Porphyrin Amino Acids – Amide Coupling, Redox and Photophysical Properties of Bis(porphyrin) amides

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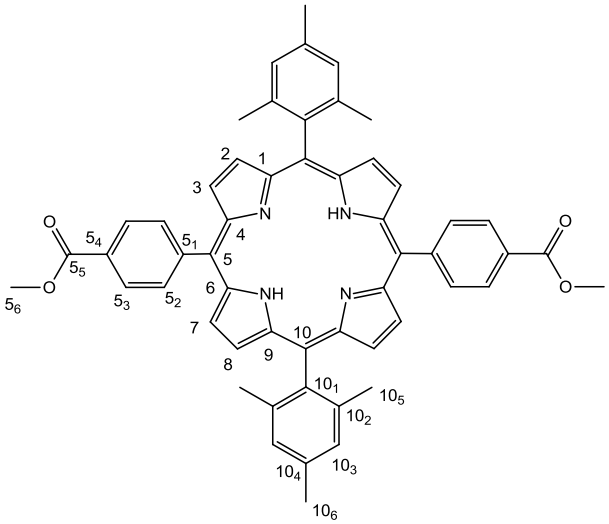
Supporting Information

Experimental Section

Porphyrins **1a**, **2a**, **Boc-3a** and **3a** were prepared by published procedures and characterised as follows.[S1][S2]

10,20-Bis(2,4,6-trimethylphenyl)-5,15-bis[4-(methoxycarbonyl)] porphyrin (1a)[S1][S2]



^{1}H-NMR ($CDCl_3$): δ = –2.63 (s, 2 H, $H^{pyrrole\text{-}NH}$), 1.83 (s, 12 H, $H^{10}{}_5$), 2.63 (s, 6 H, $H^{10}{}_6$), 4.11 (s, 6 H, $H^5{}_6$), 8.31 (d, $^3J_{HH}$ = 8.1 Hz, 4 H, $H^5{}_2$), 8.43 (d, $^3J_{HH}$ = 8.1 Hz, 4 H, $H^5{}_3$), 8.71 (d, $^3J_{HH}$ = 4.7 Hz, 4 H, $H^{pyrrole}$), 8.74 (d, $^3J_{HH}$ = 4.7 Hz, 4 H, $H^{pyrrole}$) ppm.

IR (KBr): $\tilde{\nu}$ [cm^{-1}] = 3425 (b, NH), 2922 (w, CH), 2850 (w, CH), 1722 (vs, CO), 1608 (s), 1386 (vs), 1278 (vs, C-O-C), 1114 (s), 800 (w).

UV/Vis (CH_2Cl_2): λ [nm] (ε / [10^4 $M^{-1}cm^{-1}$]) = 419 (36.88), 516 (1.99), 548 (1.13), 593 (0.82), 651 (1.38).

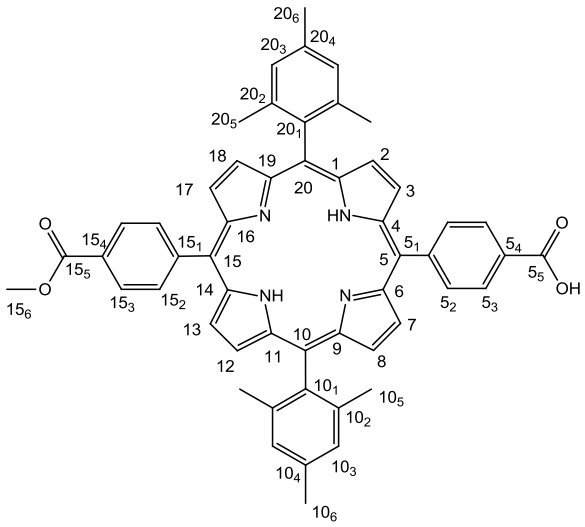
Fluorescence (CH_2Cl_2): λ [nm] (relative intensity) = 654 (1.00), 716 (0.20).

Quantum yield: Φ = 0.0774.

Lifetime: τ [ns] = 9.87 (100%).

CV (Fc/Fc^+, 100 mV s^{-1}, CH_2Cl_2): $E_{½}$[V] = –2.020, –1.670, 0.600, 1.030.

5-(4-Carboxyphenyl)-15-(4-carbomethoxyphenyl)-10,20-bis(2,4,6-trimethylphenyl) porphyrin (2a)[S1][S2]



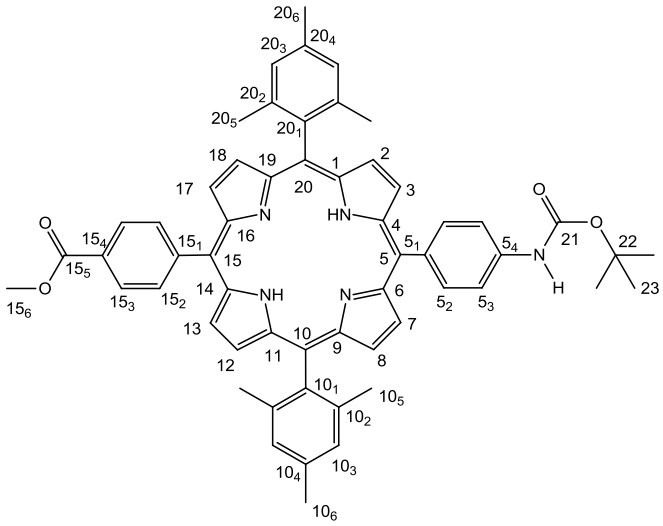
UV/Vis (CH_2Cl_2): λ [nm] (ε / [10^4 $M^{-1}cm^{-1}$]) = 419 (13.58), 515 (0.70), 549 (0.34), 592 (0.24), 650 (0.30).

Fluorescence (CH_2Cl_2): λ [nm] (relative intensity) = 652 (1.00), 716 (0.26).

Quantum yield: Φ = 0.1187.

CV (Fc/Fc^+, 100 mV s^{-1}, CH_2Cl_2): $E_{½}$[V] = –2.090, –1.705, 0.600, 1.060.

15-(4-Carbomethoxyphenyl)-5-(*N*-*tert*-butoxycarbonyl-4-aminophenyl)-10,20-bis(2,3,4,5,6-pentafluorophenyl) porphyrin (Boc-3a)[S1][S2]



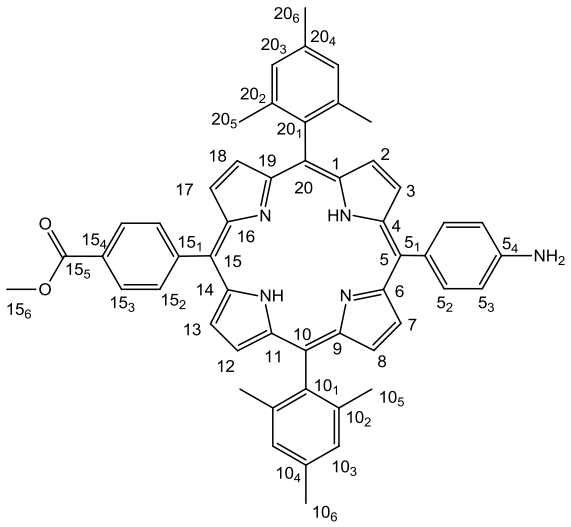
UV/Vis (CH_2Cl_2): λ [nm] (ε / [10^4 $M^{-1}cm^{-1}$]) = 420 (68.60), 516 (3.48), 550 (1.91), 594 (1.36), 651 (2.25).

Fluorescence (CH_2Cl_2): λ [nm] (relative intensity) = 654 (1.00), 719 (0.20).

Quantum yield: Φ = 0.1112.

CV (Fc/Fc^+, 100 mV s^{-1}, CH_2Cl_2): $E_{½}$[V] = –2.130, –1.745, 0.535, 0.945.

15-(4-Carbomethoxyphenyl)-5-(4-aminophenyl)-10,20-bis(2,4,6-trimethylphenyl) porphyrin (3a)[S1][S2]



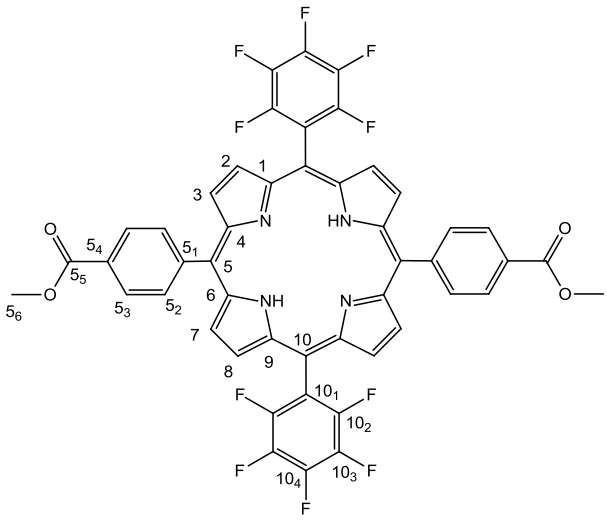
UV/Vis (CH_2Cl_2): λ [nm] (ε / [10^4 $M^{-1}cm^{-1}$]) = 421 (34.07), 517 (1.91), 552 (1.10), 593 (0.74), 651 (1.01).

Fluorescence (CH_2Cl_2): λ [nm] (relative intensity) = 654 (1.00), 719 (0.21).

Quantum yield: Φ = 0.0882.

CV (Fc/Fc^+, 100 mV s^{-1}, CH_2Cl_2): $E_{½}$[V] = –2.100, –1.760, 0.455, 0.600.

10,20-Bis(2,3,4,5,6-pentafluorophenyl)-5,15-bis[4-(methoxycarbonylphenyl)] porphyrin (1b). Following a standard procedure[S3] a solution of pentafluorophenyldipyrromethane (2.00 g, 6.4 mmol) and methyl 4-formylbenzoate (1.02 g, 6.4 mmol) in CH_2Cl_2 (700 mL) was treated with TFA (1.2 mL, 15.6 mmol) at room temperature. After 40 min, DDQ (2.1 g, 9.57 mmol) was added and after further 60 min TEA (1.2 mL) was added. The reaction mixture was concentrated under reduced pressure and chromatographed [silica, CH_2Cl_2/petroleum ether b.p. 40/60 (5:1), R_f = 0.32] affording a purple powder (200 mg, 0.22 mmol, 7%). $C_{48}H_{24}F_{10}N_4O_4$ (910.71).



^{1}H-NMR ($CDCl_3$): δ = –2.86 (s, 2 H, $H^{pyrrole\text{-}NH}$), 4.13 (s, 6 H, $H^5{}_6$), 8.31 (d, $^3J_{HH}$ = 8.2 Hz, 4 H, $H^5{}_2$), 8.47 (d, $^3J_{HH}$ = 8.2 Hz, 4 H, $H^5{}_3$), 8.83 (d, $^3J_{HH}$ = 4.7 Hz, 4 H, $H^{pyrrole}$), 8.90 (d, $^3J_{HH}$ = 4.8 Hz, 4 H, $H^{pyrrole}$) ppm.

^{1}H-NMR (d_8-THF): δ = –2.80 (s, 2 H, $H^{pyrrole\text{-}NH}$), 4.07 (s, 6 H, $H^5{}_6$), 8.37 (d, $^3J_{HH}$ = 8.2 Hz, 4 H, $H^5{}_2$), 8.47 (d, $^3J_{HH}$ = 8.2 Hz, 4 H, $H^5{}_3$), 8.93 (d, $^3J_{HH}$ = 4.7 Hz, 4 H, $H^{pyrrole}$), 9.05 (d, $^3J_{HH}$ = 4.8 Hz, 4 H, $H^{pyrrole}$) ppm.

^{13}C{^{1}H}-NMR (d_8-THF): δ = 52.7 (s, $C^5{}_6$), 121.4 (s, C^5), 129.1 (s, $C^5{}_3$), 131.4 (s, $C^5{}_4$), 131.4, 133.3 (m, $C^{2,3,7,8,12,13,17,18}$), 135.6 (s, $C^5{}_2$), 147.1 (s, $C^5{}_1$), 167.3 (s, $C^5{}_5$) ppm. $C^{10}{}_1$ – $C^{10}{}_4$ are not observed.

^{19}F-NMR (d_8-THF): δ = –162.9 (ddd, $^3J_{FF}$ = 23 Hz, $^3J_{FF}$ = 21 Hz, $^5J_{FF}$ = 8 Hz, 4 F, $F^{10/20}{}_{3/3}$,), –153.4 (t, $^3J_{FF}$ = 21 Hz, 2 F, $F^{10/20}{}_{4/4}$), –138.0 (dd, $^3J_{FF}$ = 24 Hz, $^5J_{FF}$ = 8 Hz, 4 F, $F^{10/20}{}_{2/2}$) ppm.

IR (KBr): $\tilde{\nu}$ [cm^{-1}] = 3435 (w, crystal water), 3327 (w, NH), 2923 (w, CH), 2850 (w, CH), 1718 (s, CO), 1605 (w), 1519 (vs), 1496 (m), 1281 (s, C-O-C), 1114 (m, CF), 987 (s), 804 (w).

MS (FD): *m/z* (%) = 909.7 (100), 910.7 (55) $[M]^+$.

MS (ESI): *m/z* (%) = 911.17 (100) $[M+H]^+$.

HR-MS (ESI): obs. *m/z* = 911.1700; calcd. for $[M+H]^+$ 911.1716.

UV/Vis (CH_2Cl_2): λ [nm] (ε / [10^4 $M^{-1}cm^{-1}$]) = 415 (55.69), 510 (3.09), 543 (0.73), 587 (0.95), 641 (0.34).

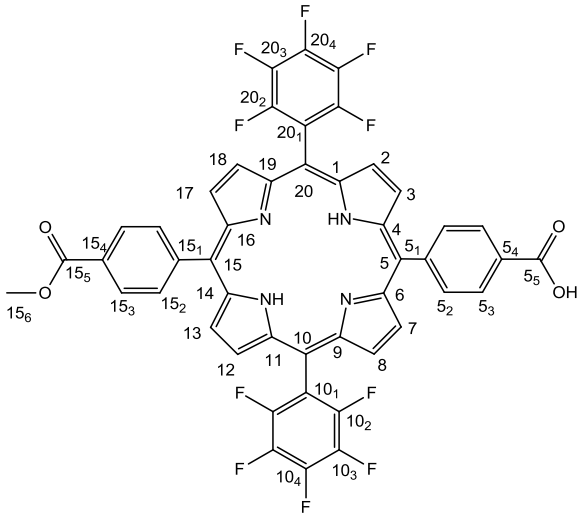
Fluorescence (CH_2Cl_2): λ [nm] (relative intensity) = 645 (1.00), 711 (0.62).

Quantum yield: Φ = 0.0520.

Lifetime: τ [ns] = 10.05 (100%).

CV (Fc/Fc^+, 100 mV s^{-1}, CH_2Cl_2): $E_{½}$[V] = –1.750, –1.350, 0.890, 1.140.

5-(4-Carboxyphenyl)-15-(4-carbomethoxyphenyl)-10,20-bis(2,3,4,5,6-pentafluorophenyl) porphyrin (2b). Porphyrin **1b** (400 mg, 0.447 mmol) was dissolved in 80 mL TFA and 160 mL concentrated HCl_{aq}. The mixture was heated to 60°C. When TLC indicated beginning formation of the diacid the reaction was cooled down, diluted with CH_2Cl_2 (100 mL) and neutralised with a saturated aqueous solution of $NaHCO_3$. The organic layer was washed with water (3×), dried over Na_2SO_4 and concentrated under reduced pressure. Porphyrins **1b** (289 mg) and **2b** (101 mg, 25% yield, purple powder, $C_{47}H_{22}F_{10}N_4O_4$ (896.69)) were isolated by column chromatography [silica, CH_2Cl_2/MeOH (20:1), R_f = 1.0 (**1b**) and R_f = 0.29 (**2b**)].



^{1}H-NMR (CD_2Cl_2 + 1 drop MeOD): δ = –2.94 (s, 2 H, $H^{pyrrole\text{-}NH}$), 4.07 (s, 3 H, $H^{15}{}_6$), 8.29 (d, $^3J_{HH}$ = 8.1 Hz, 2 H, $H^{15}{}_2$), 8.30 (d, $^3J_{HH}$ = 8.1 Hz, 2 H, $H^{5}{}_2$), 8.43 (d, $^3J_{HH}$ = 8.2 Hz, 2 H, $H^{15}{}_3$), 8.44 (d, $^3J_{HH}$ = 8.2 Hz, 2 H, $H^{5}{}_3$), 8.86 (br. s, 4 H, $H^{pyrrole}$), 8.91 (br. s, 4 H, $H^{pyrrole}$) ppm.

^{13}C{^{1}H}-NMR (CD_2Cl_2 + 1 drop MeOD): δ = 52.6 (s, $C^{15}{}_6$), 120.6 (s, C^{5}), 120.8 (s, C^{15}), 128.2 (s, $C^{15}{}_3$), 128.5 (s, $C^{5}{}_3$), 130.3 (s, $C^{15}{}_4$), 130.7 (s, $C^{5}{}_4$), 134.8 (s, $C^{15}{}_2$), 134.8 (s, $C^{5}{}_2$), 136.3, 138.8, 145.3, 147.8 (m, $C^{10,20}$, $^{10,20/10,20/10,20/10,20}{}_{1/2/3/4}$), 145.9 (s, $C^{15}{}_1$), 146.0 (s, $C^{5}{}_1$), 167.5 (s, $C^{15}{}_5$), 168.8 (s, $C^{5}{}_5$) ppm.

^{19}F-NMR (CD_2Cl_2 + 1 drop MeOD): δ = –162.1 (ddd, $^3J_{FF}$ = 23 Hz, $^3J_{FF}$ = 21 Hz, $^5J_{FF}$ = 8 Hz, 4 F, $F^{10/20}{}_{3/3}$,), –153.3 (t, $^3J_{FF}$ = 21 Hz, 2 F, $F^{10/20}{}_{4/4}$), –137.2 (dd, $^3J_{FF}$ = 24 Hz, $^5J_{FF}$ = 8 Hz, 4 F, $F^{10/20}{}_{2/2}$) ppm.

IR (KBr): $\tilde{\nu}$ [cm^{-1}] = 3431 (b, OH), 3314 (w, NH), 2925 (w, CH), 2856 (w, CH), 1725 (s, CO), 1698 (s, CO), 1524 (m), 1489 (vs), 1281 (m, C-O-C), 1108 (s, CF), 990 (s), 920 (s).

MS (FD): *m*/*z* (%) = 895.58 (100) $[M]^+$.

MS (ESI): *m*/*z* (%) = 897.17 (100) $[M+H]^+$.

HR-MS (ESI): obs. *m*/*z* = 897.1547; calcd. for $[M+H]^+$ 897.1560.

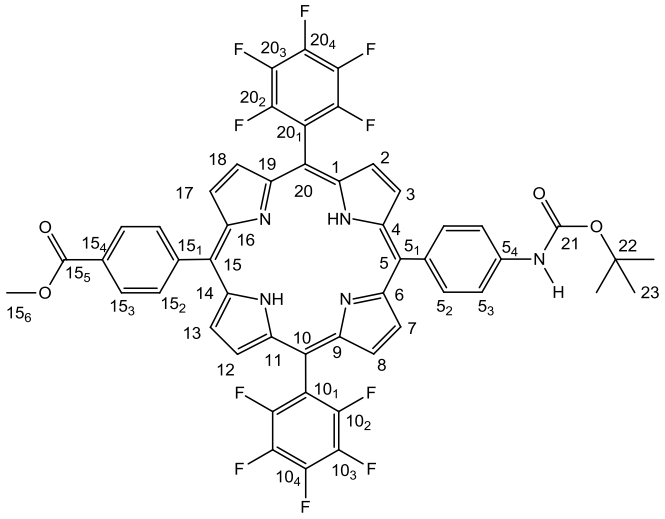
UV/Vis (CH_2Cl_2): λ [nm] (ε / [10^4 $M^{-1}cm^{-1}$]) = 415 (13.74), 510 (0.83), 543 (0.25), 587 (0.30), 641 (0.15).

Fluorescence (CH_2Cl_2): λ [nm] (relative intensity) = 645 (1.00), 712 (0.63).

Quantum yield: Φ = 0.0604.

CV (Fc/Fc^+, 100 mV s^{-1}, CH_2Cl_2): $E_{½}$[V] = –1.810, –1.380, 0.890, 1.120.

15-(4-Carbomethoxyphenyl)-5-(*N*-*tert*-butoxycarbonyl-4-aminophenyl)-10,20-bis(2,3,4,5,6-pentafluorophenyl) porphyrin (Boc-3b). Porphyrin **2b** (100 mg, 0.11 mmol) was dissolved in 15 mL of dry *tert*-butyl alcohol and 22 µL (0.16 mmol) TEA. Diphenylphosphoryl azide (DPPA) (29 µL (0.14 mmol)) was added and this solution was heated to 80°C for two days. The mixture was diluted with 50 mL CH_2Cl_2, washed with diluted aqueous citric acid, a saturated solution of $NaHCO_3$, and water (3×). After drying with Na_2SO_4 the solvent was evaporated under reduced pressure and the product isolated by column chromatography as purple powder [silica, toluene/ethyl acetate (20:1), R_f = 0.47]. Yield 40% (43.2 mg, 0.045 mmol). $C_{51}H_{31}F_{10}N_5O_4$ (967.81).



^{1}H-NMR ($CDCl_3$): δ = –2.84 (s, 2 H, $H^{pyrrole\text{-}NH}$), 1.65 (s, 9 H, H^{23}), 4.13 (s, 3 H, $H^{15}{}_6$), 6.86 (s, 1 H, $H^{Boc\text{-}NH}$), 7.81 (d, $^3J_{HH}$ = 8.3 Hz, 2 H, $H^5{}_3$), 8.14 (d, $^3J_{HH}$ = 8.3 Hz, 2 H, $H^5{}_2$), 8.30 (d, $^3J_{HH}$ = 8.1 Hz, 2 H, $H^{15}{}_2$), 8.47 (d, $^3J_{HH}$ = 8.1 Hz, 2 H, $H^{15}{}_3$), 8.81 (pt, $^3J_{HH}$ = 4.5 Hz, 4 H, $H^{pyrrole}$), 8.89 (d, $^3J_{HH}$ = 4.8 Hz, 2 H, $H^{pyrrole}$), 9.00 (d, $^3J_{HH}$ = 4.8 Hz, 2 H, $H^{pyrrole}$) ppm.

^{13}C{^{1}H}-NMR ($CDCl_3$): δ = 28.5 (s, C^{23}), 52.6 (s, $C^{15}{}_6$), 81.1 (s, C^{22}), 116.9 (s, $C^5{}_3$), 119.8 (s, C^{15}), 121.5 (s, C^5), 128.1 (s, $C^{15}{}_3$), 129.8, 132.3, 132.5 ($C^{2,3,7,8,12,13,17,18}$), 130.0 (s, $C^{15}{}_4$), 134.6 (s, $C^{15}{}_2$), 135.2 (s, $C^5{}_2$), 136.3, 138.8, 145.3, 147.8 (4 C), (m, $C^{10}{}_1$, $C^{10}{}_2$, $C^{10}{}_3$, $C^{10}{}_4$), 135.7 (s, $C^5{}_1$), 138.6 (s, $C^5{}_2$), 146.0 (s, $C^{15}{}_1$), 153.0 (s, C^{21}), 167.2 (s, $C^{15}{}_5$) ppm.

^{19}F-NMR ($CDCl_3$): δ = –162.3 (ddd, $^3J_{FF}$ = 23 Hz, $^3J_{FF}$ = 21 Hz, $^5J_{FF}$ = 7 Hz, 4 F, $F^{10/20}{}_{3/3}$,), –152.6 (t, $^3J_{FF}$ = 21 Hz, 2 F, $F^{10/20}{}_{4/4}$), –137.19 (dd, $^3J_{FF}$ = 24 Hz, $^5J_{FF}$ = 8 Hz, 4 F, $F^{10/20}{}_{2/2}$) ppm.

IR (KBr): $\tilde{\nu}$ [cm^{-1}] = 3435 (b w,NH^{Boc}), 3320 (w, $NH^{pyrrole}$), 2928 (w, CH), 2862 (w, CH), 1724 (m, CO), 1708 (m, CO), 1520 (m), 1494 (m), 1282 (m, C-O-C), 1151 (s, CF), 807 (vs).

MS (FD): *m*/*z* (%) = 866.8 (12) $[M–COOC(CH_3)_3]^+$, 966.7 (100) $[M]^+$.

MS (ESI): *m*/*z* (%) = 968.24 (100) $[M+H]^+$, 1936.49 (4) $[2M+H]^+$.

HR-MS (ESI): obs. *m*/*z* = 968.2295; calcd. for $[M+H]^+$ 968.2336.

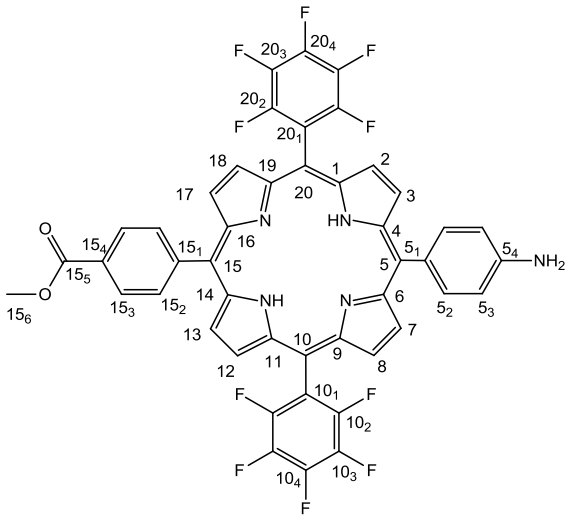
UV/Vis (CH_2Cl_2): λ [nm] (ε / [10^4 $M^{-1}cm^{-1}$]) = 417 (62.07), 511 (1.56), 545 (1.01), 588 (1.46), 643 (0.68).

Fluorescence (CH_2Cl_2): λ [nm] (relative intensity) = 648 (1.00), 713 (0.50).

Quantum yield: Φ = 0.0377.

CV (Fc/Fc^+, 100 mV s^{-1}, CH_2Cl_2): $E_{½}$[V] = –1.820, –1.410, 0.820, 1.020.

15-(4-Carbomethoxyphenyl)-5-(4-aminophenyl)-10,20-bis(2,3,4,5,6-pentafluorophenyl) porphyrin (**3b**). Porphyrin **Boc-3b** (40 mg, 0.041 mmol) was dissolved in 10 mL of CH_2Cl_2 and 10 mL of TFA was added. The solution was stirred at room temperature for 40 min. The solution was neutralised with saturated solution of $NaHCO_3$ and diluted with 10 mL CH_2Cl_2. The organic layer was separated, washed with water (3×), dried with Na_2SO_4 and concentrated under reduced pressure. The yield of **3b** was 95% (33.8 mg, 0.039 mmol, purple powder). $C_{46}H_{23}F_{10}N_5O_2$ (867.69).



^{1}H-NMR ($CDCl_3$): δ = –2.82 (s, 2 H, $H^{pyrrole\text{-}NH}$), 4.06 (s, 2 H, $H^{amine\text{-}NH}$), 4.10 (s, 3 H, $H^{15}{}_6$), 7.08 (d, $^3J_{HH}$ = 8.1 Hz, 2 H, $H^5{}_3$), 7.97 (d, $^3J_{HH}$ = 8.1 Hz, 2 H, $H^5{}_2$), 8.28 (d, $^3J_{HH}$ = 8.0 Hz, 2 H, $H^{15}{}_2$), 8.44 (d, $^3J_{HH}$ = 8.0 Hz, 2 H, $H^{15}{}_3$), 8.76 (pt, $^3J_{HH}$ = 4.5 Hz, 4 H, $H^{pyrrole}$), 8.85 (d, $^3J_{HH}$ = 4.8 Hz, 2 H, $H^{pyrrole}$), 9.04 (d, $^3J_{HH}$ = 4.8 Hz, 2 H, $H^{pyrrole}$) ppm.

^{13}C{^{1}H}-NMR ($CDCl_3$): δ = 113.6 (s, $C^5{}_3$), 52.5 (s, $C^{15}{}_6$), 122.7 (s, C^5), 119.5 (s, C^{15}), 128.1 (s, $C^{15}{}_3$), 129.6, 132.2, 133.1 ($C^{2,3,7,8,12,13,17,18}$), 130.0 (s, $C^{15}{}_4$), 131.2 (s, $C^5{}_1$), 134.6 (s, $C^{15}{}_2$), 135.9 (s, $C^5{}_2$), 146.1 (s, , $C^{15}{}_1$), 146.5 (s, $C^5{}_4$), 167.2 (s, $C^{15}{}_5$) ppm.

^{19}F-NMR ($CDCl_3$): δ = –162.0 (ddd, $^3J_{FF}$ = 23 Hz, $^3J_{FF}$ = 21 Hz, $^5J_{FF}$ = 8 Hz, $F^{10/20}{}_{3/3}$), –152.3 (t, $^3J_{FF}$ = 21 Hz, 2 F, $F^{10/20}{}_{4/4}$), –137.19 (dd, $^3J_{FF}$ = 24 Hz, $^5J_{FF}$ = 8 Hz, 4 F, $F^{10/20}{}_{2/2}$) ppm.

IR (KBr): $\tilde{\nu}$ [cm^{-1}] = 3417 (b m, NH^{amine}), 3314 (w, $NH^{pyrrole}$), 2919 (w, CH), 2849 (w, CH), 1725 (m, CO), 1614 (m), 1517 (vs), 1496 (vs), 1274 (s, C-O-C), 1108 (s, CF), 990 (vs), 920 (m), 802 (m).

MS (FD): *m*/*z* (%) = 867.27 (100) $[M]^+$.

MS (ESI): *m*/*z* (%) = 868.17 (100) $[M+H]^+$.

HR-MS (ESI): obs. *m*/*z* = 868.1777; calcd. for $[M+H]^+$ 868.1770.

UV/Vis (CH_2Cl_2): λ [nm] (ε / [10^4 $M^{-1}cm^{-1}$]) = 419 (73.13), 513 (2.59), 549 (0.95), 590 (0.98), 645 (0.43).

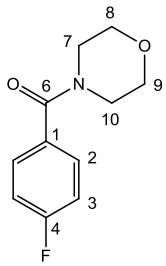
Fluorescence (CH_2Cl_2): λ [nm] (relative intensity) = 654 (1.00), 717 (0.42).

Quantum yield: Φ = 0.0802.

CV (Fc/Fc$^+$, 100 mV s^{-1}, CH_2Cl_2): $E_{½}$[V] = –1.82 (qrev.), –1.39 (qrev.), 0.65 (irr.), 0.79 (irr.).

***N*-(4-trifluoromethylbenzoyl)morpholine** was prepared according to the literature.[S4]

***N*-(4-fluorobenzoyl)morpholine** was synthesised according to a general procedure for the preparation of *N*-arylmorpholines[S4]. 33.6 g (0.24 mol) of 4-fluorobenzoic acid was dissolved in 38 mL (0.48 mol) thionyl chloride and heated under reflux overnight. The excess of thionyl chloride was removed under reduced pressure. The residue was dissolved in 100 mL dry CH_2Cl_2 and cooled down to 0°C. A solution of morpholine (60.00 g, 0.70 mol) in 70 ml CH_2Cl_2 was added slowly to the acid chloride solution, so that the temperature remains below 5°C. The colourless suspension was warmed to room temperature and stirred for 10 min. The mixture was washed with water (3×), 2M HCl (3×) and again with water (3×). The organic layer was dried with Na_2SO_4 and the solvent was removed under reduced pressure giving the product as yellow liquid (28.3 g, 0.135 mol, 56%). $C_{11}H_{12}FNO_2$ (209.22).



^{1}H-NMR ($CDCl_3$): δ = 3.63 (br. m, 2 H, $H^{7,8,9,10}$), 7.03 (m, $^3J_{HH/FH}$ = 8.6 Hz, 2 H, H^3), 7.69 (dd, $^3J_{HH}$ = 8.4 Hz, $^3J_{FH}$ = 5.4 Hz, 2 H, H^2) ppm.

^{13}C{^{1}H}-NMR ($CDCl_3$): δ = 66.6 (s, $C^{7,8,9,10}$), 115.4 (d, $^2J_{FH}$ = 21.8 Hz, C^3), 129.2 (d, $^3J_{FH}$ = 8.5 Hz, C^2), 131.1 (d, $^4J_{FH}$ = 3.4 Hz, C^1), 163.2 (d, $^1J_{FH}$ = 250.0 Hz, C^4), 169.2 (s, C^6) ppm.

^{19}F-NMR ($CDCl_3$): δ = –110.0 (tt, $^3J_{FH}$ = 8.6 Hz, $^4J_{FH}$ = 5.4 Hz) ppm.

IR (KBr): $\tilde{\nu}$ [cm^{-1}] = 3064 (w, CH), 2967 (w, CH), 2918 (w, CH), 2856 (w, CH), 1635 (vs, CO), 1510 (w), 1433 (s), 1281 (s, C-O-C), 1121 (s), 1108 (s, CF), 837 (s), 754 (s).

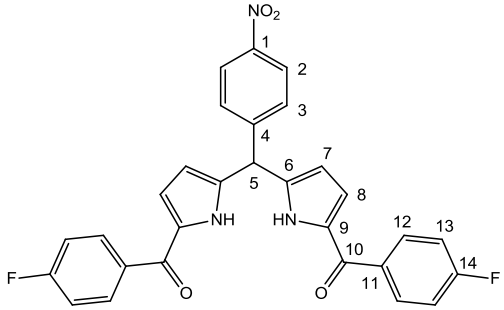
MS (FD): *m*/*z* (%) = 209.3 (100) $[M]^+$.

MS (ESI): *m*/*z* (%) = 210.09 (21, $[M]^+$), 210.09 (100, $[M+H]^+$).

HR-MS (ESI): obs. *m*/*z* = 210.0930; calcd. for $[M+H]^+$ 210.0930.

General procedure for the preparation of 1,9-diacyldipyrromethanes.[S4] *N*-aroylmorpholine (1 eq.) and phosphorous oxytrichloride (2 eq.) were heated at 65°C under nitrogen for 3 h. The dark solution was cooled to room temperature and diluted with 1,2-dichloroethane. 5-(4-nitrophenyl)dipyromethane[S6] (0.25 eq.) was added and the solution was stirred under reflux for 2 h and quenched by addition of a saturated aqueous solution of sodium acetate and heated to reflux for 1 h. After cooling to room temperature the mixture was diluted with CH_2Cl_2 and the organic layer was separated. After washing with water (3×) and drying with Na_2SO_4 and the solvent was removed under reduced pressure. The residue was purified by chromatography [silica, CH_2Cl_2/ethyl acetate (15:1), R_f = 0.60].

1,9-bis(4-fluorobenzoyl)-5-(4-nitrophenyl)dipyrromethane. 28.30 g, (0.14 mol) *N*-(4-fluorobenzoyl)morpholine, 41.5 g, (0.28 mol) phosphorous oxytrichloride, 200 mL 1,2-dichloroethane, 18.70 (0.07 mol) 5-(4-nitrophenyl)dipyromethane[S6], 150 mL CH_2Cl_2 and 360 mL saturated aqueous solution of sodium acetate. Yield 16.90 g (0.033 mol, 47%), red-brown solid. $C_{29}H_{21}F_2N_3O_4$ (511.49).



^{1}H-NMR ($CDCl_3$): δ = 5.83 (s, 1H, H^5), 5.93 (ps. t, $^3J_{HH}$ = 3.0 Hz, 2 H, H^7), 6.48 (dd, $^3J_{HH}$ = 3.8 Hz, $^4J_{HH}$ = 2.3 Hz, 2 H, H^8), 7.08 (t, $^3J_{HH}$ = 8.6 Hz, 4 H, H^{13}), 7.74 (dd, $^3J_{HH}$ = 8.8 Hz, $^3J_{HF}$ = 5.4 Hz, 4 H, H^{12}), 7.80 (d, $^3J_{HH}$ = 8.7 Hz, 2 H, H^3), 8.24 (d, $^3J_{HH}$ = 8.7 Hz, 2 H, H^2), 12.18 (br. s, 2 H, NH) ppm.

^{13}C{^{1}H}-NMR ($CDCl_3$): δ = 44.8 (s, C^5), 111.5 (s, C^7), 115.3 (d, $^2J_{FH}$ = 21.7 Hz, C^{13}), 120.8 (s, C^8), 124.1 (s, C^2), 129.8 (s, C^3), 131.1 (s, C^9), 132.0 (d, $^2J_{FH}$ = 9.0 Hz, C^{12}), 133.9 (d, $^4J_{FH}$ = 2.9 Hz, C^{11}), 139.6 (s, C^6), 147.4 (s, C^4), 147.6 (s, C^1), 165.4 (d, $^1J_{FH}$ = 253.9 Hz, C^{14}), 183.2 (s, C^{10}) ppm.

^{19}F-NMR ($CDCl_3$): δ = –106.6 (tt, $^3J_{FH}$ = 8.6 Hz, $^4J_{FH}$ = 5.4 Hz) ppm.

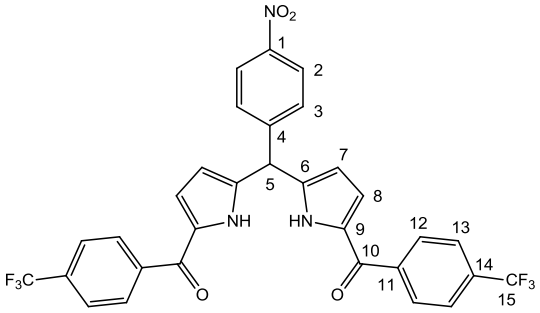
IR (KBr): $\tilde{\nu}$ [cm^{-1}] = 3230 (b, NH), 3099 (w, CH), 1611 (vs), 1600 (vs), 1517 (m, NO), 1476 (vs), 1344 (vs, NO), 1232 (s, C-O-C), 1149 (s, CF), 886 (m), 754 (m).

MS (FD): *m*/*z* (%) = 511.3 (100) $[M]^+$, 255.8 (1.07) $[M]^{2+}$.

MS (ESI): *m*/*z* (%) = 512.14 (16, $[M+H]^+$), 1023.30 (5) $[2M+H]^+$.

HR-MS (ESI): obs. *m*/*z* = 512.1406; calcd. for $[M+H]^+$ 512.1422.

1,9-bis(4-trifluoromethylbenzoyl)-5-(4-nitrophenyl)dipyrromethane. 50.0 g, (0.24 mol) *N*-(4-trifluoromethylbenzoyl)morpholine, 76.7 g, (0.58 mol) phosphorous oxytrichloride, 350 mL 1,2-dichloroethane, 16.0 (0.06 mol) 5-(4-nitrophenyl)dipyromethane[S6], 150 mL CH_2Cl_2 and 360 mL saturated aqueous solution of sodium acetate. Yield 27.0 g (0.044 mol, 74%), red-brown solid. $C_{31}H_{19}F_6N_3O_4$ (611.49).



^{1}H-NMR ($CDCl_3$): δ = 5.86 (s, 1H, H^5), 6.03 (m, 2 H, H^7), 6.57 (m, 2 H, H^8), 7.68 (d, $^3J_{HH}$ = 8.0 Hz, 4 H, H^{12}), 7.80 (m, 6 H, $H^{3/13}$), 8.28 (d, $^3J_{HH}$ = 8.5 Hz, 2 H, H^2), 12.09 (s, 2 H, NH) ppm.

^{13}C{^{1}H}-NMR ($CDCl_3$): δ = 44.8 (s, C^5), 112.0 (s, C^7), 121.5 (s, C^8), 122.1 (s, C^{11}), 124.3 (s, C^2), 125.3 (s, C^{12}), 129.8 (s, $C^{3/13}$), 131.1 (s, C^9), 133.6 (q, $^1J_{CF}$ = 32.7 Hz, C^{15}), 140.1 (s, C^6), 140.6 (s, C^{14}), 147.0 (s, C^4), 147.6 (s, C^1), 183.4 (s, C^{10}) ppm.

^{19}F-NMR ($CDCl_3$): δ = –62.9 (s) ppm.

IR (KBr): $\tilde{\nu}$ [cm^{-1}] = 3255 (b, NH), 3107 (w, CH), 1708 (w, CO), 1618 (s), 1528 (m, NO), 1331 (vs, NO), 1249 (w, C-O-C), 1169 (m, CF), 889 (m), 767 (m).

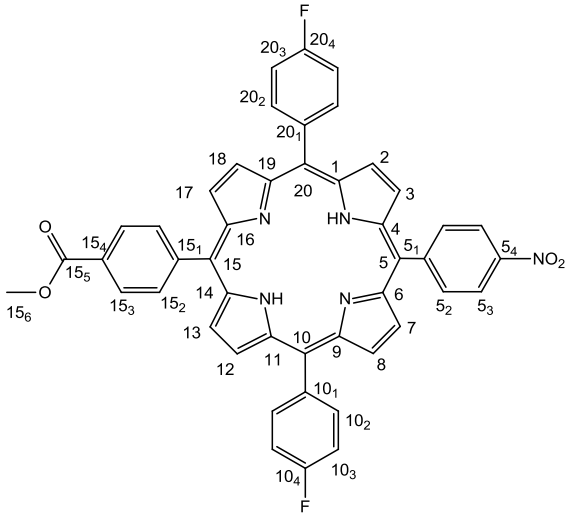
MS (FD): *m*/*z* (%) = 611.22 (100) $[M]^+$.

MS (ESI): *m*/*z* (%) = 610.15 (9, $[M–H]^+$).

HR-MS (ESI): obs. *m*/*z* = 610.1175; calcd. for $[M–H]^+$ 610.1166.

General procedure for the preparation of porphyrins 2c and 2d.[S5] To a stirred solution of 1,9-diacyldipyrromethane in THF/methanol (10 : 1) $NaBH_4$ (20 eq.) was added under nitrogen at room temperature and the mixture was stirred until TLC indicated consumption of starting material. The reaction was quenched with a saturated solution of NH_4Cl_{aq} and diluted with CH_2Cl_2. The organic layer was separated, washed with water (3×) and dried with $NaSO_4$. After removing the solvent the dipyrromethane-dicarbinol was obtained as a foamlike solid. To this brown residue was added 5-(4-benzoic acid methylester)dipyrromethane[S6] (1.2 eq.) and acetonitrile. The suspension was dipped in an ultrasonic bath to dissolve the compounds. This solution was added to a pre-cooled solution of DMF and TFA in acetonitrile (0°C) in small portions over 30 min. After stirring for 10 min 2,3-dicyano-5,6-dichloro-1,4-benzoquinone (DDQ) was added and the mixture was stirred for 1 h. TEA was added to quench the reaction and the mixture was concentrated under reduced pressure. The products were purified by column chromatography [silica, CH_2Cl_2].

4-[15-(4-nitro-phenyl)-10,20-di-(4-fluoro)phenylporphyrin-5-yl]methyl benzoate (2c). 6.81 g (180 mmol) $NaBH_4$, 440 mL THF/methanol (10:1), 9.37 g (0.033 mol) 1,9-bis(4-fluorobenzoyl)-5-(4-nitrophenyl)dipyrromethane, 17.09 g (0.040 mol) 5-(4-methyl benzoate)dipyrromethane, 2 L acetonitrile, 22 mL DMF, 30.8 mL TFA, 28.60 g (0.13 mol) DDQ, 31 mL TEA. [silica, CH_2Cl_2, R_f = 0.78]. Yield 2.37 g (3.14 mmol, 9.5%), purple powder. $C_{46}H_{29}F_2N_5O_4$ (753.75).



^{1}H-NMR ($CDCl_3$): δ = –2.81 (s, 2 H, $H^{pyrrole\text{-}NH}$), 4.12 (s, 3 H, $H^{15}{}_6$), 7.47 (t, $^3J_{HH}$ = 8.6 Hz, 4 H, $H^{10/20}{}_{3/3}$), 8.17 (dd, $^3J_{HH}$ = 8.4 Hz, $^3J_{HF}$ = 3.1 Hz, 4 H, $H^{10/20}{}_{2/2}$), 8.30 (d, $^3J_{HH}$ = 8.1 Hz, 2 H, $H^{15}{}_2$), 8.39 (d, $^3J_{HH}$ = 8.5 Hz, 2 H, $H^5{}_2$), 8.46 (d, $^3J_{HH}$ = 8.1 Hz, 2 H, $H^{15}{}_3$), 8.65 (d, $^3J_{HH}$ = 8.6 Hz, 2 H, $H^5{}_3$), 8.76 (d, $^3J_{HH}$ = 4.7 Hz, 2 H, $H^{pyrrole}$), 8.85 (m, 6 H, $H^{pyrrole}$) ppm.

^{13}C{^{1}H}-NMR ($CDCl_3$): δ = 52.5 (s, $C^{15}{}_6$), 113.9 (d, $^2J_{CF}$ = 21.3 Hz , $C^{10/20}{}_{3/3}$), 117.4 (s, C^5), 119.6 (s, $C^{10/20}$), 119.6 (s, C^{15}) 121.9 (s, $C^5{}_3$), 128.0 (s, $C^{15}{}_3$), 129.8 (s, $C^{15}{}_4$), 134.5 (s, $C^{15}{}_2$), 131.8 (br. S, $C^{pyrrole}$), 135.1 (s, $C^5{}_2$), 135.7 (d, $^3J_{CF}$ = 8.8 Hz , $C^{10/20}{}_{2/2}$), 137.6 (d, $^4J_{CF}$ = 3.4 Hz, $C^{10/20}{}_{1/1}$), 146.6 (s, $C^{15}{}_1$), 147.4 (s, $C^5{}_1$), 147.8 (s, $C^5{}_4$), 148.9 (s, $C^{pyrrole}$), 165.7 (d, $^1J_{FH}$ = 248.1 Hz, $C^{10/20}{}_{4/4}$), 167.2 (s, $C^{15}{}_5$) ppm.

^{19}F-NMR ($CDCl_3$): δ = –114.2 (tt, $^3J_{FH}$ = 8.6 Hz, $^4J_{FH}$ = 5.4 Hz).

IR (KBr): $\tilde{\nu}$ [cm^{-1}] = 3433 (w, NH), 3315 (w, CH), 1724 (s, CO), 1504 (s), 1525 (s, NO), 1348 (vs, NO), 1282 (s, C-O-C), 1105 (s, CF), 798 (vs).

MS (FD): *m*/*z* (%) = 753.4 (100) $[M]^+$.

MS (ESI): *m*/*z* (%) = 754.25 (100) $[M+H]^+$.

HR-MS (ESI): obs. *m*/*z* = 754.2260; calcd. for $[M+H]^+$ 754.2266.

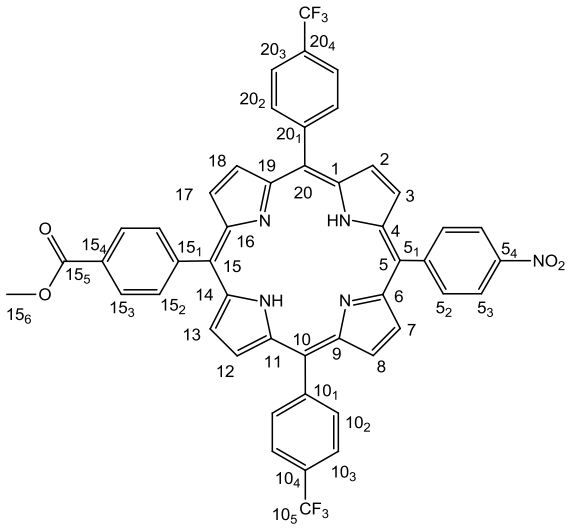
UV/Vis (CH_2Cl_2): λ [nm] (ε / [10^4 $M^{-1}cm^{-1}$]) = 421 (29.55), 517 (1.35),553 (0.58), 592 (0.41), 648 (0.32).

Fluorescence (CH_2Cl_2): λ [nm] (relative intensity) = 652 (1.00), 716 (0.36).

Quantum yield: Φ = 0.1024.

CV (Fc/Fc^+, 100 mV s^{-1}, CH_2Cl_2): $E_{½}$[V] = –2.150, –1.445 (2e), 0.690, 0.950.

4-[15-(4-nitro-phenyl)-10,20-di-(4-trifluoromethyl)phenylporphyrin-5-yl]methyl benzoate (2d). 1.96 g, (51.80 mmol) $NaBH_4$, 30.8 mL THF/methanol (10:1), 1.00 g (1.64 mmol) 1,9-bis(4- trifluoromethylbenzoyl)-5-(4-nitrophenyl)dipyrromethane, 21.22 g (2.38 mmol) 5-(4-methyl benzoate)dipyrromethane, 568 mL acetonitrile, 2.4 mL DMF, 3.4 mL TFA, 3.12 g (13.74 mmol) DDQ, 3.6 mL TEA. [silica, CH_2Cl_2, R_f = 0.68]. Yield 308 mg (0.37 mmol, 22%), purple powder. $C_{48}H_{29}F_6N_5O_4$ (853.77).



^{1}H-NMR ($CDCl_3$): δ = –2.82 (s, 2 H, $H^{pyrrole\text{-}NH}$), 4.13 (s, 3 H, $H^{15}{}_6$), 8.05 (d, $^3J_{HH}$ = 8.0 Hz, 4 H, $H^{10/20}{}_{3/3}$), 8.30 (d, $^3J_{HH}$ = 8.1 Hz, 2 H, $H^{15}{}_2$), 8.34 (d, $^3J_{HH}$ = 8.3 Hz, 4 H, $H^{10/20}{}_{2/2}$), 8.41 (d, $^3J_{HH}$ = 8.4 Hz, 2 H, $H^5{}_2$), 8.47 (d, $^3J_{HH}$ = 8.1 Hz, 2 H, $H^{15}{}_3$), 8.66 (d, $^3J_{HH}$ = 8.5 Hz, 4 H, $H^5{}_3$), 8.78 (s, $^3J_{HH}$ = 4.6 Hz, 2 H, $H^{pyrrole}$), 8.91 (m, 4 H, $H^{pyrrole}$) ppm.

^{13}C{^{1}H}-NMR ($CDCl_3$): δ = 52.5 (s, $C^{15}{}_6$), 117.6 (d, C^5), 119.2 (s, $C^{10/20}$), 120.0 (s, C^{15}), 122.0 (s, $C^5{}_3$), 123.9 (d, $^4J_{CF}$ = 3.3 Hz, $C^{10/20}{}_{3/3}$), 125.9 (s, $C^{10/20}{}_{4/4}$), 128.1 (s, $C^{15}{}_3$), 129.9 (s, $C^{15}{}_4$), 130.6 (q, $^1J_{CF}$ = 32.6 Hz, $C^{10/20}{}_{5/5}$), 131.5 (br. s, $C^{pyrrole\ 2,3,7,8,12,13,17,18}$), 134.5 (s, $C^{15}{}_2$), 134.6 (s, $C^{10/20}{}_{2/2}$), 135.1 (s, $C^5{}_2$), 145.4 (s, $C^{10/20}{}_{1/1}$), 146.4 (s, $C^{15}{}_1$), 147.9 (s, $C^5{}_4$), 148.7 (s, $C^5{}_1$), 167.2 (s, $C^{15}{}_5$) ppm.

^{19}F-NMR ($CDCl_3$): δ = –62.0 (s) ppm.

IR (KBr): $\tilde{\nu}$ [cm^{-1}] = 3433 (w, NH), 3320 (w, CH), 2925 (w, CH), 2849 (w, CH), 1718 (w, CO), 1504 (s), 1524 (w, NO), 1322 (vs, NO), 1274 (w, C-O-C), 1164 (w, CF), 1066 (s), 796 (vs).

MS (FD): *m*/*z* (%) = 853.4 (100) [M^+].

MS (ESI): *m*/*z* (%) = 854.25 (100) $[M+H]^+$.

HR-MS (ESI): obs. *m*/*z* = 854.2200; calcd. for $[M+H]^+$ 854.2202.

UV/Vis (CH_2Cl_2): λ [nm] (ε / [10^4 $M^{-1}cm^{-1}$]) = 419 (15.1), 515 (0.42), 549 (0.17), 589 (0.13), 644 (0.07).

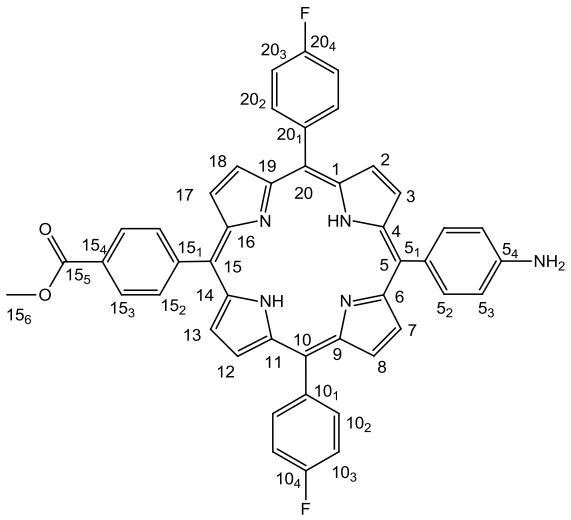
Fluorescence (CH_2Cl_2): λ [nm] (relative intensity) = 650 (1.00), 715 (0.44).

Quantum yield: Φ = 0.0608

CV (Fc/Fc^+, 100 mV s^{-1}, CH_2Cl_2): $E_{½}$[V] = –2.020, –1.470 (2e), 0.750, 1.030.

General procedure for the prepation of porphyrins 3c and 3d[S5]. Under nitrogen 1 eq. nitro-porphyrin **2c** or **2d** was suspended in conc. aqueous HCl and $SnCl_2$ (14 eq.) was added. The mixture was stirred under reflux for 1 – 2 h until TLC indicated consumption of starting material. After cooling to room temperature the solution was neutralised with conc. aqueous ammonia and extracted with ethyl acetate. The combined organic phases ware dried with $NaSO_4$ and the solvent was removed under reduced pressure. The products were purified by column chromatography [silica, toluene : ethyl acetate = 20 : 1].

15-(4-Carbomethoxyphenyl)-5-(4-aminophenyl)-10,20-bis-(4-fluorophenyl)porphyrin (3c). 1.00 g (1.33 mmol) porphyrin **1c**, 424 mL conc. aquaeous HCl, 4.33 g (0.019 mol) $SnCl_2$. [silica, toluene : ethyl acetate = 20 : 1, R_f = 0.36]. Yield 470 mg (0.65 mmol, 49%), purple powder. $C_{46}H_{31}F_2N_5O_2$ (723.77).



^{1}H-NMR ($CDCl_3$): δ = –2.79 (s, 2 H, $H^{pyrrole\text{-}NH}$), 4.11 (s, 3 H, $H^{15}{}_6$), 7.02 (d, $^3J_{HH}$ = 8.2 Hz, 2 H, $H^5{}_3$), 7.44 (ps. t, $^3J_{HH}$ = 8.6 Hz, 4 H, $H^{10/20}{}_{3/3}$), 7.99 (d, $^3J_{HH}$ = 8.2 Hz, 2 H, $H^5{}_2$), 8.17 (dd, $^3J_{HH}$ = 8.3 Hz, $^3J_{HF}$ = 5.4 Hz, 4 H, $H^{10/20}{}_{2/2}$), 8.29 (d, $^3J_{HH}$ = 8.1 Hz, 2 H, $H^{15}{}_2$), 8.44 (d, $^3J_{HH}$ = 8.1 Hz, 2 H, $H^{15}{}_3$), 8.80 (m, 6 H, $H^{pyrrole}$), 8.96 (d, $^3J_{HH}$ = 8.1 Hz, 2 H, $H^{pyrrole}$) ppm.

^{13}C{^{1}H}-NMR ($CDCl_3$): δ = 52.4 (s, $C^{15}{}_6$), 113.5 (s, $C^5{}_3$), 113.7 (d, $^2J_{CF}$ = 21.4 Hz , $C^{10/20}{}_{3/3}$), 118.3 (s, C^{15}), 118.9 (s, $C^{10/20}$), 121.5 (s, C^5), 127.9 (s, $C^{15}{}_3$), 128.5 (s, $C^{pyrrole}$), 129.6 (s, $C^{15}{}_4$), 131.0 (br. s, $C^{pyrrole}$), 132.1 (s, $C^5{}_1$), 134.6 (s, $C^{15}{}_2$), 135.7 (d, $^3J_{CF}$ = 8.8 Hz , $C^{10/20}{}_{2/2}$), 135.7 (s, $C^5{}_2$), 138.0 (d, $^4J_{CF}$ = 3.2 Hz, $C^{10/20}{}_{1/1}$), 146.2 (s, $C^5{}_4$), 146.9 (s, $C^{15}{}_1$), 162.9 (d, $^1J_{FH}$ = 247.3 Hz, $C^{10/20}{}_{4/4}$), 167.3 (s, $C^{15}{}_5$) ppm.

^{19}F-NMR ($CDCl_3$): δ = –114.7 (tt, $^3J_{FH}$=8.6 Hz, $^4J_{FH}$=5.4 Hz) ppm.

IR (KBr): $\tilde{\nu}$ [cm^{-1}] = 3452 (b, NH^{amine}), 3386 (b, NH^{amine}), 3315 (b, $NH^{pyrrole}$), 1724 (s, CO), 1504 (s), 1280 (vs, C-O-C), 1155 (s, CF), 802 (vs).

MS (FD): *m*/*z* (%) = 723.4 (100) $[M]^+$.

MS (ESI): *m*/*z* (%) = 724.2 (100) $[M+H]^+$, 1448.5 (1) $[2M+H]^+$.

HR-MS (ESI): obs. *m*/*z* = 724.2522; calcd. for $[M+H]^+$ 724.2524.

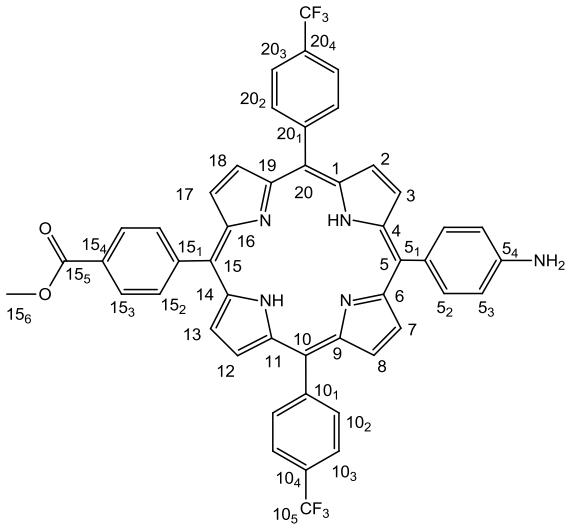
UV/Vis (CH_2Cl_2): λ [nm] (ε / [10^4 $M^{-1}cm^{-1}$]) = 421 (30.42), 517 (1.54), 554 (0.90), 593 (0.51), 649 (0.44).

Fluorescence (CH_2Cl_2): λ [nm] (relative intensity) = 656 (1.00), 719 (0.29).

Quantum yield: Φ = 0.1405.

CV (Fc/Fc^+, 100 mV s^{-1}, CH_2Cl_2): $E_{½}$[V] = –1.980, –1.650, 0.51 (irr.).

15-(4-carbomethoxyphenyl)-5-(4-aminophenyl)-10,20-bis-(4-trifluoromethylphenyl) porphyrin (3d). 0.66 g (0.77 mmol) porphyrin **2d**, 100 mL conc. aqueous HCl, 3.00 g (13.2 mmol) $SnCl_2$. [silica, toluene : ethyl acetate = 20 : 1, R_f = 0.41]. Yield 310 mg (0.38 mmol, 49%), purple powder. $C_{48}H_{31}F_6N_5O_2$ (823.75).



^{1}H-NMR ($CDCl_3$): δ = –2.78 (s, 2 H, $H^{pyrrole\text{-}NH}$), 4.07 (br. s, 2 H, $H^{amine\text{-}NH}$), 4.12 (s, 3 H, $H^{15}{}_6$), 7.09 (d, $^3J_{HH}$ = 8.2 Hz, 2 H, $H^5{}_3$), 7.99 (d, $^3J_{HH}$ = 8.2 Hz, 2 H, $H^5{}_2$), 8.03 (d, $^3J_{HH}$ = 8.0 Hz, 4 H, $H^{10/20}{}_{3/3}$), 8.29 (d, $^3J_{HH}$ = 8.1 Hz, 2 H, $H^{15}{}_2$), 8.34 (d, $^3J_{HH}$ = 7.8 Hz, 4 H, $H^{10/20}{}_{2/2}$), 8.45 (d, $^3J_{HH}$ = 8.1 Hz, 2 H, $H^{15}{}_3$), 8.78 (m, 6 H, $H^{pyrrole}$), 8.98 (d, $^3J_{HH}$ = 4.7 Hz, 2 H, $H^{pyrrole}$) ppm.

^{13}C{^{1}H}-NMR ($CDCl_3$): δ = 52.5 (s, $C^{15}{}_6$), 113.5 (s, $C^5{}_3$), 118.5 (d, $C^{10/20}$), 118.7 (s, C^{15}), 121.9 (s, C^5), 123.7 (d, $^4J_{CF}$ = 3.2 Hz, $C^{10/20}{}_{3/3}$), 125.9 (s, $C^{10/20}{}_{4/4}$), 128.0 (s, $C^{15}{}_3$), 129.7 (s, $C^{15}{}_4$), 130.1 (q, $^1J_{CF}$ = 32.6 Hz, $C^{10/20}{}_{5/5}$), 130.9 (br.s, $C^{2,3,7,8,12,13,17,18}$), 131.9 (s, $C^5{}_1$), 134.6 (s, $C^{10/20/15}{}_{2/2/2}$), 135.7 (s, $C^5{}_2$), 145.8 (s, $C^{10/20}{}_{1/1}$), 146.3 (s, $C^5{}_4$), 146.7 (s, $C^{15}{}_1$), 167.3 (s, $C^{15}{}_5$) ppm.

^{19}F-NMR ($CDCl_3$): δ = –62.0 (s) ppm.

IR (KBr): $\tilde{\nu}$ [cm^{-1}] = 3460 (b, NH^{amine}), 3386 (b, NH^{amine}), 3321 (b, $NH^{pyrrole}$), 1724 (s, CO), 1609 (s), 1315 (vs), 1274 (vs, C-O-C), 1167 (s, CF), 807 (vs).

MS (FD): *m*/*z* (%) = 823.4 (100) $[M]^+$.

MS (ESI): *m*/*z* (%) = 824.30 (100) $[M+H]^+$.

HR-MS (ESI): obs. *m*/*z* = 824.2468; calcd. for $[M+H]^+$ 824.2460.

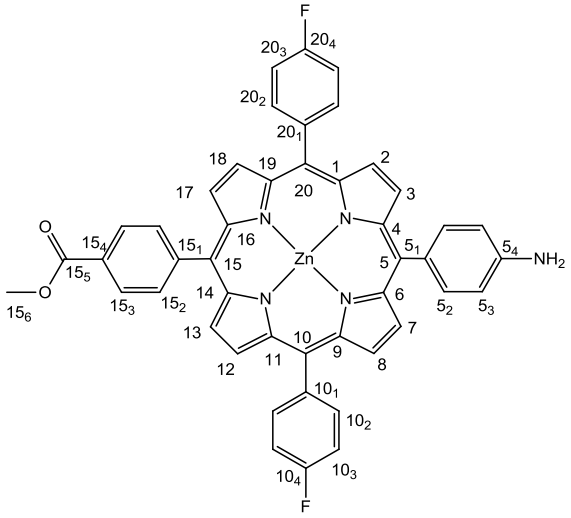
UV/Vis (CH_2Cl_2): λ [nm] (ε / [10^4 $M^{-1}cm^{-1}$]) = 421 (19.9), 517 (0.38), 553 (0.20), 592 (0.11), 650 (0.10).

Fluorescence (CH_2Cl_2): λ [nm] (relative intensity) = 656 (1.00), 719 (0.28).

Quantum yield: Φ = 0.1189.

CV (Fc/Fc^+, 100 mV s^{-1}, CH_2Cl_2): $E_{½}$[V] = –1.900, –1.560, 0.53 (irr.).

[15-(4-Carbomethoxyphenyl)-5-(4-aminophenyl)-10,20-bis-(4-fluorophenyl) porphyrinato]zinc(II) (**Zn-3c**). Porphyrin **3c** (94 mg, 0.13 mmol) and zinc acetate dihydrate (110.2 mg, 0.65 mmol) were stirred overnight in of CH_2Cl_2 (10 mL). After concentration under reduced pressure the product was isolated by column chromatography [silica, toluene : ethyl acetate = 20 : 1, R_f = 0.36]. Yield 102 mg (0.13 mmol, 97%), purple powder. $C_{46}H_{29}F_2N_5O_2Zn$ (787.16).



^{1}H-NMR (d$_8$-THF): δ = 4.05 (s, 3 H, $H^{15}{}_6$), 4.90 (s, 2 H, NH_2), 6.96 (d, $^3J_{HH}$ = 8.1 Hz, 4 H, $H^5{}_3$), 7.48 (ps. t, $^3J_{HH}$ = 8.6 Hz, 4 H, $H^{10/20}{}_{3/3}$), 7.86 (d, $^3J_{HH}$ = 8.1 Hz, 2 H, $H^5{}_2$), 8.20 (dd, $^3J_{HH}$ = 8.1 Hz, $^3J_{HF}$ = 5.6 Hz, 4 H, $H^{10/20}{}_{2/2}$), 8.30 (d, $^3J_{HH}$ = 8.0 Hz, 2 H, $H^{15}{}_2$), 8.41 (d, $^3J_{HH}$ = 8.0 Hz, 2 H, $H^{15}{}_3$), 8.82 (m, 6 H, $H^{pyrrole}$), 9.00 (d, 2 H, $^3J_{HH}$ = 4.6 Hz $H^{pyrrole}$) ppm.

^{13}C{^{1}H}-NMR (d$_8$-THF): δ = 52.5 (s, $C^{15}{}_6$), 113.3 (s, $C^5{}_3$), 114.2 (d, $^2J_{CF}$ = 21.4 Hz , $C^{10/20}{}_{3/3}$), 119.7 (s, C^{15}), 120.3 (s, $C^{10/20}$), 123.9 (C^5), 128.5 (s, $C^{15}{}_3$), 130.5 (s, $C^{15}{}_4$), 131.9, 131.9, 132.4, 133.2, (8 C), (s, $C^{pyrrole}{}_{2,3,7,8,12,13,17,18}$), 132.3 (s, $C^5{}_1$), 135.6 (s, $C^{15}{}_2$), 136.5 (s, $C^5{}_2$), 136.8 (d, $^3J_{CF}$ = 7.9 Hz, $C^{10/20}{}_{2/2}$), 140.8 (d, $^4J_{CF}$ = 3.2 Hz, $C^{10/20}{}_{1/1}$), 149.2 (s, $C^5{}_4$), 149.5 (s, $C^{15}{}_1$), 150.6, 151.0, 151.3, 152.2 (8 C), (s, $C^{1,4,6,9,11,14,16,19}$), 163.9 (d, $^1J_{FH}$ = 245.6 Hz, $C^{10/20}{}_{4/4}$), 167.5 (s, $C^{15}{}_5$) ppm.

^{19}F-NMR (d$_8$-THF): δ = –118.7 (m, $^3J_{FH}$=8.6 Hz, $^4J_{FH}$=5.4 Hz).

IR (KBr): $\tilde{\nu}$ [cm^{-1}] = 3438 (b, NH^{amine}), 3386 (b, NH^{amine}), 2918 (w, CH), 2849 (w, CH), 1725 (vs, CO), 1607 1503 (m), 1274 (vs, C-O-C), 1156 (s, CF), 1109 (m), 802 (s).

MS (FD): *m*/*z* (%) = 785.4 (100) $[M]^+$.

MS (ESI): *m*/*z* (%) = 785.17 (100) $[M]^+$.

HR-MS (ESI): obs. *m*/*z* = 785.1579; calcd. for $[M]^+$ 785.1581.

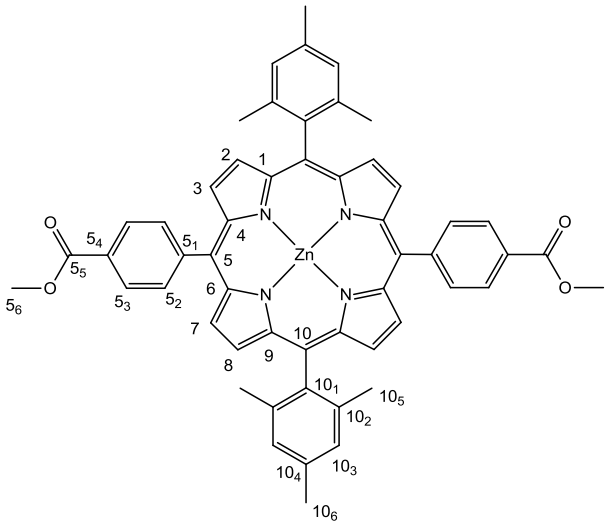
UV/Vis (CH_2Cl_2): λ [nm] (ε / [10^4 $M^{-1}cm^{-1}$]) = 424 (38.11), 551 (2.00), 593 (0.53).

Fluorescence (CH_2Cl_2): λ [nm] (relative intensity) = 606 (1.00), 652 (0.63).

Quantum yield: Φ = 0.0194.

CV (Fc/Fc$^+$, 100 mV s^{-1}, CH_2Cl_2): $E_{½}$[V] = –2.060, –1.730, 0.415 (irr.).

[10,20-Bis(2,4,6-trimethylphenyl)-5,15-bis[4-(methoxycarbonyl)] porphyrinato]zinc(II) (Zn-1a). Porphyrin **1a** (35 mg, 0.042 mmol) and zinc acetate dihydrate (46.67 mg, 0.21 mmol) were stirred overnight in CH_2Cl_2 (5 mL). After concentration under reduced pressure the product was isolated by column chromatography [silica, CH_2Cl_2, R_f = 0.80]. Yield 30 mg (0.034 mmol, 81%), purple powder. $C_{54}H_{44}N_4O_4Zn$ (878.35).



^{1}H-NMR (d_8-THF): δ = 1.84 (s, 12 H, $H^{10}{}_5$), 2.61 (s, 6 H, $H^{10}{}_6$), 4.04 (s, 6 H, $H^5{}_6$), 7.30 (s, 4 H, $H^{10/20}{}_{3/3}$), 8.31 (d, $^3J_{HH}$ = 6.8 Hz, 4 H, $H^5{}_2$), 8.39 (d, $^3J_{HH}$ = 7.9 Hz, 4 H, $H^5{}_3$), 8.68 (d, $^3J_{HH}$ = 4.4 Hz, 4 H, $H^{pyrrole}$), 8.75 (d, $^3J_{HH}$ = 4.3 Hz, 4 H, $H^{pyrrole}$) ppm.

^{13}C{^{1}H}-NMR (d_8-THF): δ = 21.7 (s, $C^{10/20}{}_{6/6}$), 22.1 (s, $C^{10/20}{}_{5/5}$), 52.5 (s, $C^5{}_6$), 119.9 (s, C^5), 128.4 (s, $C^5{}_3$), 128.7 (s, $C^{10/20}{}_{3/3}$), 130.5 ($C^5{}_4$), 131.3, 132.6 ($C^{2,3,7,8,12,13,17,18}$), 135.5 (s, $C^5{}_2$), 138.4 ($C^{10/20}{}_{4/4}$), 140.0 ($C^{10/20}{}_{2/2}$), 140.7 ($C^{10/20}{}_{1/1}$), 149.4 ($C^5{}_1$), 150.5, 150.9 ($C^{1,4,6,9,11,14,16,19}$), 167.5 (s, $C^5{}_5$) ppm.

IR (KBr): $\tilde{\nu}$ [cm^{-1}] = 3425 (b, $NH^{pyrrole}$), 2922 (w, CH), 2850 (w, CH), 1722 (vs, CO), 1608 (s), 1386 (vs), 1278 (vs, C-O-C), 1114 (s), 800 (w).

MS (ESI): *m*/*z* (%) = 877.33 (29) $[M+H]^+$.

HR-MS (ESI): obs. *m*/*z* = 877.2725; calcd. for $[M]^+$ 877.2732.

UV/Vis (CH_2Cl_2): λ [nm] (ε / [10^4 $M^{-1}cm^{-1}$]) = 421 (44.4), 548 (1.88), 590 (0.36).

Fluorescence (CH_2Cl_2): λ [nm] (relative intensity) = 598 (0.97), 647(1.00).

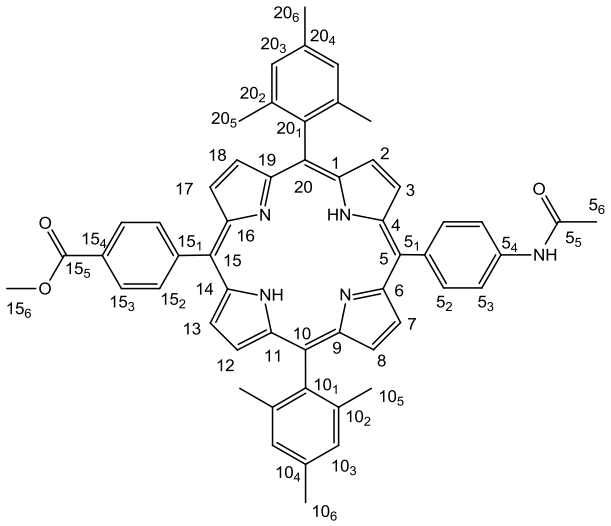
Quantum yield: Φ = 0.1001.

Lifetime: τ [ns] = 2.53 (100%).

CV (Fc/Fc$^+$, 100 mV s^{-1}, CH_2Cl_2): $E_{½}$[V] = –2.150, –1.780, 0.439, 0.739.

General procedure for *N*-acylation[S7]: To a mixture of the amino porphyrin (1 eq.) and acetyl chloride (35 eq.) iodine (1 eq.) was added and the mixture was stirred at room temperature over night. The iodine was destroyed by addition of a saturated aqueous $Na_2S_2O_3$ solution. CH_2Cl_2 was added and the organic phase was separated, washed with saturated aqueous $NaHCO_3$ solution (2×), brine (1×), water (2×) and dried with Na_2SO_4. The solvent was removed under reduced pressure and the residue was filtered over a silica pad.

5-(4-(*N*-Acetylaminophenyl))-10,20-bis(2,4,6-trimethylphenyl)-15-(4-(methoxycarbonyl-phenyl)) porphyrin (Ac-3a). 40.0 mg (0.052 mmol) Porphyrin **3a**, 12.9 mL (0.182 mol) acetyl chloride, 13.1 mg (0.052 mmol) iodine. [silica, toluene : ethyl acetate = 1 : 1, R_f = 0.38]. Yield: 34 mg (0.042 mmol, 81%), purple powder. $C_{54}H_{47}N_5O_3$ (813.98).



^{1}H-NMR (d_8-THF): δ = –2.50 (s, 2 H, $H^{pyrrole\text{-}NH}$), 1.83 (s, 12 H, $H^{10/20}{}_{5/5}$), 2.19 (s 3H, $H^5{}_6$), 2.59 (s, 6 H, $H^{10/20}{}_{6/6}$), 4.04 (s, 3 H, $H^{15}{}_6$), 7.30 (s, 4 H, $H^{10/20}{}_{3/3}$), 8.03 (d, $^3J_{HH}$ = 8.4 Hz, 2 H, $H^5{}_3$), 8.10 (d, 2 H, $^3J_{HH}$ = 8.4 Hz, $H^5{}_2$), 8.32 (d, $^3J_{HH}$ = 8.2 Hz, 2 H, $H^{15}{}_2$), 8.41 (d, $^3J_{HH}$ = 8.1 Hz, 2 H, $H^{15}{}_3$), 8.66 (ps. t, $^3J_{HH}$ = 4.5 Hz, 4 H, $H^{pyrrole}$), 8.74 (d, $^3J_{HH}$ = 4.6 Hz, 2 H, $H^{pyrrole}$), 8.84 (d, $^3J_{HH}$ = 4.6 Hz, 2 H, $H^{pyrrole}$), 9.40 (s, 1 H, $H^{amide\text{-}NH}$) ppm.

^{13}C{^{1}H}-NMR (d_8-THF): δ = 21.2 (s, $C^{10/20}{}_{5/5}$), 21.7 (s, $C^{10/20}{}_{6/6}$), 24.4 (s, $C^5{}_6$), 52.5 (s, $C^{15}{}_6$), 118.2 (s, $C^5{}_3$), 119.0 (s, C^{15}), 119.3 (s, $C^{10/20}$), 121.1 (C^5), 128.8 (s, $C^{15}{}_3$), 128.9 (s, $C^{10/20}{}_{3/3}$), 130.9 ($C^{15}{}_4$), 135.6 ($C^5{}_2$), 135.7 (s, $C^{15}{}_2$), 137.4, ($C^5{}_1$), 138.8 (s, $C^{10/20}{}_{4/4}$), 139.6 (s, $C^{10/20}{}_{2/2}$), 140.1 (s, $C^{10/20}{}_{1/1}$), 141.0 ($C^5{}_4$) 148.0 (s, $C^{15}{}_1$), 167.4 (s, $C^{15}{}_5$) 168.8 (s, $C^5{}_5$) ppm.

IR (KBr): $\tilde{\nu}$ [cm^{-1}] = 3406 (b, $NH^{pyrrole}$, NH^{amide}), 2954 (m, CH), 2921 (m, CH), 1723 (s, CO), 1702 (s, CO), 1513 (vs), 1381 (m), 1276 (vs, C-O-C), 968 (m).

MS (FD): *m*/*z* (%) = 814.2 (100) $[M]^+$.

MS (ESI): *m*/*z* (%) = 407.69 (2) $[M+H]^{2+}$, 814.37 (100) $[M]^+$.

HR-MS (ESI): obs. *m*/*z* = 814.3725; calcd. for $[M+H]^+$ 814.3757.

UV/Vis (CH_2Cl_2): λ [nm] (ε / [10^4 $M^{-1}cm^{-1}$]) = 420 (36.29), 516 (1.24), 550 (0.37), 593 (0.28), 652 (0.55).

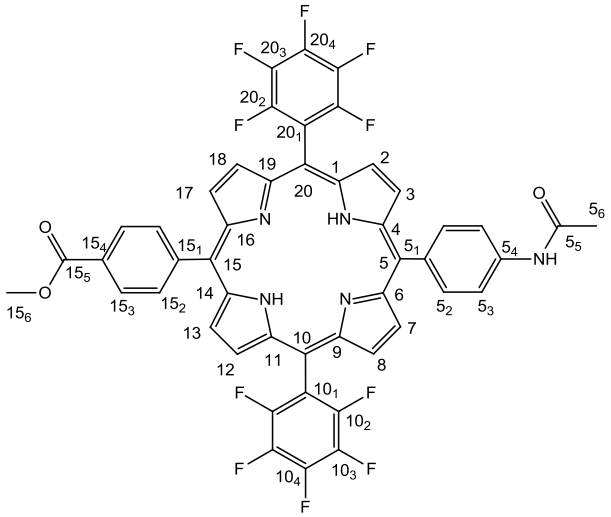
Fluorescence (CH_2Cl_2): λ [nm] (relative intensity) = 654 (1.00), 718 (0.21).

Quantum yield: Φ = 0.0778.

Lifetime: τ [ns] = 10.90 (100%).

CV (Fc/Fc^+, 100 mV s^{-1}, CH_2Cl_2): $E_{½}$[V] = –2.060, –1.710, 0.540, 0.960.

5-(4-(*N*-Acetylaminophenyl))- 10,20-bis(2,3,4,5,6-pentafluorophenyl)-15-(4-(methoxycarbonyl-phenyl)) porphyrin (Ac-3b). 27.5 mg (0.046 mmol) Porphyrin **3b**, 11.4 mL (0.159 mol) acetyl chloride, 5.8 mg (0.046 mmol) iodine. [silica, toluene : ethyl acetate = 1 : 1, R_f = 0.32]. Yield: 27 mg (0.030 mmol, 65%), purple powder. $C_{48}H_{25}F_{10}N_5O_3$ (909.73).



^{1}H-NMR (d$_8$-THF): δ = –2.78 (s, 2 H, H$^{pyrrole\text{-}NH}$), 2.21 (s, 3H, H$^5{}_6$), 4.05 (s, 3 H, H$^{15}{}_6$), 8.08 (m, 2 H, $^3J_{HH}$ = 8.3 Hz H$^5{}_3$), 8.14 (d, 2 H, $^3J_{HH}$ = 8.3 Hz, H$^5{}_2$), 8.36 (d, 2 H, $^3J_{HH}$ = 8.0 Hz, H$^{15}{}_2$), 8.46 (d, 2 H, $^3J_{HH}$ = 8.0 Hz, H$^{15}{}_3$), 8.91 (d, 2 H, $^3J_{HH}$ = 4.5 Hz, H^{pyrrole}), 9.01 (m, 6 H, H^{pyrrole}), 9.43 (s, 1 H$^{amide\text{-}NH}$) ppm.

^{13}C{^{1}H}-NMR (d$_8$-THF): δ = 24.4 (C$^5{}_6$), 52.6 (C$^{15}{}_6$), 118.2 (C$^5{}_3$), 120.9 (C^{15}), 122.9 (C^5), 129.0 (C$^{15}{}_3$), 131.0 (8 C) (br. s, C$^{2/3/7/8/12/13/17/18}$), 131.3 (C$^{15}{}_4$), 135.6 (C$^{15}{}_2$), 135.9 (C$^5{}_2$), 136.7 (C$^5{}_1$),141.4 (C$^5{}_4$), 137.7, 140.2, 146.6, 149.1 (m, C$^{10/20}{}_{1/1/2/2/3/3/4/4}$), 147.2 (C$^{15}{}_1$), 167.3 (C$^{15}{}_5$), 168.9 (C$^5{}_5$) ppm.

^{19}F-NMR (d$_8$-THF): δ = –166.7 (ddd, $^3J_{FF}$ = 23 Hz, $^3J_{FF}$ = 21 Hz, $^5J_{FF}$ = 8 Hz, 4 F, F$^{10/20}{}_{3/3}$,), –157.8 (t, $^3J_{FF}$ = 21 Hz, 2 F, F$^{10/20}{}_{4/4}$), –141.3 (dd, $^3J_{FF}$ = 24 Hz, $^5J_{FF}$ = 8 Hz, 4 F, F$^{10/20}{}_{2/2}$) ppm.

IR (KBr): $\tilde{\nu}$ [cm^{-1}] = 3417 (b, NH^{amide}, NH^{pyrrole}), 2924 (w, CH), 1719 (m, CO), 1699 (m, CO), 1518 (vs), 1496 (vs), 1276 (m), 1109 (w, CF), 1044 (w, CF), 1037 (w, CF), 987 (vs), 918 (s).

MS (FD): *m*/*z* (%) = 909.67 (100) [M]$^+$.

MS (ESI): *m*/*z* (%) = 910.21 (100) [M]$^+$, 1820.41 (49) [2M+H]$^+$.

HR-MS (ESI): obs. *m*/*z* = 910.1898; calcd. for [M+H]$^+$ 910.1876.

UV/Vis (CH_2Cl_2): λ [nm] (ε / [10^4 M^{-1}cm^{-1}]) = 418 (39.31), 512 (2.38), 545 (0.84), 587 (0.93), 642 (0.56).

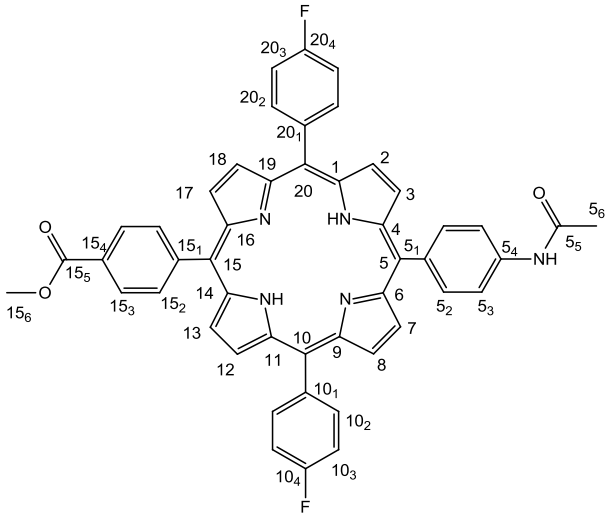
Fluorescence (CH_2Cl_2): λ [nm] (relative intensity) = 647 (1.00), 713 (0.50).

Quantum yield: Φ = 0.0696.

Lifetime: τ [ns] = 9.83 (100%)

CV (Fc/Fc$^+$, 100 mV s^{-1}, CH_2Cl_2): $E_{½}$[V] = –1.810, –1.410, 0.820, 1.030

5-(4-(*N*-Acetylaminophenyl))-10,20-bis(4-fluorophenyl)-15-(4-(methoxycarbonylphenyl)) porphyrin (Ac-3c). 33.0 mg (0.046 mmol) Porphyrin **3c**, 11.4 mL (0.159 mol) acetyl chloride, 5.8 mg (0.046 mmol) iodine. [silica, toluene : ethyl acetate = 1 : 1, R_f = 0.35]. Yield: 24 mg (0.031 mmol, 70%), purple powder. $C_{48}H_{33}F_2N_5O_3$ (765.80).



^{1}H-NMR (d$_8$-THF): δ = –2.71 (s, 2 H, H$^{\text{pyrrole-NH}}$), 2.21 (s, 3 H, H$^5{}_6$), 4.05 (s, 3 H, H$^{15}{}_6$), 7.53 (t, $^3J_{HH}$ = 8.6 Hz, 4 H, H$^{10/20}{}_{3/3}$), 8.06 (d, $^3J_{HH}$ = 8.4 Hz, 2 H, H$^5{}_3$), 8.10 (d, $^3J_{HH}$ = 8.4 Hz, 2 H, H$^5{}_2$), 8.21 (dd, $^3J_{HH}$ = 7.9 Hz, $^3J_{HF}$ = 2.3 Hz, 4 H, H$^{10/20}{}_{2/2}$), 8.32 (d, $^3J_{HH}$ = 8.0 Hz, 2 H, H$^{15}{}_2$), 8.44 (d, $^3J_{HH}$ = 7.9 Hz, 2 H, H$^{15}{}_3$), 8.82 (m, 6 H, H$^{\text{pyrrole}}$), 8.91(d, $^3J_{HH}$ = 4.3 Hz, 2 H, H$^{\text{pyrrole}}$), 9.46 (s, 1 H, H$^{\text{amide-NH}}$) ppm.

^{13}C{^{1}H}-NMR (d$_8$-THF): δ = 24.4 (s, C$^5{}_6$), 52.6 (s, C$^{15}{}_6$), 114.7 (d, $^2J_{CF}$ = 21.6 Hz , C$^{10/20}{}_{3/3}$), 118.1 (s, C$^5{}_3$), 119.7 (s, C^{15}), 120.1 (s, C$^{10/20}$), 121.8 (s, C^5), 128.9 (s, C$^{15}{}_3$), 131.0 (s, C$^{15}{}_4$), 131.9 (br. s C$^{\text{pyrrole}}$), 135.6 (s, C$^{15}{}_2$), 135.8 (s, C$^5{}_2$), 136.9 (d, $^3J_{CF}$ = 8.1 Hz, C$^{10/20}{}_{2/2}$), 137.5 (s, C$^5{}_1$), 139.4 (d, $^4J_{CF}$ = 3.1 Hz, C$^{10/20}{}_{1/1}$), 141.1 (s, C$^5{}_4$), 148.0 (s, C$^{15}{}_1$), 164.1(d, $^1J_{FH}$ = 246.5 Hz, C$^{10/20}{}_{4/4}$), 167.4 (s, C$^{15}{}_5$), 168.9 (s, C$^5{}_5$) ppm.

^{19}F-NMR (d$_8$-THF): δ = –117.7 (tt, $^3J_{FH}$ = 8.6 Hz, $^4J_{FH}$ = 5.4 Hz) ppm.

IR (KBr): $\tilde{\nu}$ [cm^{-1}] = 3419 (b, NH$^{\text{amide}}$), 3321 (w, NH$^{\text{pyrrole}}$), 2927 (w, CH), 2853 (w, CH), 1715 (m, CO), 1593 (m), 1503 (m), 1282 (m, C-O-C), 1151 (s, CF), 800 (vs).

MS (FD): *m*/*z* (%) = 765.2 (100) [M]$^+$.

MS (ESI): *m*/*z* (%) = 766.26 (100) [M+H]$^+$.

HR-MS (ESI): obs. *m*/*z* = 766.2621; calcd. for [M+H]$^+$ 766.2630.

UV/Vis (CH_2Cl_2): λ [nm] (ε / [10^4 M^{-1}cm^{-1}]) = 419 (50.42), 515 (2.16), 551 (1.07), 591 (0.72), 647 (0.61).

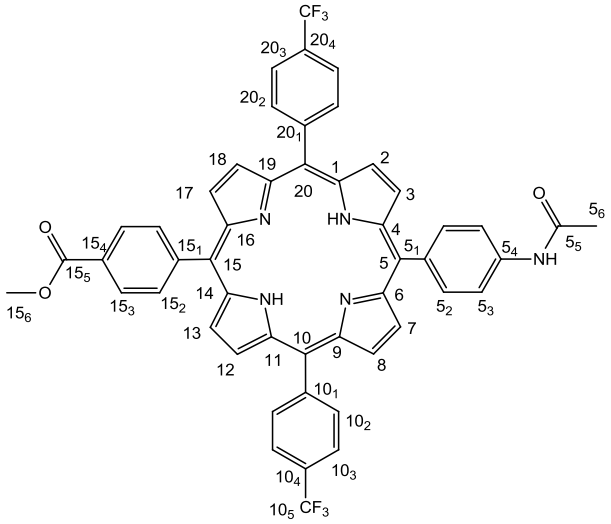
Fluorescence (CH_2Cl_2): λ [nm] (relative intensity) = 652 (1.00), 717 (0.32).

Quantum yield: Φ = 0.1003.

Lifetime: τ [ns] = 9.64 (100%).

CV (Fc/Fc$^+$, 100 mV s^{-1}, CH_2Cl_2): $E_{½}$[V] = –1.920, –1.590, 0.590, 0.870.

5-(4-(*N*-Acetylaminophenyl))-10,20-bis((4-trifluoromethyl)phenyl)-15-(4-(methoxycarbonylphenyl)) porphyrin (Ac-3d). 50.0 mg (0.069 mmol) Porphyrin **3d**, 17.2 mL (0.240 mol) acetyl chloride, 8.8 mg (0.069 mmol) iodine. [silica, toluene : ethyl acetate = 1 : 1, R_f = 0.45]. Yield: 40 mg (0.046 mmol, 67%), purple powder. $C_{50}H_{33}F_6N_5O_3$ (865.82).



^{1}H-NMR (d$_8$-THF): δ = –2.71 (s, 2 H, H$^{\text{pyrrole-NH}}$), 2.21 (s, 3 H, H$^{5}{}_{6}$), 4.05 (s, 3 H, H$^{15}{}_{6}$), 8.08 (m, 4 H, H$^{5/5}{}_{2/3}$), 8.11 (d, $^3J_{HH}$ = 8.1 Hz, 4 H, H$^{10/20}{}_{3/3}$), 8.32 (d, $^3J_{HH}$ = 8.1 Hz, 2 H, H$^{15}{}_{2}$), 8.41 (d, $^3J_{HH}$ = 7.9 Hz, 4 H, H$^{10/20}{}_{2/2}$), 8.44 (d, $^3J_{HH}$ = 8.1 Hz, 2 H, H$^{15}{}_{3}$), 8.81 (m, 6 H, H$^{\text{pyrrole}}$), 8.93 (d, $^3J_{HH}$ = 4.5, 2 H, H$^{\text{pyrrole}}$), 9.45 (s, 1 H, H$^{\text{amide-NH}}$) ppm.

^{13}C{^{1}H}-NMR (d$_8$-THF): δ = 23.2 (s, C$^{5}{}_{6}$), 52.7 (s, C$^{15}{}_{6}$), 118.3 (s, C$^{5}{}_{3}$), 119.8 (s, C$^{10/20}$), 120.2 (s, C^{15}), 122.3 (s, C^{5}), 124.8 (s, C$^{10/20}{}_{4/34}$), 124.9 (d, $^4J_{CF}$ = 3.3 Hz, C$^{10/20}{}_{3/3}$), 127.5 (s, C$^{10/20}{}_{4/4}$), 129.0 (s, C$^{15}{}_{3}$), 130.4 (q, $^1J_{CF}$ = 32.2 Hz, C$^{10/20}{}_{5/5}$), 131.2 (s, C$^{15}{}_{4}$), 132.1 (br. s, C^{2,3,7,8,12,13,17,18}), 135.7 (s, C$^{15}{}_{2}$), 136.0 (m, C$^{5/10/20}{}_{2/2/2}$), 137.4 (s, C$^{5}{}_{1}$), 141.3 (s, C$^{5}{}_{4}$), 147.4 (s, C$^{10/20}{}_{1/1}$), 147.9 (s, C$^{15}{}_{1}$), 167.5 (s, C$^{15}{}_{5}$), 169.0 (s, C$^{5}{}_{5}$) ppm.

^{19}F-NMR (d$_8$-THF): δ = –65.0 (s).

IR (KBr): $\tilde{\nu}$ [cm^{-1}] = 3419 (b, NH$^{\text{amide}}$), 3321 (w, NH$^{\text{pyrrole}}$), 2952 (w, CH), 1724 (s, CO), 1609 (m), 1511 (m), 1282 (s, C-O-C), 1127 (s, CF), 808 (s).

MS (FD): *m*/*z* (%) = 865.6 (100) [M]$^+$.

MS (ESI): *m*/*z* (%) = 866.27 (100) [M+H]$^+$.

HR-MS (ESI): obs. *m*/*z* = 866.2566; calcd. for [M+H]$^+$ 866.2563.

UV/Vis (CH$_2$Cl$_2$): λ [nm] (ε / [10^4 M^{-1}cm^{-1}]) = 419 (41.4), 515 (1.78), 550 (0.79), 590 (0.57), 646 (0.40).

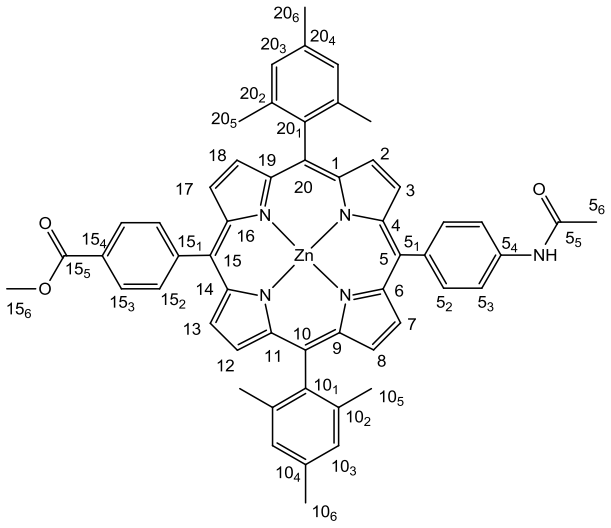
Fluorescence (CH$_2$Cl$_2$): λ [nm] (relative intensity) = 650 (1.00), 716 (0.36).

Quantum yield: Φ = 0.1080.

Lifetime: τ [ns] = 9.98 (100%).

CV (Fc/Fc$^+$, 100 mV s^{-1}, CH$_2$Cl$_2$): $E_{½}$[V] = –1.900, –1.550, 0.640, 0.890.

[5-(4-(*N*-Acetylaminophenyl))-10,20-bis(2,4,6-trimethylphenyl)-15-(4-(methoxycarbonyl-phenyl)) porphyrinato]zinc(II) (Zn-Ac-3a). Porphyrin **Ac-3a** (25 mg, 0.031 mmol) and zinc acetate dihydrate (34 mg, 0.15 mmol) were stirred overnight in CH_2Cl_2 (5 mL). After concentration under reduced pressure the product was isolated by column chromatography [silica, toluene : ethyl acetate = 1 : 1, R_f = 0.50]. Yield 23 mg (0.026 mmol, 85%), purple powder. $C_{54}H_{45}N_5O_3Zn$ (877.35).



^{1}H-NMR (d_8-THF): δ = 1.85 (s, 12 H, $H^{10/20}{}_{5/5}$), 2.20 (s 3H, $H^5{}_6$), 2.61 (s, 6 H, $H^{10/20}{}_{6/6}$), 4.04 (s, 3 H, $H^{15}{}_6$), 7.29 (s, 4 H, $H^{10/20}{}_{3/3}$), 8.00 (d, $^3J_{HH}$ = 8.2 Hz, 2 H, $H^5{}_3$), 8.10 (d, 2 H, $^3J_{HH}$ = 8.4 Hz, $H^5{}_2$), 8.31 (d, $^3J_{HH}$ = 8.2 Hz, 2 H, $H^{15}{}_2$), 8.39 (d, $^3J_{HH}$ = 8.0 Hz, 2 H, $H^{15}{}_3$), 8.66 (ps. t, $^3J_{HH}$ = 4.6 Hz, 4 H, $H^{pyrrole}$), 8.74 (d, $^3J_{HH}$ = 4.6 Hz, 2 H, $H^{pyrrole}$), 8.84 (d, $^3J_{HH}$ = 4.6 Hz, 2 H, $H^{pyrrole}$), 9.38 (s, 1 H, $H^{amide\text{-}NH}$) ppm.

^{13}C{^{1}H}-NMR (d_8-THF): δ = 21.7 (s, $C^{10/20}{}_{6/6}$), 22.1 (s, $C^{10/20}{}_{5/5}$), 24.4 (s, $C^5{}_6$), 52.5 (s, $C^{15}{}_6$), 117.6 ($C^5{}_3$), 119.4 (s, C^{15}) 119.6 ($C^{10/20}$), 121.4 (s, C^5), 128.4 (s, $C^{15}{}_3$), 128.7 (s, $C^{10/20}{}_{3/3}$), 130.4 (s, $C^{15}{}_4$), 130.9, 131.2, 132.4, 133.3 (s, $C^{2,3,7,8,12,13,17,18}$), 135.6 (s, $C^{15}{}_2$), 135.6 (s, $C^5{}_2$), 138.3 (s, $C^5{}_1$), 140.0 (s, $C^{10/20}{}_{2/2}$), 140.6 (s, $C^5{}_4$), 140.8 (s, $C^{10/20}{}_{1/1}$), 149.6 (s, $C^{15}{}_1$), 150.4, 150.7, 150.9, 151.3 (s, $C^{1,4,6,9,11,14,16,19}$), 167.5 (s, $C^{15}{}_5$), 168.7 (s, $C^5{}_5$) ppm.

IR (KBr): $\tilde{\nu}$ [cm^{-1}] = 3404 (b, NH^{amide}), 2922 (w, CH), 2853 (w, CH), 1732 (m, CO), 1668 (m, CO), 1495 (m), 1398 (m), 1278 (s), 995 (vs), 798 (m).

MS (FD): *m*/*z* (%) = 875.79 (100) $[M]^+$.

MS (ESI): *m*/*z* (%) = 875.31 (88), 877.31 (100), 879.31 (68), $[M]^+$.

HR-MS (ESI): obs. *m*/*z* = 877.2823; calcd. for $[M]^+$ 875.2814.

UV/Vis (CH_2Cl_2): λ [nm] (ε / [10^4 $M^{-1}cm^{-1}$]) = 423 (45.12), 551 (1.92), 592 (0.45).

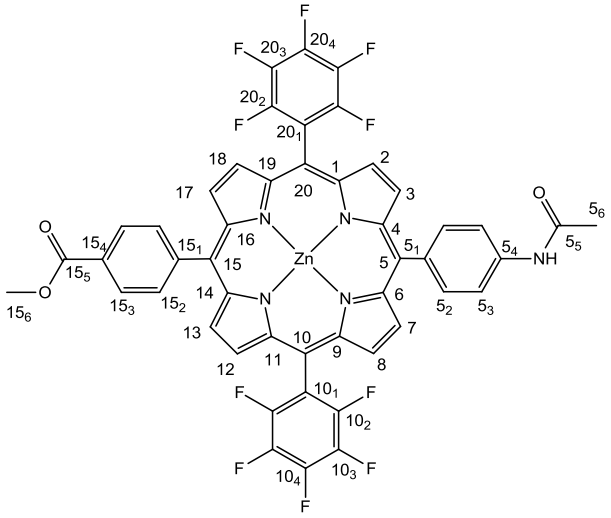
Fluorescence (CH_2Cl_2): λ [nm] (relative intensity) = 604 (1.00), 652 (0.99).

Quantum yield: Φ = 0.1343.

Lifetime: τ [ns] = 2.17 (100%).

CV (Fc/Fc^+, 100 mV s^{-1}, CH_2Cl_2): $E_{½}$[V] = –1.860, 0.335, 0.750.

[5-(4-(*N*-Acetylaminophenyl))-10,20-bis(2,3,4,5,6-pentafluorophenyl)-15-(4-(methoxycarbonyl-phenyl)) porphyrinato]zinc(II) (Zn-Ac-3b). Porphyrin **Ac-3b** (15 mg, 0.016 mmol) and zinc acetate dihydrate (18 mg, 0.08 mmol) were stirred overnight in CH_2Cl_2 (5 mL). After concentration under reduced pressure the product was isolated by column chromatography [silica, toluene : ethyl acetate = 1 : 1, R_f = 0.48]. Yield 14 mg (0.014 mmol, 87%), purple powder. $C_{48}H_{23}F_{10}N_5O_3Zn$ (973.09).



^{1}H-NMR (d$_8$-THF): δ = 2.21 (s, 3H, $H^5{}_6$), 4.06 (s, 3 H, $H^{15}{}_6$), 8.05 (m, 2 H, $^3J_{HH}$ = 8.3 Hz $H^5{}_3$), 8.10(d, 2 H, $^3J_{HH}$ = 8.3 Hz, $H^5{}_2$), 8.33 (d, 2 H, $^3J_{HH}$ = 8.0 Hz, $H^{15}{}_2$), 8.43 (d, 2 H, $^3J_{HH}$ = 8.0 Hz, $H^{15}{}_3$), 8.89 (d, 2 H, $^3J_{HH}$ = 4.6 Hz, $H^{pyrrole}$), 8.98 (m, 6 H, $H^{pyrrole}$), 9.42 (s, 1 $H^{amide\text{-}NH}$) ppm.

^{13}C{^{1}H}-NMR (d$_8$-THF): δ = 24.4 ($C^5{}_6$), 52.6 ($C^{15}{}_6$), 117.8 ($C^5{}_3$), 121.3 (C^{15}), 123.2 (C^5), 128.6 ($C^{15}{}_3$), 131.0, 131.3, 133.6, 134.3 ($C^{2,3,7,8,12,13,17,18}$), 130.8 ($C^{15}{}_4$), 135.6 ($C^{15}{}_2$), 135.9 ($C^5{}_2$), 138.2 ($C^5{}_1$), 140.9 ($C^5{}_4$), 137.5, 140.0, 146.6, 149.0 (m, $C^{10/20}{}_{1/1/2/2/3/3/4/4}$), 148.8 ($C^{15}{}_1$), 150.5, 150.7, 151.3, 152.3 ($C^{1,4,6,9,11,14,16,19}$), 167.4 ($C^{15}{}_5$), 168.8 ($C^5{}_5$) ppm.

^{19}F-NMR (d$_8$-THF): δ = –167.2 (ddd, $^3J_{FF}$ = 24 Hz, $^3J_{FF}$ = 21 Hz, $^5J_{FF}$ = 8 Hz, 4 F, $F^{10/20}{}_{3/3}$,), –158.6 (t, $^3J_{FF}$ = 21 Hz, 2 F, $F^{10/20}{}_{4/4}$), –141.5 (dd, $^3J_{FF}$ = 24 Hz, $^5J_{FF}$ = 8 Hz, 4 F, $F^{10/20}{}_{2/2}$) ppm.

IR (KBr): $\tilde{\nu}$ [cm^{-1}] = 3442 (b, NH^{amide}), 2926 (w, CH), 2851 (w, CH), 1720 (m, CO), 1518 (vs), 1493 (vs), 1282 (m), 1114 (w, CF), 1074 (w, CF), 1053 (w, CF), 989 (vs), 918 (vs), 939 (s).

MS (FD): *m*/*z* (%) = 971.35 (100) $[M]^+$.

MS (ESI): *m*/*z* (%) = 971.10 (43) $[M]^+$), 972.11 (100) $[M+H]^+$.

HR-MS (ESI): obs. *m*/*z* = 971.0931; calcd. for $[M]^+$ 971.0933.

UV/Vis (CH_2Cl_2): λ [nm] (ε / [10^4 $M^{-1}cm^{-1}$]) = 422 (51.09), 552 (2.01), 593 (0.36).

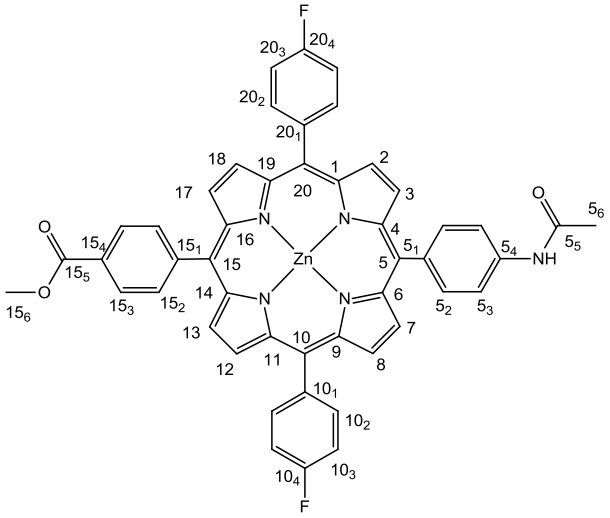
Fluorescence (CH_2Cl_2): λ [nm] (relative intensity) = 602 (1.00), 652 (0.92).

Quantum yield: Φ = 0.0771.

Lifetime: τ [ns] = 1.94 (100%).

CV (Fc/Fc$^+$, 100 mV s^{-1}, CH_2Cl_2): $E_{½}$[V] = –1.980, –1.580, 0.600, 0.940.

[5-(4-(*N*-Acetylaminophenyl))-10,20-bis(4-fluorophenyl)-15-(4-(methoxycarbonyl-phenyl)) porphyrinato]zinc(II) (Zn-Ac-3c). Porphyrin **Ac-3c** (12 mg, 0.016 mmol) and zinc acetate dihydrate (15 mg, 0.15 mmol) were stirred overnight in CH_2Cl_2 (5 mL). After concentration under reduced pressure the product was isolated by column chromatography [silica, toluene : ethyl acetate = 1 : 1, R_f = 0.50]. Yield 13 mg (0.015 mmol, 94%), purple powder. $C_{48}H_{31}F_2N_5O_3Zn$ (829.20).



^{1}H-NMR (d$_8$-THF): δ = 2.20 (s, 3 H, $H^5{}_6$), 4.05 (s, 3 H, $H^{15}{}_6$), 7.50 (t, $^3J_{HH}$ = 8.6 Hz, 4 H, $H^{10/20}{}_{3/3}$), 8.03 (d, $^3J_{HH}$ = 8.3 Hz, 2 H, $H^5{}_3$), 8.08 (d, $^3J_{HH}$ = 8.4 Hz, 2 H, $H^5{}_2$), 8.18 (dvd, $^3J_{HH}$ = 8.1 Hz, $^3J_{HF}$ = 2.4 Hz, 4 H, $H^{10/20}{}_{2/2}$), 8.30 (d, $^3J_{HH}$ = 8.0 Hz, 2 H, $H^{15}{}_2$), 8.41 (d, $^3J_{HH}$ = 8.0 Hz, 2 H, $H^{15}{}_3$), 8.83 (m, 6 H, $H^{pyrrole}$), 8.92 (d, $^3J_{HH}$ = 4.6 Hz, 2 H, $H^{pyrrole}$), 9.41 (s, 1 H, $H^{amide\text{-}NH}$) ppm.

^{13}C{^{1}H}-NMR (d$_8$-THF): δ = 24.4 (s, $C^5{}_6$), 52.5 (s, $C^{15}{}_6$), 114.2 (d, $^2J_{CF}$ = 21.4 Hz , $C^{10/20}{}_{3/3}$), 117.8 (s, $C^5{}_3$), 120.2 (s, C^{15}), 120.6 (s, $C^{10/20}$), 122.3 (s, C^5), 128.5 (s, $C^{15}{}_3$), 130.5 (s, $C^{15}{}_4$), 132.1, 132.2, 132.5, 132.8 (s, $C^{pyrrole\ 2,3,7,8,12,13,17,18}$), 135.6 (s, $C^{15}{}_2$), 135.7 (s, $C^5{}_2$), 136.8 (d, $^3J_{CF}$ = 7.9 Hz, $C^{10/20}{}_{2/2}$), 138.8 (s, $C^5{}_1$), 140.7 (d, $^4J_{CF}$ = 2.9 Hz, $C^{10/20}{}_{1/1}$), 140.7 (s, $C^5{}_4$), 149.4 (s, $C^{15}{}_1$), 150.7, 151.2, 151.3, 151.6 (s, $C^{1,4,6,9,11,14,16,19}$), 163.9 (d, $^1J_{FH}$ = 245.7 Hz, $C^{10/20}{}_{4/4}$), 167.5 (s, $C^{15}{}_5$), 168.7 (s, $C^5{}_5$) ppm.

^{19}F-NMR (d$_8$-THF): δ = –118.6 (tt, $^3J_{FH}$ = 8.6 Hz, $^4J_{FH}$=5.4 Hz).

IR (KBr): $\tilde{\nu}$ [cm^{-1}] = 3432 (b, NH^{amide}), 2926 (w, CH), 1698 (m, CO) 1598 (m), 1507 (m), 1283 (m, C-O-C), 1159 (s, CF), 993 (vs), 802 (vs).

MS (FD): *m*/*z* (%) = 827.3 (92) $[M]^+$.

MS (ESI): *m*/*z* (%) = 828.18 (4) $[M+H]^+$.

HR-MS (ESI): obs. *m*/*z* = 827.1695; calcd. for $[M]^+$ 827.1686.

UV/Vis (CH_2Cl_2): λ [nm] (ε / [10^4 $M^{-1}cm^{-1}$]) = 420 (41.45), 548 (1.87), 587 (0.50).

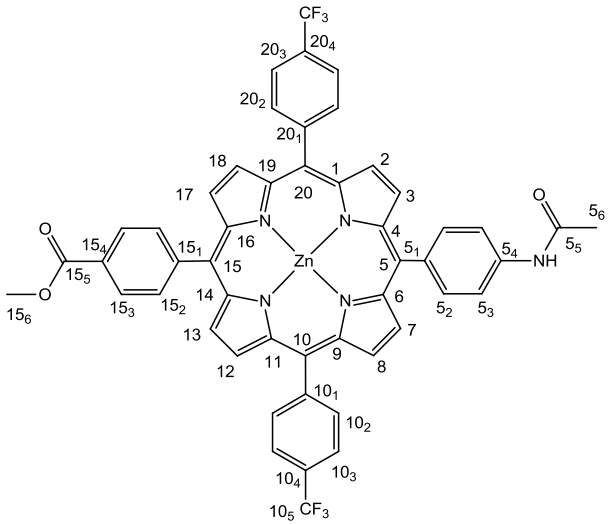
Fluorescence (CH_2Cl_2): λ [nm] (relative intensity) = 598 (0.97), 646 (1.00).

Quantum yield: Φ = 0.0569.

Lifetime: τ [ns] = 1.85 (100%).

CV (Fc/Fc$^+$, 100 mV s^{-1}, CH_2Cl_2): $E_{½}$[V] = –2.110, –1.750, 0.380, 0.780.

[5-(4-(*N*-Acetylaminophenyl))-10,20-bis((4-trifluoromethyl)phenyl)-15-(4-(methoxycarbonylphenyl)) porphyrinato]zinc(II) (Zn-Ac-3d). Porphyrin **Ac-3d** (20 mg, 0.023 mmol) and zinc acetate dihydrate (25 mg, 0.11 mmol) were stirred overnight in CH_2Cl_2 (10 mL). After concentration under reduced pressure the product was isolated by column chromatography [silica, toluene : ethyl acetate = 1 : 1, R_f = 0.40]. Yield 18 mg (0.019 mmol, 82%), purple powder. $C_{50}H_{31}F_6N_5O_3Zn$ (929.18).



^{1}H-NMR (d$_8$-THF): δ = 2.19 (s, 3 H, $H^5{}_6$), 4.04 (s, 3 H, $H^{15}{}_6$), 8.02 (d, $^3J_{HH}$ = 8.3 Hz, 2 H, $H^5{}_3$), 8.08 (m, 6 H, $H^{10/20/5}{}_{3/3/2}$), 8.30 (d, $^3J_{HH}$ = 7.99 Hz, 2 H, $H^{15}{}_2$), 8.40 (m, 4 H, $H^{15/10/20}{}_{3/2/2}$), 8.82 (m, 6 H, $H^{pyrrole}$), 8.93 (d, $^3J_{HH}$ = 4.5 Hz, 2 H, $H^{pyrrole}$), 9.40 (s, 1 H, $H^{amide\text{-}NH}$) ppm.

^{13}C{^{1}H}-NMR (d$_8$-THF): δ = 24.6 (s, $C^5{}_6$), 52.7 (s, $C^{15}{}_6$), 117.9 (s, $C^5{}_3$), 120.3 (s, $C^{10/20}$), 120.7 (s, C^{15}), 122.8 (s, C^5), 124.5 (d, $^4J_{CF}$ = 3.4 Hz, $C^{10/20}{}_{2/2}$), 127.6 (s, $C^{10/20}{}_{4/4}$), 128.7 (s, $C^{15}{}_3$), 130.5 (q, $^1J_{CF}$ = 38.2 Hz, $C^{10/20}{}_{5/5}$), 130.8 (s, $C^5{}_4$), 132.3, 132.6, 132.6, 133.3 (s, $C^{pyrrole\ 2,3,7,8,12,13,17,18}$), 135.7 (s, $C^5{}_2$), 135.9 (s, $C^{15}{}_2$), 136.0 (m, $C^{10/20}{}_{2/2}$), 138.7 (s, $C^5{}_4$) 140.9 (s, $C^5{}_4$), 148.8 (m, $C^{10/20}{}_{1/1}$), 149.3 (s, $C^{15}{}_1$), 150.8, 150.9, 151.0, 151.9 (s, $C^{pyrrole\ 1,4,6,9,11,14,16,19}$), 167.6 (s, $C^{15}{}_5$), 168.9 (s, $C^5{}_5$) ppm.

^{19}F-NMR (d$_8$-THF): δ = –64.9 (s) ppm.

IR (KBr): $\tilde{\nu}$ [cm^{-1}] = 3433 (b, NH^{amide}), 2929 (w, CH), 2854 (w, CH), 1724 (w, CO), 1703 (w, CO), 1610 (m), 1517 (w), 1387 (w), 1283 (m, C-O-C), 1163 (m, CF), 1126 (s), 997 (s), 792 (s).

MS (FD): *m*/*z* (%) = 927.2 (100) $[M]^+$.

MS (ESI): *m*/*z* (%) = 927.19 (40) $[M]^+$, 950.17 (97) $[M+Na]^+$.

HR-MS (ESI): obs. *m*/*z* = 950.1512; calcd. for $[M+Na]^+$ 950.1512.

UV/Vis (CH_2Cl_2): λ [nm] (ε / [10^4 $M^{-1}cm^{-1}$]) = 420 (28.3), 548 (1.17), 588 (0.21).

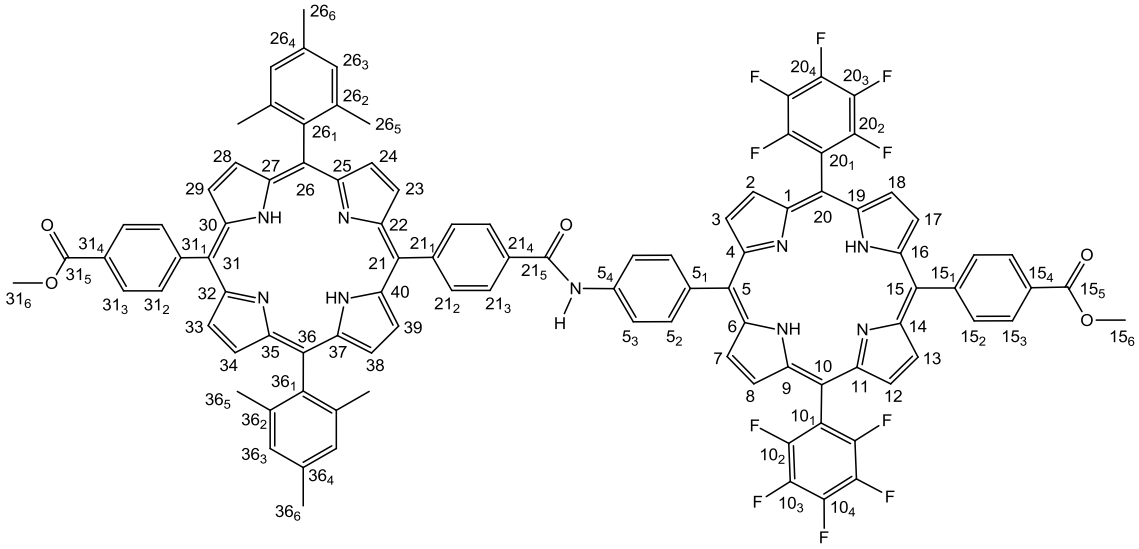
Fluorescence (CH_2Cl_2): λ [nm] (relative intensity) = 597 (0.81), 645 (1.00).

Quantum yield: Φ = 0.0838.

Lifetime: τ [ns] = 2.07 (100%).

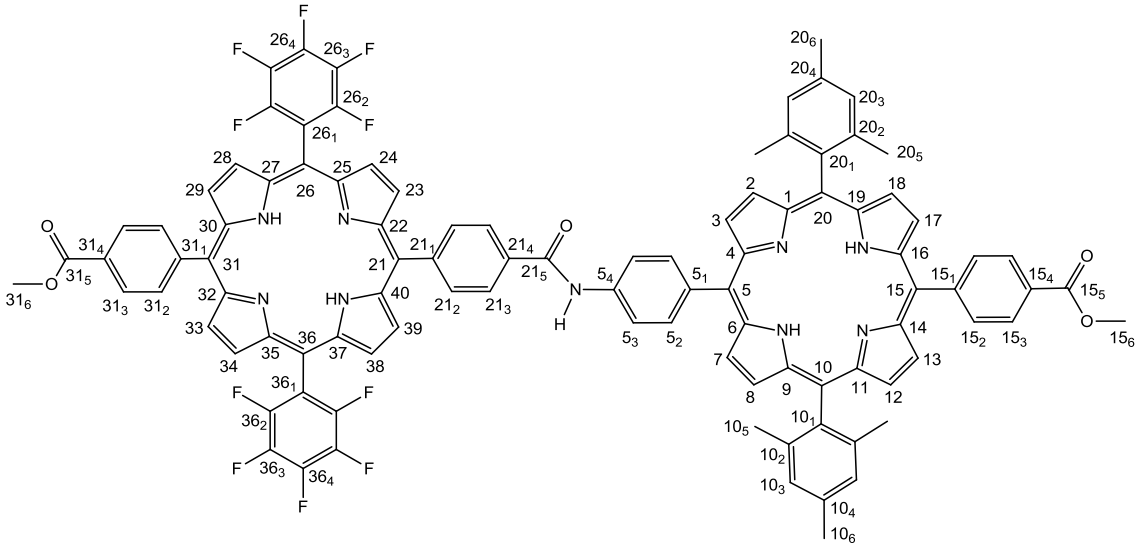
CV (Fc/Fc$^+$, 100 mV s^{-1}, CH_2Cl_2): $E_{½}$[V] = –2.010, –1.560, 0.420, 0.850.

General synthesis of bis(porphyrins) 4a, 4b, 4c, 4d, Zn^2-4d: The porphyrin acid component was dissolved in anhydrous CH_2Cl_2, 1-chloro-*N*,*N*,2-trimethylpropenylamine (Ghosez' reagent) was added and the reaction mixture was stirred under nitrogen for 3h at room temperature. After the acid chloride formed (TLC control) excess of Ghosez' reagent and solvent were removed by evaporation under reduced pressure. In order to remove the *N*,*N*-dimethyl amide byproduct anhydrous CH_2Cl_2 was added and the volatiles were again evaporated. The acid chloride was dissolved in CH_2Cl_2 (with 1 drop of triethylamine) and the solution was added dropwise to a solution of the porphyrin amino component in CH_2Cl_2 (with 1 drop of triethylamine). The reaction mixture was stirred for 12h at room temperature, washed with water and the organic phase was concentrated under reduced pressure. After column chromatography (silica, CH_2Cl_2/ethyl acetate 100:1) the respective dyad was isolated.



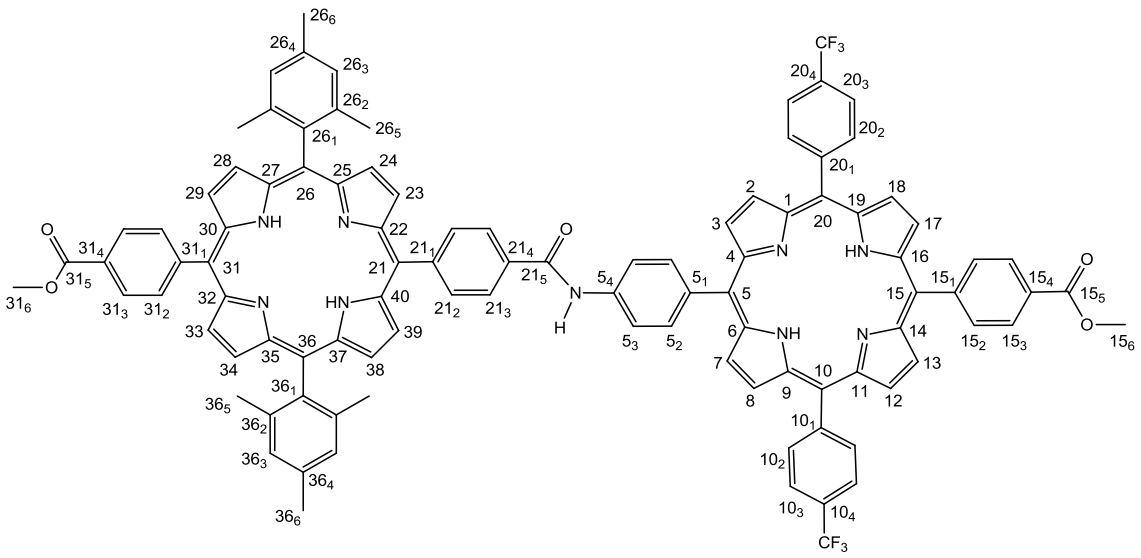
4a: 2a (10.0 mg, 0.012 mmol), CH_2Cl_2 (3×5 mL), 1-chloro-*N*,*N*,2-trimethylpropenylamine (7 µL, 0.048 mmol), triethylamine (2×1 drop), **3b** (8.7 mg, 0.010 mmol). Yield: 6.1 mg (0.0037 mmol, 37%), purple powder. $C_{99}H_{65}F_{10}N_9O_5$ (1650.61). R_f = 0.35 (silica, CH_2Cl_2/ethyl acetate 100:1). ^{1}H NMR ($CDCl_3$): δ = –2.80 (s, 2 H, $H^{C6F5\text{-}pyrroleNH}$), –2.56 (s, 2 H, $H^{Mes\text{-}pyrroleNH}$), 1.87 (s, 12 H, $H^{26/36}{}_{5/5}$), 2.65 (s, 6 H, $H^{26/36}{}_{6/6}$), 4.12 (s, 3 H, $H^{31}{}_6$), 4.14 (s, 3 H, $H^{15}{}_6$), 7.31 (s, 4 H, $H^{26/36}{}_{3/3}$), 8.22 (d, $^3J_{HH}$ = 8.3 Hz, 2 H, $H^5{}_3$), 8.34 (m, 6 H, $H^{5/15/31}{}_{2/2/2}$), 8.44 (d, $^3J_{HH}$ = 8.2 Hz, 2 H, $H^{21}{}_2$), 8.47 (m, 6 H, $H^{15/21/31}{}_{3/3/3}$), 8.72 (d, $^3J_{HH}$ = 4.8 Hz, 2 H, $H^{pyrrole}$), 8.74 (m, 4 H, $H^{pyrrole}$), 8.85 (d, $^3J_{HH}$ = 4.7 Hz, 2 H, $H^{pyrrole}$), 8.89 (d, $^3J_{HH}$ = 4.5 Hz, 2 H, $H^{pyrrole}$), 8.92 (d, $^3J_{HH}$ = 4.7 Hz, 4 H, $H^{pyrrole}$), 9.00 (d, $^3J_{HH}$ = 4.7 Hz, 2 H, $H^{pyrrole}$) ppm; $H^{amide\text{-}NH}$ not observed. $^{13}C\{^1H\}$ NMR ($CDCl_3$): δ = 21.5 ($C^{10/20}{}_{6/6}$), 21.7 ($C^{10/20}{}_{5/5}$), 52.4, 52.5 ($C^{15/31}{}_{6/6}$), 118.6, 119.0, 120.0 ($C^{5/10/15/20/21/26/31/36}$), 118.6 ($C^5{}_3$), 127.8, 127.9, 128.1 ($C^{15/21/31}{}_{3/3/3}$), 127.8 ($C^{26/36}{}_{3/3}$), 130.2, 137.8 ($C^{15/31}{}_{4/4}$), 130.2 ($C^{pyrrole\ 2,3,7,8,12,13,17,18}$), 134.6, 135.0, 135.3, ($C^{5/15/31/21}{}_{2/2/2/2}$), 138.3 ($C^{26/36}{}_{1/1}$), 138.6 ($C^5{}_1$), 139.4 ($C^{26/36}{}_{2/2}$), 145.8 ($C^5{}_4$), 147.0 ($C^{21}{}_4$), 165.9 ($C^{21}{}_5$), 167.1, 167.4 ($C^{15/31}{}_{5/5}$) ppm. ^{19}F NMR ($CDCl_3$): δ = –162.0 (ddd, $^3J_{FF}$ = 23 Hz, $^3J_{FF}$ = 21 Hz, $^5J_{FF}$ = 8 Hz, 4 F, $F^{10/20}{}_{3/3}$), –152.0 (t, $^3J_{FF}$ = 21 Hz, 2 F, $F^{10/20}{}_{4/4}$), –136.7 (dd, $^3J_{FF}$ = 24 Hz, $^5J_{FF}$

= 8 Hz, 4 F, $F^{10/20}{}_{2/2}$) ppm. MS (FD): *m/z* (%) = 1650.1 (100) $[M]^+$. MS (ESI): *m/z* (%) = 825.8 (83) $[M+H]^{2+}$, 1650.1 (87) $[M]^+$, 1651.5 (100) $[M+H]^+$. HR-MS (ESI): obs. *m/z* = 1650.4983; calcd. for $[M+H]^+$ 1650.5027. IR (KBr): $\tilde{\nu}$ [cm^{-1}] = 3439 (b, NH^{amide}/$NH^{pyrrole}$), 2924 (s, CH), 2850 (m, CH), 1730 (m, CO), 1517 (s), 1281 (m, C-O-C), 1109 (s, CF). UV/Vis (CH_2Cl_2): λ (ε / M^{-1} cm^{-1}) = 421 (684600), 513 (38500), 549 (14100), 590 (12500), 649 (9500).

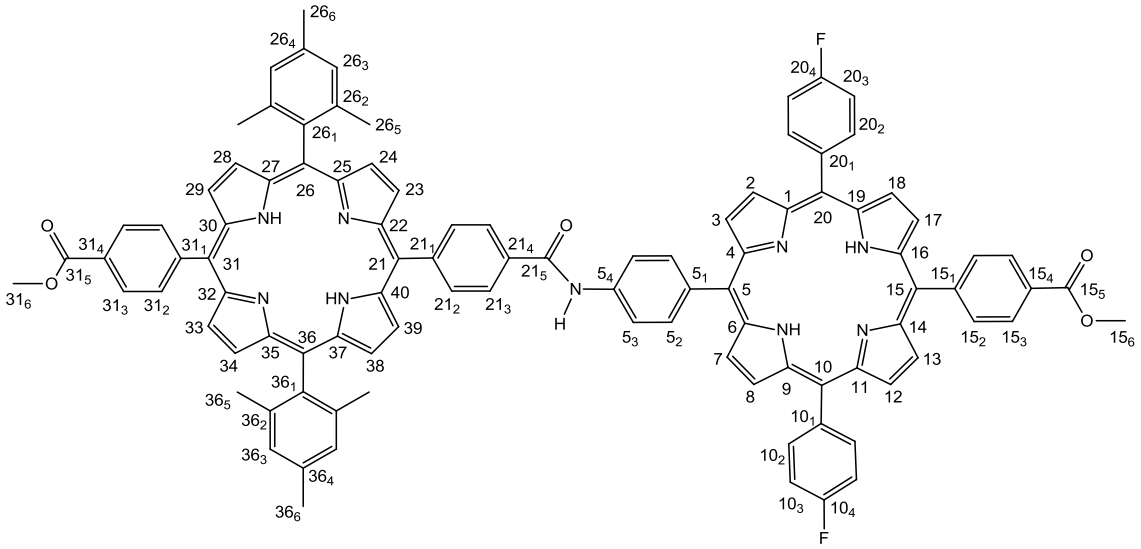


4b: 2b (35 mg, 0.039 mmol), CH_2Cl_2 (3×10 mL), 1-chloro-*N*,*N*,2-trimethylpropenylamine (20 µL, 0.156 mmol), triethylamine (2×1 drop), **3a** (27.0 mg, 0.035 mmol). Yield: 28.4 mg (0.017 mmol, 49%), purple powder. $C_{99}H_{65}F_{10}N_9O_5$ (1650.61). R_f = 0.34 (silica, CH_2Cl_2/ethyl acetate 100:1). ^1H NMR ($CDCl_3$): δ = –2.80 (s, 2 H, $H^{C6F5pyrroleNH}$), –2.59 (s, 2 H, $H^{MespyrroleNH}$), 1.87 (s, 12 H, $H^{10/20}{}_{5/5}$), 2.65 (s, 6 H, $H^{10/20}{}_{6/6}$), 4.12 (s, 3 H, $H^{15}{}_6$), 4.14 (s, 3 H, $H^{31}{}_6$), 7.31 (s, 4 H, $H^{10/20}{}_{3/3}$), 8.27 (d, $^3J_{HH}$ = 8.5 Hz, 2 H, $H^5{}_3$), 8.32 (m, 6 H, $H^{5/15/31}{}_{2/2/2}$), 8.44 (d, $^3J_{HH}$ = 7.3 Hz, 4 H, $H^{15/21}{}_{3/2}$), 8.48 (d, 4 H, $^3J_{HH}$ = 7.9 Hz, $H^{21/31}{}_{3/3}$), 8.54 (s, 1 H, $H^{amide\text{-}NH}$), 8.74 (d, $^3J_{HH}$ = 4.7 Hz, 2 H, $H^{pyrrole}$), 8.78 (m, 4 H, $H^{pyrrole}$), 8.84 (d, $^3J_{HH}$ = 4.3 Hz, 4 H, $H^{pyrrole}$), 8.87 (d, $^3J_{HH}$ = 4.5 Hz, 2 H, $H^{pyrrole}$), 8.91 (d, $^3J_{HH}$ = 4.7 Hz, 2 H, $H^{pyrrole}$), 9.09 (d, $^3J_{HH}$ = 4.7 Hz, 2 H, $H^{pyrrole}$) ppm. $^{13}C\{^1H\}$ NMR ($CDCl_3$): δ = 21.5 ($C^{10/20}{}_{6/6}$), 21.7 ($C^{10/20}{}_{5/5}$), 52.4, 52.5 ($C^{15/31}{}_{6/6}$), 117.9, 118.3, 118.8, 118.9, 120.0, 121.2 ($C^{5/10/15/20/21/26/31/36}$), 118.8 ($C^5{}_3$), 125.6, 128.1 ($C^{15/21/31}{}_{3/3/3}$), 127.8 ($C^{10/20}{}_{3/3}$), 127.9, 134.6, 134.6 ($C^{5/15/31}{}_{2/2/2}$), 129.6, 130.0, 135.4, 138.3 ($C^{15/21/31}{}_{4/4/4}$), 134.2, 136.3, 137.9, 146.0 ($C^{15/21/31/26/36}{}_{1/1/1/1/1}$), 135.0 ($C^{21}{}_2$), 137.5 ($C^5{}_1$), 138.2 ($C^{10/20}{}_{1/1}$), 139.4 ($C^{10/20}{}_{2/2}$), 146.2 ($C^5{}_4$), 146.8 ($C^{21}{}_4$), 145.4, 147.7 ($C^{26/36}{}_{2/2}$, $C^{26/36}{}_{3/3}$, $C^{26/36}{}_{4/4}$), 166.2 ($C^{21}{}_5$), 167.2, 167.3 ($C^{15/31}{}_{5/5}$) ppm. ^{19}F NMR ($CDCl_3$): δ = –162.0 (ddd, $^3J_{FF}$ = 23 Hz, $^3J_{FF}$ = 21 Hz, $^5J_{FF}$ = 8 Hz, 4 F, $F^{26/36}{}_{3/3}$), –152.0 (t, $^3J_{FF}$ = 21 Hz, 2 F, $F^{26/36}{}_{4/4}$,), –136.7 (dd, $^3J_{FF}$ = 24 Hz, $^5J_{FF}$ = 8 Hz, 4 F, $F^{26/36}{}_{2/2}$) ppm. MS (FD): *m/z* (%) = 1649.8 (50) $[M]^+$, 1651.9 (100) $[M+2H]^+$. MS (ESI): *m/z* (%) = 826.3 (100) $[M+H]^{2+}$, 1650.5 (50) $[M]^+$, 1651.5 (82) $[M+H]^+$. HR-MS (ESI): obs. *m/z* = 1650.5067; calcd. for $[M+H]^+$ 1650.5027. IR (KBr): $\tilde{\nu}$ [cm^{-1}] = 3441 (b, NH^{amide}), 3324 (w, $NH^{pyrrole}$), 2926 (s, CH), 2860 (m, CH), 1723 (m, CO), 1515 (m), 1503

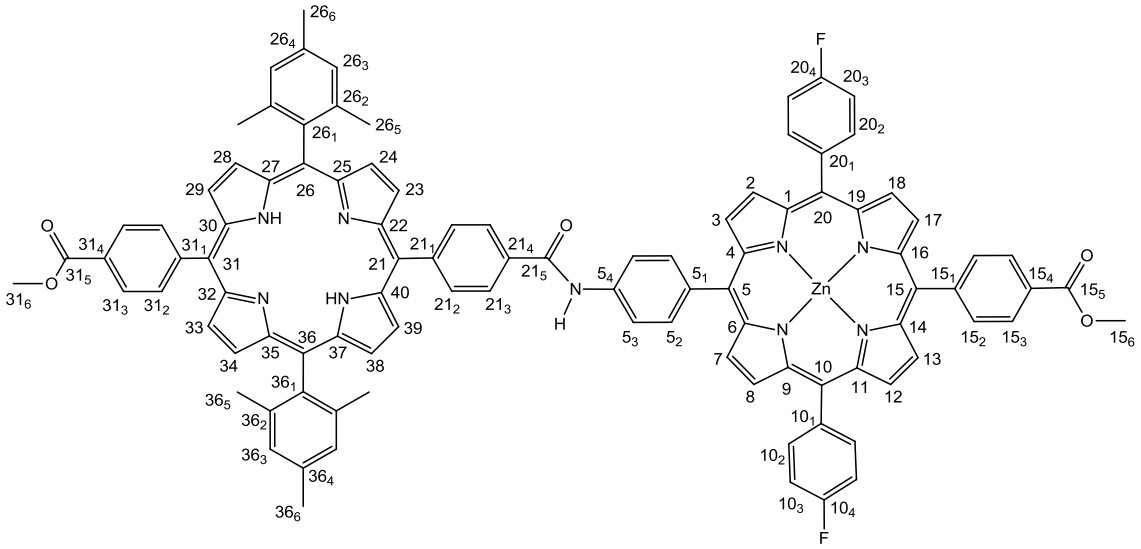
(m), 1266 (m, C-O-C), 1109 (s, CF). UV/Vis (CH_2Cl_2): λ (ε / M^{-1} cm^{-1}) = 420 (787000), 513 (46700), 549 (18000), 590 (15500), 649 (11200).



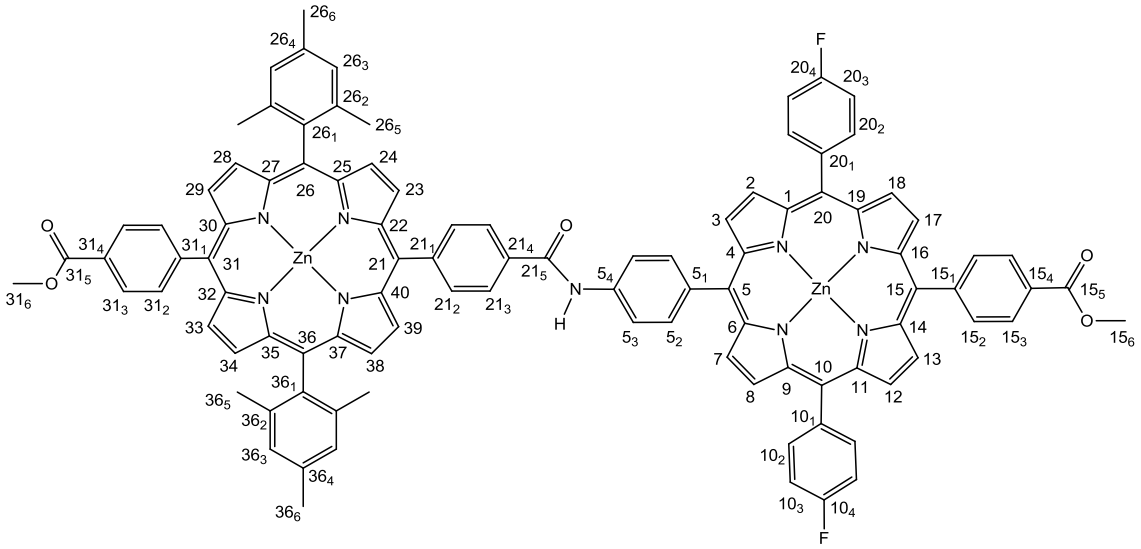
4c: 2a (23.4 mg, 0.026 mmol), CH_2Cl_2 (3 × 10 mL), 1-chloro-*N*,*N*,2-trimethylpropenylamine (14 µL, 0.104 mmol), triethylamine (2×1 drop), **3d** (17.2 mg, 0.021 mmol). Yield: 6.1 mg (0.0145 mmol, 69%), purple powder. $C_{95}H_{51}F_{16}N_9O_5$ (1702.45). R_f = 0.32 (silica, CH_2Cl_2/ethyl acetate 100:1). ^{1}H NMR ($CDCl_3$): δ = –2.81 (s, 2 H, $H^{C6F5pyrroleNH}$), –2.76 (s, 2 H, $H^{CF3pyrroleNH}$), 4.13, 4.14 (2s, 2×3 H, $H^{15/31}{}_{6/6}$), 8.06 (d, $^3J_{HH}$ = 8.0 Hz, 4 H, $H^{10/20}{}_{3/3}$), 8.26 (d, $^3J_{HH}$ = 8.4 Hz, 2 H, $H^{5}{}_{3}$), 8.32 (m, 6 H, $H^{5/15/31}{}_{2/2/2}$), 8.37 (d, $^3J_{HH}$ = 8.0, 4 H, $H^{10/20}{}_{2/2}$), 8.48 (m, 8 H, $H^{15/21/21/31}{}_{3/2/3/3}$), 8.54 (s, 1H, $H^{amide\text{-}NH}$), 8.84 (m, 8 H, $H^{pyrrole}$), 8.90 (d, $^3J_{HH}$ = 4.7 Hz, 2 H, $H^{pyrrole}$), 8.93 (d, $^3J_{HH}$ = 4.8 Hz, 2 H, H^{pyrrol}), 9.01 (pt, $^3J_{HH}$ = 6.3 Hz, 4 H, $H^{pyrrole}$) ppm. ^{13}C{^{1}H} NMR ($CDCl_3$): δ = 52.5, 52.6 ($C^{15/31}{}_{6/6}$), 118.7 ($C^{5}{}_{3}$), 118.8, 119.2, 120.0, 120.4, 123.2 ($C^{5/10/15/20/21/26/31/36}$), 123.8 (d, $^1J_{CF}$ = 3.3 Hz, $C^{10/20}{}_{3/3}$), 134.6 ($C^{10/20}{}_{3/3}$), 125.8 ($C^{10/20}{}_{4/4}$), 125.8, 125.9, 128, 128.2 ($C^{5/15/21/31}{}_{3/3/3/3}$), 130.1 (q, $^1J_{CF}$ = 32.2 Hz, $C^{10/20}{}_{5/5}$), 130.1, 130.9, 131.2 ($C^{2,3,7,8,12,13,17,18}$), 134.6, 135.0, 135.4 ($C^{5/15/21/31}{}_{2/2/2/2}$), 134.6, 134.8, 138.0 ($C^{15/21/31}{}_{4/4/4}$), 136.3, 138.8, 145.4, 147.8 ($C^{26/36}{}_{2/2}$, $C^{26/36}{}_{3/3}$, $C^{26/36}{}_{4/4}$), 138.3 ($C^{5}{}_{1}$), 145.2, 145.7, 145.8, 146.6 ($C^{5/10/20/15/21/31}{}_{4/1/1/1/1/1}$), 166.0 ($C^{21}{}_{5}$), 167.2, 167.3 ($C^{15}{}_{5}$, $C^{31}{}_{5}$) ppm. ^{19}F NMR ($CDCl_3$): δ = –162.6 (ddd, $^3J_{FF}$ = 23 Hz, $^3J_{FF}$ = 23 Hz, $^5J_{FF}$ = 8 Hz, 4 F, $F^{10/20}{}_{3/3}$,), –152.32 (t, $^3J_{FF}$ = 21 Hz, 2 F, $F^{10/20}{}_{4/4}$,), –137.19 (dd, $^3J_{FF}$ = 24 Hz, $^5J_{FF}$ = 8 Hz, 4 F, $F^{10/20}{}_{2/2}$), –62.0 (s, 6 F, $F^{10/20}{}_{5/5}$) ppm. MS (FD): *m/z* (%) = 1703.3 (100) $[M+H]^+$. MS (ESI): *m/z* (%) = 851.7 (72) $[M+H]^{2+}$, 1702.4 (75) $[M]^+$, 1703.4 (100) $[M+H]^+$. HR-MS (ESI): obs. *m/z* = 1702.3815; calcd. for $[M+H]^+$ 1702.3836. IR (KBr): $\tilde{\nu}$ [cm^{-1}] = 3443 (b, NH^{amide}), 3320 (w, $NH^{pyrrole}$), 2952 (w, CH), 2927 (w, CH), 2854 (w, CH), 1724 (m, CO), 1609 (w), 1494 (m), 1266 (s, C-O-C), 1102 (s, CF). UV/Vis (CH_2Cl_2): λ (ε / M^{-1} cm^{-1}) = 420 (745000), 512 (16100), 549 (5300), 590 (5000), 645 (2600).



4d: 2a (21.0 mg, 0.029 mmol), CH_2Cl_2 (3×10 mL), 1-chloro-*N*,*N*,2-trimethylpropenylamine (15 µL, 0.116 mmol), triethylamine (2×1 drop), **3c** (20.0 mg, 0.027 mmol). Yield: 25.0 mg (0.017 mmol, 63%), purple powder. $C_{99}H_{73}F_2N_9O_5$ (1506.69). R_f = 0.41 (silica, CH_2Cl_2/ethyl acetate 100:1). ^{1}H NMR ($CDCl_3$): δ = –2.76 (s, 2 H, $H^{PhFpyrroleNH}$), –2.58 (s, 2 H, $H^{MespyrroleNH}$), 1.87 (s, 12 H, $H^{26/36}{}_{5/5}$), 2.65 (s, 6 H, $H^{26/36}{}_{6/6}$), 4.12, 4.13 (2 s, 2 × 3 H, $H^{15/36}{}_{6/6}$), 7.31 (s, 4 H, $H^{26/36}{}_{3/3}$), 7.47 (t, ^3J = 8.6 Hz, 4 H, $H^{10/20}{}_{3/3}$), 8.20 (dd, ^3J = 8.5 Hz, ^3J = 5.4 Hz, 4 H, $H^{10/20}{}_{2/2}$), 8.24 (d, $^3J_{HH}$ = 8.4 Hz, 2 H, $H^5{}_3$), 8.32 (m, 6 H, $H^{5/15/31}{}_{2/2/2}$), 8.46 (m, 8 H, $H^{15/21/21/31}{}_{3/2/3/3}$), 8.52 (s, 1 H, $H^{amide\text{-}NH}$), 8.74 (d, $^3J_{HH}$ = 4.8 Hz, 2 H, $H^{pyrrole}$), 8.78 (m, 4 H, $H^{pyrrole}$), 8.82 (d, $^3J_{HH}$ = 4.7 Hz, 2 H, $H^{pyrrole}$), 8.85 (m, 4 H, $H^{pyrrole}$), 8.89 (d, $^3J_{HH}$ = 4.7 Hz, 2 H, $H^{pyrrole}$), 9.00 (d, $^3J_{HH}$ = 4.7 Hz, 4 H, $H^{pyrrole}$) ppm. ^{13}C{^{1}H} NMR ($CDCl_3$): δ = 52.5 ($C^{15/31}{}_{6/6}$), 113.8 (d, $^2J_{CF}$ = 21.3 Hz , $C^{10/20}{}_{3/3}$), 118.6 ($C^5{}_3$), 117.9, 118.3, 118.8, 118.9, 119.2, 120.1 ($C^{5/10/15/20/21/26/31/36}$), 125.6, 128.0, 128.0, 135.0 ($C^{15/21/21/31}{}_{3/2/3/3}$), 127.9 ($C^{26/36}{}_{3/3}$), 129.7, 134.3, 138.0 ($C^{15/26/36/31}{}_{4/1/1/4}$), 131.0 ($C^{2,3,7,8,12,13,17,18,23,24,28,29,33,34,38,39}$), 134.6 (d, $^4J_{CF}$ = 3.2 Hz, $C^{10/20}{}_{1/1}$), 134.6, 135.0, 135.4 ($C^{5/15/31}{}_{2/2/2}$), 135.7 (d, $^3J_{CF}$ = 8.0 Hz, $C^{10/20}{}_{2/2}$), 138.4 ($C^5{}_1$), 138.2 ($C^{26/36}{}_{1/1}$), 139.4, 146.1 146.8, 146.9 ($C^{15/21/21/31}{}_{1/1/4/1}$), 162.9 (d, $^1J_{CF}$ = 247.4 Hz, $C^{10/20}{}_{4/4}$), 166.2 ($C^{21}{}_5$), 167.3, 167.4 ($C^{15}{}_5$, $C^{31}{}_5$) ppm. ^{19}F NMR ($CDCl_3$): δ = –114.5 (tt, $^3J_{HF}$ = 8.6 Hz, $^4J_{HF}$ = 5.4 Hz) ppm. MS (FD): *m/z* (%) = 1506.9 (100) $[M]^+$. MS (ESI): *m/z* (%) = 753.8 (90) $[M+H]^{2+}$, 754.3 (100) $[M+2H]^{2+}$, 1506.6 (37) $[M]^+$. HR-MS (ESI): obs. *m/z* = 1506.5826; calcd. for $[M]^+$ 1506.5781. IR (KBr): $\tilde{\nu}$ [cm^{-1}] = 3443 (b, NH^{amide}), 3320 (w, $NH^{pyrrole}$), 2927 (w, CH), 2853 (w, CH), 1724 (m, CO), 1609 (m), 1512 (s), 1274 (s, C-O-C), 1103 (s, CF). UV/Vis (CH_2Cl_2): λ (ε / M^{-1} cm^{-1}) = 421 (459800), 513 (23400), 550 (11600), 592 (73000), 649 (8000).



Zn^2-4d: 2a (26.0 mg, 0.033 mmol), CH_2Cl_2 (3×10 mL), 1-chloro-*N*,*N*,2-trimethylpropenylamine (17 µL, 0.132 mmol), triethylamine (2×1 drop), **Zn-3c** (22.0 mg, 0.028 mmol). Yield: 17.0 mg (0.011 mmol, 40%), purple powder. $C_{99}H_{71}F_2N_9O_5Zn$ (1570.07). R_f = 0.41 (silica, CH_2Cl_2/ethyl acetate 100:1). ^{1}H NMR (d$_8$-THF): δ = –2.47 (s, 2 H, $H^{MespyrroleNH}$), 1.87 (s, 12 H, $H^{26/36}{}_{5/5}$), 2.63 (s, 6 H, $H^{26/36}{}_{6/6}$), 4.06 (s, 6 H, $H^{15/31}{}_{6/6}$), 7.35 (s, 4 H, $H^{26/36}{}_{3/3}$), 7.52 (t, ^3J = 8.5 Hz, 4 H, $H^{10/20}{}_{3/3}$), 8.22 (dd, ^3J = 8.2 Hz, ^3J = 5.9 Hz, 4 H, $H^{10/20}{}_{2/2}$), 8.25 (d, $^3J_{HH}$ = 8.6 Hz, 2 H, $H^5{}_3$), 8.39 (m) and 8.54 (d, $^3J_{HH}$ = 7.9 Hz, 14 H / 2 H, $H^{5/15/15/21/21/31/31}{}_{2/2/3/2/3/2/3}$), 8.71 (d, $^3J_{HH}$ = 4.6 Hz, 2 H, $H^{pyrrole}$), 8.75 (d, $^3J_{HH}$ = 4.6 Hz, 2 H, $H^{pyrrole}$), 8.78 (d, $^3J_{HH}$ = 4.5, 2 H, $H^{pyrrole}$), 8.84 (d, $^3J_{HH}$ = 4.5 Hz, 2 H, $H^{pyrrole}$), 8.86 (d, $^3J_{HH}$ = 4.7 Hz, 2 H, $H^{pyrrole}$), 8.89 (d, $^3J_{HH}$ = 4.3 Hz, 4 H, $H^{pyrrole}$), 9.03 (d, $^3J_{HH}$ = 4.6 Hz, 2 H, H^{pyrrol}), 10.16 (s, 1 H, $H^{amide\text{-}NH}$) ppm. ^{13}C{^{1}H} NMR ($CDCl_3$): δ = 21.7 ($C^{26/36}{}_{6/6}$), 21.9 ($C^{26/36}{}_{5/5}$), 52.5 ($C^{15/31}{}_{6/6}$), 114.2 (d, $^2J_{CF}$ = 21.5 Hz, $C^{10/20}{}_{3/3}$), 119.0 ($C^5{}_3$), 119.6, 119.9, 120.2, 120.6 ($C^{5/10/15/20/21/26/31/36}$), 128.9 (4 C, $C^{26/36}{}_{3/3}$), 136.8 (d, $^3J_{CF}$ = 7.9 Hz, $C^{10/20}{}_{2/2}$), 128.5, 128.8, 128.9, 135.6, 135.9, 136.8, 136.9 ($C^{5/15/15/21/21/31/31}{}_{2/2/3/2/3/2/3}$), 130.6, 131.0, 132.2, 132.3, 132.5, 132.9 ($C^{2,3,7,8,12,13,17,18,23,24,28,29,33,34,38,39}$), 150.7, 151.2, 151.4, 151.6 ($C^{1/4/6/9/11/14/16/19}$), 139.5 ($C^{26/36}{}_{1/1}$), 139.0, 139.8, 136.6, 140.1, 140.7, 146.3, 147.8, 149.4 ($C^{5/5/15/15/21/21/31/31}{}_{1/4/1/4/1/4/1/4}$), 140.7 ($C^{10/20}{}_{1/1}$), 163.9 (d, $^1J_{CF}$ = 245.8 Hz, $C^{10/20}{}_{4/4}$), 166.7 ($C^{21}{}_5$), 167.4, 167.5 ($C^{15/31}{}_{5/5}$) ppm. ^{19}F NMR (d$_8$-THF): δ = –114.5 (m) ppm. MS (FD): *m/z* (%) = 1568.2 (100) $[M]^+$. MS (ESI): *m/z* (%) = 784.8 (34) $[M+H]^{2+}$, 1568.6 (17) $[M]^+$, 1569.6 (21) $[M+H]^+$. HR-MS (ESI): obs. *m/z* = 1568.4926; calcd. for $[M–H]^+$ 1568.4916. IR (KBr): $\tilde{\nu}$ [cm^{-1}] = 3435 (b, NH^{amide}/$NH^{pyrrole}$), 2919 (w, CH), 2853 (w, CH), 1724 (m, CO), 1602 (m), 1511 (m), 1274 (s, C-O-C), 1103 (s, CF). UV/Vis (CH_2Cl_2): λ (ε / M^{-1} cm^{-1}) = 423 (816300), 515 (27000), 549 (32500), 593 (11800), 651 (15300).



Synthesis of Zn^1Zn^2-4d: To porphyrin **4d** (7.0 mg, 0.0045 mmol) in CH_2Cl_2 (5 mL) was added zinc acetate dihydrate (9.88 mg, 0.045 mmol) and the solution was stirred for 12 h at room temperature. The mixture was concentrated in vacuum. After column chromatography (silica, toluene/ethyl acetate 20:1) **Zn^1Zn^2-4d** was isolated as purple powder. Yield: 6.4 mg (0.0039 mmol, 88%). $C_{99}H_{69}F_2N_9O_5Zn_2$ (1633.44). R_f = 0.37 (silica, toluene/ethyl acetate 20:1). ^{1}H NMR (d_8-THF): δ = 1.88 (s, 12 H, $H^{26/36}{}_{5/5}$), 2.63 (s, 6 H, $H^{26/36}{}_{6/6}$), 4.05 (s), 4.06 (s, $H^{15/31}{}_{6/6}$), 7.32 (s, 4 H, $H^{26/36}{}_{3/3}$), 7.52 (t, ^3J = 8.7 Hz, 4 H, $H^{10/20}{}_{3/3}$), 8.22 (dd, ^3J = 8.4 Hz, ^3J = 5.6 Hz, 4 H, $H^{10/20}{}_{2/2}$), 8.25 (d, $^3J_{HH}$ = 8.6 Hz, 2 H, $H^5{}_3$), 8.32 (m, 4 H); 8.41 (m, 8 H,); 8.51 (d, $^3J_{HH}$ = 8.1 Hz, 2 H) ($H^{5/15/15/21/2131/31}{}_{2/2/3/2/3/2/3}$), 8.71 (d, $^3J_{HH}$ = 4.6 Hz, 2 H, $H^{pyrrole}$), 8.74 (d, $^3J_{HH}$ = 4.6 Hz, 2 H, $H^{pyrrole}$), 8.77 (d, $^3J_{HH}$ = 4.6 Hz, 2 H, $H^{pyrrole}$), 8.84 (d, $^3J_{HH}$ = 4.6 Hz, 2 H, $H^{pyrrole}$), 8.87 (d, $^3J_{HH}$ = 4.7 Hz, 2 H, $H^{pyrrole}$), 8.88 (d, $^3J_{HH}$ = 4.6 Hz, 2 H, $H^{pyrrole}$), 8.89 (d, $^3J_{HH}$ = 4.6 Hz, 2 H, $H^{pyrrole}$), 9.04 (d, $^3J_{HH}$ = 4.6 Hz, 2 H, $H^{pyrrole}$), 10.15 (s, 1 H, $H^{amide\text{-}NH}$) ppm. ^{13}C{^{1}H} NMR (d_8-THF): δ = 21.8 ($C^{26/36}{}_{6/6}$), 22.2 ($C^{26/36}{}_{5/5}$), 52.5 ($C^{15/31}{}_{6/6}$), 114.2 (d, $^2J_{CF}$ = 21.5 Hz , $C^{10/20}{}_{3/3}$), 119.0 (s, 1 C, $C^5{}_3$), 119.9, 120.3, 120.6, 122.3 ($C^{5/10/15/20/21/26/31/36}$), 126.7, 128.4, 128.5, 135.6, 135.6, 135.9, 138.4, 139.6 ($C^{5/15/15/21/21/31/31}{}_{2/2/3/2/3/2/3}$), 128.7 ($^{26/36}{}_{3/3}$), 130.5 (d, $^4J_{CF}$ = 3.2 Hz, $C^{10/20}{}_{1/1}$), 131.3, 131.3, 140.7, 140.8, 147.9, 149.4 ($C^{5/5/15/15/21/21/31/31}{}_{1/4/1/4/1/4/1/4}$), 132.2, 132.3, 132.6, 132.7, 132.8, 132.9 ($C^{2,3,7,8,12,13,17,18,23,24,28,29,33,34,38,39}$), 136.9 (d, $^3J_{CF}$ = 7.9 Hz, $C^{10/20}{}_{2/2}$), 150.6, 150.7, 150.7, 151.0, 151.0, 151.2, 151.4, 151.6 ($C^{1/4/6/9/11/14/16/19/22/25/27/30/32/35/37/40}$), 163.1 (d, $^1J_{CF}$ = 245.2 Hz, $C^{10/20}{}_{4/4}$), 166.8 ($C^{21}{}_5$), 167.5 ($C^{15}{}_5$, $C^{31}{}_5$) ppm. ^{19}F NMR (d_8-THF): δ = –118.7 (br.s) ppm. MS (FD): *m/z* (%) = 1632.6 (100) $[M]^+$. HR-MS (ESI): obs. *m/z* = 1630.4067; calcd. for $[M+H]^+$ 1630.4051. IR (KBr): $\tilde{\nu}$ [cm^{-1}] = 3425 (b, NH^{amide}), 2925 (s, CH), 2856 (w, CH), 1726 (m, CO), 1602 (m), 1512 (m), 1278 (m, C-O-C), 1101 (s, CF). UV/Vis (CH_2Cl_2): λ (ε / M^{-1} cm^{-1}) = 423 (806700), 549 (45600), 588 (13000).

Discussion of relevant NMR data of bis(porphyrins): The pyrrole NH proton resonances are indicative of the electron withdrawing nature of the porphyrin substituents: δ = –2.80 (C_6F_5), –2.76 (4-$C_6H_4CF_3$), –2.76 (4-C_6H_5F), –2.6 (2,4,6-$C_6H_2(CH_3)_3$). Their correct integral ratio confirms the composition of **4a** – **4d**. The presence of two methyl ester groups is confirmed by the presence of two resonances of the CH_3 groups again in the correct integral ratio at δ = 4.12 – 4.14 ppm. Particularly informative is the ^{19}F NMR spectrum of **4c** which displays the expected ^{19}F resonances of the C_6F_5 and $C_6H_4CF_3$ substituents in the correct intensity ratio (Supporting Information, Figure S1).

The zinc porphyrins **Zn^2-4d** and **Zn^{1}Zn^2-4d** are less soluble in chloroform than their parent free-base bis(porphyrin) **4d**. In tetrahydrofuran their amide protons resonate at δ = 10.1 ppm due to hydrogen-bonding to the solvent. In the bis(metalated) complex **Zn^{1}Zn^2-4d** pyrrole-NH resonances are absent as expected. **Zn^2-4d** shows a single resonance at δ = –2.5 ppm corresponding to the pyrrole-NH nuclei of the mesityl substituted free-base porphyrin proving the presence of the correct isomer **Zn^2-4d**.

References

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[S6] T. Rohand, E. Dolusic, T. H. Ngo, W. Maes and W. Dehaen, *ARKIVOC*, 2007**, (x)**, 307-324.

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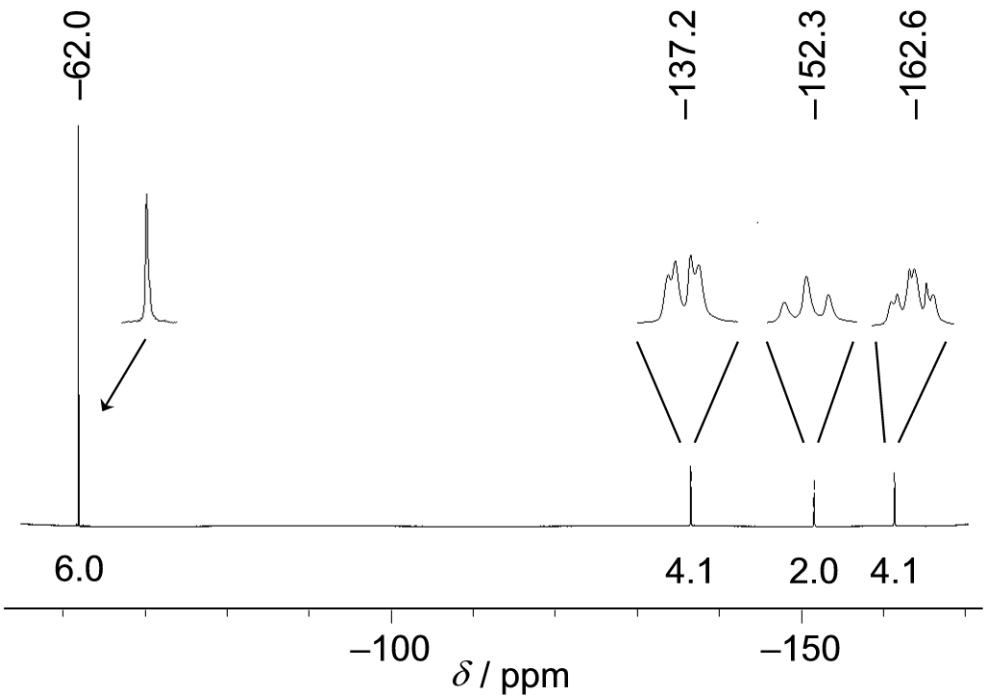
Fig. S1 ^{19}F NMR spectrum of bis(porphyrin) **4c** in $CDCl_3$.



DFT Section

Fig. S2 DFT calculated spin densities of radical ions **4c**$^{+}$ and **4c**$^{-}$ (isosurface value at 0.01 a.u.; B3LYP/LANL2DZ, PCM CH_2Cl_2).

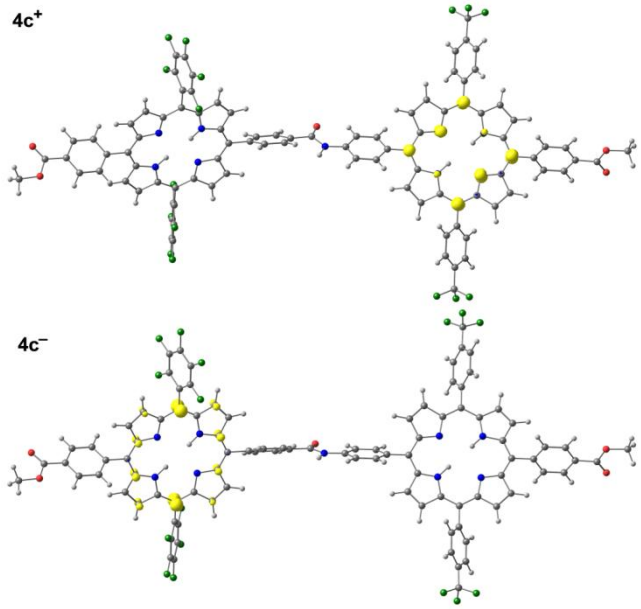


Fig. S3 Frontier orbitals of **4b** isosurface value at 0.05 a.u.; B3LYP/LANL2DZ, PCM CH_2Cl_2.

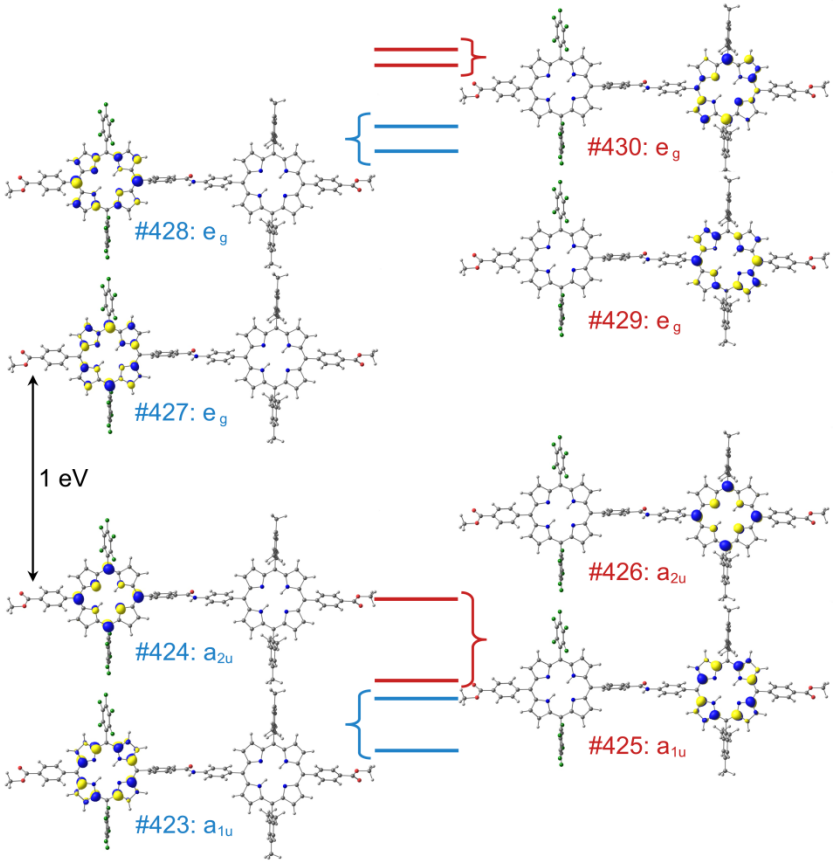


Fig. S4 Frontier orbitals of **4c** isosurface value at 0.05 a.u.; B3LYP/LANL2DZ, PCM CH_2Cl_2.

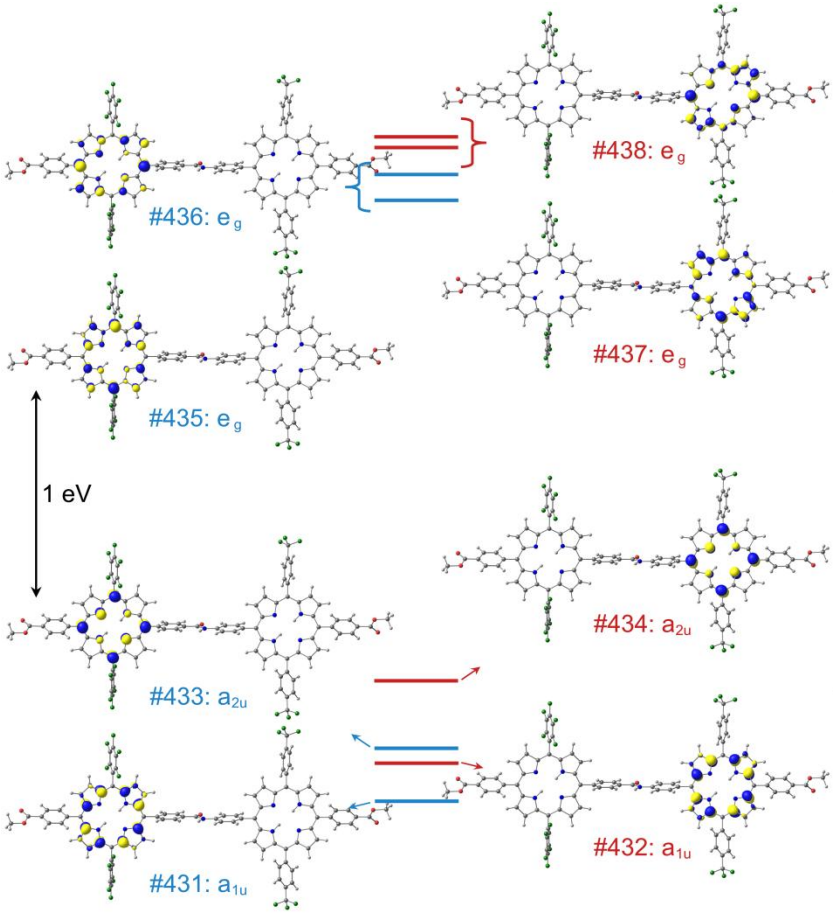


Fig. S5 Frontier orbitals of **Zn^2-4d** isosurface value at 0.05 a.u.; B3LYP/LANL2DZ, gasphase.

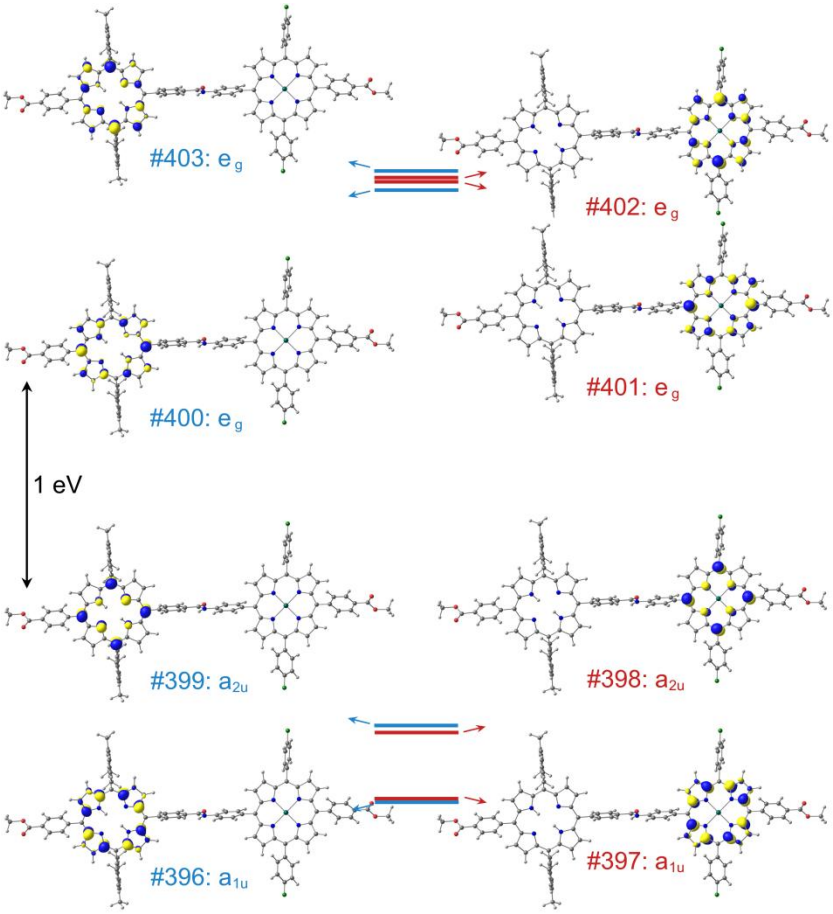


Fig. S6 EPR spectra of **4b**$^{+/-}$, **Zn^2-4d**$^{+/-}$ and their reference compounds in CH_2Cl_2 at 77 K (9.4 GHz).

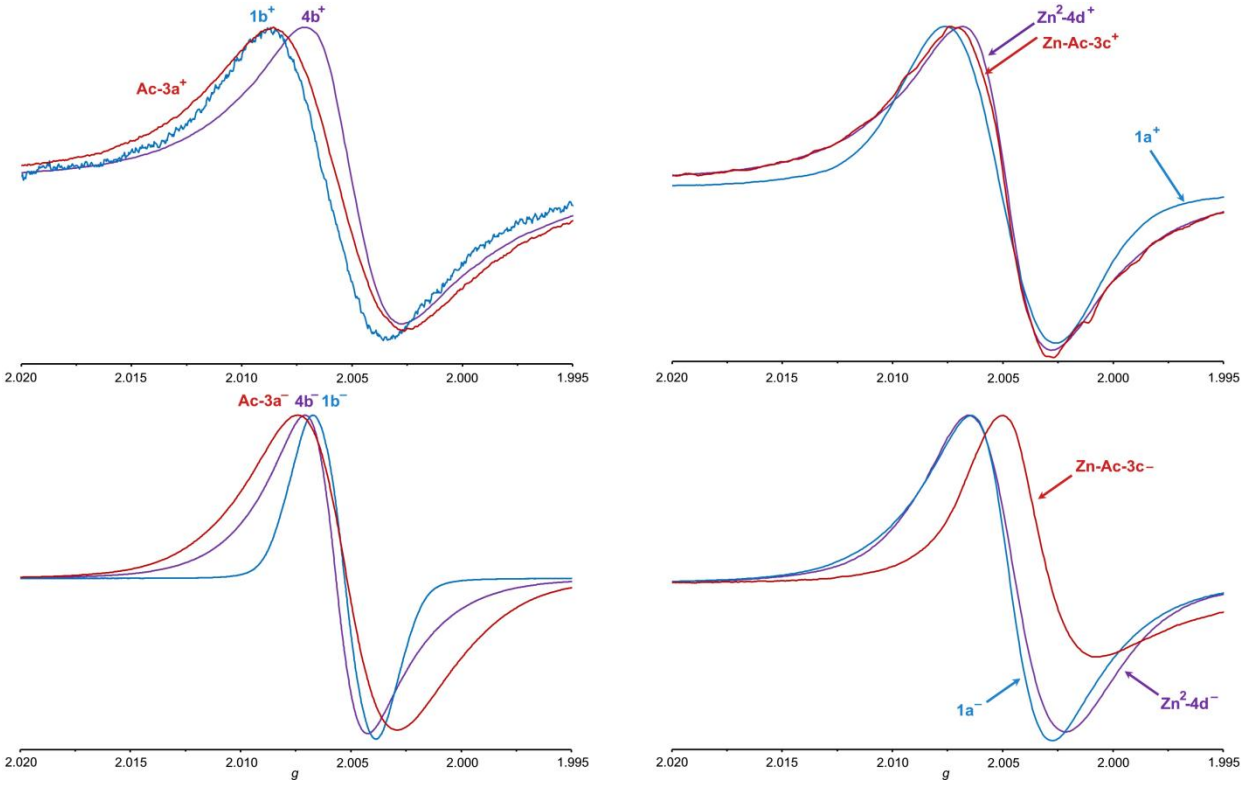


Fig. S7. Normalised Soret bands of **4a** – **4d**, **Zn^2-4d** and **Zn^{1}Zn^2-4d** and their constituent reference porphyrins in CH_2Cl_2.

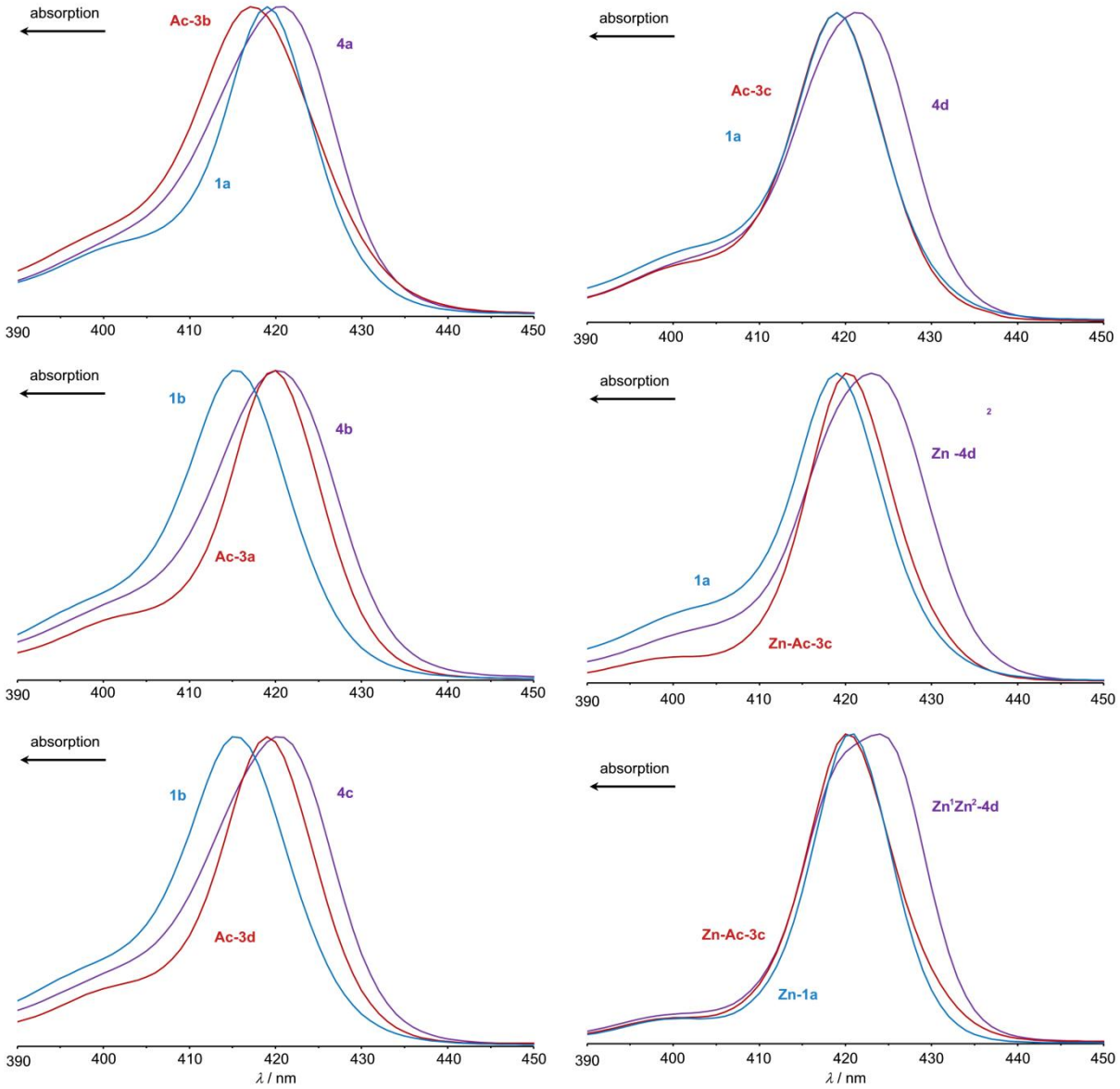


Fig. S8. Normalised (to Q(0,0)) emission spectra of **Ac-3a** – **Ac-3d** in CH_2Cl_2.

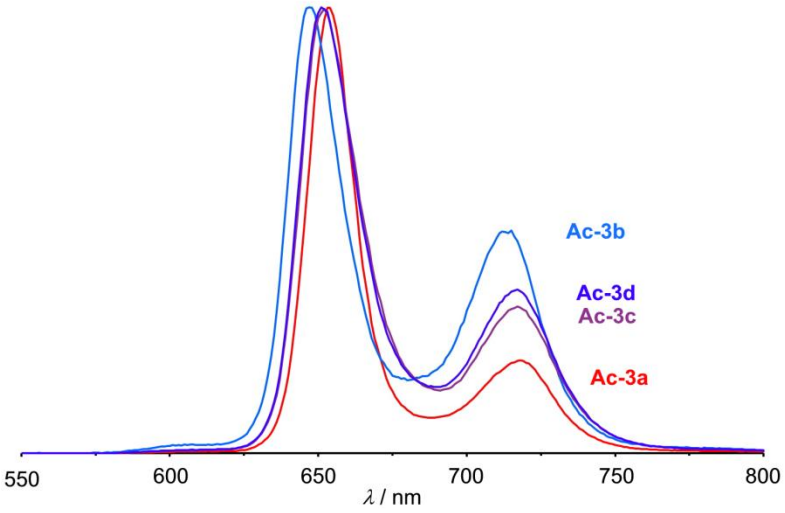


Fig. S9. Normalised (logarithmic) fluorescence decays of **Zn^1Zn^2-4d**, **Zn-1a** and **Zn-Ac-3c** in CH_2Cl_2.

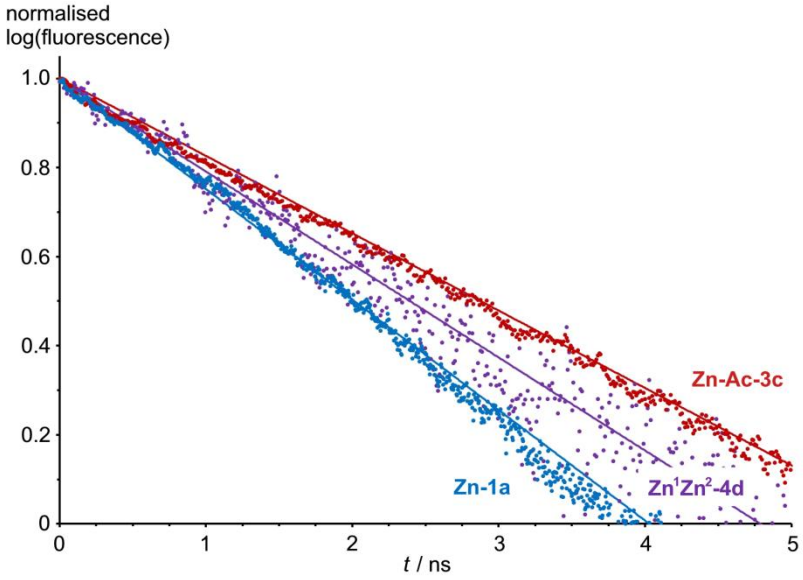
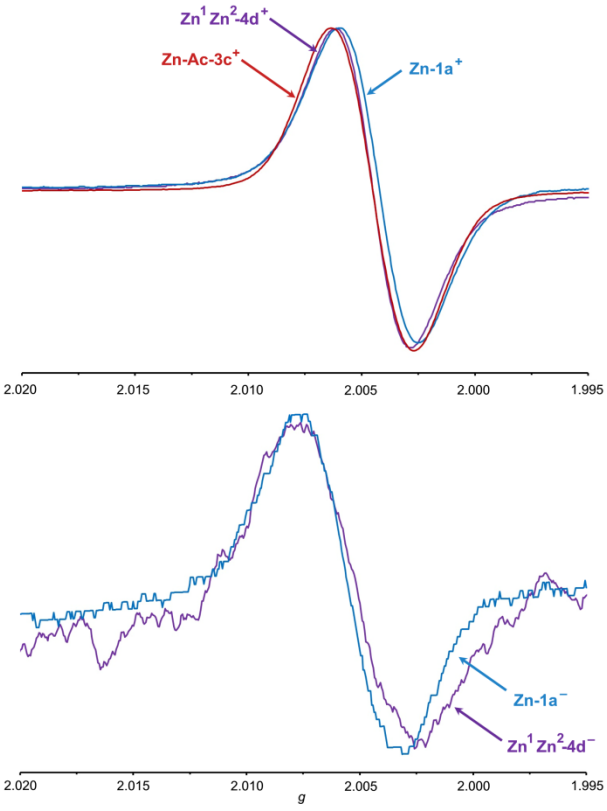


Fig. S10. X-band EPR spectra of radical ions **Zn^1Zn^2-4d$^{+/-}$** and reference radicals in CH_2Cl_2 at 295 K (9.4 GHz).



Cartesian coordinates of DFT optimised geometries (B3LYP/LANL2DZ, PCM CH_2Cl_2):

4a

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1	11.452490000	4.802852000	1.716813000
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1	8.760251000	-4.657054000	-1.390512000
1	10.500969000	-4.717386000	-1.659582000
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6	9.256207000	3.440854000	-0.723079000
6	5.787731000	0.055494000	0.302735000
6	11.772804000	3.488355000	-1.050178000
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6	6.843612000	-3.378592000	0.869474000
6	5.845365000	-2.451190000	0.747730000

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1	8.875201000	-6.279569000	-1.741254000
6	9.095010000	9.140205000	-2.036227000
1	8.443226000	9.703105000	-1.355216000
1	10.099429000	9.578894000	-1.956220000
1	8.739453000	9.306117000	-3.059239000
6	9.755093000	5.462563000	1.400889000
1	8.946084000	4.863344000	1.838393000
1	10.666373000	4.852389000	1.455910000
1	9.902107000	6.344966000	2.032914000
6	8.578086000	4.285389000	-3.446515000
1	9.413413000	3.586668000	-3.585506000
1	7.695385000	3.679275000	-3.204015000
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7	-0.779204000	-0.011091000	0.796115000
1	-0.345364000	-0.298768000	-0.074480000
6	0.073389000	0.279891000	1.841258000
8	-0.329935000	0.546232000	3.013357000
1	-11.031971000	5.423981000	-0.589331000
1	-9.516478000	4.453989000	3.333745000
1	-9.631125000	6.874661000	3.977997000
1	-11.141139000	7.846061000	0.051095000
9	-10.455428000	8.827073000	2.403292000
1	-8.684078000	-4.564579000	-2.971184000
1	-8.584890000	-6.991325000	-3.595373000
1	-10.962080000	-7.979611000	-0.128931000
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7	-8.196924000	1.538326000	0.496333000
7	-11.135913000	1.402057000	0.061650000
7	-8.122872000	-1.348900000	0.136548000
7	-11.068920000	-1.490999000	-0.245436000
6	-6.826454000	1.349322000	0.646627000
6	-6.246441000	2.659694000	0.840345000
6	-7.268046000	3.590906000	0.810556000
6	-8.513193000	2.890867000	0.592452000
1	-5.192828000	2.851945000	0.974673000
1	-7.183441000	4.661492000	0.922221000
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6	-6.144886000	0.114630000	0.595055000
6	-12.308472000	3.430262000	0.234696000
6	-13.236773000	2.453168000	-0.005080000
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1	-12.478982000	4.486972000	0.381926000
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6	-8.267805000	-2.724411000	-0.020362000

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6	-6.042875000	-2.418599000	0.367727000
6	-6.766791000	-1.138867000	0.366926000
1	-6.809779000	-4.462248000	0.056796000
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6	-13.001319000	-2.599127000	-0.711534000
6	-11.978474000	-3.528689000	-0.687255000
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6	-9.865933000	4.976024000	0.662973000
6	-10.021033000	5.547463000	1.954149000
6	-10.092142000	6.950935000	2.080816000
6	-10.015823000	7.803329000	0.959932000
6	-9.855104000	7.214800000	-0.311506000
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6	-2.731767000	0.476267000	2.284853000
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1	-4.787164000	0.717823000	2.895870000
6	-9.393858000	-4.923381000	-0.456941000
6	-9.142966000	-5.475485000	-1.741937000
6	-9.070607000	-6.876664000	-1.885757000
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6	-9.566598000	-5.780164000	0.662228000
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6	-16.576106000	0.494381000	-1.903642000
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6	-16.841330000	-0.796474000	0.149930000
6	-15.452063000	-0.762958000	0.343776000
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1	-15.020807000	-1.239779000	1.219467000
6	-9.781339000	5.815905000	-0.479567000
6	-18.879727000	-0.183355000	-1.228904000
8	-19.444082000	0.359345000	-2.204567000
1	-8.861912000	0.786610000	0.324147000
1	-10.406941000	-0.741073000	-0.054857000
1	-2.323338000	0.709070000	3.263349000
7	11.239670000	1.420332000	-0.324218000
7	8.304471000	1.532519000	-0.258656000
7	11.138072000	-1.496870000	-0.003325000
7	8.208041000	-1.370667000	0.161047000
6	12.605076000	1.150133000	-0.406611000
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1	14.382097000	2.472335000	-0.871284000
1	12.554126000	4.424797000	-1.051315000
6	9.841738000	3.487787000	-0.568564000
6	13.216031000	-0.120041000	-0.248099000
6	7.306785000	3.630221000	-0.314847000
6	6.303259000	2.706897000	-0.133299000
6	6.925262000	1.388044000	-0.106325000
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1	7.205593000	4.704249000	-0.362998000
1	5.248404000	2.902173000	-0.010020000
6	6.227990000	0.166127000	0.071226000
6	10.881310000	-2.848682000	0.224466000
6	12.149714000	-3.557036000	0.360328000
6	13.155142000	-2.632419000	0.199895000
6	12.522390000	-1.338990000	-0.038202000
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1	14.219030000	-2.808454000	0.257057000
6	6.114705000	-2.374540000	0.255831000
6	7.051527000	-3.379586000	0.322895000
6	8.367293000	-2.751227000	0.276164000
6	6.837915000	-1.111172000	0.163235000
1	5.040126000	-2.480468000	0.250490000
1	6.867293000	-4.442039000	0.380614000
6	9.601464000	-3.448177000	0.329788000
6	9.892637000	4.975570000	-0.777523000
6	10.509350000	5.818885000	0.176420000
6	10.560609000	7.212623000	-0.009451000
6	9.990280000	7.740077000	-1.171135000
6	9.372649000	6.950556000	-2.144947000
6	14.715429000	-0.179468000	-0.315440000
6	15.365326000	-0.888805000	-1.353960000
6	16.764832000	-0.940580000	-1.421753000
6	17.548923000	-0.289892000	-0.443091000
6	16.910735000	0.416920000	0.600587000
6	15.509970000	0.473184000	0.657133000
1	14.770751000	-1.385421000	-2.115478000
1	17.258878000	-1.478009000	-2.225663000
1	15.026585000	1.012359000	1.466933000
6	9.548108000	-4.939084000	0.517313000
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6	9.449580000	-7.708971000	0.865172000
6	9.010938000	-6.891075000	1.910042000
6	9.061161000	-5.497486000	1.722430000
6	4.731774000	0.225739000	0.188728000
6	3.922458000	0.631691000	-0.897506000
6	2.525787000	0.670026000	-0.783006000
6	1.893002000	0.314883000	0.432495000
6	2.690245000	-0.079877000	1.532345000
6	4.087547000	-0.127003000	1.395187000
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1	1.925752000	0.973151000	-1.638689000

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1	4.687362000	-0.431193000	2.249216000
6	9.325257000	5.560272000	-1.934353000
1	17.509649000	0.913121000	1.356396000
9	9.399232000	-9.107441000	1.040660000
9	10.040201000	9.135344000	-1.370174000
6	19.030350000	-0.371434000	-0.547475000
8	19.651629000	-0.977501000	-1.448576000
8	19.675950000	0.300873000	0.467187000
6	21.153699000	0.286213000	0.462593000
1	21.530761000	0.736172000	-0.460316000
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1	21.519117000	-0.741077000	0.550183000
8	-19.580114000	-0.869365000	-0.261234000
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1	-10.164302000	-9.645310000	-1.296577000
1	-8.455554000	-9.537922000	-1.736098000
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1	10.261326000	-7.882020000	-1.130530000
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1	8.946951000	7.404687000	-3.034070000
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6	-0.373046000	0.142280000	1.537860000
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Zn^{2}-4d^{+}

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6	12.452549000	-1.144982000	0.069041000
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6	9.866600000	-6.925687000	1.840058000
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6	1.845550000	0.220770000	1.545891000
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6	-13.310865000	2.143402000	0.894352000
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1	-7.175179000	4.245614000	1.760853000
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1	-14.644902000	1.894018000	-1.766271000
1	-17.113064000	1.925889000	-2.094821000
1	-14.993782000	-1.846926000	0.377384000
6	-9.887177000	4.437128000	2.126854000
6	-10.530266000	5.519387000	1.476412000
6	-10.577481000	6.791999000	2.068491000
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6	-9.296484000	4.653609000	3.396677000
6	-4.725987000	-0.129685000	0.559265000
6	-3.897715000	-0.504106000	-0.532484000
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6	-2.696874000	0.240240000	1.906619000
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1	-17.457900000	-1.795449000	0.059306000
9	-10.043784000	8.219467000	3.932928000
9	-9.341268000	-8.439007000	-3.792093000
6	-18.919142000	0.134314000	-1.256878000
8	-19.505713000	1.051691000	-1.870490000
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1	-21.323751000	-1.010251000	-1.913347000
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1	21.135666000	0.857833000	-2.500541000
1	21.345952000	1.470412000	-0.821498000
1	21.387371000	-0.297152000	-1.156586000
1	10.339642000	-6.074963000	5.104475000
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1	9.722266000	-9.251374000	3.183845000
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6	10.228820000	-3.453679000	4.414375000

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6	9.096379000	8.707566000	-3.396970000
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1	8.569570000	8.723890000	-4.357714000
6	9.957184000	5.632742000	0.549840000
1	9.187815000	5.078301000	1.102481000
1	10.894823000	5.072775000	0.664151000
1	10.085816000	6.607065000	1.033227000
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Zn^2-4d$^-$

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6	-9.062313000	-7.276031000	-2.866891000
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Zn^1Zn^2-4d

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6	-6.498107000	0.177559000	0.324139000
6	-11.357087000	2.827666000	-0.026887000
6	-12.679941000	3.443160000	-0.030946000
6	-13.600973000	2.435441000	-0.196893000
6	-12.860879000	1.181615000	-0.296189000
1	-12.880414000	4.496657000	0.095544000
1	-14.676051000	2.532335000	-0.226347000
6	-6.581574000	2.725584000	0.330884000
6	-7.591812000	3.657891000	0.278883000
6	-8.853232000	2.928369000	0.205097000
6	-7.203872000	1.407072000	0.292474000
1	-5.518918000	2.912719000	0.373720000
1	-7.489218000	4.732858000	0.270960000
6	-10.135651000	3.529850000	0.127760000
6	-9.748592000	-4.953697000	-0.295648000
6	-10.357139000	-5.757739000	0.696459000
6	-10.295055000	-7.162071000	0.633635000

6	-9.620219000	-7.740425000	-0.444870000
6	-9.006818000	-6.991116000	-1.452549000
6	-14.938623000	-0.158463000	-0.639487000
6	-15.551996000	0.431351000	-1.771111000
6	-16.941405000	0.370432000	-1.948567000
6	-17.753580000	-0.275387000	-0.989814000
6	-17.152882000	-0.862354000	0.146236000
6	-15.760987000	-0.806195000	0.313203000
1	-14.935309000	0.922874000	-2.518224000
1	-17.405999000	0.815684000	-2.823207000
1	-15.307822000	-1.252721000	1.193719000
6	-10.204106000	5.028760000	0.222162000
6	-10.638351000	5.803764000	-0.878666000
6	-10.704038000	7.207124000	-0.799409000
6	-10.334870000	7.813264000	0.404473000
6	-9.902878000	7.092888000	1.521426000
6	-9.836756000	5.691376000	1.416953000
6	-5.003838000	0.233500000	0.468113000
6	-4.160613000	-0.195679000	-0.583276000
6	-2.766276000	-0.152995000	-0.454558000
6	-2.168335000	0.309283000	0.742412000
6	-2.997682000	0.740867000	1.803665000
6	-4.394891000	0.704922000	1.651816000
1	-4.598722000	-0.553772000	-1.510987000
1	-2.140702000	-0.482038000	-1.281948000
1	-2.553382000	1.086455000	2.727023000
1	-5.019981000	1.032662000	2.478622000
6	-9.074131000	-5.588471000	-1.365096000
1	-17.773746000	-1.353569000	0.887441000
9	-10.401627000	9.218976000	0.496778000
9	-9.555120000	-9.147210000	-0.520241000
6	-19.223645000	-0.314832000	-1.212298000
8	-19.812562000	0.194218000	-2.191771000
8	-19.898040000	-0.982590000	-0.213524000
6	-21.367992000	-1.079893000	-0.330427000
1	-21.638077000	-1.596518000	-1.255906000
1	-21.680861000	-1.653373000	0.542338000
1	-21.811768000	-0.080147000	-0.320961000
8	19.169834000	-0.181340000	-0.905608000
6	20.624541000	-0.266079000	-1.151668000
1	20.882959000	0.274827000	-2.066618000
1	21.083480000	0.200597000	-0.279841000
1	20.929915000	-1.312654000	-1.241326000
1	9.204818000	-7.469246000	2.862016000
1	8.379823000	-7.735879000	-1.358617000
1	9.206113000	7.572067000	-2.422746000
1	10.248365000	7.759311000	1.753759000
6	8.704372000	-9.299880000	0.880116000
1	8.338474000	-9.754042000	-0.047473000
1	9.690916000	-9.733032000	1.097022000
1	8.033839000	-9.603505000	1.694638000
6	9.449482000	-4.774810000	3.059571000
1	10.374570000	-4.193606000	2.949130000
1	8.647610000	-4.056663000	3.275578000
1	9.562700000	-5.428064000	3.931472000
6	8.473929000	-5.092406000	-1.960471000
1	7.658188000	-4.358110000	-1.939107000
1	9.373716000	-4.557604000	-2.292688000
1	8.231464000	-5.846460000	-2.717019000
6	9.873937000	9.360194000	-0.444419000
1	9.490104000	9.852628000	0.457564000
1	10.925533000	9.661706000	-0.555433000
1	9.326480000	9.754241000	-1.308313000
6	10.173356000	5.106127000	2.311994000
1	9.301022000	4.537644000	2.660680000
1	11.008702000	4.396680000	2.245987000
1	10.420769000	5.848899000	3.078067000
6	8.932135000	4.883523000	-2.654918000
1	9.702903000	4.145817000	-2.913749000
1	7.995682000	4.327739000	-2.513393000
1	8.801553000	5.551944000	-3.512767000
1	-10.914267000	5.310994000	-1.806387000
1	-9.510404000	5.109838000	2.274252000
1	-9.630315000	7.607241000	2.437473000
1	-11.029211000	7.808556000	-1.642339000
1	-8.610706000	-4.985424000	-2.140491000
1	-8.497988000	-7.484769000	-2.274382000
1	-10.752851000	-7.784917000	1.395512000
1	-10.870106000	-5.285772000	1.529363000
7	-0.747353000	0.313405000	0.795727000
1	-0.288994000	0.012119000	-0.057744000
6	0.080875000	0.597245000	1.866075000
8	-0.351197000	0.864448000	3.025881000
30	-9.978056000	0.038433000	-0.046138000
30	9.257174000	0.029571000	0.168468000

$Zn^{1}Zn^{2}$-4d^{+}

7	7.759470000	-1.140578000	0.943664000
7	10.617473000	-1.463660000	0.318887000
7	7.871979000	1.629918000	0.008909000
7	10.742205000	1.324854000	-0.560181000
6	6.417251000	-0.811487000	1.121863000
6	5.700060000	-1.989155000	1.604650000
6	6.617039000	-3.008621000	1.720266000
6	7.909402000	-2.480408000	1.301858000
1	4.642210000	-2.035018000	1.817169000
1	6.438895000	-4.022949000	2.047351000
6	9.108669000	-3.230952000	1.261287000
6	5.828876000	0.450583000	0.849765000
6	11.594957000	-3.515230000	0.804125000
6	12.584487000	-2.700822000	0.303273000
6	11.970788000	-1.412618000	-0.009730000
6	10.359472000	-2.741623000	0.814925000
1	11.689811000	-4.537038000	1.142591000
1	13.628036000	-2.945158000	0.170115000
6	12.656614000	-0.288631000	-0.537778000
6	8.144484000	2.926783000	-0.427104000
6	6.925395000	3.722007000	-0.346947000

6	5.929716000	2.899773000	0.128864000
6	6.521225000	1.582264000	0.347730000
1	6.848130000	4.766697000	-0.612123000
1	4.901079000	3.163858000	0.326103000
6	12.766791000	2.125001000	-1.372333000
6	11.856367000	3.152700000	-1.463636000
6	10.584884000	2.653418000	-0.954384000
6	12.070994000	0.977443000	-0.795212000
1	13.803380000	2.140685000	-1.675215000
1	12.022991000	4.149712000	-1.845482000
6	9.392678000	3.413028000	-0.884152000
6	9.046414000	-4.667480000	1.719919000
6	9.237767000	-4.987122000	3.091243000
6	9.172833000	-6.335468000	3.499702000
6	8.924266000	-7.378782000	2.583150000
6	8.731504000	-7.039362000	1.228494000
6	4.351980000	0.589381000	1.087270000
6	3.470331000	0.792569000	0.000393000
6	2.084540000	0.885633000	0.201012000
6	1.542736000	0.789156000	1.503641000
6	2.421602000	0.620794000	2.596585000
6	3.804716000	0.512086000	2.389557000
1	3.871148000	0.865914000	-1.006515000
1	1.449002000	1.064784000	-0.663000000
1	4.466461000	0.375749000	3.240255000
6	9.457577000	4.852372000	-1.333049000
6	9.160775000	5.193485000	-2.678794000
6	9.228546000	6.545942000	-3.078155000
6	9.586006000	7.569511000	-2.177326000
6	9.871750000	7.209247000	-0.843390000
6	9.816197000	5.869355000	-0.407189000
6	14.118332000	-0.451593000	-0.845510000
6	14.547609000	-1.325134000	-1.873052000
6	15.910926000	-1.475429000	-2.164572000
6	16.879410000	-0.759774000	-1.425842000
6	16.462139000	0.110706000	-0.394283000
6	15.095827000	0.263692000	-0.113766000
1	13.809685000	-1.874161000	-2.451145000
1	16.235353000	-2.140203000	-2.959531000
1	17.203420000	0.657060000	0.178620000
1	14.783072000	0.929087000	0.686022000
6	8.791419000	-5.701892000	0.780979000
6	18.315513000	-0.949111000	-1.763719000
8	18.744404000	-1.700957000	-2.667044000
1	2.009828000	0.570120000	3.599837000
7	-11.297882000	-1.509910000	-0.602008000
7	-8.356119000	-1.277319000	-0.391459000
7	-11.566904000	1.328973000	0.157523000
7	-8.648607000	1.481954000	0.610079000
6	-12.664356000	-1.359572000	-0.820272000
6	-13.181959000	-2.549293000	-1.477786000
6	-12.124881000	-3.417006000	-1.637171000
6	-10.948703000	-2.767443000	-1.079153000
1	-14.200094000	-2.695708000	-1.803883000
1	-12.142580000	-4.383798000	-2.115970000
6	-9.638222000	-3.331670000	-1.054023000
6	-13.437727000	-0.214397000	-0.476554000
6	-7.157452000	-3.265251000	-0.467564000
6	-6.281526000	-2.272199000	-0.089870000
6	-7.032069000	-1.026829000	-0.056105000
6	-8.454420000	-2.639892000	-0.667439000
1	-6.946323000	-4.319404000	-0.559792000
1	-5.243422000	-2.388351000	0.179443000
6	-6.486123000	0.243643000	0.312329000
6	-11.502469000	2.599556000	0.720820000
6	-12.849878000	3.074950000	0.993629000
6	-13.720014000	2.094916000	0.571352000
6	-12.914629000	1.005675000	0.042470000
1	-13.103661000	4.008774000	1.470853000
1	-14.796509000	2.101814000	0.646534000
6	-6.709166000	2.747179000	0.777538000
6	-7.771094000	3.600346000	0.979431000
6	-8.984431000	2.805468000	0.881584000
6	-7.259743000	1.418513000	0.563503000
1	-5.663114000	3.008287000	0.742064000
1	-7.728647000	4.666794000	1.138270000
6	-10.307118000	3.322453000	1.008515000
6	-9.497831000	-4.761613000	-1.465242000
6	-10.236004000	-5.775713000	-0.806170000
6	-10.101251000	-7.123464000	-1.177780000
6	-9.235461000	-7.430869000	-2.232059000
6	-8.495124000	-6.464977000	-2.920777000
6	-14.918400000	-0.294999000	-0.675002000
6	-15.577566000	0.629154000	-1.522184000
6	-16.962272000	0.550044000	-1.721532000
6	-17.719720000	-0.441537000	-1.060480000
6	-17.072802000	-1.359719000	-0.204625000
6	-15.683813000	-1.291867000	-0.023079000
1	-15.002108000	1.390247000	-2.040585000
1	-17.464736000	1.248497000	-2.383403000
1	-15.195523000	-1.996242000	0.643782000
6	-10.449243000	4.733187000	1.480845000
6	-11.149983000	5.688917000	0.704263000
6	-11.276315000	7.018685000	1.138492000
6	-10.709363000	7.364759000	2.369086000
6	-10.017994000	6.455662000	3.175943000
6	-9.882241000	5.135712000	2.715557000
6	-5.009326000	0.337659000	0.443462000
6	-4.160290000	-0.104760000	-0.605372000
6	-2.771733000	-0.024764000	-0.488821000
6	-2.173006000	0.471212000	0.697870000
6	-3.006163000	0.909972000	1.757333000
6	-4.398915000	0.854182000	1.614289000
1	-4.593369000	-0.480836000	-1.527328000
1	-2.145847000	-0.349736000	-1.316607000
1	-2.561712000	1.275001000	2.672668000
1	-5.020493000	1.176792000	2.444630000
6	-8.624879000	-5.124934000	-2.520413000

1	-17.655292000	-2.116149000	0.309132000
9	-10.840515000	8.690028000	2.816171000
9	-9.102956000	-8.775140000	-2.617897000
6	-19.191532000	-0.484089000	-1.292793000
8	-19.815106000	0.303969000	-2.035940000
8	-19.811088000	-1.494861000	-0.596922000
6	-21.275710000	-1.632928000	-0.752173000
1	-21.522948000	-1.831872000	-1.798815000
1	-21.545535000	-2.478031000	-0.118949000
1	-21.774541000	-0.718160000	-0.419861000
8	19.155412000	-0.199641000	-0.969340000
6	20.607923000	-0.310071000	-1.218851000
1	20.839288000	0.015786000	-2.237095000
1	21.069228000	0.349744000	-0.483812000
1	20.935700000	-1.343958000	-1.077335000
1	9.319017000	-6.574632000	4.551775000
1	8.531395000	-7.828150000	0.505421000
1	8.997917000	6.801694000	-4.110803000
1	10.142945000	7.984909000	-0.129053000
6	8.885870000	-8.825956000	3.041579000
1	8.341678000	-9.457439000	2.329939000
1	9.901353000	-9.236874000	3.136333000
1	8.405037000	-8.922908000	4.022780000
6	9.509011000	-3.902783000	4.121074000
1	10.408242000	-3.325147000	3.869535000
1	8.678519000	-3.186968000	4.180053000
1	9.652598000	-4.336562000	5.116535000
6	8.577153000	-5.393543000	-0.691704000
1	7.736882000	-4.702650000	-0.840668000
1	9.461792000	-4.917639000	-1.135068000
1	8.367695000	-6.308374000	-1.256454000
6	9.679975000	9.015660000	-2.631037000
1	9.287993000	9.700862000	-1.869185000
1	10.724427000	9.303523000	-2.818644000
1	9.121851000	9.181390000	-3.559634000
6	10.136031000	5.537243000	1.040958000
1	9.298490000	5.023970000	1.531205000
1	11.005242000	4.870582000	1.117744000
1	10.357006000	6.446034000	1.611073000
6	8.770513000	4.131117000	-3.693057000
1	9.548074000	3.362032000	-3.789580000
1	7.847392000	3.614078000	-3.399042000
1	8.609003000	4.575002000	-4.681311000
1	-11.573811000	5.402093000	-0.253065000
1	-9.357578000	4.411312000	3.330779000
1	-9.601864000	6.769081000	4.127637000
1	-11.796238000	7.761848000	0.543091000
1	-8.066327000	-4.358020000	-3.048030000
1	-7.842404000	-6.751073000	-3.738865000
1	-10.648768000	-7.909087000	-0.667694000
1	-10.895646000	-5.516267000	0.016094000
7	-0.761037000	0.489966000	0.745126000
1	-0.301150000	0.128781000	-0.084044000
6	0.072142000	0.872277000	1.789201000
8	-0.366847000	1.239225000	2.916170000
30	-9.963017000	0.022876000	-0.094410000
30	9.249436000	0.089367000	0.183829000

$Zn^{1}Zn^{2}$-4d^{-}

7	7.802952000	-1.181428000	0.921016000
7	10.663504000	-1.469913000	0.285926000
7	7.891387000	1.606338000	0.037240000
7	10.763812000	1.334053000	-0.542461000
6	6.456675000	-0.868603000	1.100360000
6	5.747692000	-2.064736000	1.548544000
6	6.672979000	-3.078691000	1.643327000
6	7.962632000	-2.528748000	1.245387000
1	4.688857000	-2.125739000	1.751455000
1	6.501297000	-4.102758000	1.942279000
6	9.168049000	-3.268590000	1.189323000
6	5.857468000	0.394908000	0.858064000
6	11.656725000	-3.523477000	0.728458000
6	12.639874000	-2.691222000	0.244254000
6	12.016088000	-1.401862000	-0.042760000
6	10.415285000	-2.760031000	0.755324000
1	11.759657000	-4.551421000	1.045410000
1	13.685168000	-2.924967000	0.105450000
6	12.692353000	-0.262510000	-0.549801000
6	8.154836000	2.915330000	-0.366555000
6	6.932138000	3.701656000	-0.260187000
6	5.943360000	2.862276000	0.199777000
6	6.542451000	1.542664000	0.381759000
1	6.847541000	4.752310000	-0.498163000
1	4.914584000	3.115578000	0.409519000
6	12.781543000	2.168049000	-1.336854000
6	11.862772000	3.190225000	-1.405732000
6	10.595679000	2.670263000	-0.906649000
6	12.095552000	1.002933000	-0.783853000
1	13.817853000	2.198867000	-1.639639000
1	12.021280000	4.196477000	-1.766261000
6	9.398906000	3.420099000	-0.814900000
6	9.115194000	-4.716429000	1.612147000
6	9.301019000	-5.068694000	2.976564000
6	9.242769000	-6.426722000	3.351264000
6	9.005207000	-7.448964000	2.407950000
6	8.818751000	-7.077723000	1.061209000
6	4.380137000	0.517248000	1.100856000
6	3.496459000	0.765649000	0.025103000
6	2.109998000	0.844198000	0.230461000
6	1.567232000	0.683742000	1.526294000
6	2.448767000	0.469394000	2.608733000
6	3.832730000	0.378396000	2.397929000
1	3.895860000	0.885618000	-0.978055000
1	1.473854000	1.059509000	-0.624802000
1	4.494868000	0.208040000	3.242369000
6	9.455345000	4.872018000	-1.222799000
6	9.164996000	5.249869000	-2.559415000
6	9.229200000	6.614246000	-2.919852000

6	9.573495000	7.613192000	-1.987857000
6	9.855352000	7.215817000	-0.663024000
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