Supplementary Material (ESI) for Chemical Communications

Supplementary Information

for

Endocyclic extension of porphyrin π-System in etheno-bridged N-confused tetraphenylporphyrin

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1. Experimental Section

Synthesis of 21-trimethylsilylethynyl N-fused tetraphenylporphyrin (5)

To a solution of 21-bromo N-fused tetraphenylporphyrin (**4**, 59.8 mg, 0.086 mmol, 1 equiv) and $Pd(PPh_3)_4$ (29.7 mg, 0.026 mmol, 30 mol %) in 12 mL of THF, tri-*n*-butyl(trimethylsilylethynyl)tin (166 μL, 0.43 mmol, 5 equiv) was added. The reaction mixture was stirred for 12 h at 23 °C under Ar. After evaporation, the residue was separated by silica gel column chromatography with $MeOH/CH_2Cl_2$ (= 2/98). The second red fraction afforded **5** in 83% yield (49.7 mg, 0.070 mmol). **5**: ^1H NMR ($CDCl_3$, 300 MHz, ppm) δ 0.23 (s, 9H), 7.54 (m, 1H), 7.61 (d, J = 4.9 Hz, 1H), 7.67–7.75 (m, 11H), 7.99–8.07 (m, 8H), 8.13–8.16 (m, 2H), 8.63 (d, J = 4.8 Hz, 1H), 8.81 (d, J = 6.7 Hz, 2H), 9.06 (d, J = 4.8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 75 MHz, ppm) δ 0.41, 101.93, 103.53, 107.74, 116.31, 119.98, 120.12, 124.96, 125.71, 126.94, 127.56, 127.71, 127.74, 127.87, 128.16, 128.98, 129.17, 129.75, 130.95, 131.72, 131.86, 133.02, 133.25, 133.69, 134.20, 134.52, 135.13, 136.96, 137.35, 138.98, 139.17, 141.78, 146.29, 146.49, 150.85, 150.90, 154.64, 157.43; MS (MALDI, positive) m/z = 707.951 ($[M]^+$); Anal. Calcd for **5**: C, 83.02; H, 5.12; N, 7.90. Found: C, 82.76; H, 5.12; N, 7.70; UV-vis (CH_2Cl_2, λ_{max}/nm (relative intensity)) 980 (0.05), 886 (0.05), 713 (0.15), 660 (0.19), 563 (1.00), 518 (0.82), 393 (0.73), 350 (0.72).

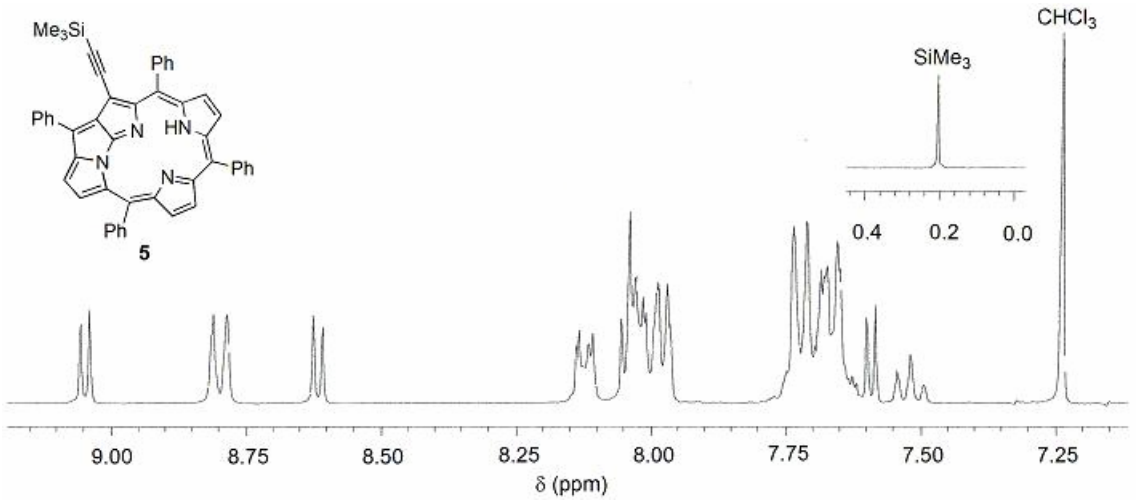

Figure S1. ^{1}H NMR spectrum of **5** at 25 °C in $CDCl_3$.

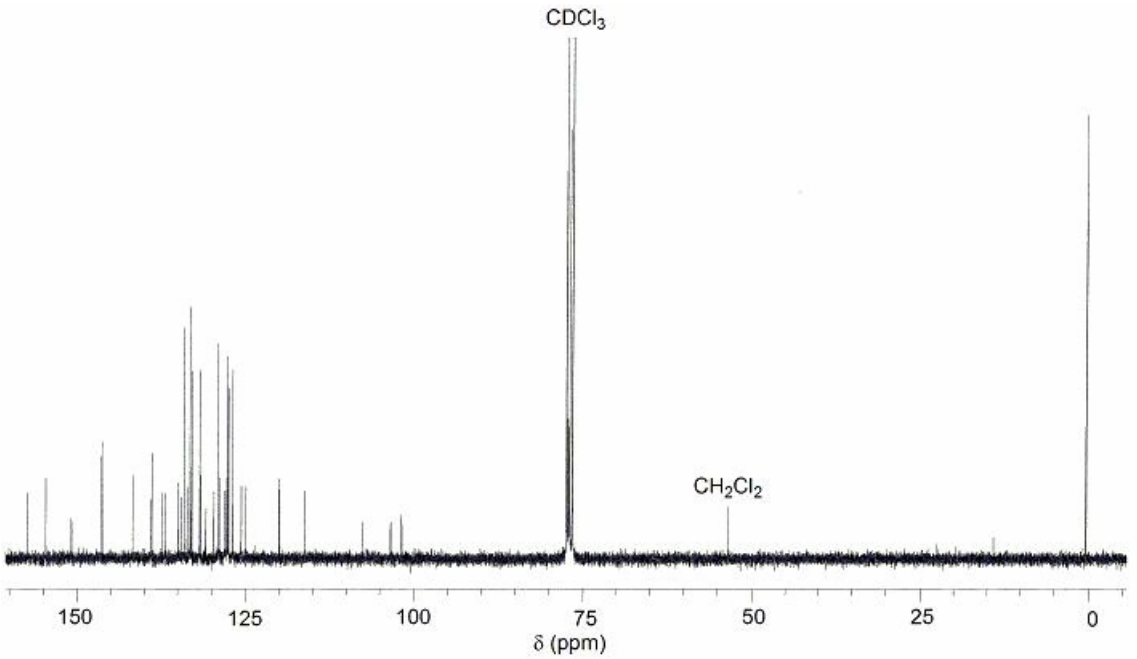

Figure S2. ^{13}C NMR spectrum of **5** at 25 °C in $CDCl_3$.

Synthesis of 3-methoxy-etheno-bridged N-confused tetraphenylporphyrin (1a)

To a THF (20 mL) solution of **5** (50 mg, 0.071 mmol), a 28% solution of NaOMe in MeOH (0.2 mL, 12 equiv) was added at 23 °C in one portion. The reaction mixture was stirred at that temperature for 4 h and then neutralized with sat. aq NH_4Cl. The organic layer was separated, washed with brine and dried over anhydrous Na_2SO_4. After evaporation, the residue was separated by silica gel column chromatography with $MeOH/CH_2Cl_2$ (= 1/99). The brown fraction afforded **1a** in 86% yield (41 mg, 0.061 mmol). **1a**: ^{1}H NMR ($CDCl_3$, 300 MHz, ppm) δ –0.78 (d, J = 7.3 Hz, 1H), –0.47 (d, J = 7.3 Hz, 1H), 3.83 (s, 3H), 7.64–7.73 (m, 13H), 7.89–7.92 (m, 2H), 8.10 (m, 5H), 8.20 (d, J = 4.9 Hz, 1H), 8.29 (s, 1H), 8.38 (d, J = 4.9 Hz, 1H), 8.55 (d, J = 4.9 Hz, 1H), 8.61 (d, J = 4.9 Hz, 1H); ^{13}C NMR ($CDCl_3$, 300 MHz, ppm) δ 55.76, 101.23, 113.02, 117.21, 120.03, 120.59, 123.33, 125.97, 126.01, 126.59, 126.98, 127.06, 127.16, 127.52, 127.63, 128.56, 128.77, 130.04, 132.24, 132.37, 133.12, 135.29, 136.13, 140.28, 141.18, 141.43, 141.77, 141.81, 143.15, 144.70, 144.76, 146.52, 152.66, 153.34, 163.57; MS (MALDI, positive) m/z = 668.216 ($[M]^+$); Anal. Calcd for **1a**•0.1CH_2Cl_2: C, 83.53; H, 4.79; N, 8.27. Found: C, 83.22; H, 5.02; N, 8.05; UV-vis (CH_2Cl_2, λ_{max}/nm (ε)) 775 (2500), 628 (6500), 579 (7300), 426 (50000), 355 (42000).

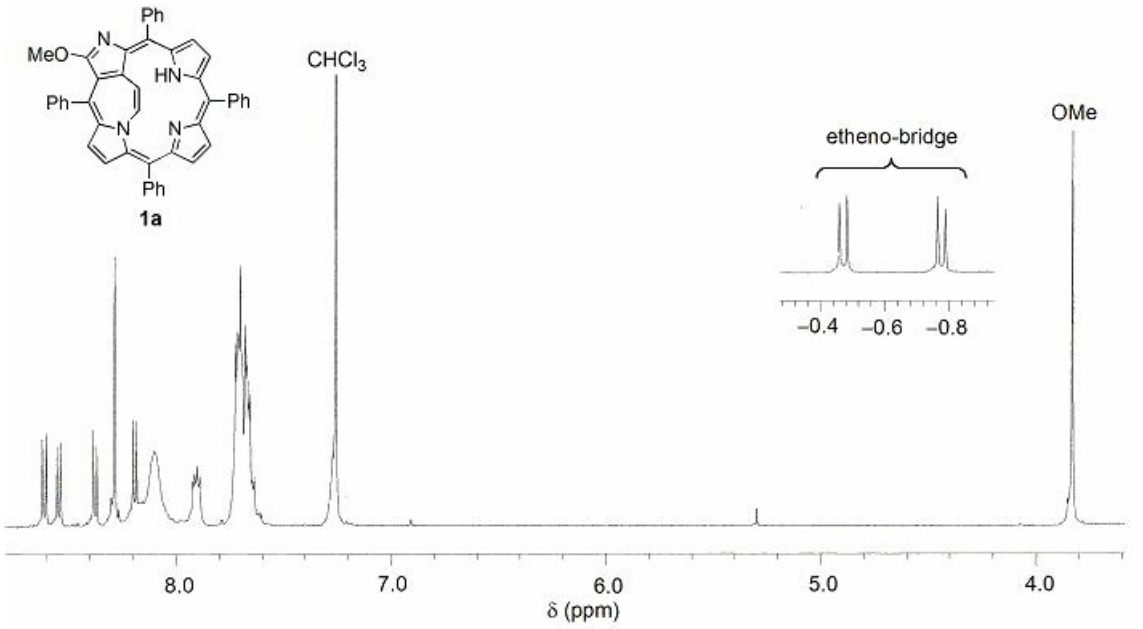

Figure S3. ^{1}H NMR spectrum of **1a** at 25 °C in $CDCl_3$.

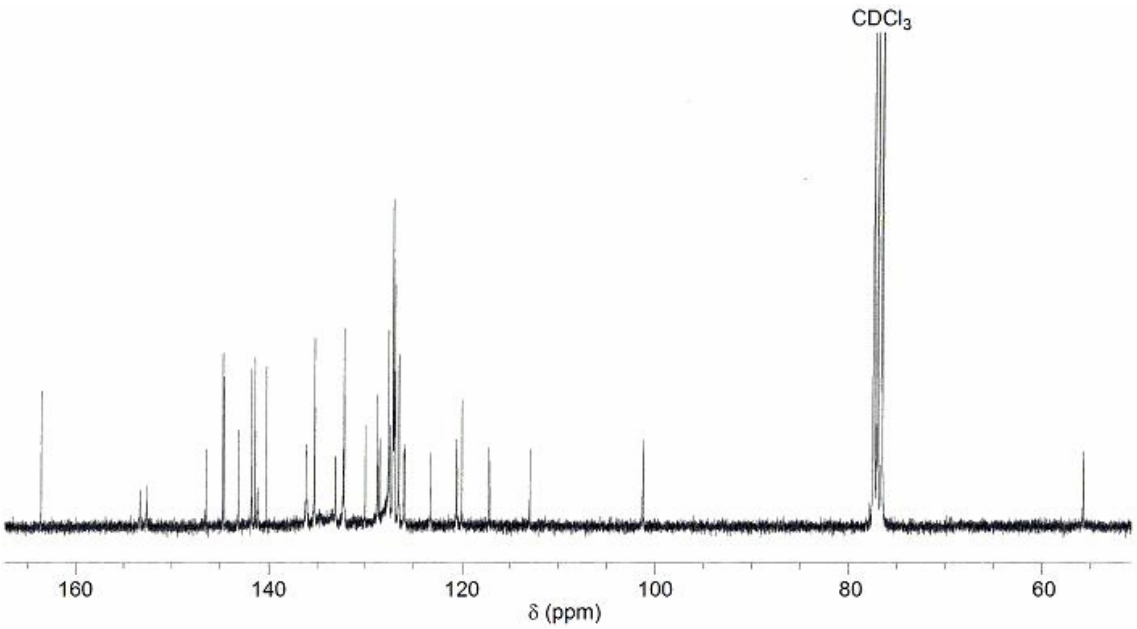

Figure S4. ^{13}C NMR spectrum of **1a** at 25 °C in $CDCl_3$.

Synthesis of 3-ethoxy-etheno-bridged N-confused tetraphenylporphyrin (1b)

To a THF (40 mL) solution of **5** (72.7 mg, 0.103 mmol), a 20% solution of NaOEt in EtOH (0.4 mL, 9.0 equiv) was added at 23 °C in one portion. The reaction mixture was stirred at 60 °C for 12 h and then neutralized with sat. aq NH_4Cl. The organic layer was separated, washed with brine and dried over anhydrous Na_2SO_4. After evaporation, the residue was separated by silica gel column chromatography with $MeOH/CH_2Cl_2$ (= 1/99) to give **1b** in 92% yield (64.5 mg, 0.0945 mmol). **1b**: ^{1}H NMR ($CDCl_3$, 300 MHz, ppm) δ –0.78 (d, J = 7.3 Hz, 1H), –0.48 (d, J = 7.3 Hz, 1H), 0.96 (t, 3H), 4.04–4.14 (dq, J = 7.0, 10.4 Hz, 1H), 4.39–4.49 (dq, J = 7.0, 10.4 Hz, 1H), 7.65–7.75 (m, 13H), 7.89–7.92 (m, 2H), 8.11 (m, 5H), 8.22 (d, J = 4.9 Hz, 1H), 8.30 (s, 2H), 8.38–8.40 (m, 1H), 8.54 (d, J = 4.9 Hz, 1H), 8.69 (d, J = 4.9 Hz, 1H); ^{13}C NMR ($CDCl_3$, 300 MHz, ppm) δ 13.94, 63.89, 101.21, 112.85, 117.11, 119.96, 120.53, 123.18, 125.93, 126.05, 126.57, 126.94, 127.02, 127.14, 127.48, 127.52, 127.57, 128.36, 128.68, 129.21, 130.14, 132.28, 132.32, 133.06, 135.28, 136.14, 140.40, 141.12, 141.40, 141.68, 141.75, 143.11, 144.53, 144.69; MS (MALDI, positive) *m/z* = 682.003 ($[M]^+$); Anal. Calcd for **1b**·0.1CH_2Cl_2: C, 83.57; H, 4.99; N, 8.10. Found: C, 83.53; H, 5.23; N, 7.92; UV-vis (CH_2Cl_2, λ_{max}/nm (relative intensity)) 771 (0.05), 629 (0.12), 582 (0.13), 426 (1.00), 355 (0.83).

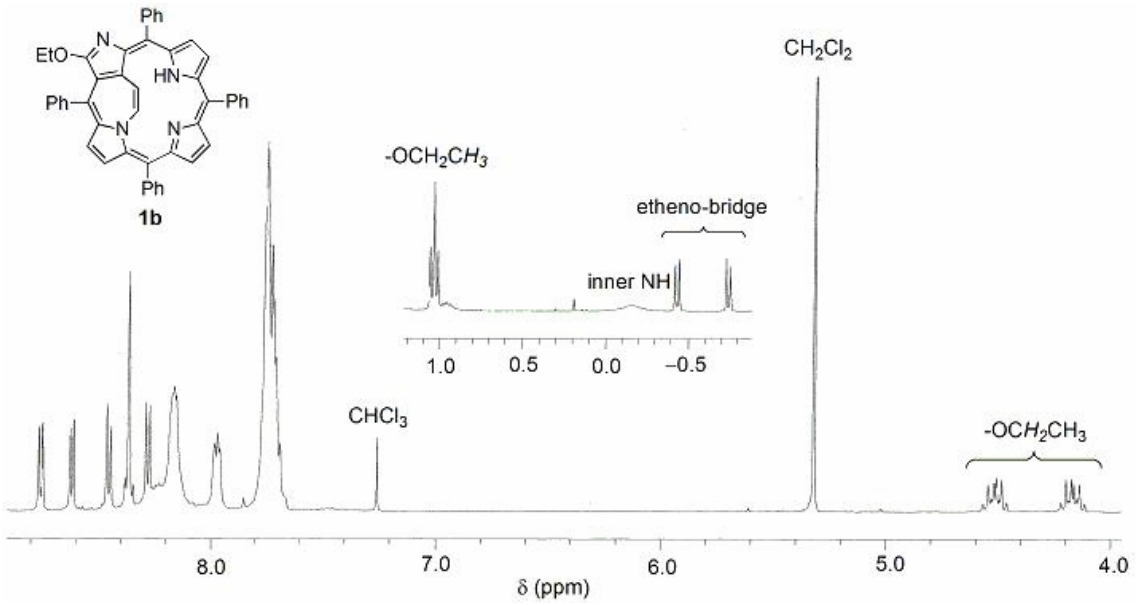

Figure S5. ^{1}H NMR spectrum of **1b** at 25 °C in $CDCl_3$.

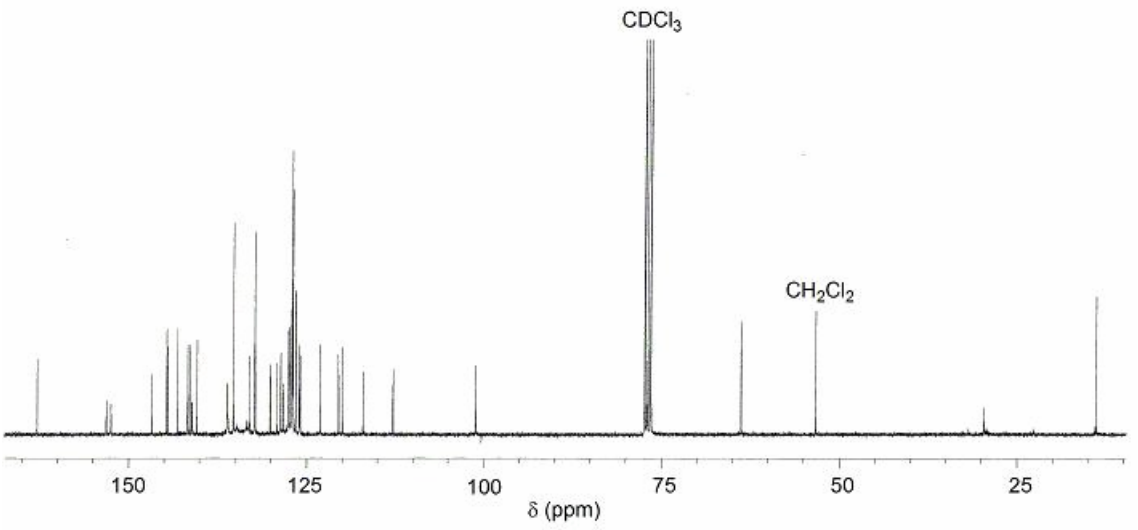

Figure S6. ^{13}C NMR spectrum of **1b** at 25 °C in $CDCl_3$.

Synthesis of 21-ethynyl N-fused tetraphenylporphyrin (7)

A solution of **5** (51.7 mg, 0.0729 mmol, 1.0 equiv) in 25 mL of CH_2Cl_2 was treated with TBAF (1 M in THF, 109 μL, 1.5 equiv) at 23 °C for 1.5 h. Then, the reaction mixture was treated with 10 μl of CH_3COOH. After removal of the solvent, the residue was recrystallized from CH_2Cl_2/MeOH to give **7** in 89% yield (41.5 mg, 0.0652 mmol). **7**: ^{1}H NMR ($CDCl_3$, 300 MHz, ppm) δ3.64 (s, 1H), 7.54 (m, 1H), 7.61-7.75 (m, 12H), 7.99-8.13 (m, 10H), 8.64 (d, J = 5.2 Hz, 1H), 8.79 (d, J = 7.9 Hz, 1H), 9.08 (d, J = 5.2 Hz, 1H); MS (MALDI, positive) m/z = 636.384 ($[M]^+$); UV-vis (CH_2Cl_2, λ_{max}/nm (relative intensity)) 966 (0.06), 872 (0.06), 710 (0.13), 656 (0.19), 557 (1.00), 514 (0.90), 389 (0.77), 352 (0.75).

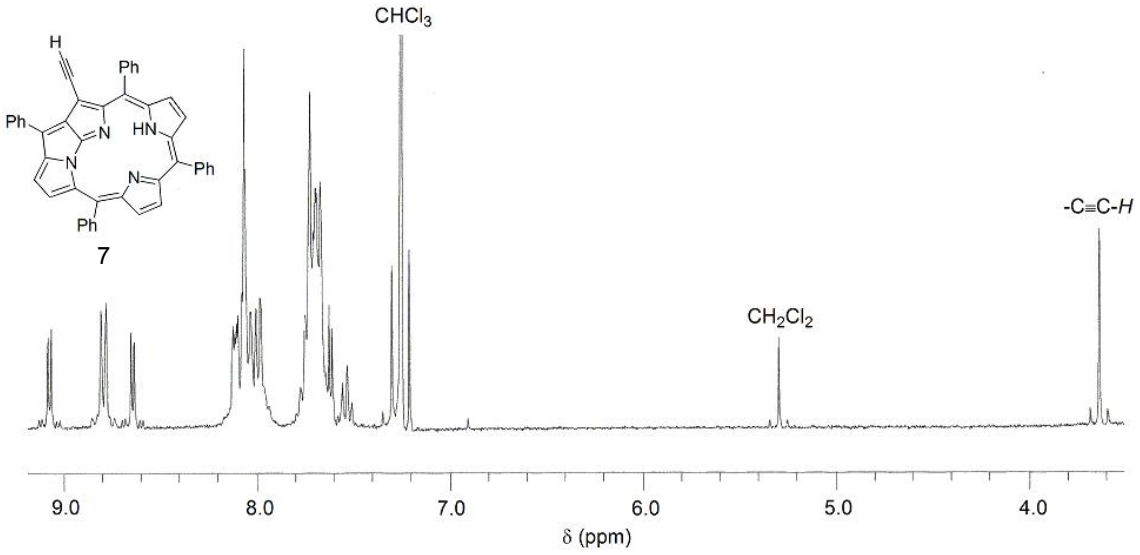

Figure S7. ^{1}H NMR spectrum of **7** at 25 °C in $CDCl_3$.

Synthesis of 1a from 7

To a THF (4.0 mL) solution of **7** (13.4 mg, 0.0210 mmol, 1.0 equiv), a 28% solution of NaOMe in MeOH (0.05 mL, 12 equiv) was added at 23 °C. The reaction mixture was stirred at that temperature for 30 min and then neutralized with sat. aq NH_4Cl. The organic layer was separated, washed with brine and dried over anhydrous Na_2SO_4. After evaporation, the residue was separated by silica gel column chromatography with MeOH/CH_2Cl_2 (= 1/99). The brown fraction afforded **1a** in 60% yield (8.4 mg, 0.0126 mmol).

Synthesis of 21-triisopropylsilylethynyl N-fused tetraphenylporphyrin (8)

To a solution of 21-bromo N-fused tetraphenylporphyrin (**4**, 100 mg, 0.145 mmol, 1 equiv) and $Pd(PPh_3)_4$ (24.5 mg, 0.0212 mmol, 15 mol %) in 20 mL of THF, tri-*n*-butyl(triisopropylsilylethynyl)tin (342 mg, 0.725 mmol, 5 equiv) was added. The reaction mixture was stirred for 18 h at 60 °C under Ar. After evaporation, the residue was separated by silica gel column chromatography with $MeOH/CH_2Cl_2$ (= 0.5/99.5). The second red fraction afforded **8** in 78% yield (90.0 mg, 0.113 mmol). **8**: ^{1}H NMR ($CDCl_3$, 300 MHz, ppm) δ1.03 (s, 21H), 7.50-7.55 (m, 1H), 7.61 (d, J = 4.3 Hz, 1H), 7.63-7.73 (m, 11H), 7.93-8.07 (m, 8H), 8.17-8.20 (m, 2H), 8.62 (d, J = 4.9 Hz, 1H), 8.66 (d, J = 7.3 Hz, 2H), 9.00 (d, J = 4.9 Hz, 1H); MS (MALDI, positive) m/z = 792.644 ($[M]^+$); UV-vis (CH_2Cl_2, λ_{max}/nm (relative intensity)) 350 (0.68), 395 (0.70), 519 (0.77), 562 (1.00), 659 (0.19), 711 (0.14), 891 (0.05), 984 (0.05).

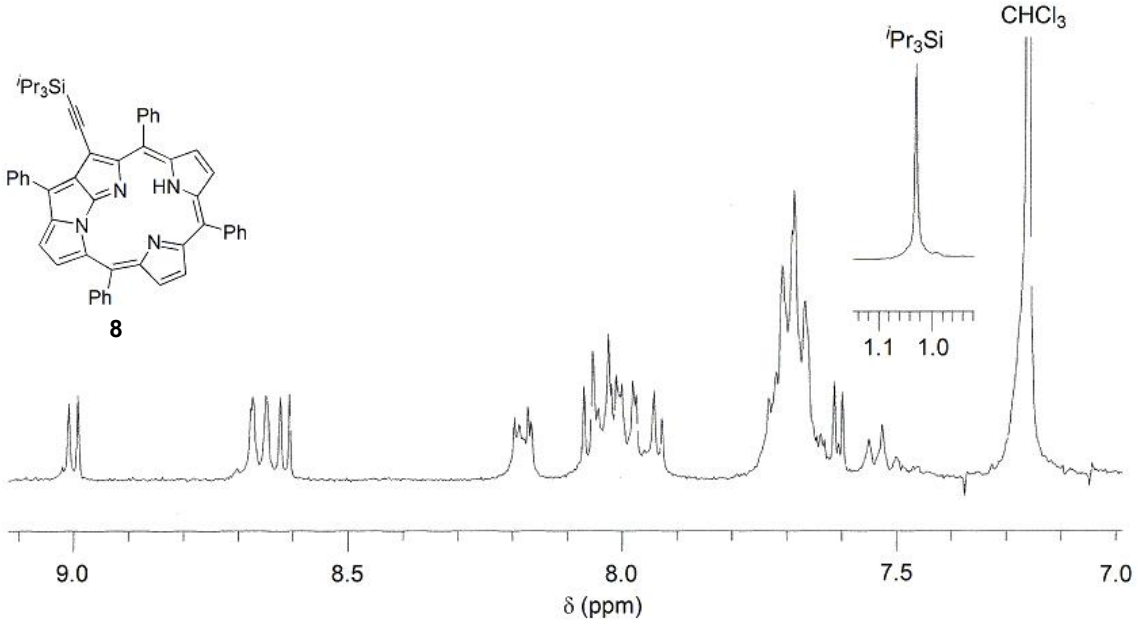

Figure S8. ^{1}H NMR spectrum of **8** at 25 °C in $CDCl_3$.

Synthesis of 3-methoxy-21-triisopropylsilylethynyl N-confused tetraphenylporphyrin (9)

To a THF (20 mL) solution of **8** (69.7 mg, 0.0879 mmol), a 28% solution of NaOMe in MeOH (0.2 mL, 12 equiv) was added at 23 °C. The reaction mixture was stirred at that temperature for 4 h and then neutralized with sat. aq NH_4Cl. The organic layer was separated, washed with brine and dried over anhydrous Na_2SO_4. After evaporation, the residue was separated by silica gel column chromatography with $MeOH/CH_2Cl_2$ (= 1/99). The brown fraction afforded **9** in 73% yield (52.8 mg, 0.0640 mmol). **9**: ^{1}H NMR

($CDCl_3$, 300 MHz, ppm) δ-1.07 (septet, J = 7.3 Hz, 3H), -0.69 (d, J = 7.3 Hz, 18H), 3.67 (s, 3H), 7.66-7.81 (m, 12H), 7.89-7.92 (m, 1H), 8.04-8.10 (m, 2H), 8.25-8.30 (m, 3H), 8.39-8.47 (m, 6H), 8.68 (d, J = 4.9 Hz, 1H), 8.80 (d, J = 5.5 Hz, 1H); MS (MALDI, positive) m/z = 823.664 ($[M]^+$); UV-vis (CH_2Cl_2, λ_{max}/nm (relative intensity)) 356 (0.22), 424 (1.00), 460 (0.87), 563 (0.12), 608 (0.11), 722 (0.06).

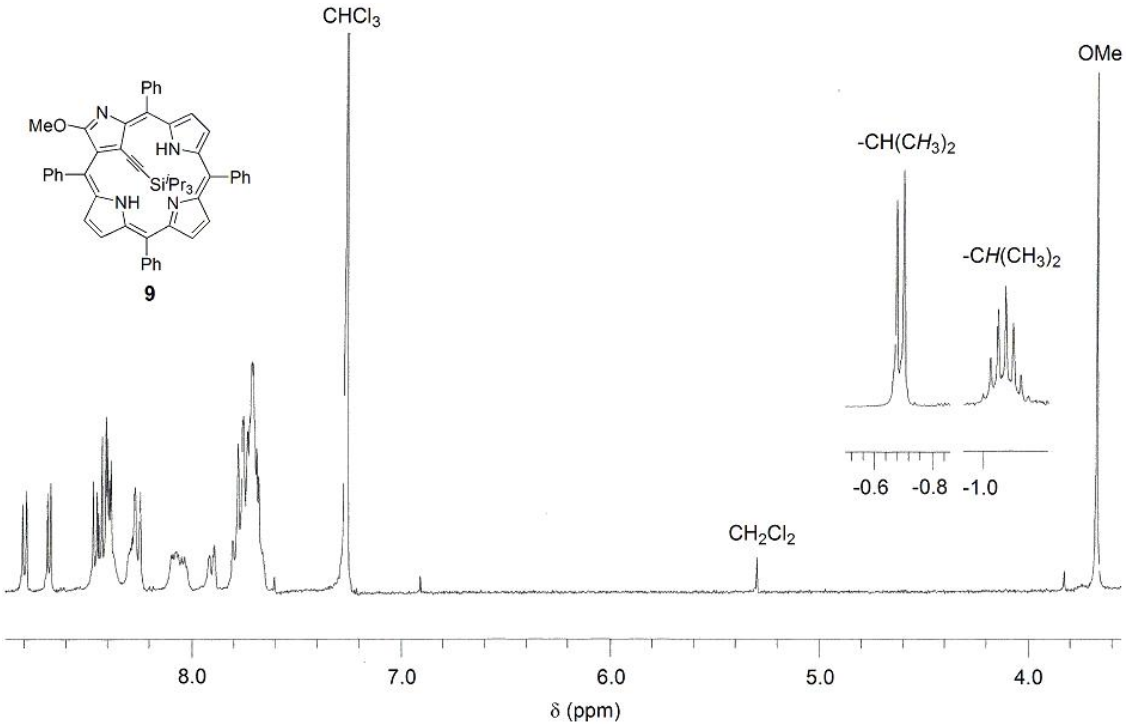

Figure S9. ^{1}H NMR spectrum of **9** at 25 °C in $CDCl_3$.

Synthesis of 1a from 9

A solution of **9 (**15.0 mg, 0.0182 mmol**)** in 5 mL of THF was treated with TBAF (1 M in THF, 37.8 μL, 2 equiv) at 23 °C for 72 h. After evaporation, the residue was separated by silica gel column chromatography with MeOH/CH_2Cl_2 (= 1/99). The brown fraction afforded **1a** in 97% yield (11.8 mg, 0.0176 mmol).

2. Cartesian Coordinates of the Optimized Structures

For 1a Energy = -2104.49404983 A.U.

Stoichiometry C47H32N4O
Framework group C1[X(C47H32N4O)]
Deg. of freedom 246
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	.424690	2.059234	-.444332
2	7	0	3.400793	-1.918659	.264052
3	7	0	-1.001250	-1.992713	.026673
4	7	0	-2.263920	.595693	.108539
5	6	0	2.075707	-1.879307	-.230154
6	6	0	1.731022	-.560962	-.631700
7	6	0	2.833960	.265098	-.299964
8	6	0	3.831482	-.693521	.215519
9	6	0	2.907159	1.670896	-.283111
10	6	0	1.763137	2.493757	-.293192
11	6	0	1.702648	3.862764	.079306
12	6	0	.381473	4.218022	.224547
13	6	0	-.436469	3.096468	-.092662
14	6	0	-1.850163	3.051018	-.001045
15	6	0	-2.671677	1.898190	.051455
16	6	0	-4.137201	1.971757	.038056
17	6	0	-4.589818	.697844	.084582
18	6	0	-3.404025	-.159095	.099924
19	6	0	-3.447186	-1.567526	.063946
20	6	0	-2.311960	-2.406148	-.026923
21	6	0	-2.286894	-3.814047	-.268220
22	6	0	-.973249	-4.205392	-.360499
23	6	0	-.138106	-3.058042	-.177754
24	6	0	1.281367	-3.043624	-.176152
25	6	0	4.236096	2.346584	-.128585
26	6	0	.036607	1.059556	-1.378407
27	1	0	-.779053	1.351781	-2.027641
28	6	0	5.135553	2.358056	-1.203702
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30	6	0	6.738199	3.602849	.111803
31	6	0	5.853557	3.589543	1.191181
32	6	0	-2.516883	4.386944	.125705
33	6	0	4.611231	2.966789	1.071800

34	1	0	4.855422	1.875407	-2.135322
35	1	0	7.058400	2.990328	-1.930632
36	1	0	7.704799	4.089520	.204238
37	1	0	6.131622	4.060209	2.129880
38	1	0	3.930540	2.944928	1.917464
39	6	0	-4.777420	-2.254360	.058810
40	1	0	-.776485	-1.009555	.160617
41	8	0	5.034783	-.307275	.655436
42	1	0	.240263	-.833817	-2.205795
43	6	0	-2.412993	5.342684	-.898768
44	6	0	-3.026695	6.589588	-.781058
45	6	0	-3.753253	6.908310	.367431
46	6	0	1.975329	-4.354888	-.030888
47	6	0	1.615756	-5.267499	.975167
48	6	0	2.270365	-6.492941	1.097149
49	6	0	3.295729	-6.831124	.213626
50	6	0	3.668578	-5.930453	-.787008
51	6	0	3.020370	-4.703779	-.903470
52	1	0	.830992	-5.002099	1.676182
53	1	0	1.982507	-7.180060	1.887746
54	6	0	.622742	-.138427	-1.464295
55	1	0	2.564438	4.472540	.301503
56	1	0	.003117	5.163579	.581455
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63	1	0	3.314331	-4.004272	-1.678439
64	6	0	-3.860354	5.971351	1.396784
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67	1	0	-2.940727	7.310337	-1.589236
68	1	0	-4.230693	7.879389	.460306
69	1	0	-4.416596	6.213142	2.297965
70	1	0	-3.325270	4.000860	2.083435
71	6	0	-5.667974	-2.106717	-1.016789
72	6	0	-6.903434	-2.754607	-1.015927
73	6	0	-7.270405	-3.565956	.058938
74	6	0	-6.392593	-3.726028	1.132223
75	6	0	-5.157569	-3.077384	1.131168
76	1	0	-5.380996	-1.485058	-1.859394
77	1	0	-7.576670	-2.629735	-1.859247
78	1	0	-8.232063	-4.070708	.059310
79	1	0	-6.670295	-4.353037	1.974700

80	1	0	-4.480006	-3.198071	1.971106
81	6	0	5.853003	-1.345038	1.211273
82	1	0	6.046926	-2.123597	.468397
83	1	0	5.360883	-1.804051	2.073065
84	1	0	6.780996	-.856808	1.509661

For 2a Energy = -2104.49812156 A.U.

Stoichiometry C47H32N4O
Framework group C1[X(C47H32N4O)]
Deg. of freedom 246
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-.166051	2.118390	.079953
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3	7	0	-.381682	-2.179199	-.527566
4	7	0	-2.325404	.159522	.095248
5	6	0	2.533724	-1.368627	-.224912
6	6	0	1.827350	-.192810	-.643364
7	6	0	2.633177	.905409	-.292423
8	6	0	3.841861	.265424	.260555
9	6	0	2.321844	2.296757	-.265193
10	6	0	1.017734	2.811973	-.156642
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13	6	0	-1.241406	2.975742	.121305
14	6	0	-2.596531	2.612262	.215242
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19	6	0	-2.877599	-2.256386	-.165438
20	6	0	-1.573114	-2.830371	-.216696
21	6	0	-1.230460	-4.156010	.148645
22	6	0	.142384	-4.292951	.098808
23	6	0	.705084	-3.048811	-.275113
24	6	0	2.071159	-2.688252	-.192415
25	6	0	3.447257	3.274092	-.326474
26	6	0	-.347442	-1.078877	-1.405944
27	1	0	-1.222997	-.994660	-2.035620

28	6	0	5.914872	.207524	1.360858
29	1	0	6.361179	-.469915	.628226
30	1	0	5.536839	-.385680	2.197590
31	1	0	6.644728	.940988	1.703910
32	6	0	-3.577418	3.741395	.309643
33	6	0	4.372633	3.204801	-1.381401
34	6	0	5.428416	4.109020	-1.466468
35	6	0	5.588305	5.095474	-.490794
36	6	0	4.684455	5.168293	.570076
37	6	0	3.624048	4.266346	.651724
38	1	0	4.249281	2.439114	-2.141481
39	6	0	-3.992574	-3.254562	-.132706
40	1	0	-.305603	1.114125	.144248
41	8	0	4.856212	.970777	.764779
42	1	0	.534568	.631063	-2.179215
43	1	0	6.126487	4.045601	-2.296361
44	1	0	6.413136	5.799211	-.555180
45	1	0	4.808668	5.923385	1.341115
46	6	0	3.057960	-3.768913	.129577
47	1	0	2.935765	4.313186	1.489668
48	6	0	3.075929	-4.394640	1.384102
49	6	0	4.008045	-5.393546	1.666277
50	6	0	4.934578	-5.782417	.697844
51	6	0	4.929164	-5.160094	-.551509
52	6	0	4.001262	-4.157542	-.831174
53	1	0	2.364281	-4.085354	2.143549
54	6	0	.650153	-.184397	-1.471474
55	1	0	1.325369	5.002313	-.454162
56	1	0	-1.312506	5.195961	-.098255
57	1	0	-5.331809	1.652005	.116240
58	1	0	-5.468537	-.996052	-.194294
59	1	0	-1.940989	-4.897122	.481787
60	1	0	.717891	-5.158348	.386933
61	1	0	4.012471	-5.864257	2.645307
62	1	0	5.658606	-6.561898	.916816
63	1	0	5.649804	-5.453189	-1.309622
64	1	0	4.002959	-3.668789	-1.800594
65	6	0	-4.164660	-4.170415	-1.184577
66	6	0	-5.195548	-5.108850	-1.156043
67	6	0	-6.070515	-5.157510	-.069173
68	6	0	-5.905663	-4.261584	.988433
69	6	0	-4.876870	-3.320366	.957622
70	1	0	-3.488315	-4.134084	-2.033249
71	1	0	-5.316911	-5.800284	-1.984961
72	1	0	-6.872045	-5.889984	-.045271
73	1	0	-6.574445	-4.298950	1.843576

74	1	0	-4.743628	-2.633152	1.787050
75	6	0	-4.440705	4.048265	-.754514
76	6	0	-5.344637	5.106679	-.659850
77	6	0	-5.398779	5.882381	.499509
78	6	0	-4.542352	5.592705	1.562633
79	6	0	-3.640211	4.532406	1.467670
80	1	0	-4.393444	3.453901	-1.662011
81	1	0	-6.002011	5.329354	-1.495552
82	1	0	-6.101807	6.707001	.572930
83	1	0	-4.578364	6.189375	2.469716
84	1	0	-2.979721	4.304525	2.299026

For 11 Energy = -2028.31776644 A.U.

Stoichiometry C45H32N4O
Framework group C1[X(C45H32N4O)]
Deg. of freedom 240
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-.030679	-2.138723	-.118440
2	7	0	-3.676608	1.304661	.400508
3	7	0	.570849	2.168373	-.040633
4	7	0	2.233839	-.271971	.072147
5	6	0	-2.363785	1.531373	-.060368
6	6	0	-1.742307	.309590	-.422683
7	6	0	-2.668143	-.718733	-.181989
8	6	0	-3.847327	.016231	.332065
9	6	0	-2.517899	-2.125531	-.267095
10	6	0	-1.260480	-2.753760	-.279668
11	6	0	-.979293	-4.156848	-.393655
12	6	0	.370724	-4.346243	-.252134
13	6	0	.985082	-3.062966	-.075472
14	6	0	2.341985	-2.764844	.122552
15	6	0	2.896974	-1.464157	.204374
16	6	0	4.330785	-1.245662	.358626
17	6	0	4.525641	.091853	.296083
18	6	0	3.212822	.695553	.094642
19	6	0	3.041762	2.085435	-.082622
20	6	0	1.803849	2.750825	-.211222
21	6	0	1.559513	4.118943	-.537379

22	6	0	.198235	4.323499	-.531171
23	6	0	-.443958	3.089954	-.209780
24	6	0	-1.832771	2.835026	-.087172
25	6	0	-3.725185	-3.001286	-.326169
26	1	0	.154796	-1.158256	.044607
27	6	0	-4.652900	-2.847114	-1.368855
28	6	0	-5.775963	-3.667064	-1.450557
29	6	0	-5.998360	-4.652128	-.485781
30	6	0	-5.088766	-4.810294	.560470
31	6	0	3.267746	-3.941194	.231206
32	6	0	-3.961281	-3.992926	.638864
33	1	0	-4.480377	-2.083291	-2.121147
34	1	0	-6.477587	-3.539058	-2.269927
35	1	0	-6.875197	-5.290050	-.548616
36	1	0	-5.258676	-5.567002	1.321111
37	1	0	-3.264012	-4.108209	1.462850
38	6	0	4.258341	2.954450	-.164256
39	1	0	.480100	1.204824	.252278
40	8	0	-4.950919	-.608913	.755036
41	6	0	3.612872	-4.692156	-.902574
42	6	0	4.467644	-5.790480	-.797955
43	6	0	4.993228	-6.154664	.442582
44	6	0	-2.743564	4.001571	.054886
45	6	0	-2.458017	5.041567	.956727
46	6	0	-3.312272	6.136767	1.081040
47	6	0	-4.467924	6.215950	.303640
48	6	0	-4.767014	5.187468	-.593097
49	6	0	-3.918249	4.090473	-.712749
50	1	0	-1.570744	4.976036	1.578103
51	1	0	-3.076880	6.924393	1.791124
52	1	0	-.809018	.212200	-.956674
53	1	0	-1.729129	-4.913960	-.562684
54	1	0	.905930	-5.283106	-.274458
55	1	0	5.074313	-2.018048	.486207
56	1	0	5.459081	.627970	.377021
57	1	0	2.327280	4.842143	-.765102
58	1	0	-.324779	5.238165	-.764497
59	1	0	-5.132830	7.069673	.397999
60	1	0	-5.664528	5.241291	-1.202677
61	1	0	-4.155497	3.292679	-1.407033
62	6	0	4.658071	-5.414752	1.577832
63	6	0	3.800950	-4.318817	1.472995
64	1	0	3.212057	-4.404819	-1.870196
65	1	0	4.726390	-6.357908	-1.687404
66	1	0	5.659534	-7.008452	.524128
67	1	0	5.060483	-5.692576	2.547817

68	1	0	3.537316	-3.747295	2.357998
69	6	0	5.184652	2.805793	-1.209387
70	6	0	6.310993	3.624862	-1.287003
71	6	0	6.532608	4.608387	-.321475
72	6	0	5.619087	4.768471	.721590
73	6	0	4.491550	3.950843	.797654
74	1	0	5.010744	2.046654	-1.965696
75	1	0	7.013097	3.497148	-2.105928
76	1	0	7.410256	5.245269	-.381865
77	1	0	5.785608	5.527519	1.480575
78	1	0	3.786966	4.073041	1.614690
79	6	0	-5.969273	.234218	1.309257
80	1	0	-6.316058	.959232	.567881
81	1	0	-5.587380	.780622	2.175826
82	1	0	-6.778012	-.436796	1.599424

No imaginary vibrations were found in vibration analyses for **1a**, **2a** and **11**.

Gaussian 03, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.