

## Supporting information

# Dye-loaded metal-organic helical capsules applied to the combination of photocatalytic H<sub>2</sub>S splitting and nitroaromatic hydrogenation

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## 1. Synthesis Methods

### Materials and Methods

Unless otherwise specified, organic solvents were dried before using in accordance with standard methods. Other chemicals were of reagent grade and were obtained from commercial sources and used without further purification.

**Elemental analyses.** The elemental analyses of C, H and N were performed on a Vario EL III elemental analyzer.

**Nuclear magnetic resonance.**  $^1\text{H}$  NMR spectra were recorded on a Varian INOVA-400M spectrometer with chemical shifts reported in ppm.  $^{13}\text{C}$  NMR spectra were also measured on a Varian INOVA-400M spectrometer. The peak frequencies were referenced versus an internal standard (tetramethylsilane (TMS)) shifts at 0.0 ppm.

**Liquid chromatograph mass spectra.** The ESI mass spectra were collected on an HPLC-Q-ToF-MS spectrometer in acetonitrile/methanol solution.

**Electrochemical experiments.** The cyclic voltammetry (CV) was performed on a CHI 660E electrochemical workstation with a three-electrode system using a Ag/AgCl electrode as the reference electrode, 0.5 mm diameter platinum silk as the counter electrode, and a glassy carbon electrode as the working electrode. The measurements were performed after degassing the solutions with argon to eliminate the effects of oxygen.

**Isothermal titration calorimetry (ITC).** The ITC was performed on a Nano ITC (TA Instruments Inc.–Waters LLC) at atmospheric parameters and at 25.0 °C, giving the association constants and the thermodynamic parameters. The solution of guest in the syringe was sequentially injected under stirring at 250 rpm into a solution of host in the sample cell.

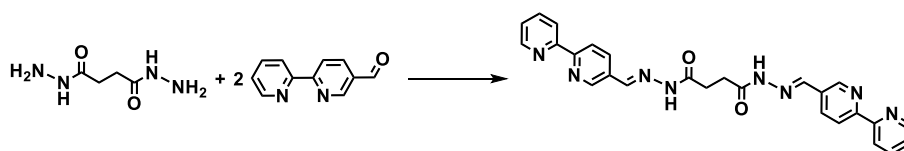
**Fluorescence spectra.** The solution fluorescence spectra was measured on Edinburgh FS920 steady-state fluorescence spectrophotometer using an excitation wavelength at 475 nm to guarantee the only excitation of FI and showing the emission intensity at 520 nm.

**Liquid UV-vis spectra.** The solution UV-vis spectra were recorded on a SHIMADZU UV 2600 UV-vis spectrophotometer.

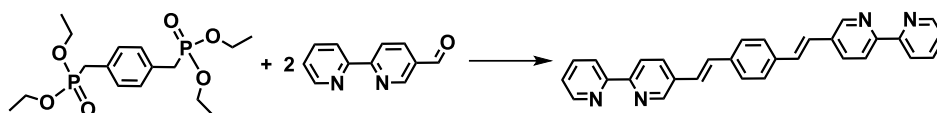
**Gas chromatography.** The generated  $\text{H}_2$  was characterized by GC 7890T instrument analysis using a 5 Å molecular sieve column (0.6 m × 3.0 mm) with thermal conductivity detector, and argon as carrier gas.

**High-performance liquid chromatography.** The HPLC analysis were performed on SHIMADZU LC 2030 Plus analyzer using a ZORBAX SB-C18 reverse phase column (250 × 4.6 mm I.D, s-5  $\mu\text{M}$ ) eluting with methanol/water to determine the yields of the catalytic reactions. (Detection:  $\lambda = 270$  nm; Temperature: 25.0 °C.

### Synthetic procedures



**Synthesis of L<sup>1</sup>.** Ten drops of acetic acid were added to a mixture of succinic dihydrazide (0.73 g, 5.0 mmol) and 2,2-bipyridine-5-carbaldehyde (1.84 g, 10.0 mmol) in a methanol solution. After the mixture was refluxed at 70 °C for 10 h, the precipitate was formed and collected by filtration. Yield: 92 %. Anal. Calc. for C<sub>26</sub>H<sub>22</sub>N<sub>8</sub>O<sub>2</sub>: H, 4.63; C, 65.26; N, 23.42. Found: H, 4.73; C, 65.28; N, 23.45. <sup>1</sup>H NMR (DMSO-d<sub>6</sub>, 400 MHz, ppm): 11.70–11.54 (m, 2H), 8.92–8.90 (dd, 2H), 8.71–8.68 (m, 2H), 8.46–8.38 (m, 4H), 8.29–8.23 (m, 3H), 8.10 (s, 1H), 7.99–7.93 (m, 2H), 7.49–7.46 (m, 2H), 2.51–2.49 (m, 4H). <sup>13</sup>C NMR (100 MHz, DMSO-d<sub>6</sub>) δ 166.7, 157.6, 155.0, 151.5, 149.2, 143.1, 137.4, 137.2, 123.7, 123.3, 121.4, 121.2, 34.2.



**Synthesis of L<sup>2</sup>.** Refluxing the mixture of 1,4-bis(bromomethyl)benzene (1.05 g, 4.0 mmol) and triethylphosphite (20 mL) at 160 °C for 6 hours. After the reaction completed, the excess triethylphosphite was removed under reduced pressure. The mixture was poured into excess hexanes and stirred for 30 minutes, then followed by filtration to obtain the 1,4-bis(diethoxyphosphinylmethyl)benzene as pale yellow solid with yield of 81 %.

A solution of 1,4-bis(diethoxyphosphinylmethyl)benzene (0.38 g, 1.0 mmol) and potassium tert-butoxide (0.45 g, 4.0 mmol) were added into 70 mL toluene and stirred for 30 minutes under Ar atmosphere. Then 30 mL toluene solution contained 2,2-bipyridine-5-carbaldehyde (0.42 g, 2.3 mmol) was added dropwise into the abovementioned solution. After stirred for 24 hours at room temperature, 100 mL 95 % ethanol was added into the reaction mixture and followed by another 1 hour stirring. After the reaction completed, the solvent was removed under reduced pressure, the residual solid was redissolved in chloroform and washed by water. The organic phase was dried over MgSO<sub>4</sub> and evaporated to dryness. The crude products were purified by recrystallization from ethanol. Yield: 70 %. Anal. Calc. for C<sub>30</sub>H<sub>22</sub>N<sub>4</sub>: H, 5.06; C, 82.17; N, 12.78. Found: H, 5.10; C, 82.19; N, 12.77. <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz, ppm): 8.81 (d, 2H), 8.73–8.71 (d, 2H), 8.49–8.47 (m, 4H), 8.05–8.03 (d, 2H), 7.90–7.86 (m, 2H), 7.59 (s, 4H), 7.37–7.34 (m, 2H), 7.21–7.17 (m, 2H). <sup>13</sup>C NMR (100 MHz, DMSO-d<sub>6</sub>) δ 155.8, 155.2, 150.2, 149.0, 137.4, 136.6, 133.9, 130.4, 129.1, 128.5, 124.3, 123.6, 121.5, 121.2.

**Synthesis of C<sub>1</sub> (Fe<sub>2</sub>L<sup>1</sup><sub>3</sub>).** The ligand L<sup>1</sup> (71.8 mg, 0.15 mmol) and Fe(BF<sub>4</sub>)<sub>2</sub>·6H<sub>2</sub>O (33.8 mg, 0.10 mmol) were mixed in CH<sub>3</sub>CN solution and refluxed at 85 °C for 20 h. After the reaction mixture was cooled to room temperature, a dark purple precipitate was formed after the addition of diethyl ether and then was collected by filtration. Yield: 65 %. The purple crystals of C<sub>1</sub> were obtained by slowly diffusing diethyl ether into a DMF/CH<sub>3</sub>CN solution of C<sub>1</sub>. Anal. Calc. for C<sub>79</sub>H<sub>64</sub>N<sub>23</sub>O<sub>7</sub>B<sub>4</sub>F<sub>16</sub>Fe<sub>2</sub>: H, 3.38; C, 49.77; N, 16.90. Found: H, 3.44; C, 49.75; N, 16.92. <sup>1</sup>H NMR (DMSO-d<sub>6</sub>, 400 MHz, ppm): 9.74–9.44 (m, 4H), 8.58–8.45 (m, 12H), 8.14–8.05 (m, 12H), 7.77–7.70 (m, 4H), 7.65–7.58 (m, 4H), 7.43–7.34 (m, 12H), 2.37–2.31 (m, 12H). <sup>13</sup>C NMR (100 MHz, DMSO-d<sub>6</sub>) δ 172.77, 164.66, 158.50, 157.94, 154.06, 149.47, 139.27, 139.00, 138.53, 127.42, 124.37, 123.63, 36.32, 28.63. ESI-MS: m/z: 386.6074, [Fe<sub>2</sub>L<sup>1</sup><sub>3</sub>]<sup>4+</sup>; 544.4782, [Fe<sub>2</sub>L<sup>1</sup><sub>3</sub>·BF<sub>4</sub>]<sup>3+</sup>; 860.2183, [Fe<sub>2</sub>L<sup>1</sup><sub>3</sub>·2BF<sub>4</sub>]<sup>2+</sup>.

**Synthesis of C<sub>2</sub> (Fe<sub>2</sub>L<sup>2</sup><sub>3</sub>).** The ligand L<sup>2</sup> (65.7 mg, 0.15 mmol) and Fe(OTf)<sub>2</sub> (35.4 mg, 0.10 mmol) were mixed in CH<sub>3</sub>CN solution and refluxed at 85 °C for 20 h. After the reaction mixture was cooled to room temperature, a dark red precipitate was formed after the addition of diethyl ether and then was collected by filtration. Yield: 60 %. The dark red crystals of C<sub>2</sub> were obtained by slowly diffusing diethyl ether into a CH<sub>3</sub>CN solution of C<sub>2</sub>. Anal. Calc. for C<sub>96</sub>H<sub>66</sub>N<sub>13</sub>O<sub>12</sub>S<sub>4</sub>F<sub>12</sub>Fe<sub>2</sub>: H, 3.23; C, 55.93; N, 8.83. Found: H, 3.25; C, 55.94; N, 8.81. <sup>1</sup>H NMR (DMSO-d<sub>6</sub>, 400 MHz, ppm): 8.56–8.53 (m, 12H), 8.34–8.32 (m, 3H), 8.13–8.09 (m, 9H), 7.45–7.37 (m, 30H), 7.09–6.92 (m, 12H). <sup>13</sup>C NMR (100 MHz, DMSO-d<sub>6</sub>) δ 158.72, 157.16, 153.89, 150.00, 138.40, 138.26, 136.33, 136.27, 132.75, 129.54, 127.20, 126.84, 123.68, 123.45, 123.11. ESI-MS: m/z: 356.8560, [Fe<sub>2</sub>L<sup>2</sup><sub>3</sub>]<sup>4+</sup>; 525.4591, [Fe<sub>2</sub>L<sup>2</sup><sub>3</sub>·OTf]<sup>3+</sup>; 862.6650, [Fe<sub>2</sub>L<sup>2</sup><sub>3</sub>·2OTf]<sup>2+</sup>.

### General procedure for catalytic reactions

All catalytic reactions were carried out under a 300 W Xenon lamp (25 mW/cm<sup>2</sup>). The reaction temperature was maintained at 25 °C by circulating water through the outer packet of the reactor. The amount of hydrogen generated was determined by a GC7890T gas chromatograph equipped with a 5 Å molecular sieve column (0.6 m × 3 mm) and a thermal conductivity detector; argon was used as the carrier gas. The amount of hydrogen generated was determined by an external standard method, and the slight effect of the generated hydrogen gas on the pressure of the flask was neglected in the calculation of the volume of hydrogen gas. The yields of the amino products were determined by HPLC analysis performed on SHIMADZU LC 2030 Plus analyzer using a ZORBAX SB-C18 reverse phase column (250 × 4.6 mm I.D, s-5 μM) eluting with methanol/water to determine

the yields of the catalytic reactions.

The photocatalytic hydrogen generation reactions using Na<sub>2</sub>S as electron donor were carried out in a 25.0 mL home-made flask containing C<sub>1F</sub> or C<sub>2F</sub> (1.0 mM), Na<sub>2</sub>S (5.0 mmol, using a 1.0 M HCl solution to adjust the pH) in a CH<sub>3</sub>CN/H<sub>2</sub>O (v/v, 1/1) solution. The flask was degassed by bubbling argon for 20 min under atmospheric pressure at room temperature. The generated photoproduct H<sub>2</sub> was characterized on a GC 7890T instrument. The amount of hydrogen was determined using an external standard. After the reaction completed, the pH value of the reaction mixture was further adjust to 8.0 and the elemental sulfur was collect by filtration of the reaction mixture and followed by washing with CH<sub>3</sub>CN and H<sub>2</sub>O. The turnover number (TON) and TOF was calculated based on the amount of the generated hydrogen and the loading amount of the photocatalyst C<sub>F</sub>.

$$TON_{H_2} = n_{H_2}/n_{CF} \quad TOF_{H_2} = TON_{H_2}/t$$

The photocatalytic nitro compounds reduction reactions using Na<sub>2</sub>S as electron donor were also carried out in a home-made flask under the same conditions of hydrogen generation reactions with addition of nitro compounds 0.50 mmol. The yields of the corresponding amino compounds were measured by HPLC eluting with methanol/water using m-toluidine as integral standard. (Detection:  $\lambda = 270$  nm; Temperature: 25.0 °C; Flow rate: 0.8 mL/min).

Kinetics experiments for Michaelis-Menten mechanism analysis were carried out at conditions: C<sub>1F</sub>/C<sub>2F</sub> (5.0  $\mu$ mol), Na<sub>2</sub>S (5.0 mmol), and nitro substrates (0.05 mmol, 0.10 mmol, 0.25 mmol and 0.5 mmol, respectively) in 5.0 mL CH<sub>3</sub>CN/H<sub>2</sub>O (v/v, 1/1) solution with pH of 10.5. After blowing Ar gas for 20 minutes, the reaction mixture was irradiated under the Xenon lamp. The yields of amino product in the initial reaction stages were regarded as the initial rate of the reactions, which were further used in the reciprocal plot fitting.

$$Rate (\mu M \cdot s^{-1}) = \frac{[substrate] \times yield}{t}$$

## 2. Crystallography

The intensities were collected on a Bruker SMART APEX CCD diffractometer equipped with a graphite-monochromated Mo-K $\alpha$  ( $\lambda = 0.71073$  Å) radiation source; the data were acquired using the SMART and SAINT programs.<sup>S1,S2</sup> The structures were solved by direct methods and refined on F<sup>2</sup> by full-matrix least-squares methods using the SHELXTL version 5.1 software.<sup>S3</sup>

### Crystal data for C<sub>1</sub>

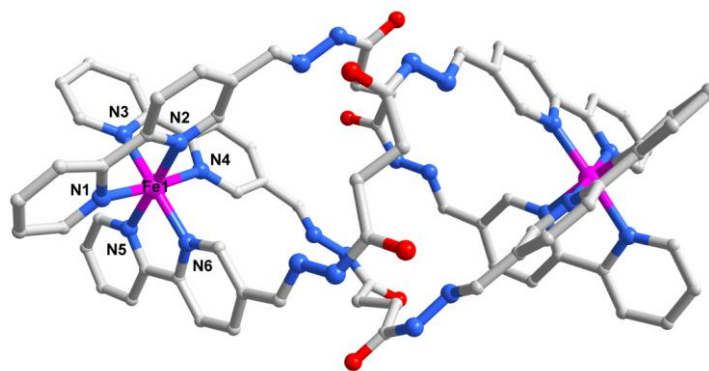
C<sub>79</sub>H<sub>64</sub>N<sub>23</sub>O<sub>7</sub>B<sub>4</sub>F<sub>16</sub>Fe<sub>2</sub>, Mr = 1906.48, Triclinic space group P-1, dark-red block, a = 12.773 (1) Å, b = 19.091 (2) Å, c = 22.774 (3) Å,  $\alpha = 104.066$  (5) °,  $\beta = 100.757$  (4) °,  $\gamma = 94.934$  (4) °, V = 5241.9 (10) Å<sup>3</sup>, Z = 2, Dc = 1.208 g cm<sup>-3</sup>, T = 120 (2) K,  $\mu$  (Mo-K $\alpha$ ) = 0.361 mm<sup>-1</sup>. [R<sub>int</sub> = 0.1043]. For 18645 unique reflects, final R<sub>1</sub>[with I > 2 $\sigma$ (I)] = 0.1133, wR<sub>2</sub> (all data) = 0.3456, GOOF = 1.023. CCDC NO. 2117502.

For the refinement of C<sub>1</sub>, except the disordered moieties and the particularly occupied counter ions and solvents non-hydrogen atoms were refined anisotropically. Except the solvent water molecules, hydrogen atoms were fixed geometrically at calculated distances and allowed to ride on the parent non-hydrogen atoms. Several bond distances in the counter BF<sub>4</sub><sup>-</sup> ions were restrained as idealized values. Thermal parameters on adjacent atoms of these counter BF<sub>4</sub><sup>-</sup> ions were restrained to be similar. The free solvent and the disordered solvent molecules have been removed out by using PLATON SQUEEZE program.

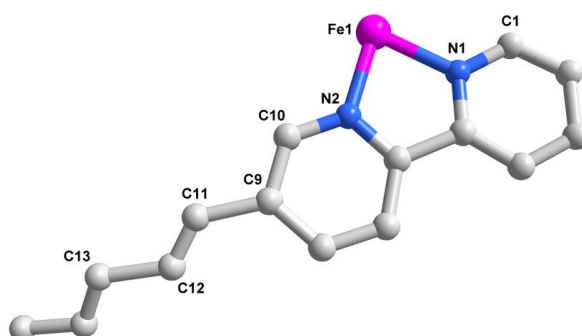
### Crystal data for C<sub>2</sub>

C<sub>96</sub>H<sub>66</sub>N<sub>13</sub>O<sub>12</sub>S<sub>4</sub>F<sub>12</sub>Fe<sub>2</sub>, Mr = 2061.53, Hexagonal space group P-3c1, dark-red block, a = 10.407 (3) Å, b = 10.407 (3) Å, c = 48.843 (12) Å,  $\alpha = \beta = 90.000$  °,  $\gamma = 120.000$  °, V = 4581 (3) Å<sup>3</sup>, Z = 2, Dc = 1.495 g cm<sup>-3</sup>, T = 223 (2) K,  $\mu$  (Mo-K $\alpha$ ) = 0.503 mm<sup>-1</sup>. [R<sub>int</sub> = 0.1290]. For 2738 unique reflects, final R<sub>1</sub>[with I > 2 $\sigma$ (I)] = 0.1199, wR<sub>2</sub> (all data) = 0.3444, GOOF = 1.158. CCDC NO. 2117508.

For the refinement of C<sub>2</sub>, except the solvent molecules, other non-hydrogen atoms were refined anisotropically, hydrogen atoms were fixed geometrically at calculated distances and allowed to ride on the parent non-hydrogen atoms. Several bond distances in benzene rings were restrained as idealized values. Thermal parameters on adjacent atoms of these atoms were restrained to be similar. And the C atom and S atom in one counter OTf<sup>-</sup> ion were disordered into three parts with the site occupied factors of each part being fixed as 0.33, respectively. The related bond distances in the counter ions were restrained as idealized values. Thermal parameters on adjacent atoms of the counter ions were restrained to be similar.



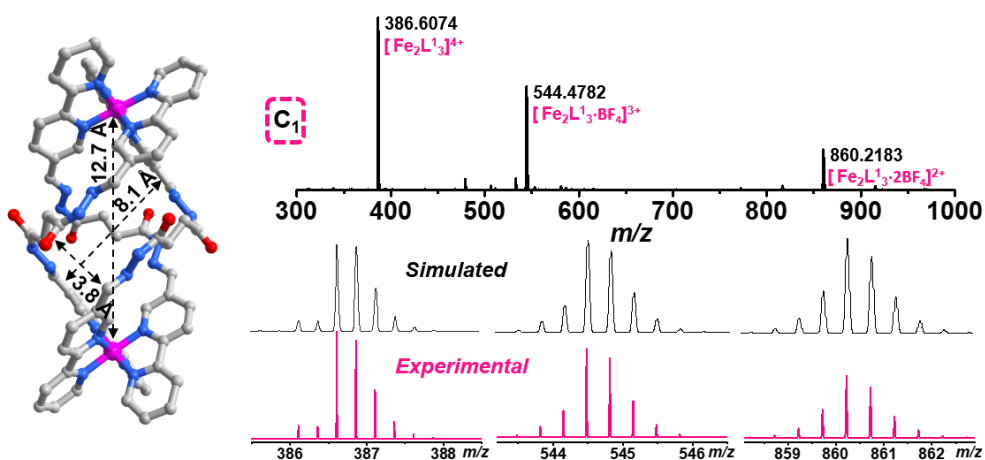
**Figure S1.** Molecular structure of  $C_1$  capsule within a unique asymmetric unit, showing the backbone of the ligand in the complex. Selected bond distances (Å) and angles ( $^\circ$ ): Fe1 – N1 1.969 (6), Fe1 – N2 1.964 (7), Fe1 – N3 1.968 (6), Fe1 – N4 1.976 (5), Fe1 – N5 1.958 (6), Fe1 – N6 1.967 (5), N1 – Fe1 – N2 81.6 (3), N1 – Fe1 – N3 94.3 (3), N1 – Fe1 – N4 176.3 (2), N1 – Fe1 – N5 93.2 (2), N1 – Fe1 – N6 89.2 (2), N2 – Fe1 – N3 91.1 (2), N2 – Fe1 – N4 97.5 (2), N2 – Fe1 – N5 172.9 (2), N2 – Fe1 – N6 93.2 (2), N3 – Fe1 – N4 82.1 (2), N3 – Fe1 – N5 94.2 (2), N3 – Fe1 – N6 174.8 (2), N4 – Fe1 – N5 88.0 (2), N4 – Fe1 – N6 94.4 (2), N5 – Fe1 – N6 81.8 (2).



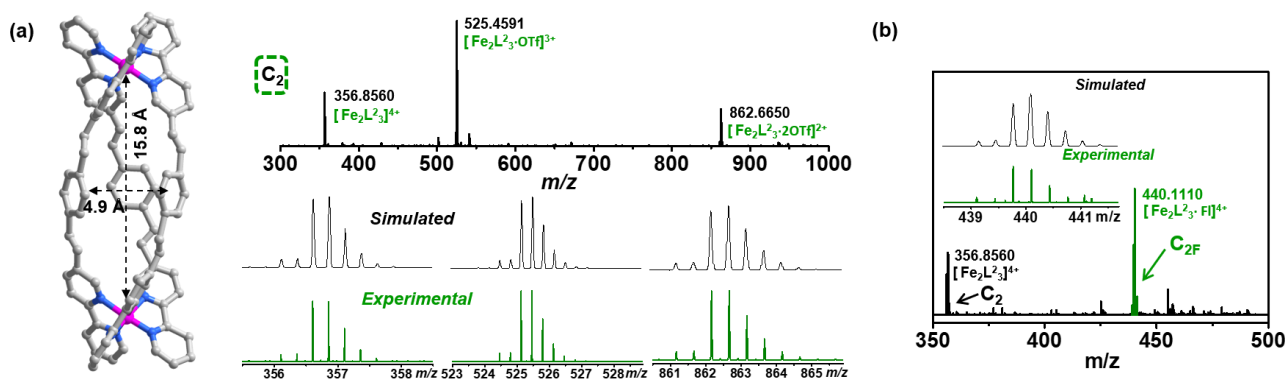
**Figure S2.** Molecular structure of  $C_2$  capsule within a unique asymmetric unit, showing the backbone of the ligand in the complex. Selected bond distances (Å) and angles ( $^\circ$ ): Fe1 – N1 1.969 (9), Fe1 – N2 1.962 (10), C9 – C11 1.504 (19), C11 – C12 1.151 (16), C12 – C13 1.537 (16), N1 – Fe1 – N2 90.3 (4), C9 – C11 – C12 128.5 (19), C12 – C13 – C14 121.0 (2).

### 3. Experimental Section

#### ESI-MS spectra data



**Figure S3.** The ESI-MS spectrum of  $C_1$  (1.0 mM) in an  $\text{CH}_3\text{CN}$  solution exhibited three intense peaks at  $m/z = 386.6074$ ,  $544.4782$ , and  $860.2183$ , which were assigned to species of  $[\text{Fe}_2\text{L}_3]^{4+}$ ,  $[\text{Fe}_2\text{L}_3\cdot\text{BF}_4]^{3+}$ , and  $[\text{Fe}_2\text{L}_3\cdot 2\text{BF}_4]^{2+}$ , respectively.

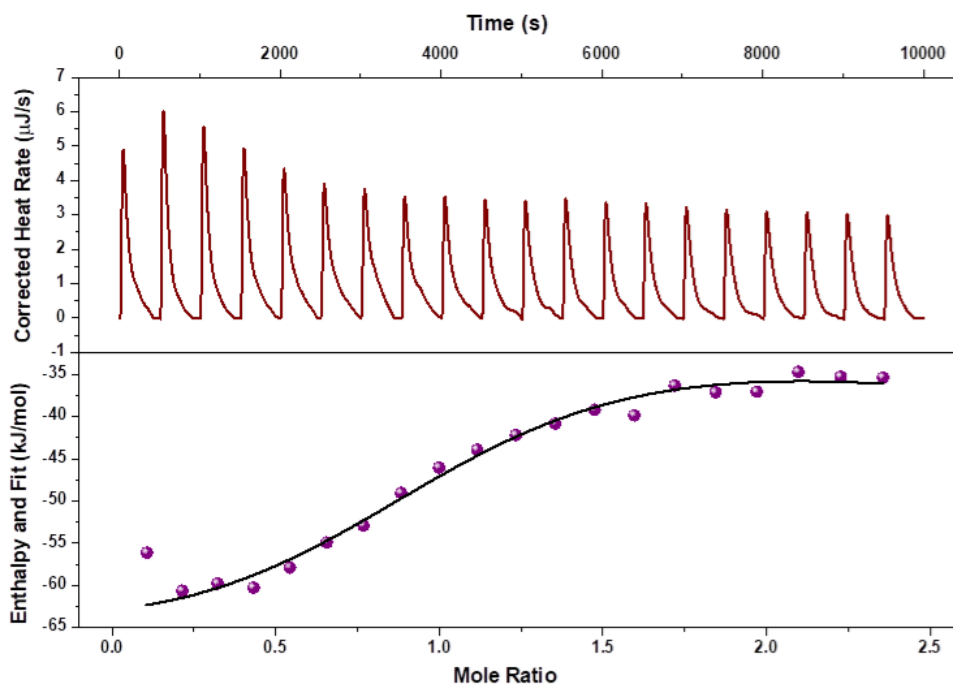


**Figure S4.** (a) The ESI-MS spectrum of  $C_2$  (1.0 mM) in an  $\text{CH}_3\text{CN}$  solution also exhibited three intense peaks at  $m/z = 356.8560$ ,  $525.4591$ , and  $862.6650$ , which were assigned to species of  $[\text{Fe}_2\text{L}_2^3]^{4+}$ ,  $[\text{Fe}_2\text{L}_2^3\cdot\text{BF}_4]^{3+}$ , and  $[\text{Fe}_2\text{L}_2^3\cdot 2\text{BF}_4]^{2+}$ , respectively. (b) The ESI-MS spectra of  $C_2$  (1.0 mM) with addition of  $\text{FI}$  (1.0 mM) in an  $\text{CH}_3\text{CN}$  solution, showing the peak corresponding to  $[\text{Fe}_2\text{L}_2^3\cdot\text{FI}]^{4+}$  at  $m/z = 440.1110$ .



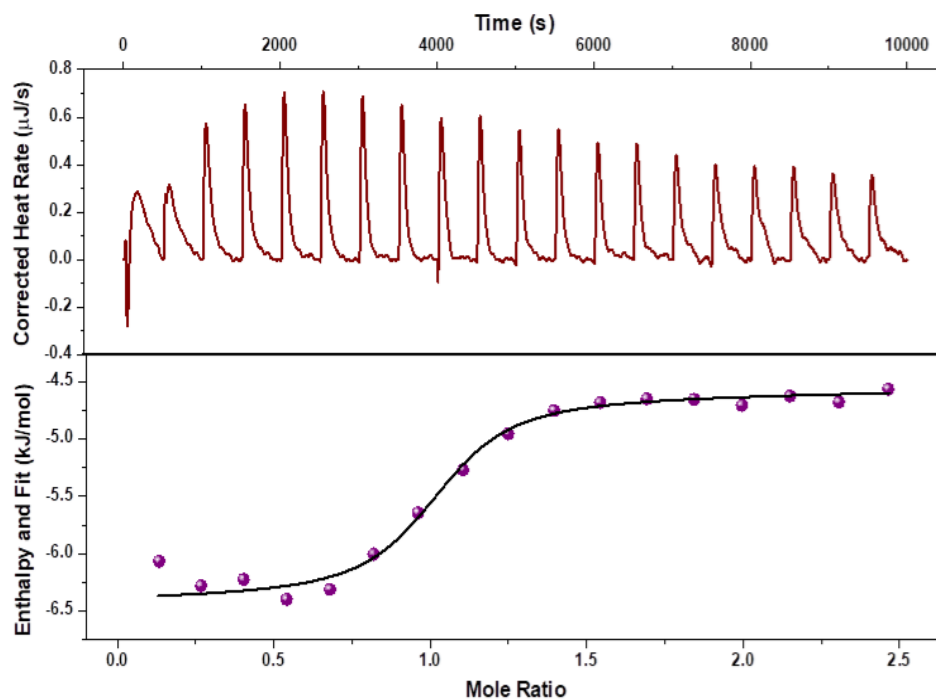
### Microcalorimetric titration experiments of the interactions between capsules and dye molecules.

The ITC was performed on a Nano ITC (TA Instruments Inc.–Waters LLC) at atmospheric parameters and at 25.0 °C, giving the association constants and the thermodynamic parameters. The solution of guest in the syringe was sequentially injected under stirring at 250 rpm into a solution of host in the sample cell.



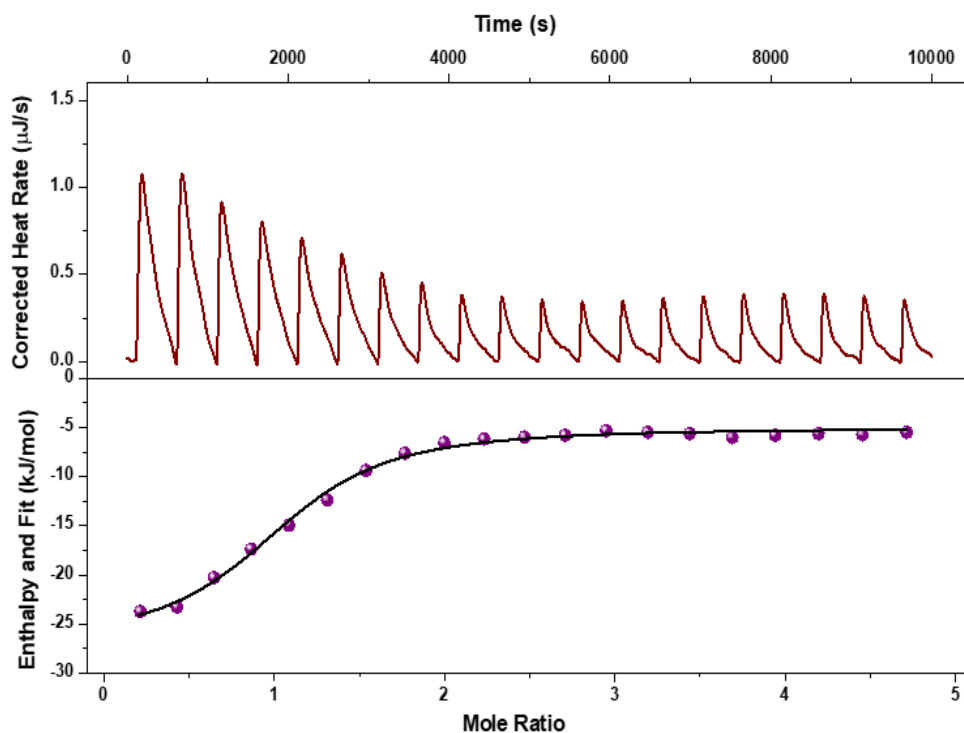
Model	Variable	Value	Conf. Interval
Independent	Kd (M)	2.199E-5	1.370E-6
	n	1.095	0.097
	$\Delta H$ (kJ/mol)	-6.189	0.180
	$\Delta S$ (J/mol·K)	118.4	
Confidence level		99%	

**Figure S5.** Microcalorimetric titration of  $C_1$  in  $CH_3CN$  solution at 298.00 K. (Top) Raw data for sequential 20 injections (10  $\mu L$  per injection) of FI solution injecting into  $C_1$  solution (0.1 mM). (Bottom) Apparent reaction heat obtained from the integration of calorimetric traces.



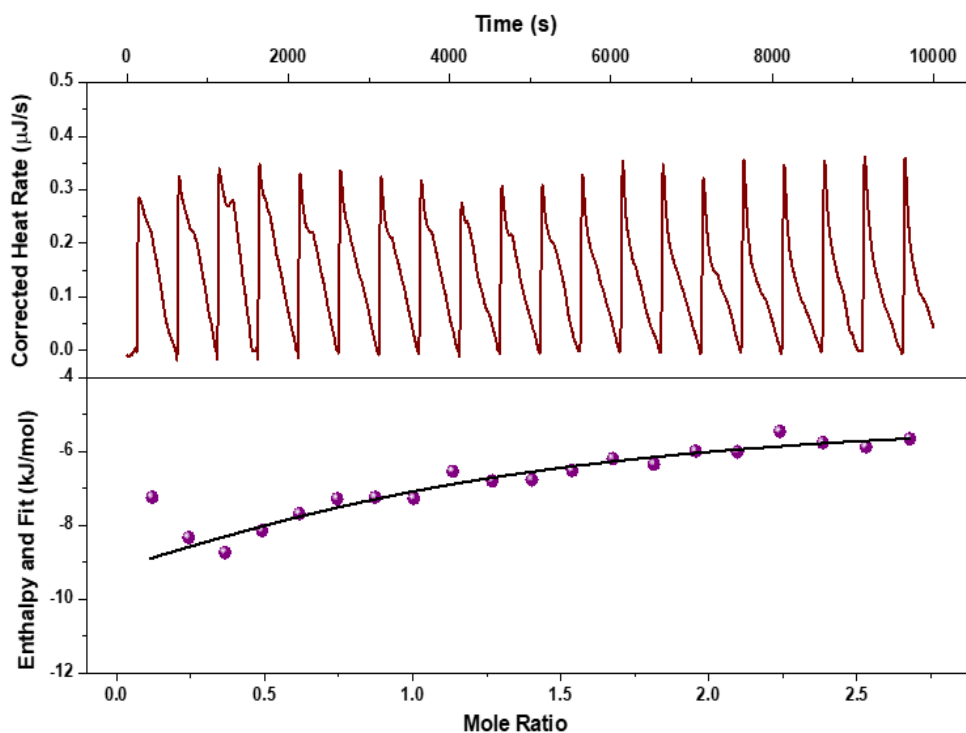
Model	Variable	Value	Conf. Interval
Independent	Kd (M)	1.162E-5	1.495E-6
	n	0.966	0.056
	$\Delta H$ (kJ/mol)	-1.690	0.491
	$\Delta S$ (J/mol·K)	107.9	
Confidence level		99%	

**Figure S6.** Microcalorimetric titration of  $C_2$  in  $CH_3CN$  solution at 298.00 K. (Top) Raw data for sequential 20 injections (10  $\mu L$  per injection) of **FI** solution injecting into  $C_2$  solution (0.1 mM). (Bottom) Apparent reaction heat obtained from the integration of calorimetric traces.



Model	Variable	Value	Conf. Interval
Independent	Kd (M)	6.247E-6	6.321E-7
	n	1.021	0.091
	$\Delta H$ (kJ/mol)	-21.99	1.479
	$\Delta S$ (J/mol·K)	25.88	
Confidence level		99%	

**Figure S7.** Microcalorimetric titration of  $C_{1F}$  in  $CH_3CN$  solution at 298.00 K. (Top) Raw data for sequential 20 injections (10  $\mu L$  per injection) of 9-nitroanthracene solution injecting into  $C_{1F}$  solution (0.1 mM). (Bottom) Apparent reaction heat obtained from the integration of calorimetric traces.

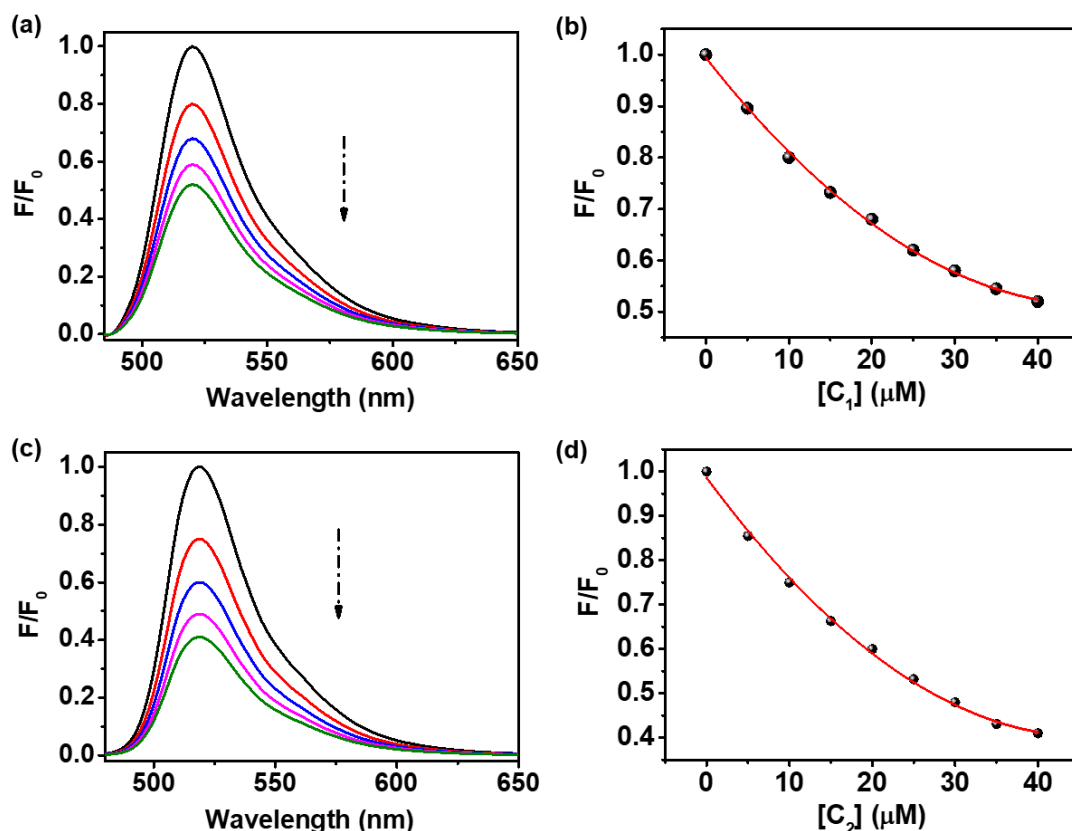


Model	Variable	Value	Conf. Interval
Independent	Kd (M)	8.860E-5	3.770E-6
	n	0.976	0.126
	$\Delta H$ (kJ/mol)	-8.432	0.987
	$\Delta S$ (J/mol·k)	49.30	
Confidence level		99%	

**Figure S8.** Microcalorimetric titration of  $C_{2F}$  in  $CH_3CN$  solution at 298.00 K. (Top) Raw data for sequential 20 injections (10  $\mu L$  per injection) of 9-nitroanthracene solution injecting into  $C_{2F}$  solution (0.1 mM). (Bottom) Apparent reaction heat obtained from the integration of calorimetric traces.

## Fluorescence titration experiment

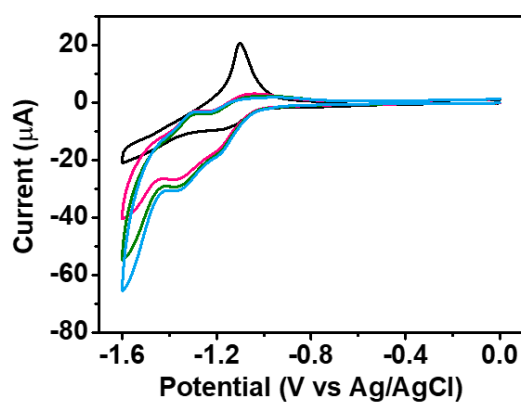
The solution fluorescence spectra was measured on Edinburgh FS920 steady-state fluorescence spectrophotometer using an excitation wavelength at 475 nm to guarantee the only excitation of **FI** and showing the emission intensity at 520 nm. In an  $\text{CH}_3\text{CN}/\text{H}_2\text{O}$  solution containing **FI** (0.10 mM) (black line) upon addition of  $\text{C}_1$  or  $\text{C}_2$  successively (up to 40.0  $\mu\text{M}$ ), the fluorescence intensity quenching process was recorded. And nonlinear fitting was used for each titration curve to determine the host-guest behavior.



**Figure S9.** (a) Emission spectra of **FI** upon addition of  $\text{C}_1$  (excited at 475 nm). (b) Nonlinear fitting of the titration curve that suggested the 1:1 host-guest behavior with a constant of  $K_{a1} = 1.07 \pm 0.035 \times 10^5$ . (c) Emission spectra of **FI** upon addition of  $\text{C}_2$  (excited at 475 nm). (d) Nonlinear fitting of the titration curve that suggested the 1:1 host-guest behavior with a constant of  $K_{a2} = 2.19 \pm 0.065 \times 10^5$ .

### Electrochemical titration experiment

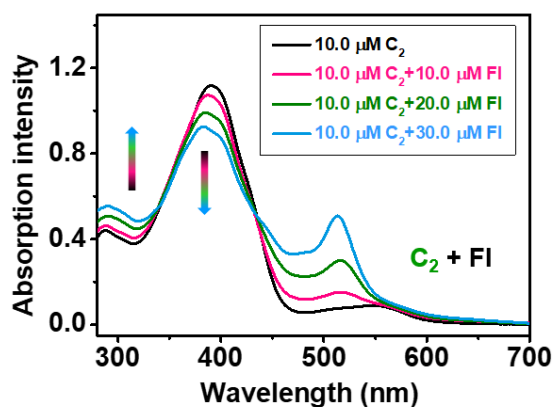
The cyclic voltammetry (CV) was performed on a CHI 660E electrochemical workstation with a three-electrode system using a Ag/AgCl electrode as the reference electrode, 0.5 mm diameter platinum silk as the counter electrode, and a glassy carbon electrode as the working electrode. The measurements were performed after degassing the solutions with argon to eliminate the effects of oxygen. The cyclic voltammetry of  $C_1$  and  $C_2$  were all displayed in acetonitrile solutions using 0.10 M (n-Bu<sub>4</sub>N)·(PF<sub>6</sub>) as supporting electrolyte with scan rate of 100 mV/s. The electrochemical titration experiments of  $C_1$  (0.1 mM) or  $C_2$  (0.1 mM) upon addition of Et<sub>3</sub>NHCl (2.0 mM) successively (up to 8.0 mM) were measured at the same conditions.



**Figure S10.** Cyclic voltammetry of  $C_2$  (0.10 mM) (black line) upon addition of Et<sub>3</sub>NHCl (colour lines). All the measurement was displayed in acetonitrile solutions containing 0.10 M (n-Bu<sub>4</sub>N)·(PF<sub>6</sub>) with a scan rate of 100 mV/s.

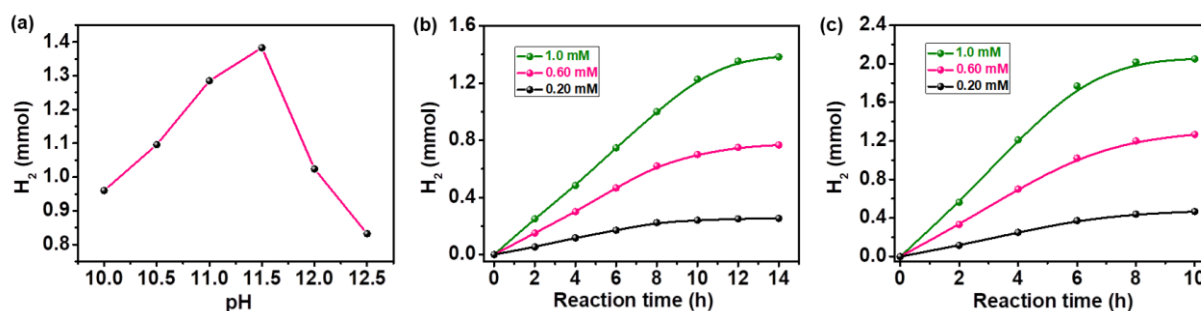
### UV/vis titration experiment

The solution UV-vis spectra were recorded on a SHIMADZU UV 2600 UV-vis spectrophotometer. UV/Vis spectra of  $C_1$  (10.0  $\mu\text{M}$ ) or  $C_2$  (10.0  $\mu\text{M}$ ) were recorded in an  $\text{CH}_3\text{CN}$  solution. The titration experiment of  $C_1$  (10.0  $\mu\text{M}$ ) or  $C_2$  (10.0  $\mu\text{M}$ ) upon addition of **FI** (10.0  $\mu\text{M}$ ) successively (up to 30.0  $\mu\text{M}$ ) were measured at the same conditions.



**Figure S11.** UV/Vis spectra of an  $\text{CH}_3\text{CN}$  solution containing  $C_2$  (10.0  $\mu\text{M}$ ) (black line) upon addition of **FI** (colored lines).

## The photocatalytic hydrogen generation using Na<sub>2</sub>S as electron donor



**Figure S12.** (a) The photocatalytic hydrogen generation in 1:1 acetonitrile/H<sub>2</sub>O (v/v) solution containing C<sub>1F</sub> (1.0 mM) and Na<sub>2</sub>S (5.0 mmol) at different pH values, showing the optimal pH value for the photocatalytic system at 11.5. (b) The kinetics of the photocatalytic hydrogen generation for systems in 1:1 acetonitrile/H<sub>2</sub>O (v/v) solution containing Na<sub>2</sub>S (5.0 mmol) at pH = 11.5 with different concentration of C<sub>1F</sub>. (c) The kinetics of the photocatalytic hydrogen generation for systems in 1:1 acetonitrile/H<sub>2</sub>O (v/v) solution containing Na<sub>2</sub>S (5.0 mmol) at pH = 11.5 with different concentration of C<sub>2F</sub>.

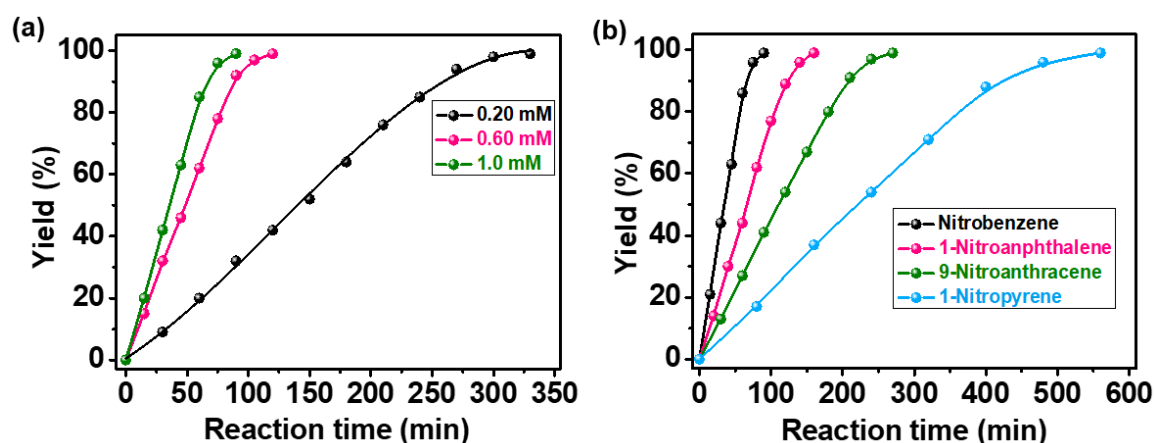


### Kinetics experiments of photocatalytic of nitro substrates reduction using $\text{Na}_2\text{S}$ as electron donor and the reciprocal (Lineweaver-Burk) plot fitting

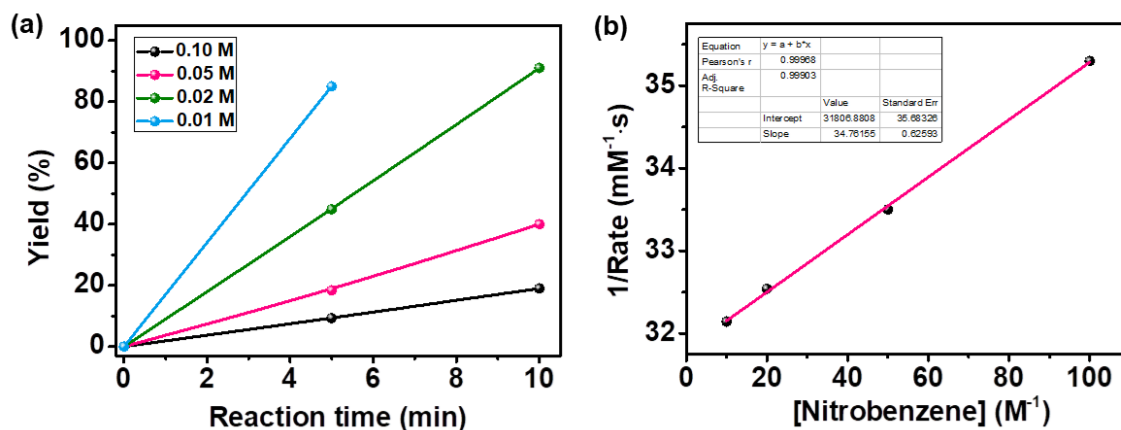
During the reaction process, the tracking of the reaction process was carried by extraction of 50  $\mu\text{L}$  reaction mixture each time with a long needle and followed by HPLC analysis after the quick flush through the silica gel. The reaction rates in the initial stage were regarded as the initial rate of the reactions, which were further used in the reciprocal (Lineweaver-Burk) plot fitting.

**Table S1.** The determined constants of  $K_m$  and  $K_{cat}$  in the catalytic process with different substrates under standard conditions of  $\text{C}_{1\text{F}}$  and  $\text{C}_{2\text{F}}$  systems.

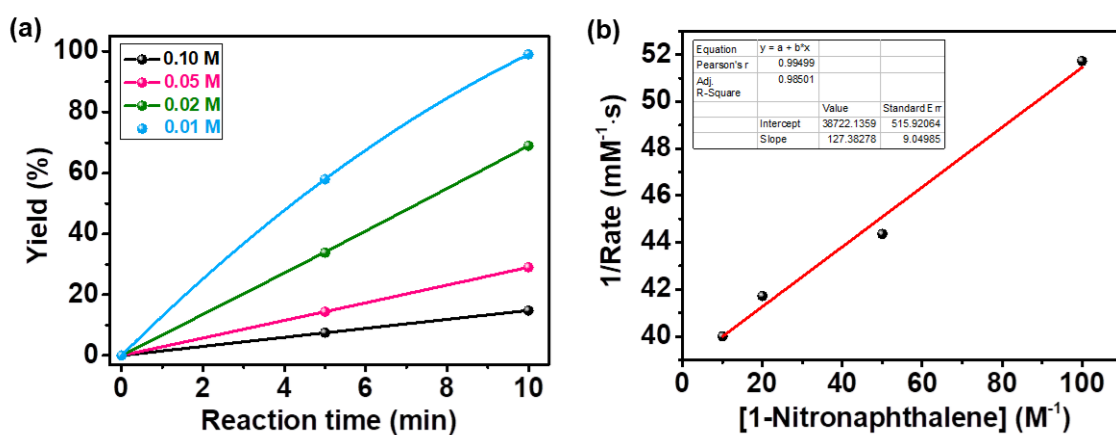
Substrates	$\text{C}_{1\text{F}}$		$\text{C}_{2\text{F}}$	
	$K_m$ (M)	$K_{\text{Cat}}$ ( $\text{s}^{-1}$ )	$K_m$ (M)	$K_{\text{Cat}}$ ( $\text{s}^{-1}$ )
Nitrobenzene	$1.09 \times 10^{-3}$	$3.14 \times 10^{-2}$	$2.49 \times 10^{-3}$	$2.39 \times 10^{-2}$
1-Nitroanthracene	$3.29 \times 10^{-3}$	$2.58 \times 10^{-2}$	$5.30 \times 10^{-3}$	$1.24 \times 10^{-2}$
9-Nitroanthracene	$1.05 \times 10^{-2}$	$1.19 \times 10^{-2}$	$1.75 \times 10^{-2}$	$8.08 \times 10^{-3}$
1-Nitropyrene	$3.48 \times 10^{-2}$	$6.33 \times 10^{-3}$	$5.77 \times 10^{-2}$	$5.73 \times 10^{-3}$



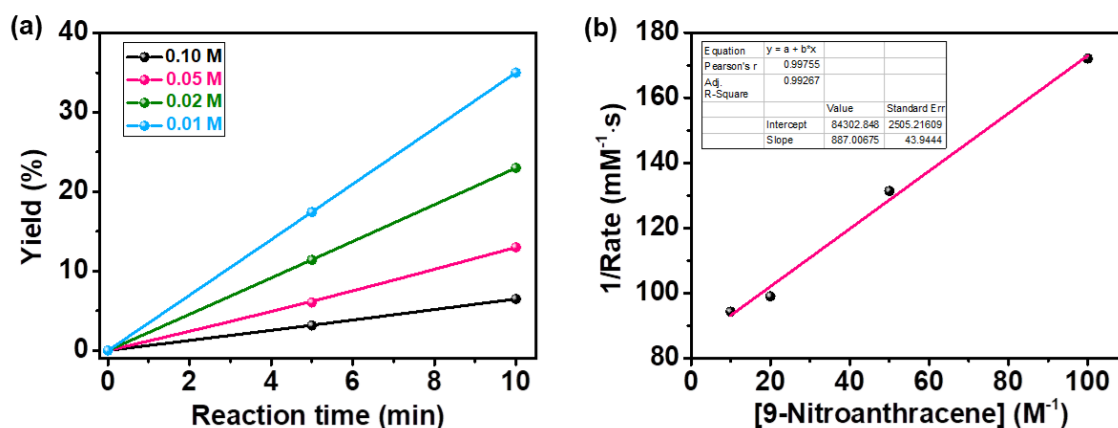
**Figure S13.** (a) Yields of photocatalytic nitrobenzene reduction under standard conditions with different loading of  $\text{C}_{2\text{F}}$ . (b) Kinetics of the aminoarene conversion with varied substrates under standard conditions of  $\text{C}_{2\text{F}}$  system.



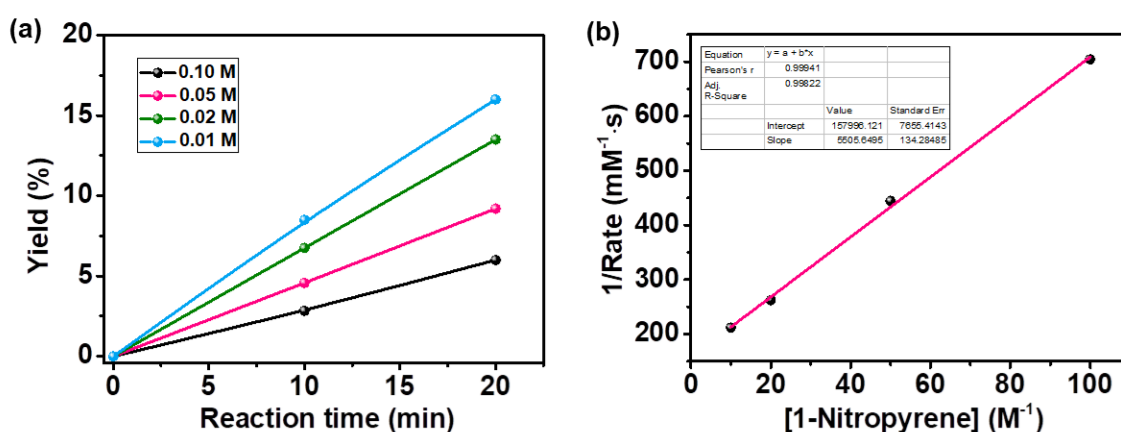
**Figure S14.** (a) Kinetics experiments of reduction reactions of nitrobenzene using Na<sub>2</sub>S as electron donor with different concentration of nitrobenzene in C<sub>1F</sub> system. (b) The reciprocal (Lineweaver-Burk) plot of the initial rate of nitrobenzene reduction and the concentration of [Nitrobenzene], suggested a Michaelis-Menten mechanism involving the catalytic process.



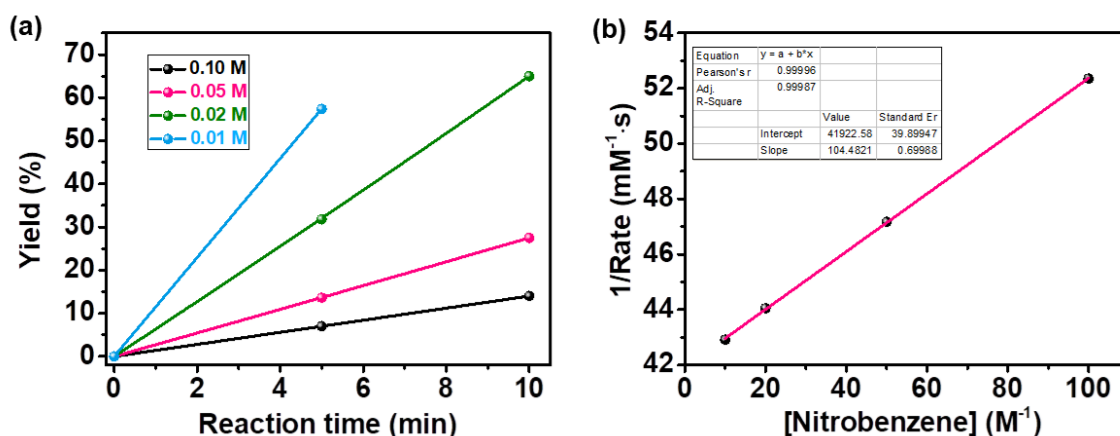
**Figure S15.** (a) Kinetics experiments of reduction reactions of 1-nitronaphthalene using Na<sub>2</sub>S as electron donor with different concentration of 1-nitronaphthalene in C<sub>1F</sub> system. (b) The reciprocal (Lineweaver-Burk) plot of the initial rate of 1-nitronaphthalene reduction and the concentration of [1-Nitronaphthalene], suggested a Michaelis-Menten mechanism involving the catalytic process.



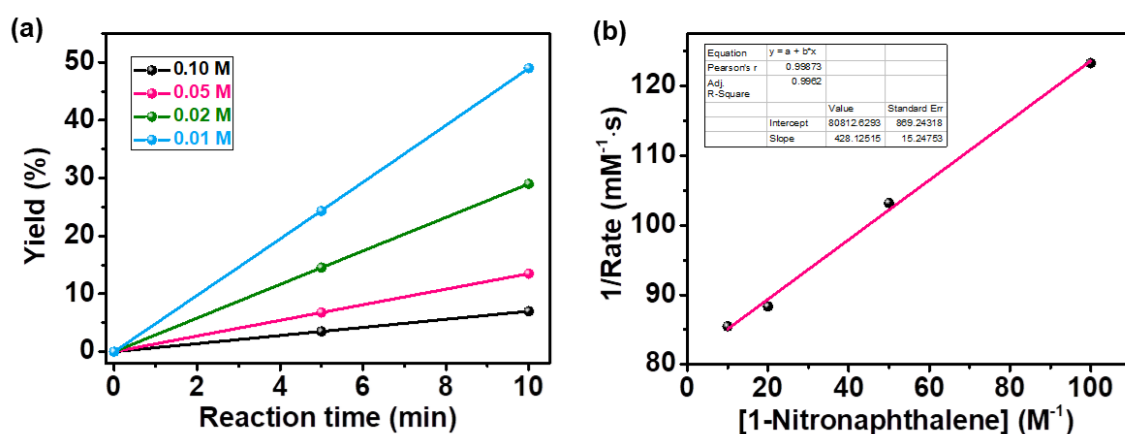
**Figure S16.** (a) Kinetics experiments of reduction reactions of 9-nitroanthracene using Na<sub>2</sub>S as electron donor with different concentration of 9-nitroanthracene in C<sub>1F</sub> system. (b) The reciprocal (Lineweaver-Burk) plot of the initial rate of 9-nitroanthracene reduction and the concentration of [9-Nitroanthracene], suggested a Michaelis-Menten mechanism involving the catalytic process.



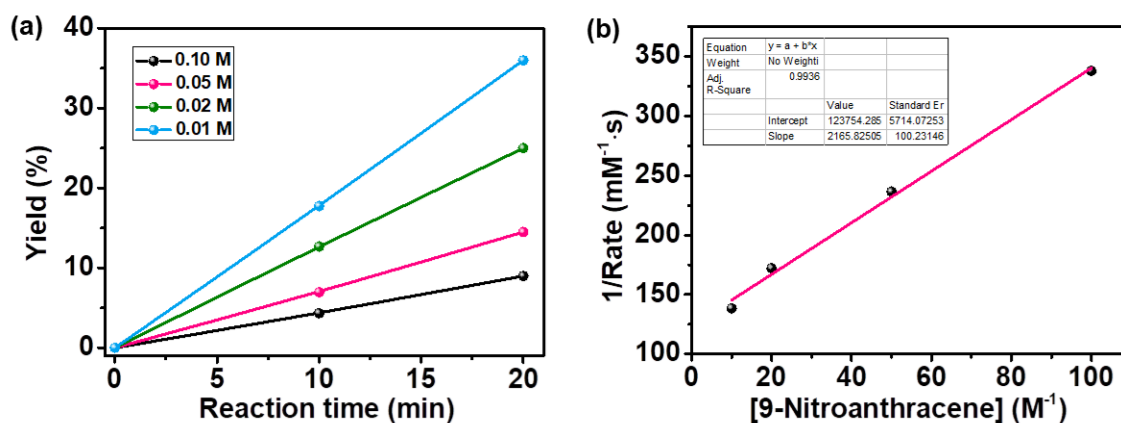
**Figure S17.** (a) Kinetics experiments of reduction reactions of 1-nitropyrene using Na<sub>2</sub>S as electron donor with different concentration of 1-nitropyrene in C<sub>1F</sub> system. (b) The reciprocal (Lineweaver-Burk) plot of the initial rate of 1-nitropyrene reduction and the concentration of [1-Nitropyrene], suggested a Michaelis-Menten mechanism involving the catalytic process.



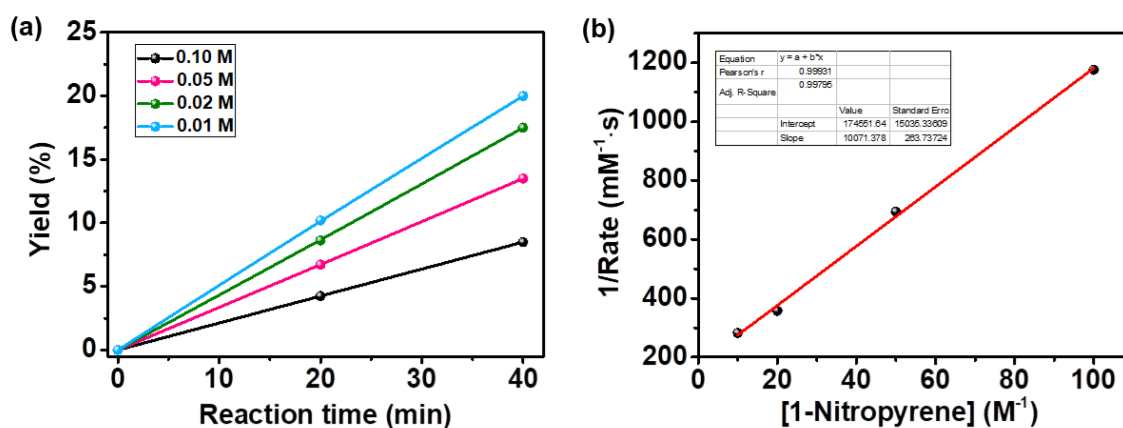
**Figure S18.** (a) Kinetics experiments of reduction reactions of nitrobenzene using Na<sub>2</sub>S as electron donor with different concentration of nitrobenzene in C<sub>2</sub>F system. (b) The reciprocal (Lineweaver-Burk) plot of the initial rate of nitrobenzene reduction and the concentration of [Nitrobenzene], suggested a Michaelis-Menten mechanism involving the catalytic process.



**Figure S19.** (a) Kinetics experiments of reduction reactions of 1-nitronaphthalene using Na<sub>2</sub>S as electron donor with different concentration of 1-nitronaphthalene in C<sub>2</sub>F system. (b) The reciprocal (Lineweaver-Burk) plot of the initial rate of 1-nitronaphthalene reduction and the concentration of [1-Nitronaphthalene], suggested a Michaelis-Menten mechanism involving the catalytic process.

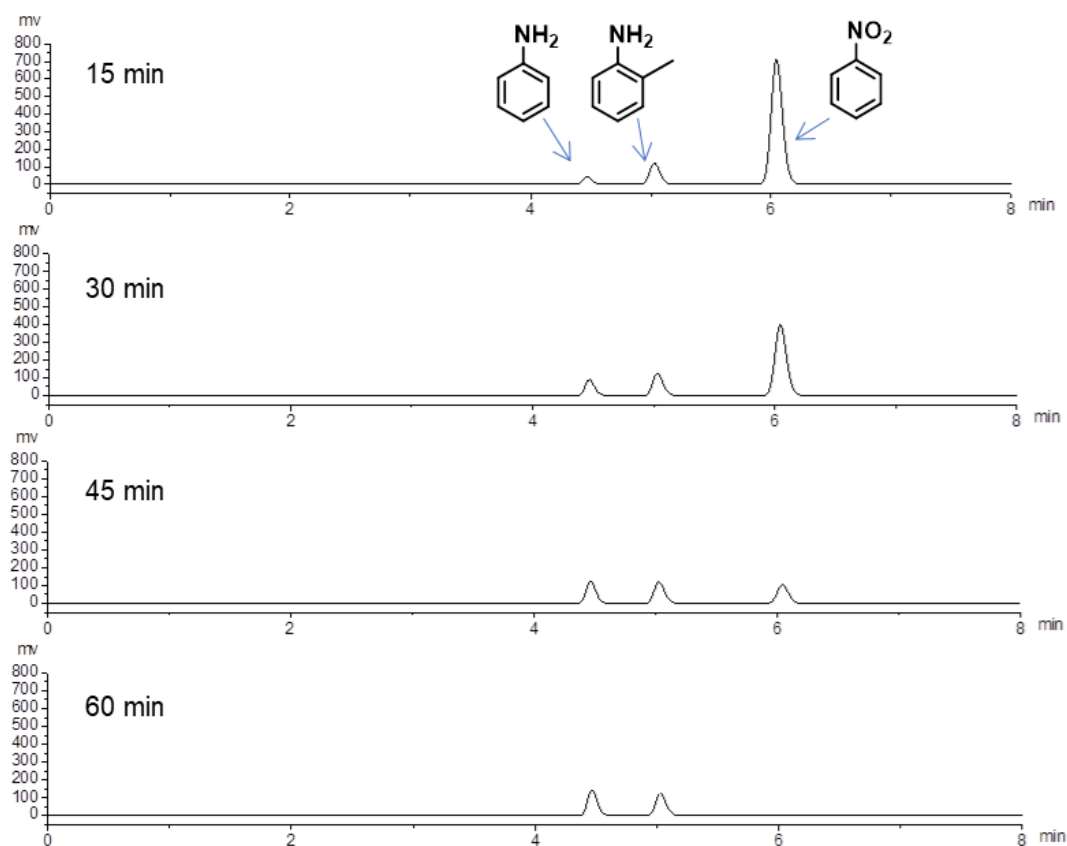


**Figure S20.** (a) Kinetics experiments of reduction reactions of 9-nitroanthracene using Na<sub>2</sub>S as electron donor with different concentration of 9-nitroanthracene in C<sub>2F</sub> system. (b) The reciprocal (Lineweaver-Burk) plot of the initial rate of 9-nitroanthracene reduction and the concentration of [9-Nitroanthracene], suggested a Michaelis-Menten mechanism involving the catalytic process.



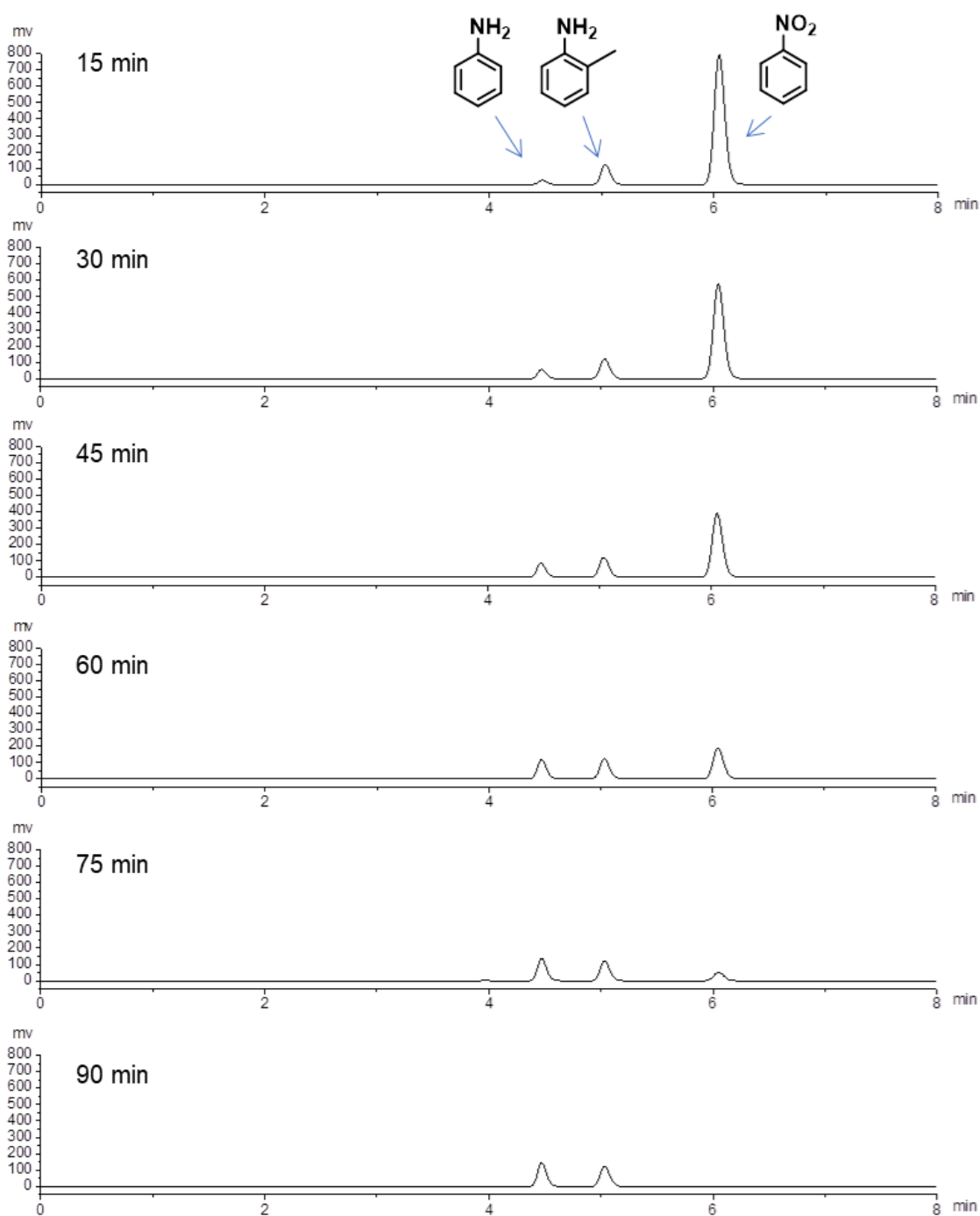
**Figure S21.** (a) Kinetics experiments of reduction reactions of 1-nitropyrene using Na<sub>2</sub>S as electron donor with different concentration of 1-nitropyrene in C<sub>1F</sub> system. (b) The reciprocal (Lineweaver-Burk) plot of the initial rate of 1-nitropyrene reduction and the concentration of [1-Nitropyrene], suggested a Michaelis-Menten mechanism involving the catalytic process.

#### 4. HPLC data for the photocatalytic reactions



Peaks	Retention time (min)	Height	Area	Area (%)
15 min				
1	4.468	44.053	253.568	4.354
2	5.029	120.920	758.014	13.016
3	6.045	711.309	4812.009	82.630
30 min				
1	4.466	90.251	519.753	12.906
2	5.028	125.016	785.000	19.492
3	6.044	402.157	2722.517	67.602
45 min				
1	4.467	126.939	729.489	33.300
2	5.029	120.444	755.161	34.472
3	6.045	104.325	705.995	32.228
60 min				
1	4.466	145.595	838.217	51.989
2	5.028	123.270	774.076	48.011

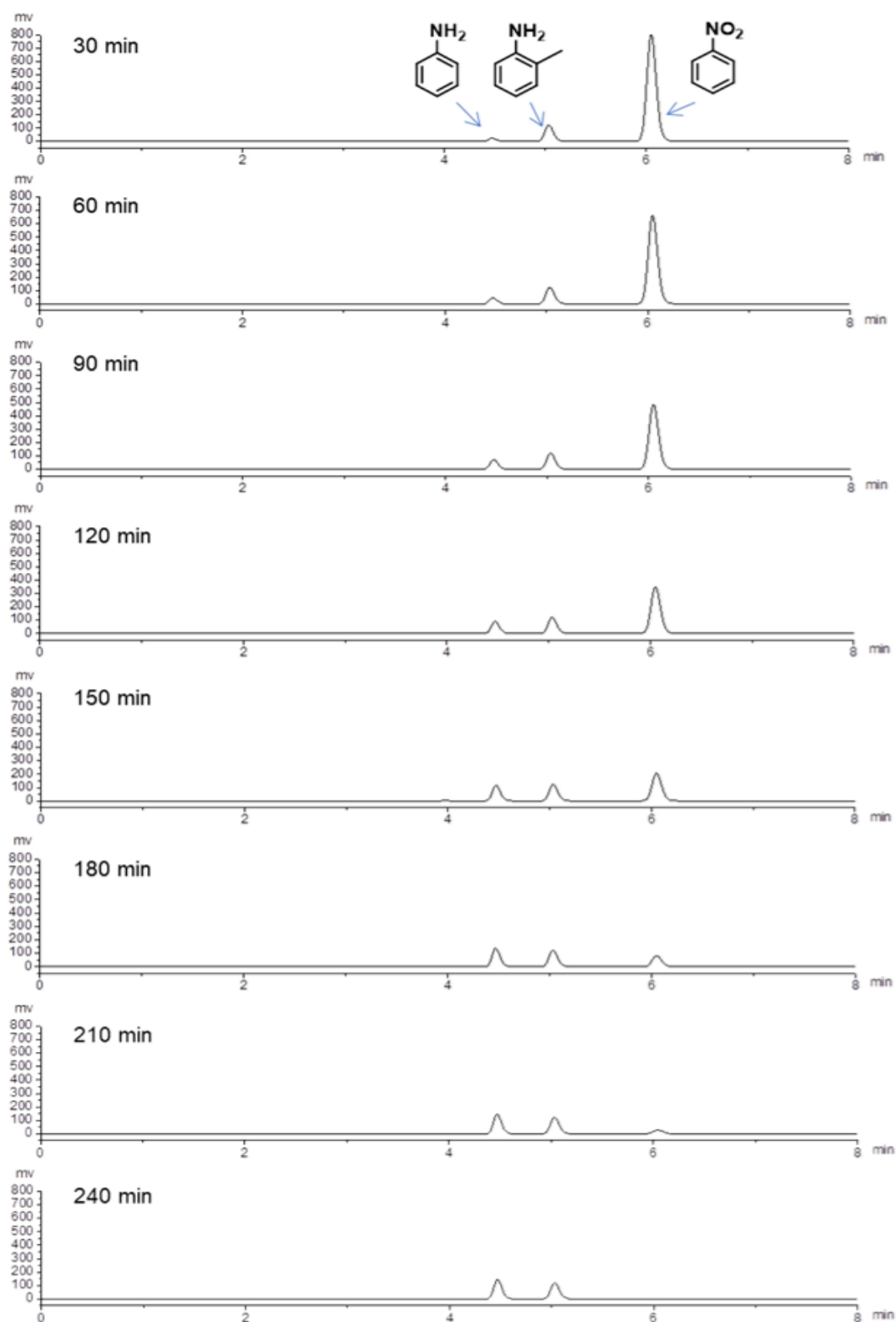
**Figure S22.** HPLC data for the yields of aniline of the photocatalytic reduction of nitrobenzene catalyzed by  $C_{1F}$  (1.0 mM) using m-toluidine as internal standard at 15 min, 30 min, 45 min, 60 min, respectively.



**Figure S23.** HPLC data for the yields of aniline of the photocatalytic reduction of nitrobenzene catalyzed by  $C_{1F}$  (0.60 mM) using m-toluidine as integral standard at 15 min, 30 min, 45 min, 60 min, 75 min, 90 min, respectively.

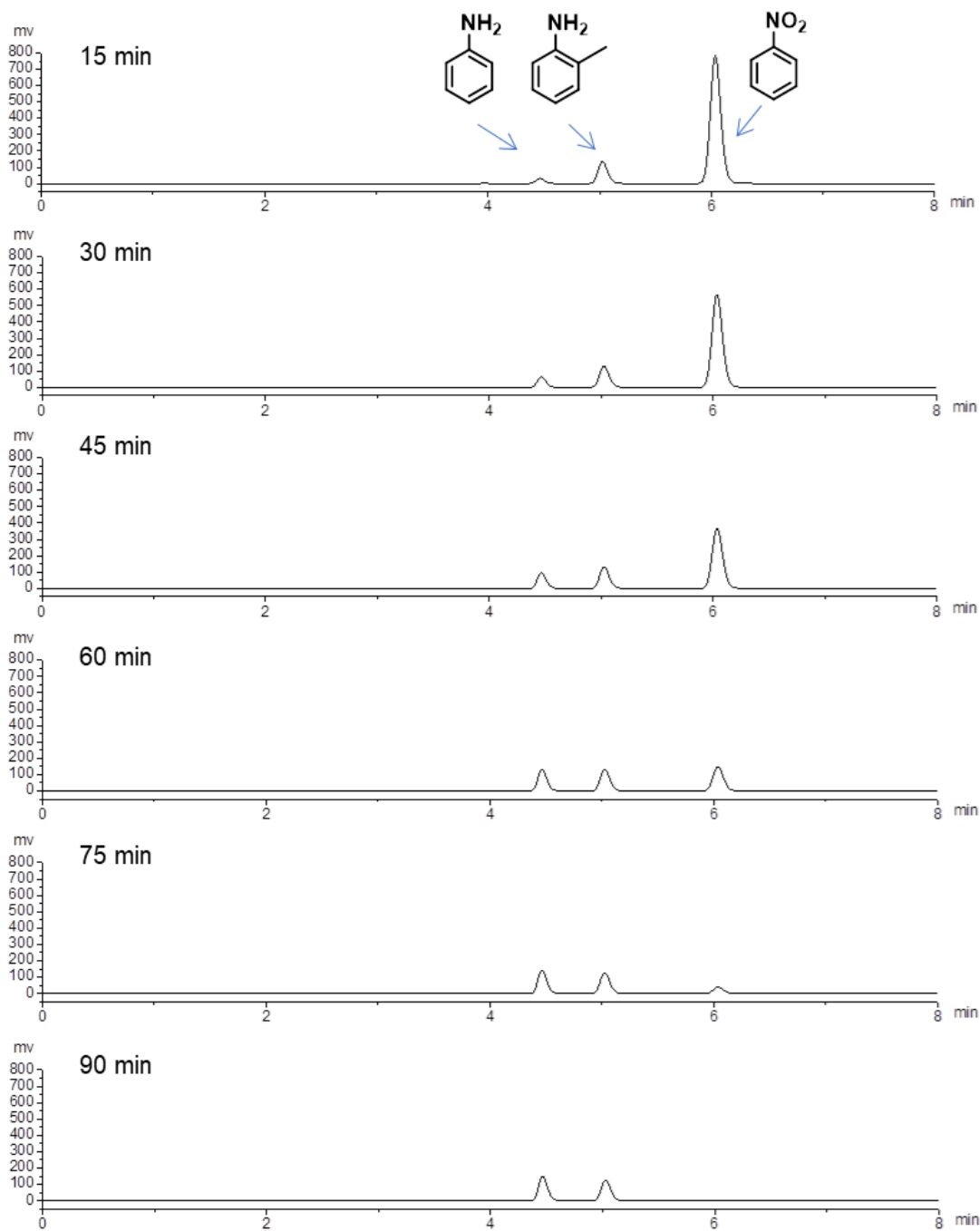
Peaks	Retention time (min)	Height	Area	Area (%)
15 min				
1	4.470	28.336	163.347	2.602
2	5.032	121.696	756.928	12.055
3	6.047	793.963	5358.528	85.343
30 min				
1	4.469	58.068	333.795	6.685
2	5.031	121.940	759.473	15.210
3	6.047	577.579	3900.050	78.105
45 min				
1	4.471	85.846	494.151	12.694
2	5.034	123.069	766.593	19.693
3	6.048	390.712	2632.053	67.613
60 min				
1	4.470	119.385	688.272	25.022
2	5.033	124.540	777.103	28.251
3	6.048	190.322	1285.329	46.727
75 min				
1	4.470	137.831	793.352	41.385
2	5.032	122.452	764.949	39.903
3	6.048	52.939	358.716	18.712
90 min				
1	4.470	146.367	843.851	52.174
2	5.032	123.785	773.538	47.826





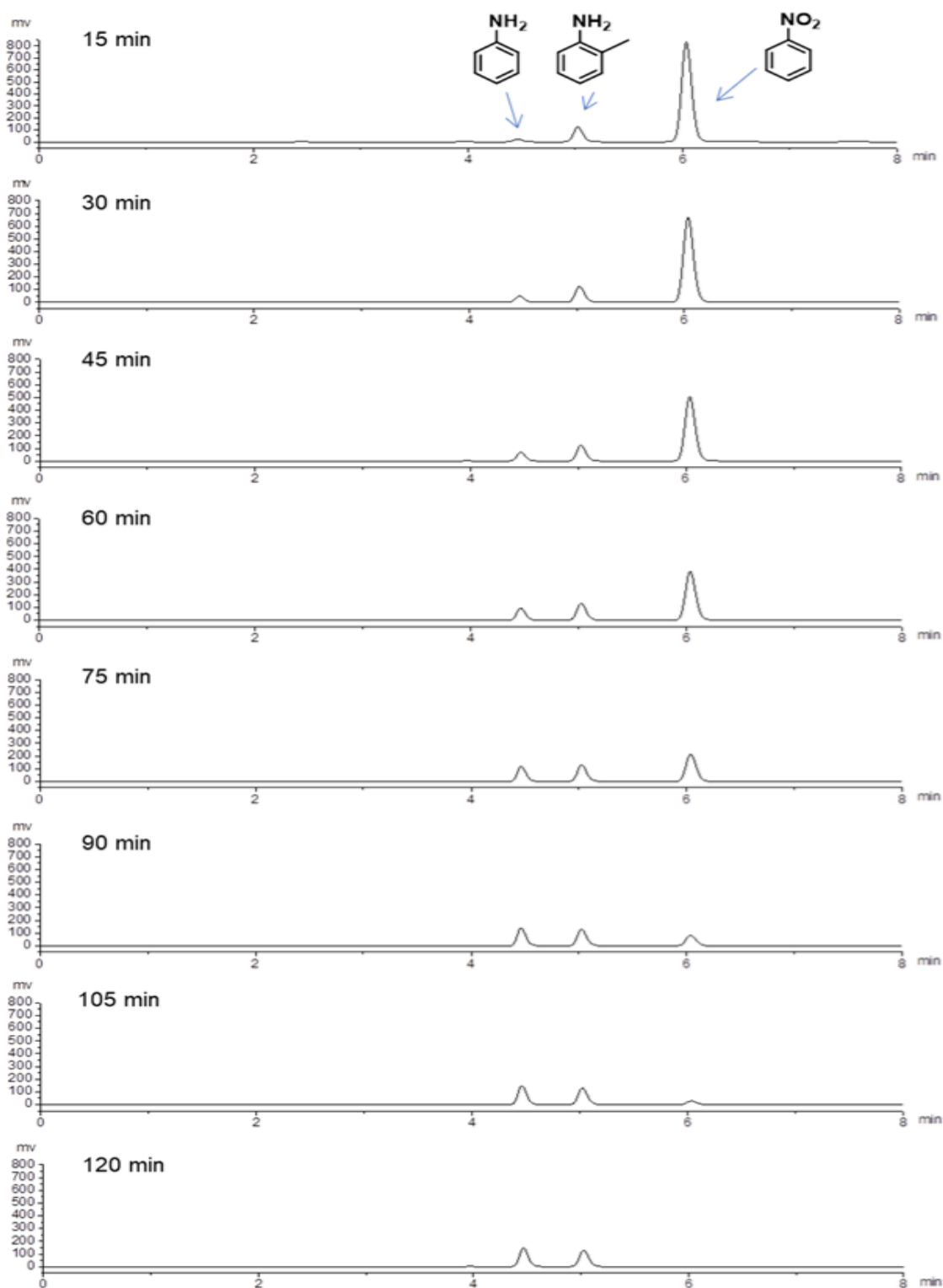
**Figure S24.** HPLC data for the yields of aniline of the photocatalytic reduction of nitrobenzene catalyzed by  $C_{1F}$  (0.20 mM) using m-toluidine as internal standard at 30 min, 60 min, 90 min, 120 min, 150 min, 180 min, 210 min, 240 min, respectively.

Peaks	Retention time (min)	Height	Area	Area (%)
30 min				
1	4.471	24.763	142.964	2.260
2	5.032	123.948	770.623	12.180
3	6.047	802.600	5413.197	85.560
60 min				
1	4.471	47.076	271.036	4.915
2	5.033	124.576	775.525	14.063
3	6.048	662.732	4468.196	81.022
90 min				
1	4.472	73.162	420.505	9.428
2	5.034	122.391	761.574	17.076
3	6.049	486.367	3277.904	73.496
120 min				
1	4.471	91.905	529.006	14.511
2	5.033	122.023	759.509	20.834
3	6.048	349.569	2356.995	64.655
150 min				
1	4.471	116.301	670.371	23.605
2	5.033	123.317	768.225	27.050
3	6.048	207.778	1401.395	49.345
180 min				
1	4.471	137.347	792.996	37.310
2	5.032	123.285	769.677	36.213
3	6.047	82.980	562.735	26.477
210 min				
1	4.470	144.872	834.444	46.323
2	5.031	123.479	772.128	42.863
3	6.044	28.384	194.796	10.814
240 min				
1	4.469	146.754	841.399	52.946
2	5.029	119.806	747.761	47.054



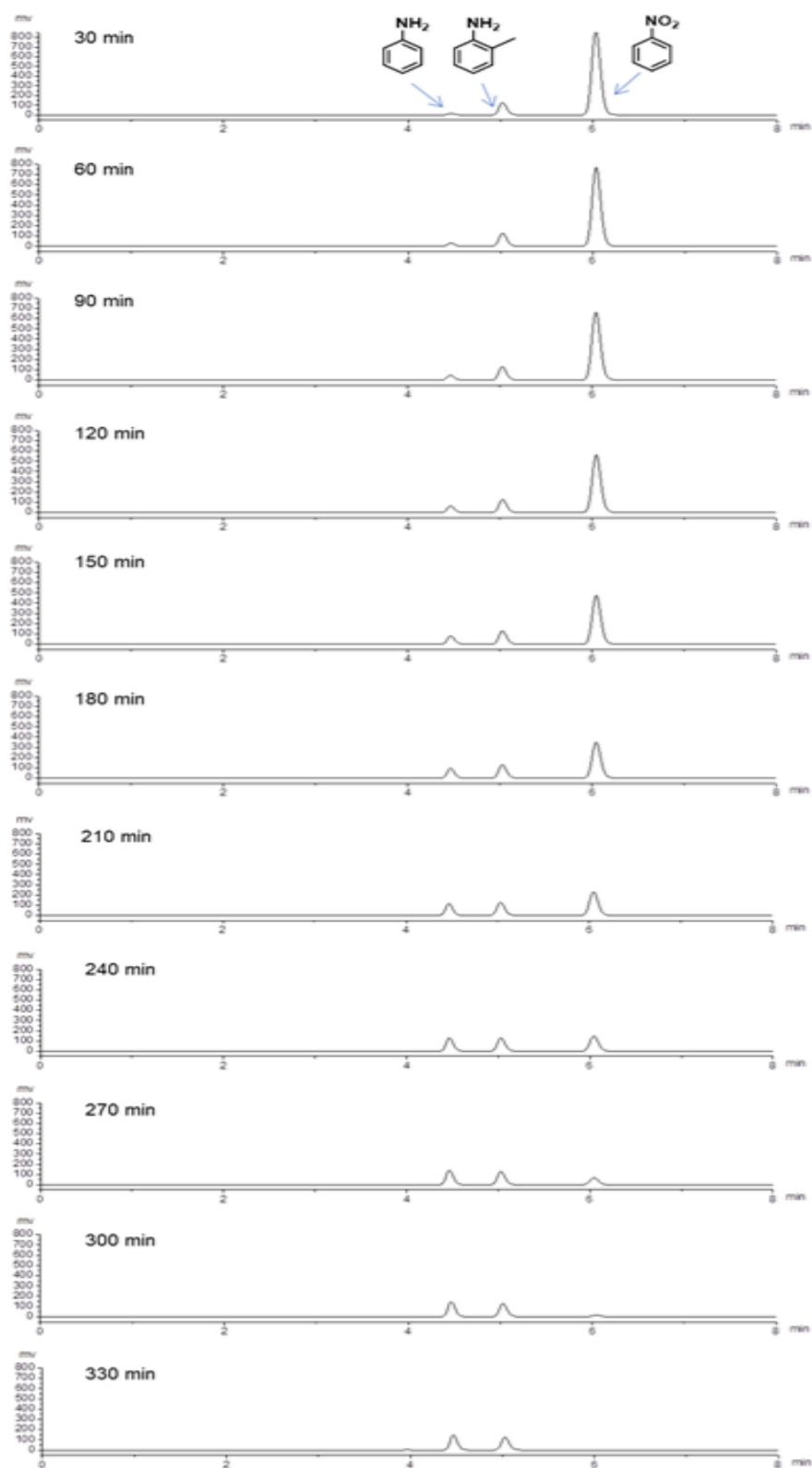
**Figure S25.** HPLC data for the yields of aniline of the photocatalytic reduction of nitrobenzene catalyzed by  $C_{2F}$  (1.0 mM) using m-toluidine as integral standard at 15 min, 30 min, 45 min, 60 min, 75 min, 90 min, respectively.

Peaks	Retention time (min)	Height	Area	Area (%)
15 min				
1	4.464	31.981	184.541	2.917
2	5.023	135.051	842.385	13.316
3	6.035	784.522	5299.372	83.767
30 min				
1	4.463	64.563	372.108	7.401
2	5.023	130.760	815.652	16.223
3	6.034	569.370	3840.109	76.376
45 min				
1	4.464	96.483	556.086	14.377
2	5.025	131.705	822.520	21.266
3	6.036	368.686	2489.160	64.357
60 min				
1	4.464	131.171	757.392	29.295
2	5.024	132.493	828.396	32.041
3	6.035	147.779	999.607	38.664
75 min				
1	4.463	143.246	827.360	43.585
2	5.023	128.269	800.680	42.179
3	6.035	39.790	270.232	14.236
90 min				
1	4.463	151.273	873.742	52.319
2	5.025	127.199	796.276	47.681



**Figure S26.** HPLC data for the yields of aniline of the photocatalytic reduction of nitrobenzene catalyzed by  $C_{2F}$  (0.60 mM) using m-toluidine as internal standard at 15 min, 30 min, 45 min, 60 min, 75 min, 90 min, 105 min, 120 min, respectively.

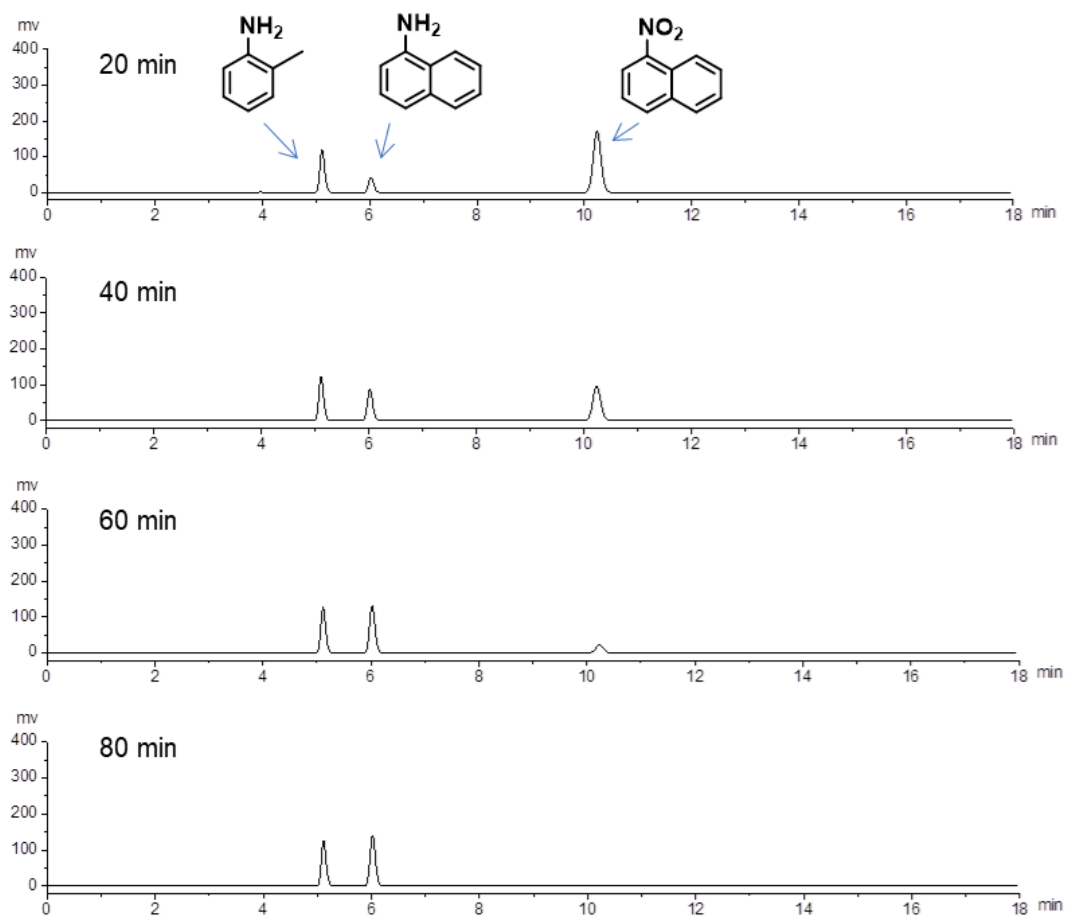
Peaks	Retention time (min)	Height	Area	Area (%)
15 min				
1	4.464	23.179	133.553	2.047
2	5.024	124.206	772.348	11.837
3	6.035	833.886	5618.723	86.116
30 min				
1	4.464	48.931	281.008	5.047
2	5.025	125.712	782.176	14.049
3	6.036	668.338	4504.406	80.904
45 min				
1	4.465	69.639	399.618	8.663
2	5.025	126.950	790.828	17.143
3	6.035	507.813	3422.558	74.194
60 min				
1	4.464	95.510	549.973	13.946
2	5.024	131.097	818.215	20.748
3	6.035	381.552	2575.455	65.306
75 min				
1	4.465	119.382	687.469	23.326
2	5.025	130.664	816.181	27.693
3	6.036	213.418	1443.626	48.981
90 min				
1	4.463	139.791	806.972	36.905
2	5.024	130.068	814.043	37.228
3	6.035	83.346	565.604	25.867
105 min				
1	4.463	149.291	863.217	45.830
2	5.023	130.479	816.425	43.346
3	6.036	29.779	203.875	10.824
120 min				
1	4.462	148.050	855.310	51.746
2	5.023	127.368	797.584	48.254



**Figure S27.** HPLC data for the yields of aniline of the photocatalytic reduction of nitrobenzene catalyzed by  $C_{2F}$  (0.20 mM) using m-toluidine as integral standard at 30 min, 60 min, 90 min, 120 min, 150 min, 180 min, 210 min, 240 min, 270 min, 300 min, 330 min, respectively.

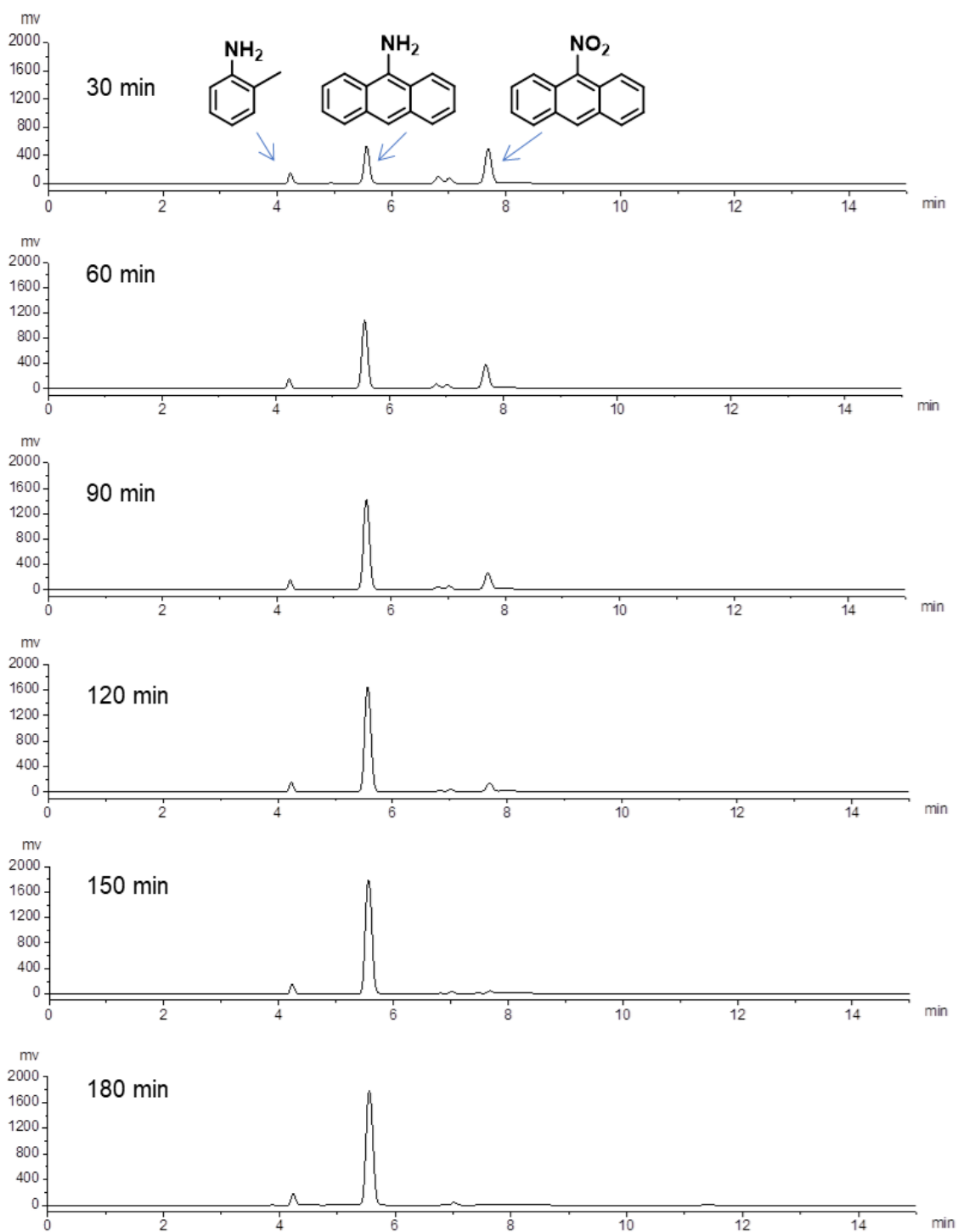
Peaks	Retention time (min)	Height	Area	Area (%)
30 min				
1	4.463	14.860	86.489	1.279
2	5.023	127.108	793.075	11.732
3	6.034	872.746	5880.406	86.989
60 min				
1	4.463	31.544	182.437	2.951
2	5.024	127.457	795.003	12.861
3	6.037	768.166	5204.007	84.188
90 min				
1	4.464	49.483	285.026	5.087
2	5.026	130.408	814.805	14.542
3	6.042	666.495	4503.301	80.371
120 min				
1	4.466	63.945	367.382	7.412
2	5.029	127.200	798.161	16.104
3	6.046	559.512	3790.791	76.484
150 min				
1	4.466	79.886	459.009	10.245
2	5.029	128.799	807.107	18.015
3	6.046	473.954	3214.150	71.740
180 min				
1	4.465	96.902	556.775	14.883
2	5.028	129.791	811.977	21.704
3	6.045	350.559	2372.342	63.413
210 min				
1	4.466	115.883	665.696	21.952
2	5.028	128.859	806.434	26.593
3	6.044	230.812	1560.401	51.455
240 min				
1	4.467	129.951	746.268	29.141
2	5.029	129.151	809.914	31.626
3	6.044	148.580	1004.693	39.233
270 min				
1	4.466	142.550	819.440	39.175
2	5.028	128.462	806.391	38.551
3	6.045	68.359	465.922	22.274
300 min				
1	4.467	146.588	841.618	51.176
2	5.029	127.984	802.942	48.824
330 min				
1	4.467	147.612	846.606	52.111
2	5.029	124.072	778.000	47.889





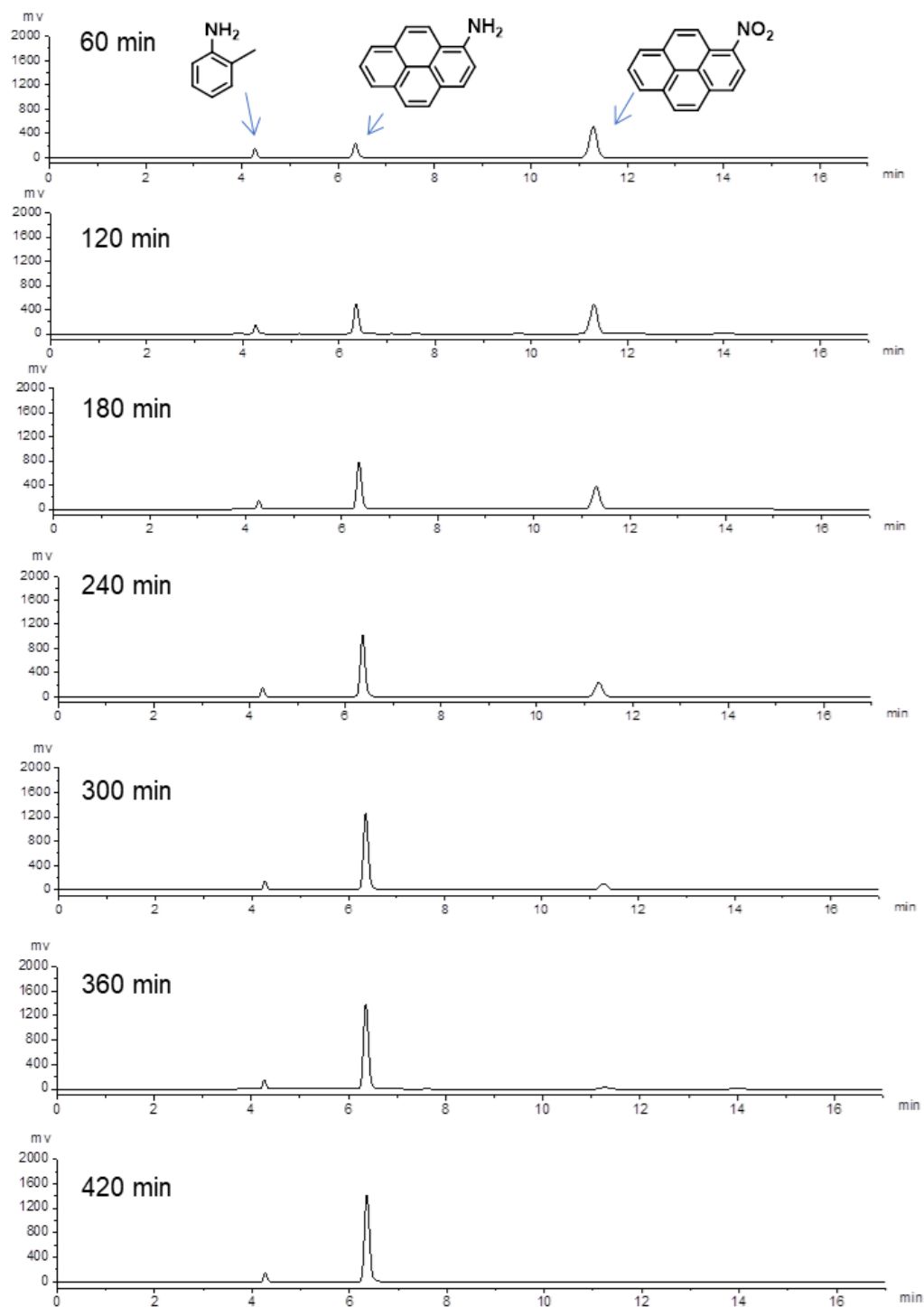
**Figure S28.** HPLC data for the yields of 1-aminoanthracene of the photocatalytic reduction of 1-nitroanthracene catalyzed by C<sub>1F</sub> (1.0 mM) using m-toluidine as integral standard at 20 min, 40 min, 60 min, 80 min, respectively.

Peaks	Retention time (min)	Height	Area	Area (%)
20 min				
1	5.111	120.884	776.183	26.972
2	6.021	42.381	305.322	10.610
3	10.239	170.638	1796.185	62.418
40 min				
1	5.114	124.613	802.193	32.900
2	6.022	86.721	625.827	25.667
3	10.238	96.537	1010.246	41.433
60 min				
1	5.114	126.908	814.353	40.574
2	6.023	131.270	948.054	47.235
3	10.236	23.366	244.675	12.191
80 min				
1	5.114	126.377	808.896	44.138
2	6.021	141.697	1023.742	55.862



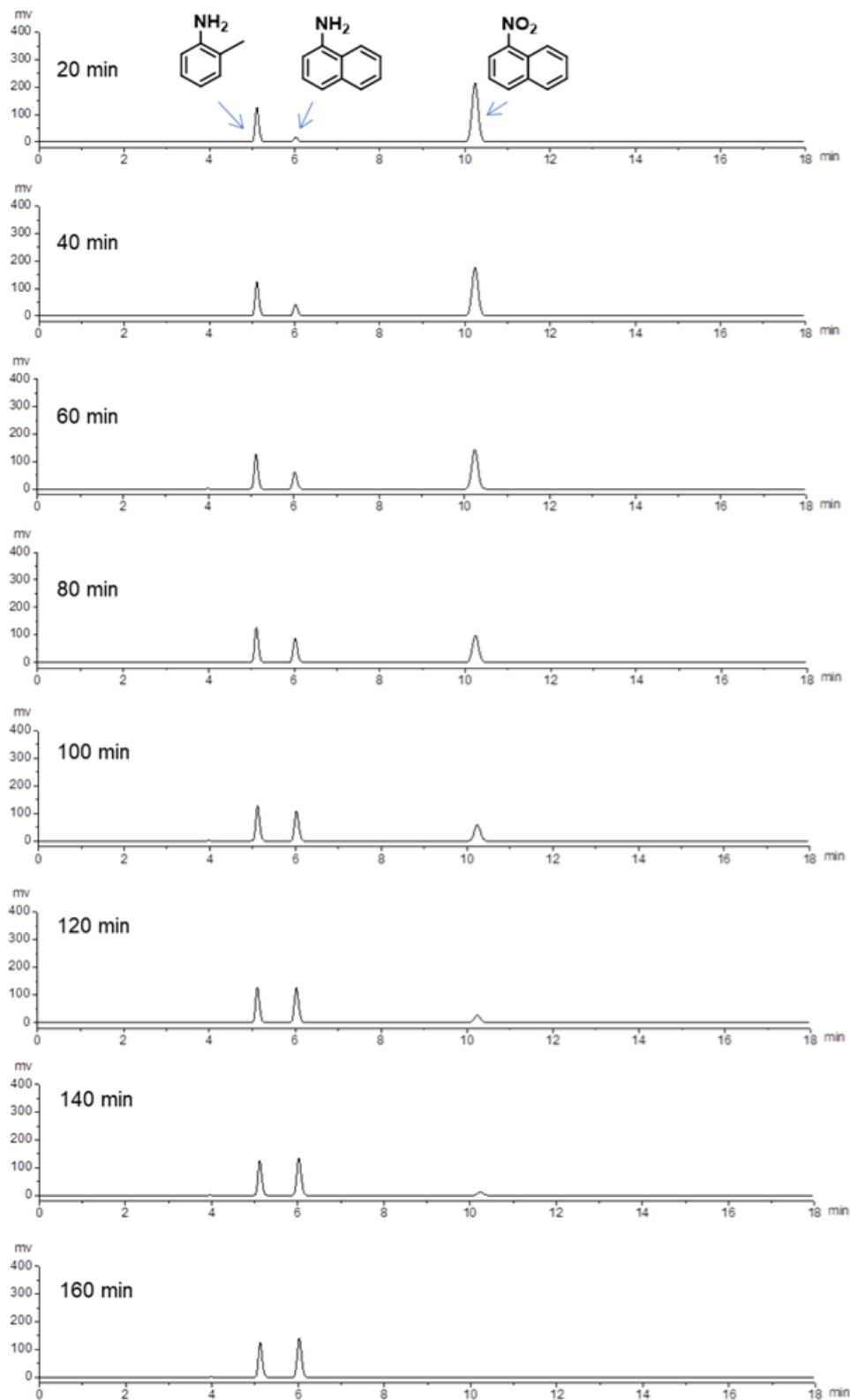
**Figure S29.** HPLC data for the yields of 9-aminoanthracene of the photocatalytic reduction of 9-nitroanthracene catalyzed by  $C_{1F}$  (1.0 mM) using m-toluidine as integral standard at 30 min, 60 min, 90 min, 120 min, 150 min, 180 min respectively.

Peaks	Retention time (min)	Height	Area	Area (%)
30 min				
1	4.229	152.735	799.694	9.558
2	5.564	530.863	3587.152	42.874
3	7.688	502.320	3979.840	47.568
60 min				
1	4.229	154.638	806.699	6.958
2	5.562	1075.461	7767.822	66.996
3	7.690	379.254	3019.906	26.046
90 min				
1	4.233	156.361	811.544	5.876
2	5.567	1424.591	10862.209	78.650
3	7.692	264.701	2137.038	15.474
120 min				
1	4.234	156.493	817.815	5.363
2	5.566	1649.179	13268.880	87.020
3	7.687	140.929	1161.425	7.617
150 min				
1	4.236	157.321	831.213	5.171
2	5.568	1784.263	14803.032	92.091
3	7.690	51.229	440.114	2.738
180 min				
1	4.238	185.129	1042.363	6.423
2	5.553	1780.352	15186.762	93.577



**Figure S30.** HPLC data for the yields of 1-aminopyrene of the photocatalytic reduction of 1-nitropyrene catalyzed by  $C_{1F}$  (1.0 mM) using m-toluidine as integral standard at 60 min, 120 min, 180 min, 240 min, 300 min, 360 min, 420 min, respectively.

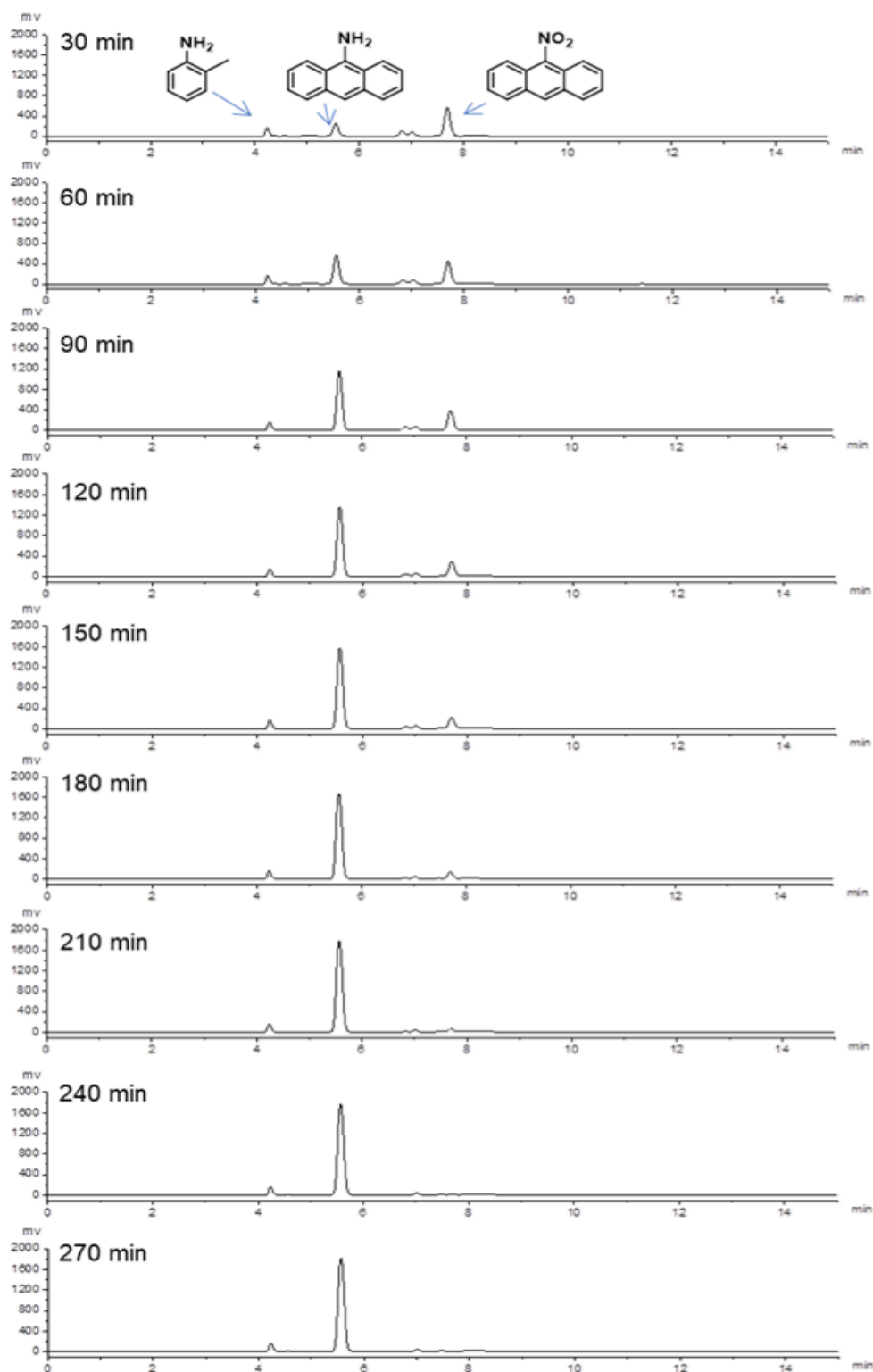
Peaks	Retention time (min)	Height	Area	Area (%)
60 min				
1	4.268	148.210	772.767	9.502
2	6.356	234.365	1679.970	20.657
3	11.299	515.103	5680.042	69.841
120 min				
1	4.267	147.054	766.943	7.876
2	6.357	505.659	3593.509	36.902
3	11.303	486.821	5377.617	55.222
180 min				
1	4.267	149.247	779.535	7.419
2	6.358	786.309	5635.706	53.638
3	11.302	370.796	4091.640	38.943
240 min				
1	4.269	150.754	792.096	7.304
2	6.359	1031.544	7416.526	68.389
3	11.299	239.165	2636.016	24.307
300 min				
1	4.268	147.115	772.105	6.987
2	6.358	1251.573	9141.182	82.716
3	11.282	103.419	1138.039	10.297
360 min				
1	4.269	148.796	781.263	6.898
2	6.359	1384.941	10195.352	90.023
3	11.282	31.725	348.628	3.079
420 min				
1	4.267	147.515	766.445	6.768
2	6.357	1413.798	10382.617	93.232



**Figure S31.** HPLC data for the yields of 1-aminoanthracene of the photocatalytic reduction of 1-nitroanthracene catalyzed by  $C_{2}F$  (1.0 mM) using m-toluidine as integral standard at 20 min, 40 min, 60 min, 80 min, 100 min, 120 min, 140 min, 160 min, respectively.

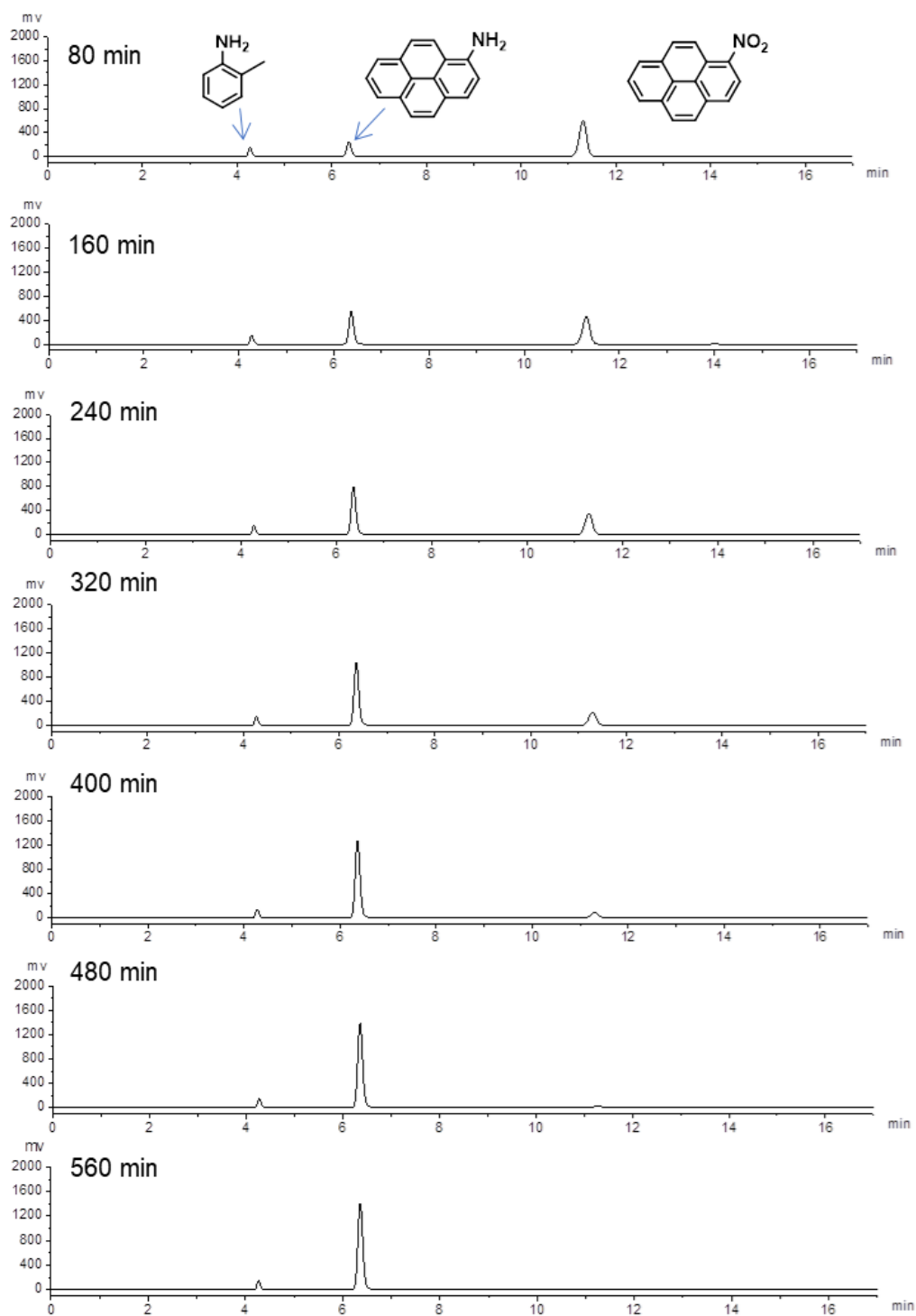
Peaks	Retention time (min)	Height	Area	Area (%)
20 min				
1	5.114	126.725	816.617	25.446
2	6.023	18.648	133.100	4.148
3	10.237	214.988	2259.436	70.406
40 min				
1	5.114	125.735	812.478	27.328
2	6.022	42.241	302.678	10.181
3	10.237	176.840	1857.957	62.491
60 min				
1	5.115	128.976	833.093	29.597
2	6.024	62.401	448.899	15.948
3	10.238	146.117	1532.781	54.455
80 min				
1	5.115	127.919	825.411	33.048
2	6.023	87.377	631.161	25.270
3	10.239	99.328	1041.051	41.682
100 min				
1	5.116	127.620	818.364	36.740
2	6.024	109.345	788.992	35.421
3	10.240	59.290	620.105	27.839
120 min				
1	5.117	128.056	820.267	40.323
2	6.026	126.457	914.895	44.975
3	10.238	28.556	299.080	14.702
140 min				
1	5.117	126.892	810.927	42.049
2	6.025	135.834	981.881	50.914
3	10.240	12.952	135.708	7.037
160 min				
1	5.117	127.609	814.230	44.433
2	6.025	140.809	1018.258	55.567





**Figure S32.** HPLC data for the yields of 9-aminoanthracene of the photocatalytic reduction of 9-nitroanthracene catalyzed by  $C_{2F}$  (1.0 mM) using m-toluidine as integral standard at 30 min, 60 min, 90 min, 120 min, 150 min, 180 min, 210 min, 240 min, 270 min, respectively.

Peaks	Retention time (min)	Height	Area	Area (%)
30 min				
1	4.236	162.618	859.753	11.806
2	5.554	248.898	1921.529	26.386
3	7.693	568.882	4501.195	61.808
60 min				
1	4.237	166.838	890.171	10.106
2	5.555	565.286	4332.523	49.188
3	7.694	450.409	3585.333	40.706
90 min				
1	4.236	163.800	857.322	6.855
2	5.567	1163.012	8535.199	68.250
3	7.691	391.662	3113.278	24.895
120 min				
1	4.236	159.468	837.972	6.180
2	5.569	1364.422	10398.886	76.687
3	7.696	289.763	2323.293	17.133
150 min				
1	4.238	164.342	869.041	5.742
2	5.570	1576.524	12497.840	82.570
3	7.696	219.223	1769.093	11.688
180 min				
1	4.238	163.648	866.510	5.572
2	5.570	1681.789	13632.091	87.666
3	7.696	128.737	1051.403	6.762
210 min				
1	4.237	163.056	868.643	5.411
2	5.568	1774.757	14679.636	91.448
3	7.695	60.266	504.080	3.141
240 min				
1	4.237	162.964	870.464	5.552
2	5.568	1767.845	14646.370	93.423
3	7.694	17.968	160.618	1.025
270 min				
1	4.237	167.383	903.208	5.579
2	5.564	1812.574	15287.627	94.421



**Figure S33.** HPLC data for the yields of 1-aminopyrene of the photocatalytic reduction of 1-nitropyrene catalyzed by C<sub>2</sub>F (1.0 mM) using m-toluidine as integral standard at 80 min, 160 min, 240 min, 320 min, 400 min, 480 min, 560 min, respectively.

Peaks	Retention time (min)	Height	Area	Area (%)
60 min				
1	4.268	146.665	765.907	8.318
2	6.358	247.216	1789.702	19.436
3	11.307	601.634	6652.390	72.246
120 min				
1	4.268	149.149	779.780	7.852
2	6.360	556.354	3997.691	40.253
3	11.307	467.744	5154.045	51.895
180 min				
1	4.268	147.304	764.874	7.406
2	6.357	801.063	5710.585	55.293
3	11.299	349.378	3852.315	37.301
240 min				
1	4.269	148.372	778.244	7.274
2	6.359	1037.144	7490.559	70.014
3	11.294	220.603	2429.850	22.712
300 min				
1	4.269	148.593	780.698	7.054
2	6.362	1271.706	9327.024	84.269
3	11.295	87.053	960.441	8.677
360 min				
1	4.268	151.463	794.827	7.002
2	6.358	1386.931	10208.962	89.936
3	11.287	31.579	347.521	3.062
420 min				
1	4.269	149.457	784.377	6.981
2	6.360	1415.446	10451.589	93.019

## 5. References

(S1) SMART, Data collection software (version 5.629) (Bruker AXS Inc., Madison, WI, **2003**).

(S2) SAINT, Data reduction software (version 6.54) (Bruker AXS Inc., Madison, WI, **2003**).

(S3) Sheldrick, G. M. SHELXTL97, Program for Crystal Structure Solution (University of Göttingen: Göttingen, Germany, **1997**).