energy and population of the interaction between catechol **1** and PEPy in the MD simulation.[a]

	Energy / kcal mol^{-1}		Population / %
	Coulomb	VDW	
Catechol-OH---N-PEPy	-1.59	0.03	10.4
Catechol-OH---O-Si (Catechol-O---HO-Si)	-1.39	0.03	4.1
Solvent-O---HO-Si	-0.27	0.00	2.0

[a] Diffusion coefficient is 0.38×10^{-5} cm^2 s^{-1}.