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### **Supporting Information**

### A New Transformation of Coumarins via Direct C-H Bond Activation

#### Utilizing an Iron-Organic Framework as a Recyclable Catalyst

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Section S1: Materials and Analytical Techniques

**Materials.** All reagents and starting materials were obtained commercially from Sigma-Aldrich, Merck, and Tokyo Chemical industry CO., LTD. (TCI) were used as received without any further purification unless otherwise noted.

**Analytical techniques.** The single crystal of VNU-20 was mounted on a cryoloop and cooled down by a nitrogen flow controlled by a Kryoflex II system. A Bruker D8 Venture diffractometer was used with X-rays generated by a monochromatic microfocus Cu K $\alpha$  radiation source ( $\lambda$  = 1.54178 Å) at 50 kV and 1.0 mA. The diffraction data was collected by a PHOTON-100 CMOS detector. The unit cell was determined using Bruker SMART APEX II software suite. The data set was reduced and data correction was carried out by a multi-scan spherical absorption method. The structure was solved by direct methods and further refinement was carried out using the full-matrix least-squares method in the SHELX-97 program package. The crystallographic information file (CIF) of VNU-20 can be obtained, free of charge, via the Cambridge Structural Database (CCDC number: 1572921).

Powder X-ray diffraction (PXRD) patterns were collected using a D8 Advance diffractometer equipped with a LYNXEYE detector. Thermogravimetric analysis (TGA) was performed using a TA Instruments Q-500 thermal gravimetric analyzer under a gas mixture of  $O_2$  (20%) and  $N_2$  (80%) with temperature ramp of 5 °C min<sup>-1</sup>. Fourier transform infrared (FT-IR) spectra were measured on a Bruker ALPHA FTIR spectrometer using Attenuated Total Reflection (ATR) sampling technique. Low-pressure  $N_2$  adsorption measurements were carried out on the Micromeritics volumetric gas adsorption analyzer (3-FLEX Surface

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Characterization). A liquid  $N_2$  bath was used for measurements at 77 K. Helium was used as estimation of dead space. Ultrahigh-purity-grade  $N_2$ , and He (99.999% purity) were used throughout adsorption experiments.

XPS analysis was performed at room temperature using a Thermo Scientific K-Alpha+ X-ray Photoelectron Spectrometer with Al Kα radiation. C 1s (284.6 eV) was used to calibrate the binding energies of the elements.

Gas chromatographic (GC) analyses were performed using a Shimadzu GC 2010-Plus equipped with a flame ionization detector (FID) and an SPB-5 column (length = 30 m, inner diameter = 0.25 mm, and film thickness = 0.25  $\mu$ m). The temperature program for GC analysis held samples at 120 °C for 0.5 min; heated them from 120 to 130 °C at 40 °C/min; held them at 130 °C for 1 min; heated them from 130 to 280 °C at 40 °C/min; and finally held them at 280 °C for 1.5 min.. Inlet and detector temperatures were set constant at 280 °C. The GC yield was calculated using diphenyl ether as the internal standard. GC-MS analyses were analyzed on a Shimadzu GCMS-QP2010Ultra with a ZB-5MS column (length = 30 m, inner diameter = 0.25 mm, and film thickness = 0.25  $\mu$ m). The temperature program for GC-MS analysis held samples at 50 °C for 2 min; heated samples from 50 to 280°C at 10 °C/min and held them at 280 °C for 10 min. Inlet temperature was set constant at 280 °C. MS spectra were compared with the spectra gathered in the NIST library. The <sup>1</sup>H NMR and <sup>13</sup>C NMR were recorded on Bruker AV 500 spectrometers using residual solvent peak as a reference.

### Section S2: Material Synthesis

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**Synthesis of VNU-20.** The mixture of  $H_2NDC$  (0.09 g, 0.42 mmol),  $H_3BTC$  (0.03 g, 0.112 mmol) and FeCl<sub>2</sub> (0.09 g, 0.705 mmol) and was dissolved in DMF (12 mL) and sonicated for 5 min to obtain a clear solution. Subsequently, this solution was divided into glass tubes, which was sealed and placed in an isothermal oven at 200 °C for 72 h to obtain the reddish crystal of VNU-20. Consequently, VNU-20 crystals were exchanged by DMF (5 x 15 mL) and methanol (5 x 15 mL). The sample was then activated under a dynamic vacuum to obtain activated VNU-20 (0.057 g, yield: 75% base on  $H_3BTC$ ).



**Figure S1.** Synthetic scheme for self-assembling the reddish-yellow crystal of VNU-20.

### Section S3: Single Crystal X-rays Diffraction Analysis

Empirical formula	$C_{39.1}H_{24.5}Fe_{3}N_{2.1}O_{15.7}$
Formula weight	942.46
Temperature (K)	93(2)
Wavelength (Å)	1.54178
Crystal system	monoclinic
Space group	P 2 <sub>1</sub> /c
	<i>a</i> = 12.6797(3)
Unit cell dimensions (Å)	<i>b</i> = 13.5123(4)
	<i>c</i> = 23.9480(7)
Volume (Å <sup>3</sup> )	4103.1(2)
Z	4
Density (g cm <sup>-1</sup> )	1.526
Absorption coefficient (mm <sup>-1</sup> )	9.046
<i>F</i> (000)	1910
Crystal size (mm)	0.356 × 0.233 × 0.154
$\theta$ range (°)	3.486 to 62.355.
Index ranges	$-14 \le h \le 14, -15 \le k \le 13, -25 \le l \le 27$
Reflections collected	25524
Independent reflections	6499 [ <i>R</i> <sub>int</sub> = 0.1849]
Completeness to $\theta$ = 62.355°	0.999
Refined as a 2-component perfect	-1 0 0 0 -1 0 0 0 1
twin	
Data / restraints / parameters	25524 / 41 / 502
S (GOF)	1.065
$R_1, wR_2[l > 2\sigma(l)]$	0. 1027, 0.2430
$R_1$ , $wR_2$ (all data)	0.1408, 0.2701
Largest diff. peak and hole $(e \cdot A^{-3})$	1.009 and -0.984

 Table S1. Crystal data and structure refinement for VNU-20 with guest molecules inside.



**Figure S2.** Thermal ellipsoid plot of the asymmetric unit of VNU-20 with 30% probability.





**Figure S3.** Powder X-ray diffraction patterns of VNU-20 after multistep-steps treatments.



**Figure S4.** The Pawley refinements of activated VNU-20: The experimental (red), refined (black), and difference (green) patterns. The Bragg positions are marked as blue bars.

### Section S5: Fourier Transform Infrared Analysis

 $H_3BTC$  and  $H_2NDC$  have the characterization peaks centered at 1720 cm<sup>-1</sup> and 1684 cm<sup>-1</sup>. Peaks of the coordinated carboxylate group of BTC<sup>3-</sup> and NDC<sup>2-</sup> were known to shifted to lower wavelengths as higher energy is needed for the stretching vibration of these functional groups. Indeed, there is only one peak observed with wavelengths ranged from 1600 to 1750 cm<sup>-1</sup> in the FT-IR spectrum of VNU-20 (centered at 1614 cm<sup>-1</sup>), thus, this peak was assigned to the v<sub>C=O</sub> stretch of the coordinated carboxylate groups."



Figure S5. Fourier transform infrared analysis (FT-IR) of activated VNU-20.

Section S6: Thermogravimetric Analysis (TGA)



Figure S6. TGA analysis of VNU-20.





**Figure S7.**  $N_2$  uptake of VNU-20 at 77 K. The closed and open circles represent the adsorption and desorption branches of the isotherm, respectively. The connecting line functions as a guide for the eye.

Section S8: SEM and TEM micrographs of VNU-20



Figure S8 SEM micrograph of VNU-20.



Figure S9 TEM micrograph of VNU-20.

Section S9: X-ray photoelectron spectroscopy (XPS)

## analysis of VNU-20



Figure S10. Fe 2p XPS spectrum of VNU-20.

## **Section S10:** Synthesis of Characterization Data of Coumarin Derivatives

In a typical reaction, coumarin (0.146 g, 1 mmol), *N*,*N*-dimethylaniline (2 mL), DABCO (0.112 g, 1 mmol), and diphenyl ether (0.1 mL) as internal standard were introduced to a vial containing the VNU-20 catalyst (0.012 g, 5 mol%). *Tert*-butyl hydroperoxide in decane (0.545 mL g, 3 mmol) as oxidant was then added to the vial. The mixture was magnetically stirred at 120 °C for 1 h. The reaction mixture was diluted with ethyl acetate (30 mL). The ethyl acetate solution was washed with HCl solution (5% in water, 3 x 5 mL), and subsequently with saturated NaHCO<sub>3</sub> solution (3 x 5 mL). The organic layer was dried utilizing anhydrous Na<sub>2</sub>SO<sub>4</sub>. Reaction yields were recorded from GC analysis results with regard to the diphenyl ether internal standard. The expected product was isolated using column chromatography. The product structure was furthermore confirmed by GC-MS, HRMS, <sup>1</sup>H NMR, and <sup>13</sup>C NMR.



Figure S11. <sup>1</sup>H-NMR spectra of 3-((methyl(phenyl)amino)methyl)-2H-chromen-2-

one.



**Figure S12**. <sup>13</sup>C-NMR spectra of 3-((methyl(phenyl)amino)methyl)-2H-chromen-2-one.

### Characterization data for 3-((methyl(phenyl)amino)methyl)-2H-chromen-2one

Prepared as shown in the general experimental procedure and purified on silica gel (230-400 mesh or 37-63  $\mu$ m, ethyl acetate/hexane = 1:3 (v./v.), TLC silica gel 60 F<sub>254</sub>, R<sub>f</sub> = 0.5): Yellow solid, 89% yield (237 mg). <sup>1</sup>H-NMR (500 MHz, CDCl<sub>3</sub>) 3.12 (s, 3H), 4.44 (s, 2H), 6.71 (d, *J* = 9.0 Hz, 2H), 6.74 (td, *J* = 7.5 Hz, 1.0 Hz, 1H), 7.22–7.26 (m, 3H), 7.34 (dd, *J* = 19.0 Hz, 8.0 Hz, 2H), 7.46–7.50 (m, 2H). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz)  $\delta$ (ppm) 38.9, 52.7, 112.0, 116.5, 117.0, 119.2, 124.4, 125.4, 127.7, 129.4, 131.0, 137.7, 148.9, 153.1, 161.1. HRMS calcd for C<sub>17</sub>H<sub>15</sub>NO<sub>2</sub> (M+H)<sup>+</sup>: 266.1176, found (M+H)<sup>+</sup>: 266.1174.



**Figure S13**. <sup>1</sup>H-NMR spectra of 3-((methyl(p-tolyl)amino)methyl)-2H-chromen-2one.



**Figure S14**. <sup>13</sup>C-NMR spectra of 3-((methyl(p-tolyl)amino)methyl)-2H-chromen-2one.

Characterization data for 3-((methyl(p-tolyl)amino)methyl)-2H-chromen-2one

Prepared as shown in the general experimental procedure and purified on silica gel (230-400 mesh or 37-63  $\mu$ m, ethyl acetate/hexane = 1:4 (v./v.), TLC silica gel 60 F<sub>254</sub>, R<sub>f</sub> = 0.5): White solid, 86% yield (239 mg). <sup>1</sup>H-NMR (500 MHz, CDCl<sub>3</sub>) 2.25 (s, 3H), 3.08 (s, 3H), 4.39 (s, 2H), 6.63 (d, *J* = 8.0 Hz, 2H), 7.04 (d, *J* = 8.5 Hz, 2H), 7.33 (dd, *J* = 19.5 Hz, 8.0 Hz, 2H), 7.46–7.49 (m, 2H). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz)  $\delta$ (ppm) 20.2, 39.1, 52.9, 112.2, 116.4, 119.3, 124.3, 125.6, 126.3, 127.7, 129.9, 130.1, 130.9, 137.7, 146.9, 153.1, 161.2. HRMS calcd for C<sub>18</sub>H<sub>17</sub>NO<sub>2</sub> (M+H)<sup>+</sup>: 280.1332, found (M+H)<sup>+</sup>: 280.1363.



**Figure S15**. <sup>1</sup>H-NMR spectra of 3-(((4-bromophenyl)(methyl)amino)methyl)-2Hchromen-2-one.



**Figure S16**. <sup>13</sup>C-NMR spectra of 3-(((4-bromophenyl)(methyl)amino)methyl)-2Hchromen-2-one.

Characterization data for 3-(((4-bromophenyl)(methyl)amino)methyl)-2Hchromen-2-one

Prepared as shown in the general experimental procedure and purified on silica gel (230-400 mesh or 37-63  $\mu$ m, ethyl acetate/hexane = 1:4 (v./v.), TLC silica gel 60 F<sub>254</sub>, R<sub>f</sub> = 0.45): White solid, 84% yield (288 mg). <sup>1</sup>H-NMR (500 MHz, CDCl<sub>3</sub>) 3.09 (s, 3H), 4.41 (s, 2H), 6.57 (d, *J* = 9.0 Hz, 2H), 7.24 (d, *J* = 7.0 Hz, 1H), 7.29 (d, *J* = 9.0 Hz, 2H), 7.34 (d, *J* = 8.5 Hz, 1H), 7.38–7.40 (m, 2H), 7.48 (td, *J* = 7.0 Hz, 1.0 Hz, 1.0 Hz, 1.1). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz)  $\overline{0}$ (ppm) 39.1, 52.6, 109.0, 113.6, 116.5, 119.1, 124.5, 124.8, 127.7, 131.2, 132.0, 137.7, 147.8, 153.1, 161.0. HRMS calcd for C<sub>17</sub>H<sub>14</sub>BrNO<sub>2</sub> (M+H)<sup>+</sup>: 344.0281, found (M+H)<sup>+</sup>: 344.0296.



**Figure S17**. <sup>1</sup>H-NMR spectra of 3-(((3-chlorophenyl)(methyl)amino)methyl)-2Hchromen-2-one.



**Figure S18**. <sup>13</sup>C-NMR spectra of 3-(((3-chlorophenyl)(methyl)amino)methyl)-2Hchromen-2-one.

### Characterization data for 3-(((3-chlorophenyl)(methyl)amino)methyl)-2Hchromen-2-one

Prepared as shown in the general experimental procedure and purified on silica gel (230-400 mesh or 37-63  $\mu$ m, ethyl acetate/hexane = 1:4 (v./v.), TLC silica gel 60 F<sub>254</sub>, R<sub>f</sub> = 0.4): White solid, 79% yield (237 mg). <sup>1</sup>H-NMR (500 MHz, CDCl<sub>3</sub>) 3.14 (s, 3H), 4.46 (s, 2H), 6.59 (d, *J* = 7.5 Hz, 1H), 6.73–6.76 (m, 2H), 7.15 (t, *J* = 8.0 Hz, 1H), 7.27–7.29 (m, 2H), 7.43–7.45 (m, 2H), 7.52 (t, *J* = 7.5 Hz, 1H). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz)  $\delta$ (ppm) 39.0, 52.5, 110.2, 111.9, 116.5, 117.0, 119.0 124.5, 124.7, 127.7, 130.3, 131.2, 135.3, 137.7, 149.8, 153.1, 161.0. HRMS calcd for C<sub>17</sub>H<sub>14</sub>CINO<sub>2</sub> (M+H)<sup>+</sup>: 300.0786, found (M+H)<sup>+</sup>: 300.0814.



**Figure S19**. <sup>1</sup>H-NMR spectra of 6-methyl-3-((methyl(phenyl)amino)methyl)-2Hchromen-2-one.



**Figure S20**. <sup>13</sup>C-NMR spectra of 6-methyl-3-((methyl(phenyl)amino)methyl)-2Hchromen-2-one.

### Characterization data for 6-methyl-3-((methyl(phenyl)amino)methyl)-2Hchromen-2-one

Prepared as shown in the general experimental procedure and purified on silica gel (230-400 mesh or 37-63  $\mu$ m, ethyl acetate/hexane = 1:4 (v./v.), TLC silica gel 60 F254, Rf = 0.55): Orange solid, 88% yield (246 mg). <sup>1</sup>H-NMR (500 MHz, CDCl<sub>3</sub>) 2.38 (s, 3H), 3.14 (s, 3H), 4.46 (s, 2H), 6.73 (d, *J* = 8.5 Hz, 2H), 6.77 (t, *J* = 7.0 Hz, 1H), 7.21 (s, 1H), 7.26–7.33 (m, 4H), 7.43 (s, 1H). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz)  $\overline{0}$ (ppm) 20.7, 38.9, 52.6, 111.9, 116.2, 117.0, 118.9, 125.1, 127.6, 129.3, 132.0, 134.0, 137.7, 148.9, 151.2, 161.4. HRMS calcd for C<sub>18</sub>H<sub>17</sub>NO<sub>2</sub> (M+H)<sup>+</sup>: 280.1332, found (M+H)<sup>+</sup>: 280.1337.



**Figure S21**. <sup>1</sup>H-NMR spectra of 3-(((3-chlorophenyl)(methyl)amino)methyl)-6methyl-2H-chromen-2-one.



**Figure S22**. <sup>13</sup>C-NMR spectra of 3-(((3-chlorophenyl)(methyl)amino)methyl)-6methyl-2H-chromen-2-one.

### Characterization data for 3-(((3-chlorophenyl)(methyl)amino)methyl)-6methyl-2H-chromen-2-one

Prepared as shown in the general experimental procedure and purified on silica gel (230-400 mesh or 37-63  $\mu$ m, ethyl acetate/hexane = 1:4 (v./v.), TLC silica gel 60 F<sub>254</sub>, R<sub>f</sub> = 0.45): Yellow solid, 71% yield (222 mg). <sup>1</sup>H-NMR (500 MHz, CDCl<sub>3</sub>) 2.29 (s, 3H), 3.03 (s, 3H), 4.35 (s, 2H), 6.47 (dd, *J* = 8.5 Hz, 2.5 Hz, 1H), 6.61 (t, *J* = 2.0 Hz, 1H), 6.63 (dd, *J* = 8.0 Hz, 1.0 Hz, 1H), 7.04 (t, *J* = 8.0 Hz, 1H), 7.13 (s, 1H), 7.17–7.19 (m, 1H), 7.22–7.24 (m, 1H), 7.26 (s, 1H). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz)  $\delta$ (ppm) 20.7, 39.0, 52.5, 110.1, 111.8, 116.2, 116.9, 118.8, 124.4, 127.6, 130.3, 132.2, 134.2, 135.3, 137.7, 149.8, 151.2, 161.2. HRMS calcd for C<sub>18</sub>H<sub>16</sub>CINO<sub>2</sub> (M+H)<sup>+</sup>: 314.0942, found (M+H)<sup>+</sup>: 314.0966.



**Figure S23**. <sup>1</sup>H-NMR spectra of 6-methyl-3-((methyl(p-tolyl)amino)methyl)-2Hchromen-2-one.



**Figure S24**. <sup>13</sup>C-NMR spectra of 6-methyl-3-((methyl(p-tolyl)amino)methyl)-2Hchromen-2-one.

Characterization data for 6-methyl-3-((methyl(p-tolyl)amino)methyl)-2Hchromen-2-one.

Prepared as shown in the general experimental procedure and purified on silica gel (230-400 mesh or 37-63  $\mu$ m, ethyl acetate/hexane = 1:4 (v./v.), TLC silica gel 60 F<sub>254</sub>, R<sub>f</sub> = 0.55): Brownish solid, 72% yield (210 mg). <sup>1</sup>H-NMR (500 MHz, CDCl<sub>3</sub>) 2.17 (s, 3H), 2.27 (s, 3H), 2.99 (s, 3H), 4.30 (s, 2H), 6.54 (d, *J* = 8.5 Hz, 2H), 6.96 (d, *J* = 8.0 Hz, 2H), 7.08 (s, 1H), 7.14–7.20 (m, 2H), 7.33 (s, 1H). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz)  $\delta$ (ppm) 20.2, 20.7, 39.0, 52.8, 112.2, 116.2, 119.0, 125.4, 126.2, 127.6, 130.0, 132.0, 134.0, 137.8, 146.9, 151.2, 161.5. HRMS calcd for C<sub>19</sub>H<sub>19</sub>NO<sub>2</sub> (M+H)<sup>+</sup>: 294.1488, found (M+H)<sup>+</sup>: 294.1468.



yl)methyl)benzamide.



**Figure S26**. <sup>13</sup>C-NMR spectra of N-methyl-N-((2-oxo-2H-chromen-3-yl)methyl)benzamide.

Characterization data for N-methyl-N-((2-oxo-2H-chromen-3yl)methyl)benzamide.

Prepared as shown in the general experimental procedure and purified on silica gel (230-400 mesh or 37-63  $\mu$ m, ethyl acetate/hexane = 1:3 (v./v.), TLC silica gel 60 F<sub>254</sub>, R<sub>f</sub> = 0.15): Yellow solid, 80% yield (235 mg). Observed as two rotamers of 64/36 ratio in <sup>1</sup>H NMR. <sup>1</sup>H-NMR (500 MHz, CDCl<sub>3</sub>) 4.16 (s, 3H), 4.64/4.45 (s, 2H), 7.27–7.53 (m, 9H), 7.88 (s, 1H). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz)  $\overline{0}$ (ppm) 39.1, 47.2, 116.5, 119.2, 124.1, 124.5, 126.4, 127.1, 128.0, 128.4, 128.6, 129.9, 131.5, 131.7, 135.7, 141.7, 153.4, 161.8. HRMS calcd for C<sub>18</sub>H<sub>15</sub>NO<sub>3</sub> (M+H)<sup>+</sup>: 294.1125, found (M+H)<sup>+</sup>: 294.1123.



Figure S27. Effect of different solvents on the reaction.



Figure S28. Effect of N,N-dimethylaniline volume on the reaction.



**Figure S29**. After 30 min reaction time, TEMPO as the radical scavenger was added to the reaction mixture. GC-MS analysis indicated the presence of *N*-methyl-*N*-((2,2,6,6-tetramethylpiperidin-1-yloxy)methyl)aniline with m/z = 276 in the reaction mixture, generated by the combination of TEMPO and *N*,*N*-dimethylaniline radical.

# Section S11: Stability of VNU-20 after Catalyst Reutilizing Studies



Figure S30. PXRD analysis of VNU-20 after 5<sup>th</sup> catalytic cycle.



Figure S31. FT-IR analysis of VNU-20 after 5<sup>th</sup> catalytic cycle.

# **Section S12:** Additional Information for other MOFs used in Table 2

- Fe(BTC) (Basolite F-300) was commercially supplied by Sigma-Aldrich.
- Fe<sub>3</sub>O(BDC)<sub>3</sub> (MOF-235) was synthesized according to literature procedure (E. Haque, J.W. Jun, S.H. Jhung, J. Hazard. Mater. 185 (2011) 507; M. Anbia, V. Hoseini, S. Sheykhi, J. Ind. Eng. Chem. 18 (2012) 1149)
- Fe<sub>3</sub>O(BPDC)<sub>3</sub> was synthesized according to literature procedure (M. Dan-Hardi, H. Chevreau, T. Devic, P. Horcajada, G. Maurin, G. Férey, D. Popov, C. Riekel, S. Wuttke, J.-C. Lavalley, A. Vimont, T. Boudewijns, D.E.D. Vos, C. Serre, Chem. Mater. 24 (2012) 2486)
- Cu(BDC) was synthesized according to literature procedure (C.G. Carson, K. Hardcastle, J. Schwartz, X. Liu, C. Hoffmann, R.A. Gerhardt, R. Tannenbaum, Eur. J. Inorg. Chem. (2009) 2338-2343)
- Fe(BDC)(DMF) was synthesized according to literature procedure (Tabatha R. Whitfield, Xiqu Wang, Lumei Liu, Allan J. Jacobson, Solid State Sci. 7 (2005) 1096).