

## ***Electronic Supplementary Information***

### **Significantly improved electrocatalytic oxygen reduction by asymmetrical Pacman dinuclear cobalt(II) porphyrin- porphyrin dyad**

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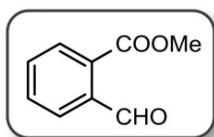
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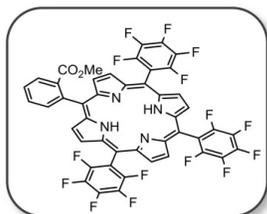
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**Synthesis of dinuclear metal complexes.** The synthetic routes of bisporphyrin macrocycles and corresponding metal complexes are depicted in Fig. 2 in the main text. Detailed synthetic conditions and characterizations are described in the following.



**Synthesis of methyl 2-formylbenzoate.** *o*-Carboxybenzaldehyde (1.5 g, 9.1 mmol) was dissolved in 200 mL methanol in a 500 mL flask, and 1 mL concentrated sulfuric acid was added with stirring.

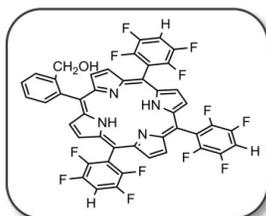
The mixture was stirred and refluxed for 4 h, and was then added dichloromethane and water for extraction. The dichloromethane layer was separated and was dried with anhydrous Na<sub>2</sub>SO<sub>4</sub>. Dichloromethane was then removed by vacuo to give methyl 2-formylbenzoate (1.55 g, yield 95%). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ = 10.62 (s, 1H), 7.97 (m, 1H), 7.94 (m, 1H), 7.65 (m, 2H), 3.98 (s, 3H) (Fig. S1).



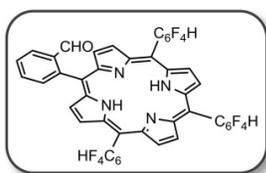
**Synthesis of a.** To a 500 mL flask containing chloroform (300 mL), were added methyl 2-formylbenzoate (0.41 g, 2.5 mmol), pentafluorobenzaldehyde (1.47 g, 7.5 mmol) and pyrrole (0.67 g, 10 mmol) at room temperature. The solution was purged with N<sub>2</sub>

for 30 min, and then BF<sub>3</sub>·OEt<sub>2</sub> (0.125 mL, 1 mmol) was added. The mixture was stirred under N<sub>2</sub> for 40 min, and then DDQ (2.04 g, 18 mmol) dissolved in benzene (20 mL) was added. The resulted solution was further stirred for 1 h, and was then dried using a rotary evaporator. The dark residue was dissolved in CH<sub>2</sub>Cl<sub>2</sub>, and purified by silica-gel column chromatography (hexanes/CH<sub>2</sub>Cl<sub>2</sub> = 5:1 v/v) to afford pure **a** as a purple solid (0.47 g yield 20%). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ = 8.94 (s, 4H), 8.83 (s, 4H), 8.49 (d, 1H),

8.18 (d, 1H), 7.87-7.97 (m, 2H), 2.89 (s, 3H), -2.67 (s, 2H) (Fig. S2). HRMS of  $[M+H]^+$ : calcd. for  $C_{46}H_{18}F_{15}N_4O_2$ , 943.1185; found, 943.1179 (Fig. S3).

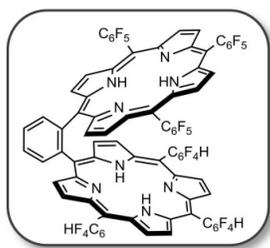


**Synthesis of b.** To a dry THF (50 mL) solution of **a** (0.8 g, 0.82 mmol) in an ice bath,  $LiAlH_4$  (150 mg, 3.5 mmol) was added slowly. The mixture was stirred for 5 h at temperature. Methanol (20 mL) and water (15 mL) were then added to quench the reaction. The resulted mixture was extracted with dichloromethane, washed with water (50 mL  $\times$  3), and dried with anhydrous  $Na_2SO_4$ . The solution was concentrated to dryness using a rotary evaporator to afford **b** as a solid (0.64 g, yield 87%).  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  = 8.92 (s, 4H), 8.82 (s, 4H), 8.08 (d, 1H), 7.98 (d, 1H), 7.88 (t, 1H), 7.70 (t, 1H), 7.65-7.57 (m, 3H), 4.35 (s, 2H), -2.78 (s, 2H) (Fig. S4). HRMS of  $[M+H]^+$ : calcd. for  $C_{45}H_{21}F_{12}N_4O$ , 861.1518; found, 861.1532 (Fig. S5).



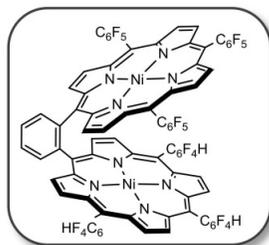
**Synthesis of c.** Dry dichloromethane (2.5 mL) was added to a dried Schlenk flask (100 mL) containing oxalyl chloride (47  $\mu$ L, 0.55 mmol) under  $N_2$  and  $-78$   $^\circ$ C. DMSO (78  $\mu$ L, 1.1 mmol) was added slowly, and the mixture was stirred for 15 min at  $-78$   $^\circ$ C. Complex **b** (460 mg, 0.5 mmol) dissolved in dry dichloromethane (30 mL) was then added slowly, and the resulted solution was stirred for 5 min. Next, dry triethylamine (605  $\mu$ L, 4.35 mmol) was added, and was stirred for another 10 min at  $-78$   $^\circ$ C. The solution was then kept stirring at room temperature for overnight. The reaction was quenched with  $CH_3OH$  and  $H_2O$ , and was extracted with dichloromethane, washed with water (50 mL  $\times$  3), and was dried with

anhydrous  $\text{Na}_2\text{SO}_4$ . The solution was concentrated to dryness using a rotary evaporator to afford **c** as a solid (0.422 g, yield 92%).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 9.50 (s, 1H), 8.92 (s, 4H), 8.76-8.85 (s, 4H), 8.44 (d, 1H), 8.23 (d, 1H), 8.03-7.93 (m, 2H), 7.68-7.57 (m, 3H), -2.73 (s, 2H) (Fig. S6). HRMS of  $[\text{M}+\text{H}]^+$ : calcd. for  $\text{C}_{45}\text{H}_{19}\text{F}_{12}\text{N}_4\text{O}$ , 859.1362; found, 859.1355 (Fig. S7).



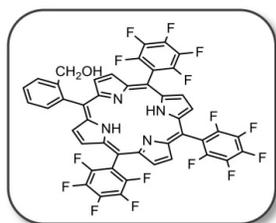
**Synthesis of 5'.** To a 500 mL flask containing chloroform (300 mL), were added **c** (0.422 g, 0.5 mmol), benzaldehyde (582  $\mu\text{L}$ , 5.5 mmol), and pyrrole (416  $\mu\text{L}$ , 6.0 mmol) at room temperature. After purging with argon for 30 min,  $\text{BF}_3\cdot\text{OEt}_2$  was added. The

mixture was stirred under argon for 40 min, and then DDQ dissolved in benzene (20 mL) was added, and the solution was stirred for 1 h. The reaction solution was dried using a rotary evaporator. The resulted dark residue was dissolved in dichloromethane, and purified by silica-gel column chromatography (hexanes/dichloromethane = 5:1 v/v) to afford pure **5'** as a purple solid (96.5 mg, yield 12%).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 9.37-9.32 (m, 4H), 8.89-8.82 (m, 2H), 8.48-8.34 (m, 14H), 7.63-7.52 (m, 2H), 7.45-7.35 (m, 1H), -4.03 (s, 4H) (Fig. S8). HRMS of  $[\text{M}+\text{H}]^+$ : calcd. for  $\text{C}_{82}\text{H}_{28}\text{F}_{27}\text{N}_8$ , 1637.2000; found, 1637.1995 (Fig. S9).

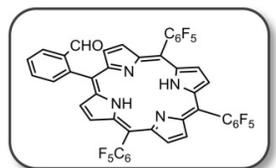


**Synthesis of 5.** The mixture of **5'** (96 mg, 60  $\mu\text{mol}$ ) in 50 mL DMF was treated with  $\text{Ni}(\text{OAc})_2\cdot 4\text{H}_2\text{O}$  (75 mg, 0.3 mmol). The reaction mixture was kept stirring and heating at 115  $^\circ\text{C}$  under argon for 4 h. The solvent was then removed under reduced

pressure, and the resulted dark solid was dissolved in dichloromethane and washed with distilled water. The organic phase was concentrated to dryness and was subjected to silica chromatography (hexane:dichloromethane = 5:1) to afford red solid of **5** (92 mg, yield 87%). HRMS of  $[M+Na]^+$ : calcd. for  $C_{82}H_{23}F_{27}N_8NaNi_2$ , 1771.0214; found, 1771.0225 (Fig. S10).

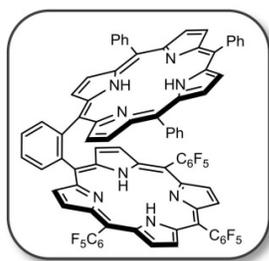


**Synthesis of d.** To a dried Schlenk flask (100mL) containing dry toluene solution (60 mL) of **a** (550 mg, 0.58 mmol) under  $N_2$  and  $-78\text{ }^\circ\text{C}$ , DIBAL-H (2 mL, 1.2 mmol) was added. The solution was stirred for 5 h under  $N_2$  and  $-78\text{ }^\circ\text{C}$ , and was quenched by 20 mL  $CH_3OH$  and 30 mL  $H_2O$ . The mixture was added 30 mL saturated sodium potassium tartrate solution and stirred for overnight. Next, the solution was extracted by dichloromethane, and was dried with anhydrous  $Na_2SO_4$ . The resulted solution was dried using a rotary evaporator to afford a purple solid compound **d** (519 mg, yield 95%).  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  = 8.91 (s, 4H), 8.82 (s, 4H), 8.08 (d, 1H), 7.98 (d, 1H), 7.88 (t, 1H), 7.70 (t, 1H), 4.35 (s, 2H),  $-2.80$  (s, 2H) (Fig. S11). HRMS of  $[M+Na]^+$ : calcd. for  $C_{45}H_{17}F_{15}N_4NaO$ , 937.1055; found, 937.1095 (Fig. S12).

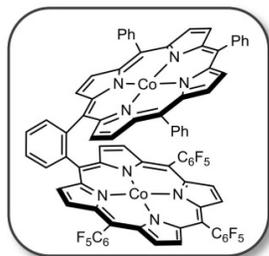


**Synthesis of e.** Dry dichloromethane (2.5 mL) was added to a dried Schlenk flask (100mL) containing oxalyl chloride (47  $\mu\text{L}$ , 0.55 mmol) under  $N_2$  and  $-78\text{ }^\circ\text{C}$ . DMSO (78  $\mu\text{L}$ , 1.1 mmol) was added slowly, and the mixture was stirred for 15 min under  $N_2$  and  $-78\text{ }^\circ\text{C}$ . Next, complex **d** (460 mg, 0.5 mmol) dissolved in dry dichloromethane (30 mL) was added to

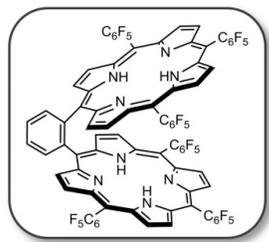
the mixture slowly and was stirred for 5 min. Dry triethylamine (605  $\mu\text{L}$ , 4.35 mmol) was added to the above solution and was stirred for 10 min under  $\text{N}_2$  and  $-78\text{ }^\circ\text{C}$ . The solution was then kept stirring at room temperature for overnight. The reaction was quenched with  $\text{CH}_3\text{OH}$  and  $\text{H}_2\text{O}$ . The mixture was extracted with dichloromethane, washed with water ( $50\text{ mL} \times 3$ ), and was dried with anhydrous  $\text{Na}_2\text{SO}_4$ . The solution was concentrated to dryness using a rotary evaporator to afford **e** as a solid (416 mg, yield 93%).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta = 9.50$  (s, 1H), 8.92 (s, 4H), 8.86-8.76 (s, 4H), 8.44 (d, 1H), 8.23 (d, 1H), 8.05-7.94 (m, 2H),  $-2.77$  (s, 2H) (Fig. S13). HRMS of  $[\text{M}+\text{H}]^+$ : calcd. for  $\text{C}_{45}\text{H}_{16}\text{F}_{15}\text{N}_4\text{O}$ , 913.1079; found, 913.1085 (Fig. S14).



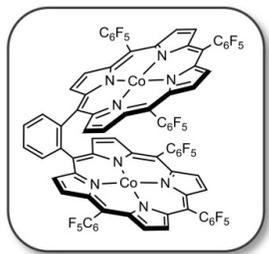
**Synthesis of 1'.** To a 500 mL flask containing chloroform (300 mL), were added **e** (0.416 g, 0.5 mmol), benzaldehyde (582  $\mu\text{L}$ , 5.5 mmol), and pyrrole (416  $\mu\text{L}$ , 6.0 mmol) at room temperature. After purging with argon for 20 min,  $\text{BF}_3 \cdot \text{OEt}_2$  was added. The mixture was stirred under argon for 40 min. Then DDQ dissolved in benzene (20 mL) was added and the solution was further stirred for 1 h. The solution was dried using a rotary evaporator, and the resulted dark residue was dissolved in dichloromethane, and purified by silica-gel column chromatography (hexanes/dichloromethane = 5:1 v/v) to afford pure **1'** as a purple solid (85 mg, yield 13%).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta = 9.49$  (d, 2H), 9.29 (d, 2H), 8.86 (m, 2H), 8.56 (d, 2H), 8.52 (d, 2H), 8.47 (s, 4H), 8.42 (s, 4H), 8.34 (m, 2H), 8.04 (s, 1H), 7.81 (m, 8H), 7.64-7.58 (m, 4H), 7.52-7.40 (m, 2H),  $-3.91$  (m, 4H) (Fig. S15). HRMS of  $[\text{M}+\text{H}]^+$ : calcd. for  $\text{C}_{82}\text{H}_{40}\text{F}_{15}\text{N}_8$ , 1421.3131; found, 1421.3137 (Fig. S16).



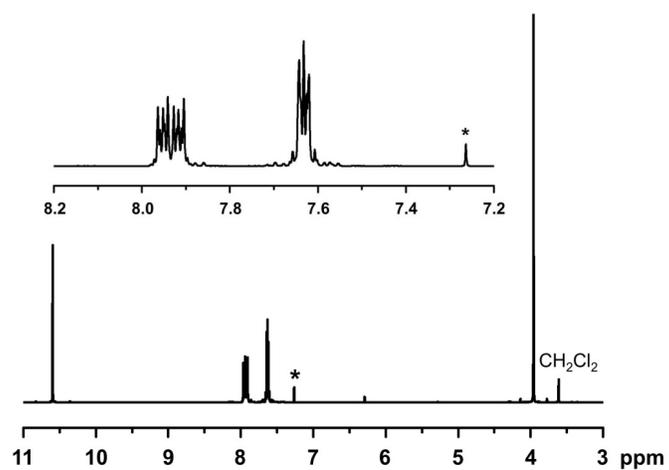
**Synthesis of 1.** Complex **1'** (85 mg, 60  $\mu\text{mol}$ ) was dissolved in 50 mL DMF, and was then treated with  $\text{CoCl}_2$  (40 mg, 0.3 mmol). The reaction solution was kept stirring and heating at 115  $^\circ\text{C}$  under argon for 4 h. Next, the solvent was removed under reduced pressure, and the resulted dark solid was dissolved in dichloromethane and washed with water. The organic phase was concentrated to dryness and subjected to silica chromatography (hexane:dichloromethane = 5:1) to afford red solid of **1** (80 mg, yield 87%). HRMS of  $[\text{M}]^+$  and  $[\text{M}+\text{H}]^+$  are overlapped: calcd. for  $\text{C}_{82}\text{H}_{35}\text{Co}_2\text{F}_{15}\text{N}_8$ , 1534.1404 and  $\text{C}_{82}\text{H}_{36}\text{Co}_2\text{F}_{15}\text{N}_8$ , 1535.1437; found, 1534.1404 and 1535.1461 (Fig. S17).



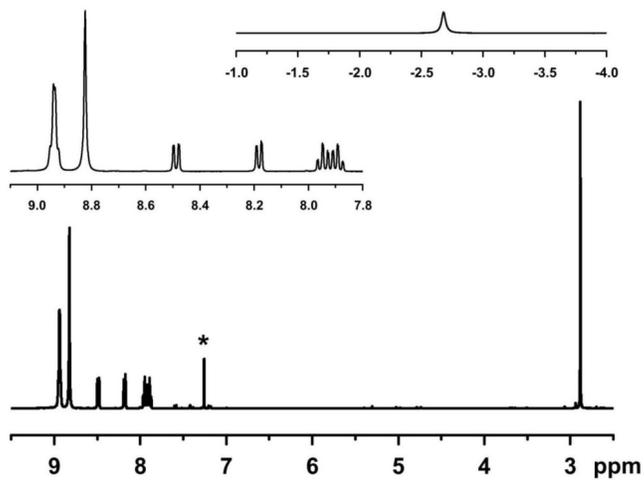
**Synthesis of 2'.** The synthetic conditions of **2'** are the same to that of **1'**, except the use of pentafluorobenzaldehyde (yield 16%).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 9.33 (t, 4H), 8.87-8.82 (m, 2H), 8.46-8.82 (m, 14H), -4.04 (s, 4H) (Fig. S18). HRMS of  $[\text{M}+\text{H}]^+$ : calcd. for  $\text{C}_{82}\text{H}_{25}\text{F}_{30}\text{N}_8$ , 1691.1718; found, 1691.1699 (Fig. S19).



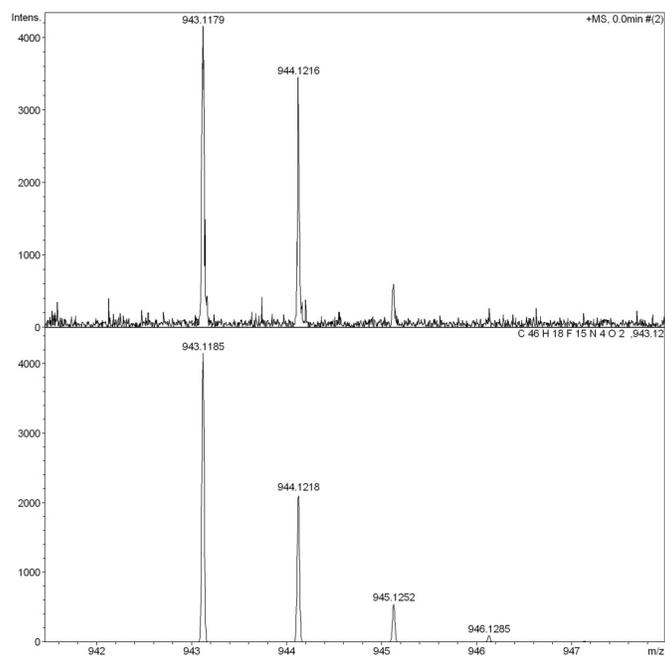
**Synthesis of 2.** The synthetic conditions of **2** are the same to that of **1** mentioned above, except the use of **2'** as the porphyrin ligand (yield 89%). HRMS of  $[\text{M}]^+$  and  $[\text{M}+\text{H}]^+$  are overlapped: calcd. for  $\text{C}_{82}\text{H}_{20}\text{Co}_2\text{F}_{30}\text{N}_8$ , 1803.9990 and  $\text{C}_{82}\text{H}_{21}\text{Co}_2\text{F}_{30}\text{N}_8$ , 1805.0023; found, 1803.9995 and 1805.0038 (Fig. S20).



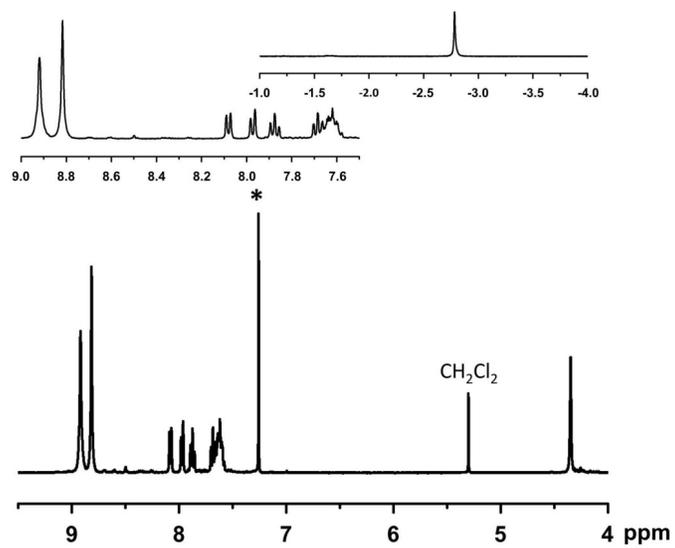
**Fig. S1** <sup>1</sup>H NMR spectrum of methyl 2-formylbenzoate in CDCl<sub>3</sub>. The solvent residue peak of CDCl<sub>3</sub> is labeled (\*).



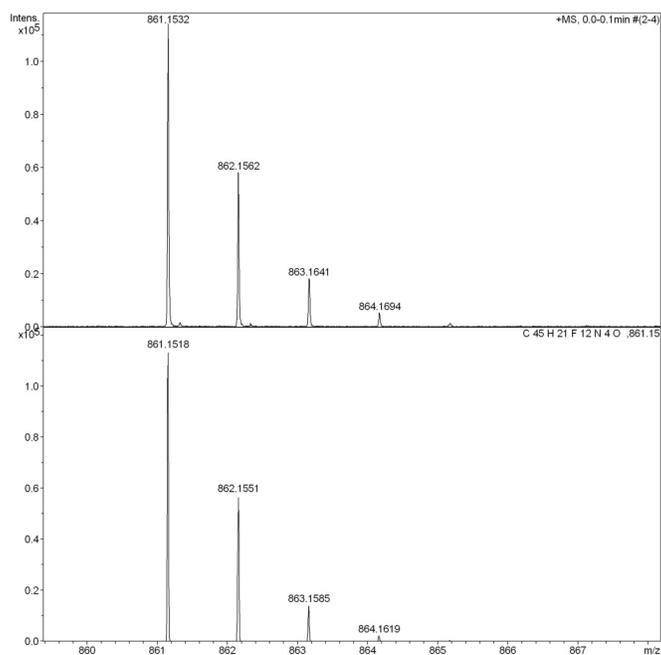
**Fig. S2** <sup>1</sup>H NMR spectrum of **a** in CDCl<sub>3</sub>. The solvent residue peak of CDCl<sub>3</sub> is labeled (\*).



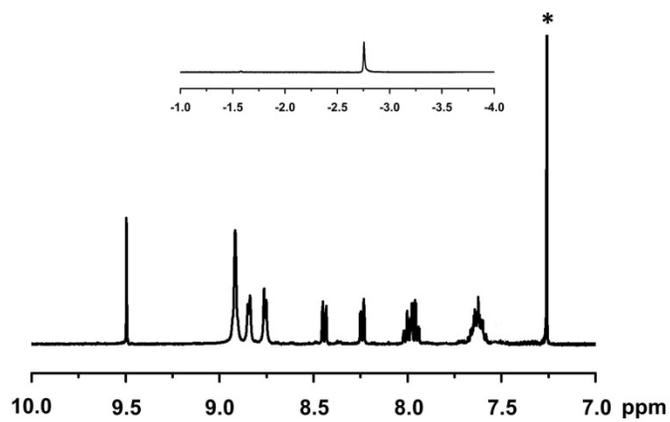
**Fig. S3** HRMS of **a**. The ion at a mass-to-charge ratio of 943.1179 matches the calculated value of 943.1185 for the monocation of  $[\text{C}_{46}\text{H}_{18}\text{F}_{15}\text{N}_4\text{O}_2]^+$  with identical isotopic distribution pattern.



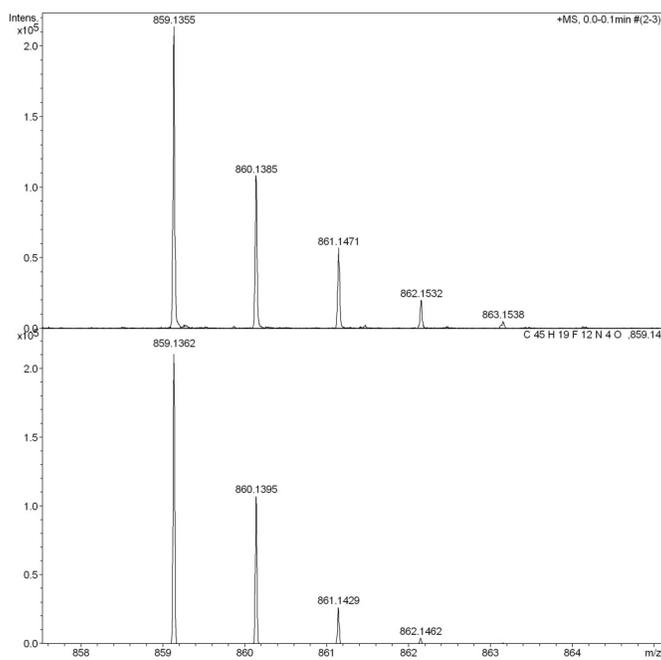
**Fig. S4**  $^1\text{H}$  NMR spectrum of **b** in  $\text{CDCl}_3$ . The solvent residue peak of  $\text{CDCl}_3$  is labeled (\*).



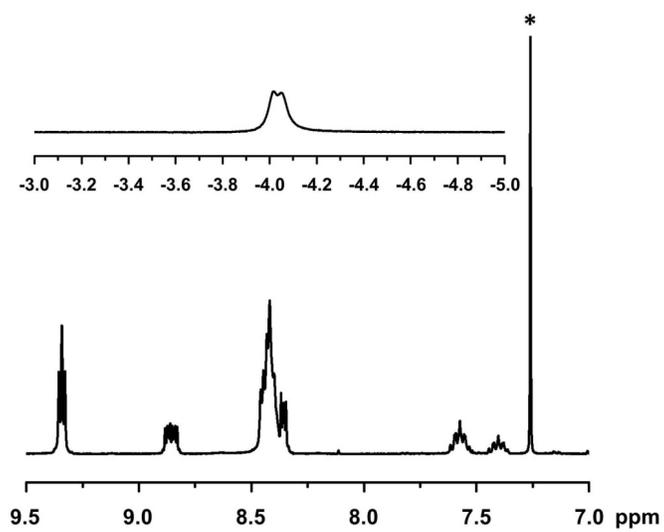
**Fig. S5** HRMS of **b**. The ion at a mass-to-charge ratio of 861.1532 matches the calculated value of 861.1518 for the monocation of  $[C_{45}H_{21}F_{12}N_4O]^+$  with identical isotopic distribution pattern.



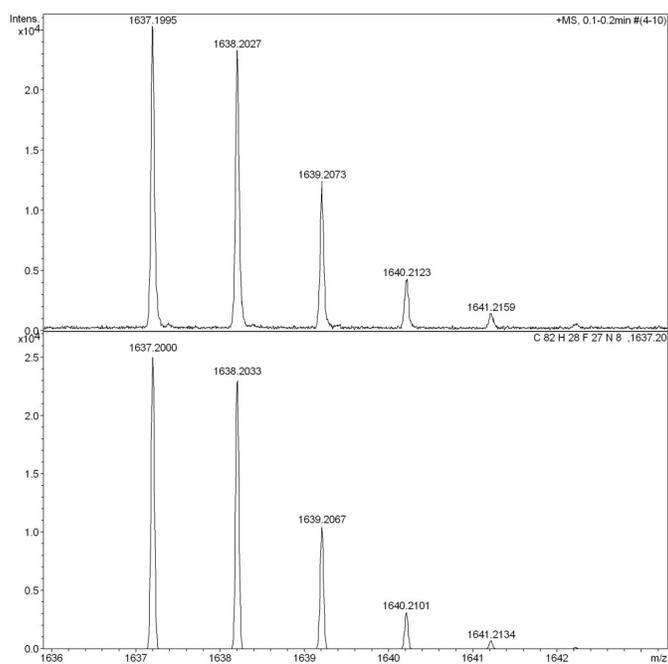
**Fig. S6** <sup>1</sup>H NMR spectrum of **c** in CDCl<sub>3</sub>. The solvent residue peak of CDCl<sub>3</sub> is labeled (\*).



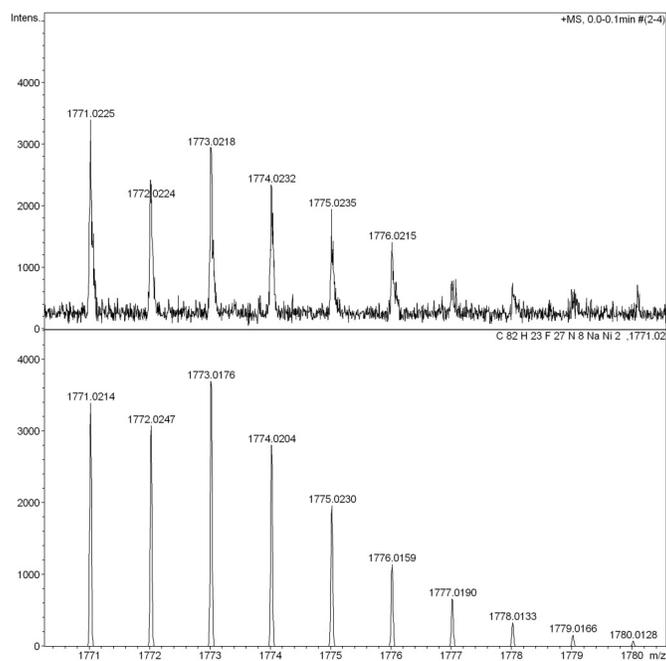
**Fig. S7** HRMS of **c**. The ion at a mass-to-charge ratio of 859.1355 matches the calculated value of 859.1362 for the monocation of [C<sub>45</sub>H<sub>19</sub>F<sub>12</sub>N<sub>4</sub>O]<sup>+</sup> with identical isotopic distribution pattern.



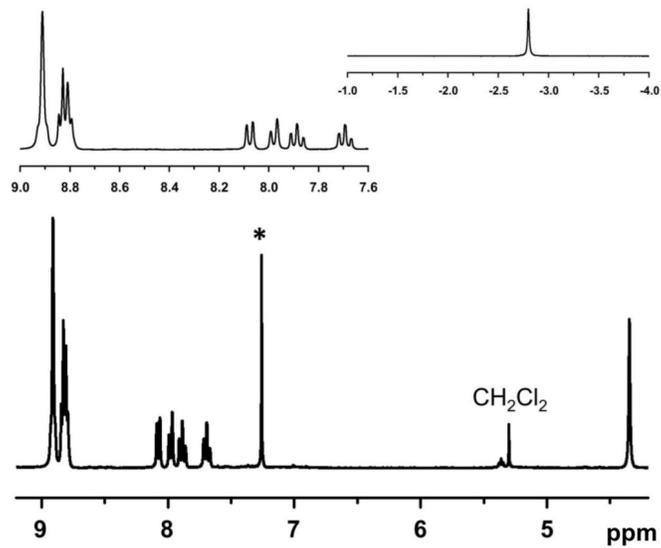
**Fig. S8**  $^1\text{H}$  NMR spectrum of **5'** in  $\text{CDCl}_3$ . The solvent residue peak of  $\text{CDCl}_3$  is labeled (\*).



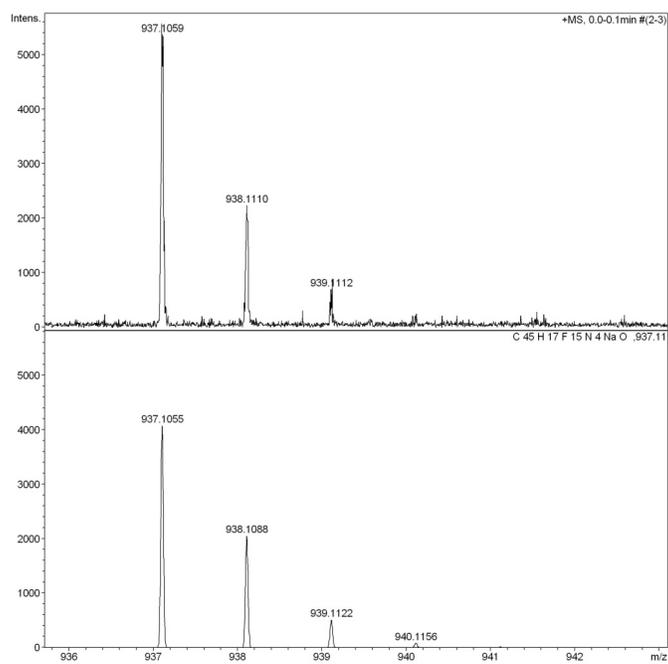
**Fig. S9** HRMS of **5'**. The ion at a mass-to-charge ratio of 1637.1995 matches the calculated value of 1637.2000 for the monocation of  $[\text{C}_{82}\text{H}_{28}\text{F}_{27}\text{N}_8]^+$  with identical isotopic distribution pattern.



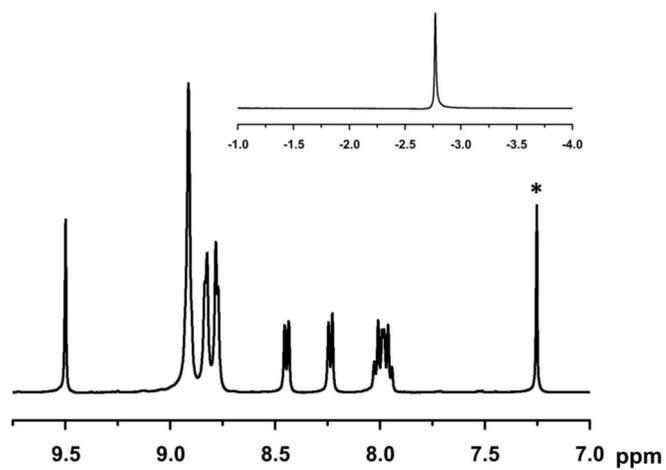
**Fig. S10** HRMS of **5**. The ion at a mass-to-charge ratio of 1771.0225 matches the calculated value of 1771.0214 for the monocation of  $[\text{C}_{82}\text{H}_{23}\text{F}_{27}\text{N}_8\text{NaNi}_2]^+$  with identical isotopic distribution pattern.



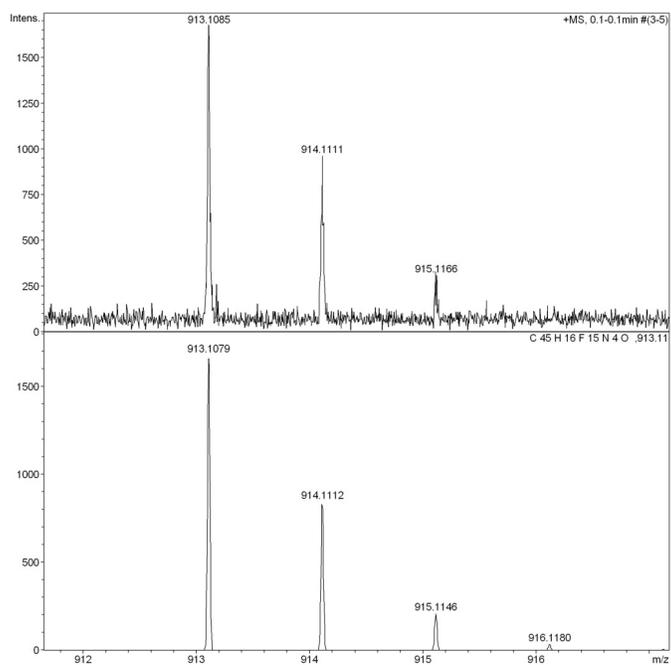
**Fig. S11** <sup>1</sup>H NMR spectrum of **d** in CDCl<sub>3</sub>. The solvent residue peak of CDCl<sub>3</sub> is labeled (\*).



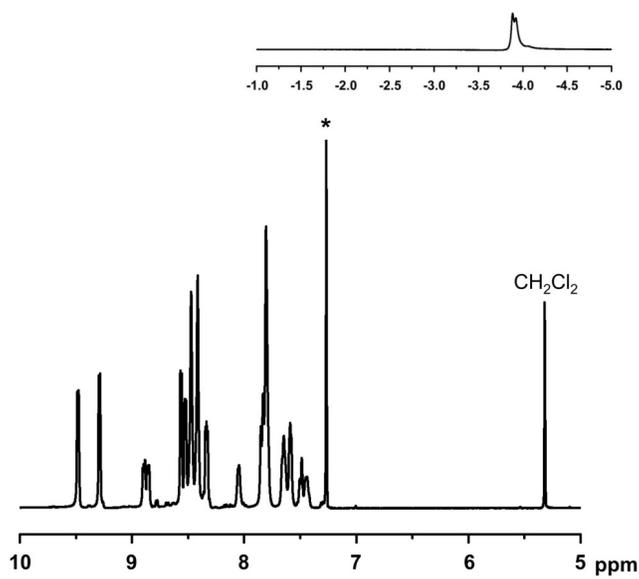
**Fig. S12** HRMS of **d**. The ion at a mass-to-charge ratio of 937.1059 matches the calculated value of 937.1055 for the monocation of  $[\text{C}_{45}\text{H}_{17}\text{F}_{15}\text{N}_4\text{NaO}]^+$  with identical isotopic distribution pattern.



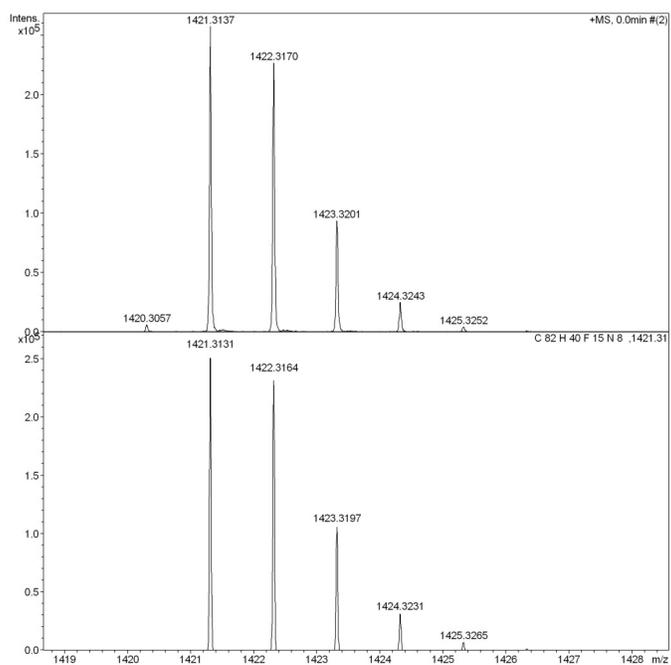
**Fig. S13**  $^1\text{H}$  NMR spectrum of **e** in  $\text{CDCl}_3$ . The solvent residue peak of  $\text{CDCl}_3$  is labeled (\*).



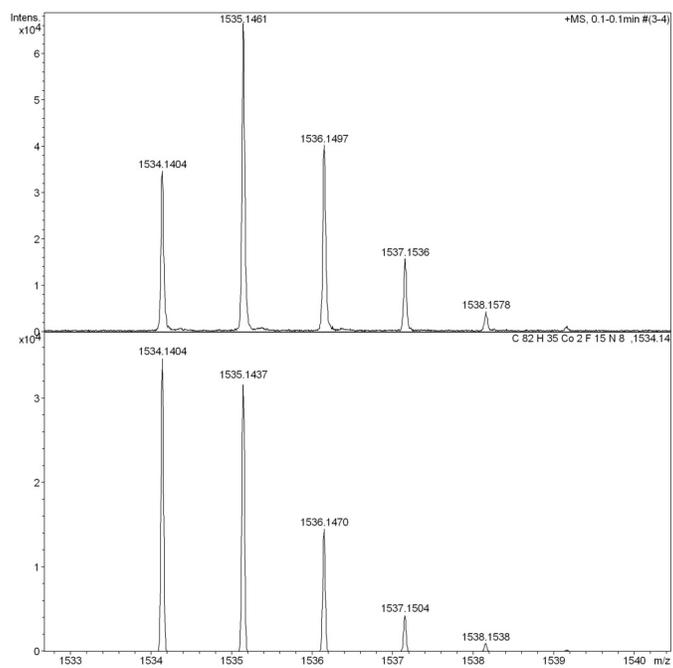
**Fig. S14** HRMS of **e**. The ion at a mass-to-charge ratio of 913.1085 matches the calculated value of 913.1079 for the monocation of  $[\text{C}_{45}\text{H}_{16}\text{F}_{15}\text{N}_4\text{O}]^+$  with identical isotopic distribution pattern.



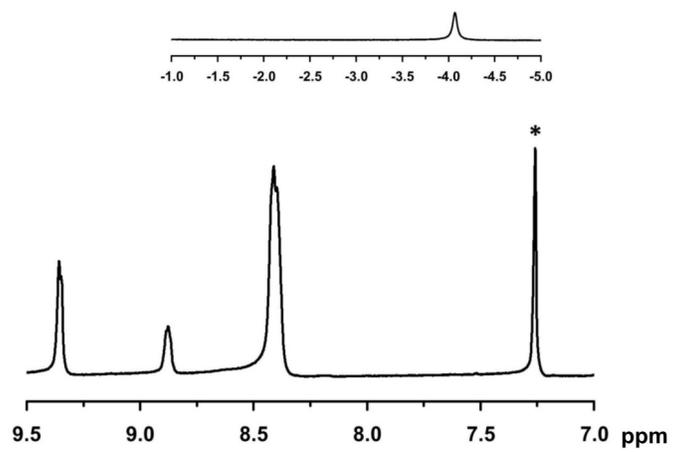
**Fig. S15**  $^1\text{H}$  NMR spectrum of **1'** in  $\text{CDCl}_3$ . The solvent residue peak of  $\text{CDCl}_3$  is labeled (\*).



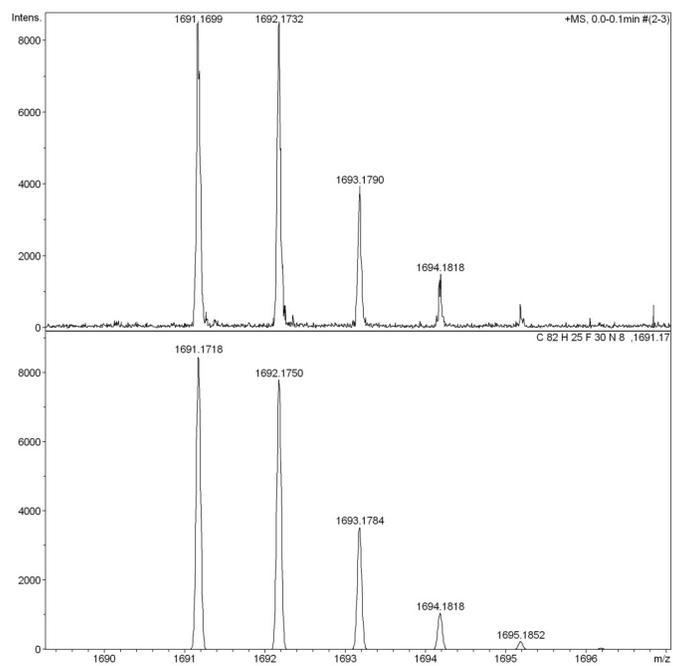
**Fig. S16** HRMS of **1'**. The ion at a mass-to-charge ratio of 1421.3137 matches the calculated value of 1421.3131 for the monocation of  $[\text{C}_{82}\text{H}_{40}\text{F}_{15}\text{N}_8]^+$  with identical isotopic distribution pattern.



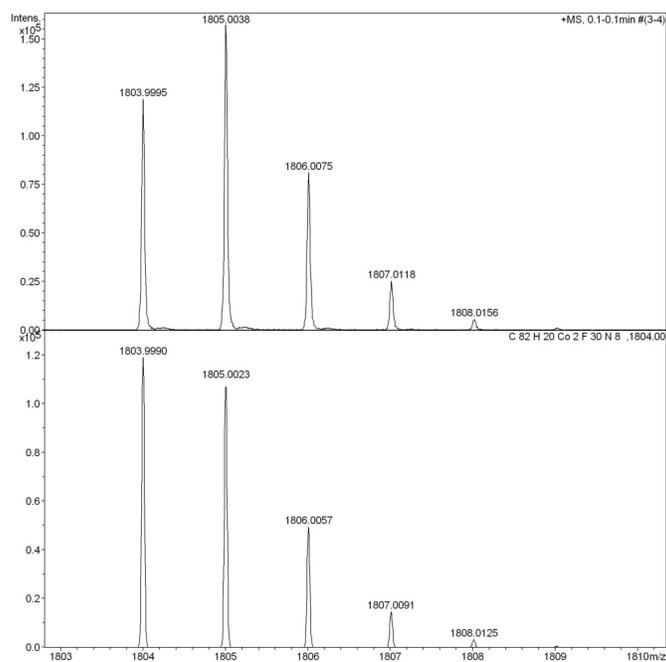
**Fig. S17** HRMS of **1**. The ions at a mass-to-charge ratio of 1534.1404 and 1535.1461 matches the calculated value of 1534.1404 and 1535.1437 for the monocation of  $[\text{C}_{82}\text{H}_{35}\text{Co}_2\text{F}_{15}\text{N}_8]^+$  and  $[\text{C}_{82}\text{H}_{36}\text{Co}_2\text{F}_{15}\text{N}_8]^+$  with identical overlapped sum of isotopic distribution patterns.



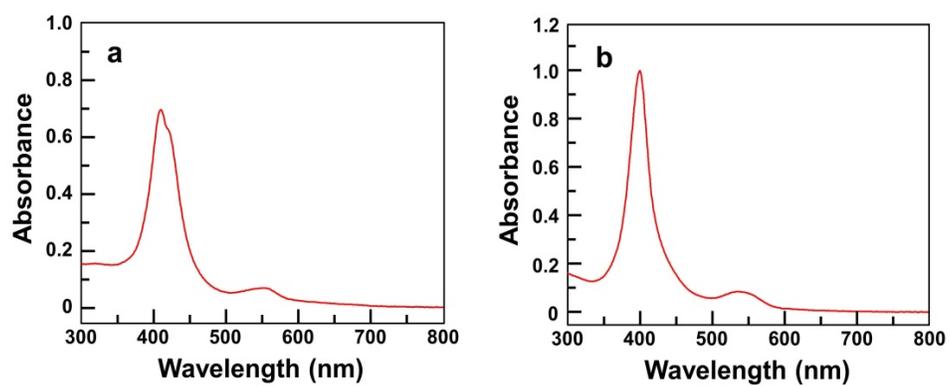
**Fig. S18** <sup>1</sup>H NMR spectrum of **2'** in CDCl<sub>3</sub>. The solvent residue peak of CDCl<sub>3</sub> is labeled (\*).



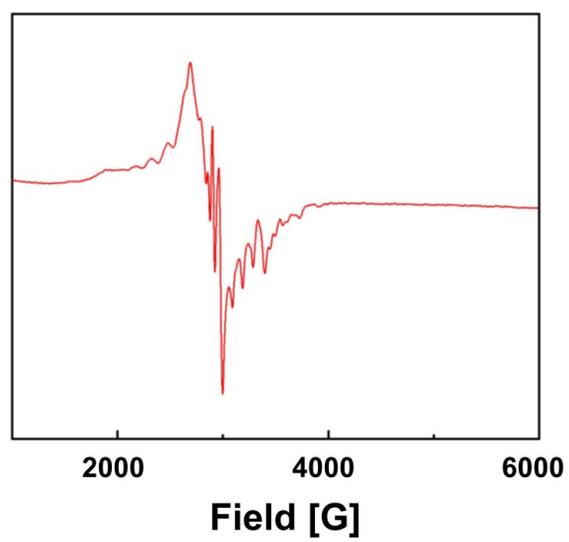
**Fig. S19** HRMS of **2'**. The ion at a mass-to-charge ratio of 1691.1699 matches the calculated value of 1691.1718 for the monocation of  $[C_{82}H_{25}F_{30}N_8]^+$  with identical isotopic distribution pattern.



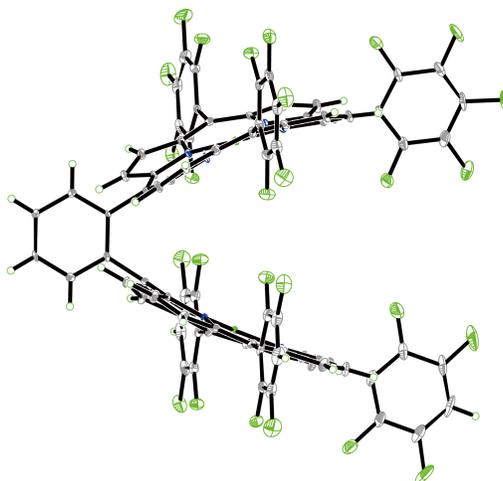
**Fig. S20** HRMS of **2**. The ions at a mass-to-charge ratio of 1803.9995 and 1805.0038 matches the calculated value of 1803.9990 and 1805.0023 for the monocation of  $[\text{C}_{82}\text{H}_{20}\text{Co}_2\text{F}_{30}\text{N}_8]^+$  and  $[\text{C}_{82}\text{H}_{21}\text{Co}_2\text{F}_{30}\text{N}_8]^+$  with identical overlapped sum of isotopic distribution patterns.



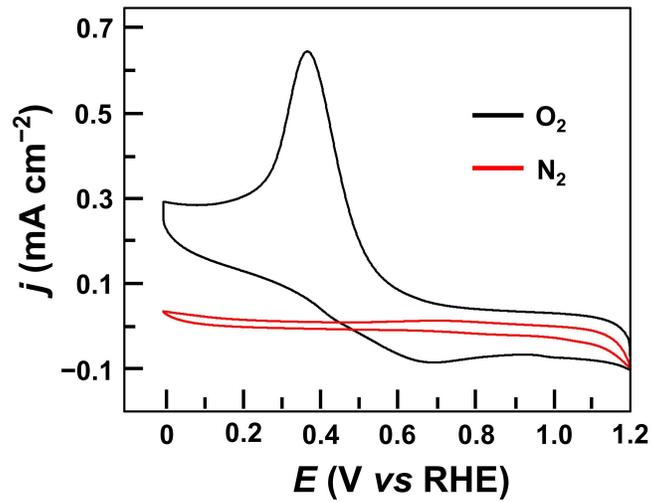
**Fig. S21** UV-vis absorption spectra of **1** (a) and **2** (b) in DMF.



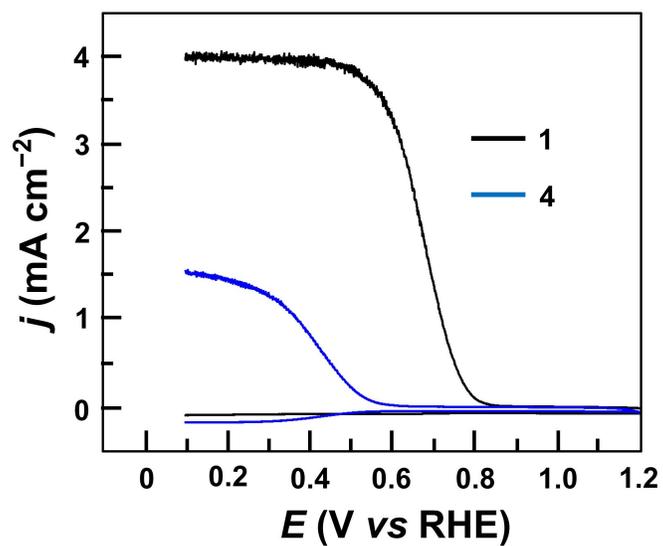
**Fig. S22** EPR spectrum of **1** in toluene at 90 K.



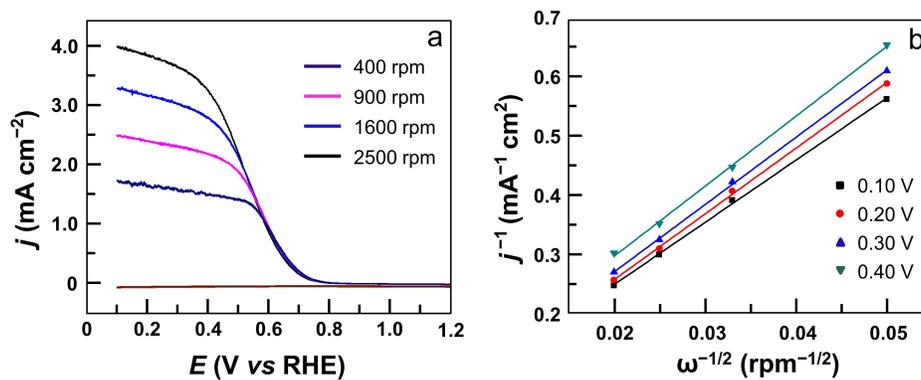
**Fig. S23** Thermal ellipsoid plot of the X-ray structure of **5** (30% probability). In the bottom porphyrin macrocycle, the F atom at the *para*-position of three pentafluorophenyl units is replaced by an H atom.



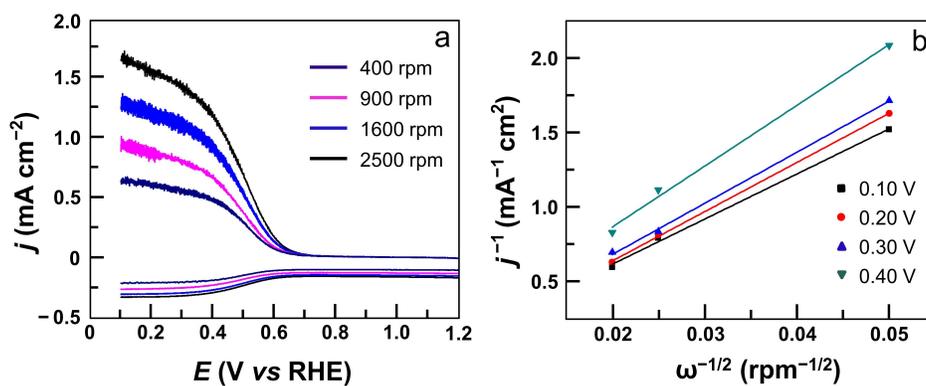
**Fig. S24** CVs of **3** in 0.5 M H<sub>2</sub>SO<sub>4</sub> under N<sub>2</sub> (red) and O<sub>2</sub> (black). Conditions: GC working electrode, scan rate 100 mV s<sup>-1</sup>, 20 °C.



**Fig. S25** RRDE measurements for ORR at the GC disk electrode coated with **1** (black) and **4** (blue) in an  $\text{O}_2$ -saturated 0.5 M  $\text{H}_2\text{SO}_4$  solution at 2500 rpm. The ring electrode was polarized at 1.0 V.



**Fig. S26** (a) RRDE measurements for ORR with **2** in O<sub>2</sub>-saturated 0.5 M H<sub>2</sub>SO<sub>4</sub> solution at various rotation rates. (d) K-L plots for ORR with **2**.



**Fig. S27** (a) RRDE measurements for ORR with **3** in O<sub>2</sub>-saturated 0.5 M H<sub>2</sub>SO<sub>4</sub> solution at various rotation rates. (d) K-L plots for ORR with **3**.

**Table S1.** Crystal data and structure refinement parameters for the X-ray structures of **2** and **5**.

complex	<b>2</b>	<b>5</b>
molecular formula	C <sub>89</sub> H <sub>28</sub> Co <sub>2</sub> F <sub>30</sub> N <sub>8</sub>	C <sub>93</sub> H <sub>48</sub> Cl <sub>3</sub> F <sub>27</sub> N <sub>8</sub> Ni <sub>2</sub>
formula wt. (g mol <sup>-1</sup> )	1897.05	2014.16
temperature (K)	173(2)	153(2)
radiation (λ, Å)	0.71073	0.71073
crystal system	Triclinic	Triclinic
space group	<i>P</i> $\bar{1}$ (#2)	<i>P</i> $\bar{1}$ (#2)
<i>a</i> (Å)	14.422(2)	14.9706(19)
<i>b</i> (Å)	15.261(3)	15.430(2)
<i>c</i> (Å)	20.632(4)	19.502(2)
$\alpha$ (°)	67.7449(10)	76.905(4)
$\beta$ (°)	84.949(2)	68.784(4)
$\gamma$ (°)	74.9246(10)	84.109(5)
Volume (Å <sup>3</sup> )	4057.6(12)	4089.3(9)
<i>Z</i>	2	2
$\rho_{\text{calcd}}$ (g cm <sup>-3</sup> )	1.553	1.636
$\mu$ (mm <sup>-1</sup> )	0.530	0.676
F(000)	1884	2024
crystal size (mm <sup>3</sup> )	0.20 × 0.20 × 0.18	0.30 × 0.30 × 0.10
Theta range	1.066 to 25.500°	2.147 to 26.416°
reflections collected	45101	69320
indep. reflections	14661 [R(int) = 0.0967]	16774 [R(int) = 0.1433]
Completeness	97.1%	99.9%
goodness-of-fit on F <sup>2</sup>	1.065	1.049
final R indices	R <sub>1</sub> <sup>a</sup> = 0.0496	R <sub>1</sub> <sup>a</sup> = 0.0791
[R > 2σ (I)]	wR <sub>2</sub> <sup>b</sup> = 0.1103	wR <sub>2</sub> <sup>b</sup> = 0.1484
R indices (all data)	R <sub>1</sub> <sup>a</sup> = 0.0572	R <sub>1</sub> <sup>a</sup> = 0.1297
	wR <sub>2</sub> <sup>b</sup> = 0.1125	wR <sub>2</sub> <sup>b</sup> = 0.1705
largest diff. peak and hole (e Å <sup>-3</sup> )	0.666 and -0.565	1.263 and -0.776

$${}^a R_1 = \Sigma ||F_o| - |F_c|| / |F_o|, {}^b wR_2 = \{ \Sigma [w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2] \}^{0.5}$$