Synthesis of New Porphyrin Trimers *via* Buchwald-Hartwig Amination Reaction

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Supporting Information

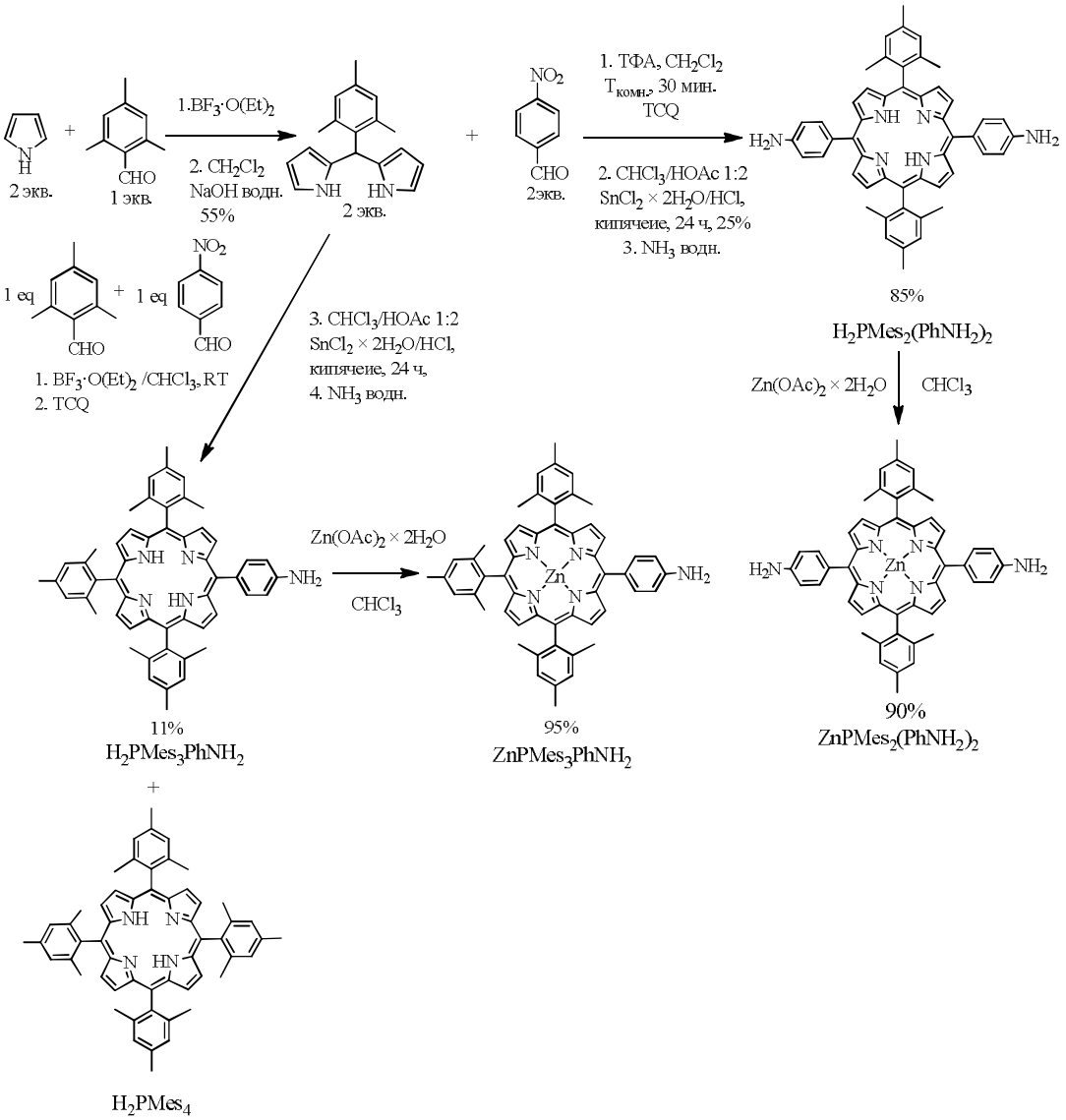


Figure 1. Synthesis of aminophenylporphyrins $ZnPMes_3PhNH_2$ и $ZnPMes_2(PhNH_2)_2$.

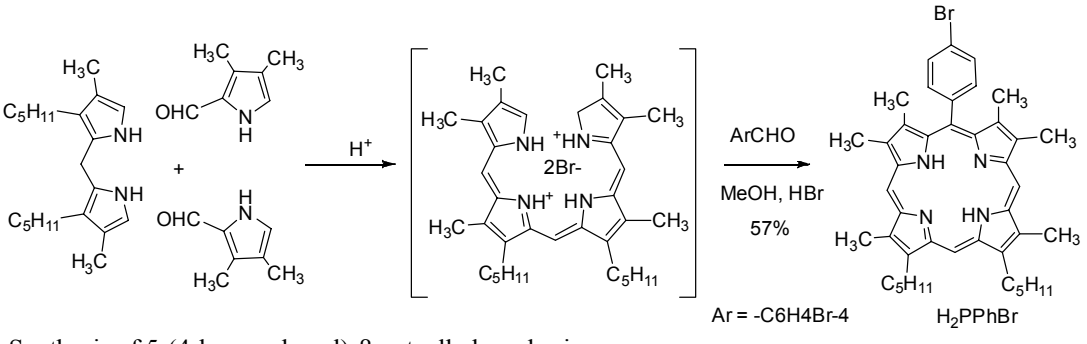


Figure 2. Synthesis of 5-(4-bromophenyl)-β-octaalkylporphyrin.

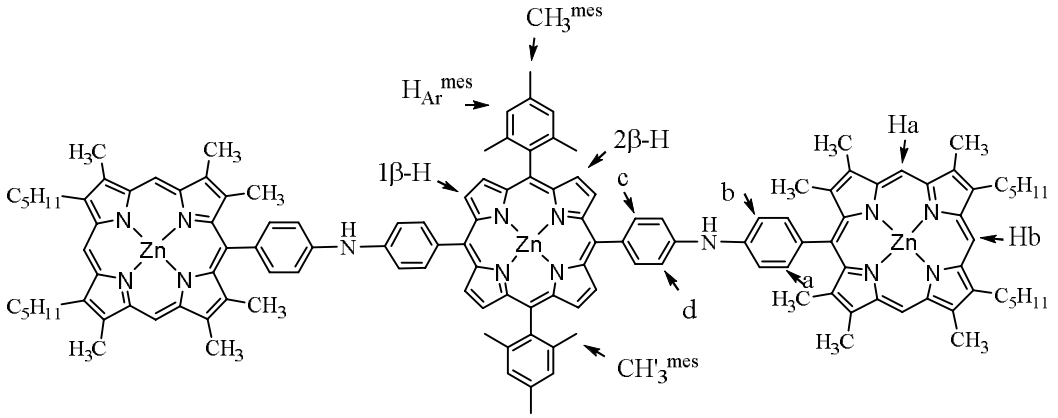


Figure 3. The structure of the porphyrin trimer $ZnPMes_2(PhNH)_2$-$(ZnPPh)_2$.

Table 1. ^{1}H NMR data of the β-unsubstituted porphyrin substrates and coupling products[a].

Compound	β-H, δ(Δδ), ppm		*meso*-H δ(Δδ), ppm		H_{Ar} δ(Δδ), ppm				H_{Ar}^{mes}	CH_3^{mes}	CH'_3^{mes}
	1	2	H_a	H_b	a	b	c	d			
ZnPPhBr	-		9.90	9.52	7.90		-	-	-	-	-
$ZnPMes_2(PhNH_2)_2$	8.85	8.65	-	-	-	-	7.98	7.05	7.41	2.61	1.86
$ZnPMes_3PhNH_2$	8.79	8.71	-	-	-	-	7.69	6.03	7.28	2.69	1.84
$ZnPMes_2(PhNH)_2$-$(ZnPPh)_2$	9.15 (0.3)	8.89 (0.24)	10.04 (0.14)	9.76 (0.24)	8.05 (0.15)	7.78 (-0.12)	8.30 (0.32)	7.74 (0.69)	7.34 (-0.07)	1.93 (-0.68)	1.54 (-0.32)
$(ZnPMes_3Ph)_2$	8.72 (-0.07)	8.55 (-0.16) 8.49 (-0.22)	-	-	-	-	8.12 (0.43)	7.58 (1.55)	7.27 (-0.01) 7.26 (-0.02)	2.54 (-0.15)	1,76 (-0,08)
$(ZnPMes_3Ph)_2NH$	8.85 (0.06)	8.78 (0.07)	-	-	-	-	8.22 (0.24)	7.49 (0.44)	7.27 (-0.01)	2.63 (-0.06)	1.84 (0)

[a]In $CDCl_3$

Table 2. ^{1}H NMR data of the β-substituted porphyrin substrates and coupling products[a].

Compound	*meso*-H δ(Δδ), ppm		H_{Ar} δ(Δδ), ppm		NCH_2	$N'CH_2$	CH_2 of diaza-18-Cr-6 δ, ppm			
	H_a	H_b	a	b			1, 1'	2, 2'	3, 3'	4, 4'
$ZnP(PhPip)_2$[b]	10.00		8.11	7.28	3.55	3.31	-	-	-	-
$ZnP(PhDiaza18C6)_2$	10.03		7.81	7.07	3.78	3.68	3.64	3.57	3.52	3.45
$ZnP(PhPip)_2$-$(ZnPPh)_2$	10.19	10.11	7.95	7.28	3.04	2.84	-	-	-	-
$ZnP(PhDiaza18C6)_2$-$(ZnPPh)_2$	10.13-9.91		7.79	6.91	3.86	3.86	3.86	3.73	3.73	3.73
$ZnP(PhDiaza18C6)_2$-ZnPPh	10.16-10.05		7.63	7.47	3.98	3.98	3.98	3.98	3.98	3.98

[a]In $CDCl_3$, [b]In DMSO-d_6

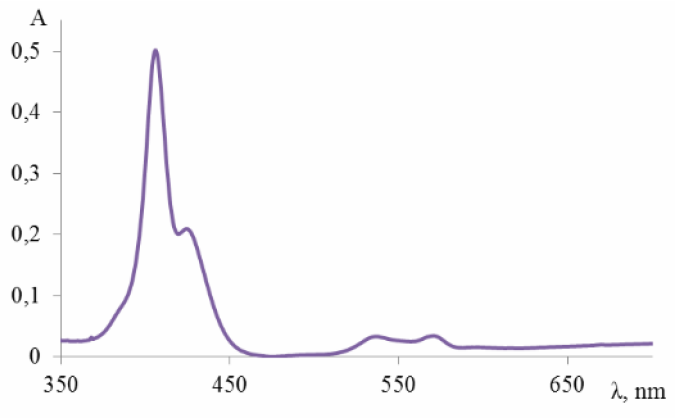


Figure 4. UV-Vis spectra of the porphyrin trimer $ZnPMes_2(PhNH)_2$-$(ZnPPh)_2$.

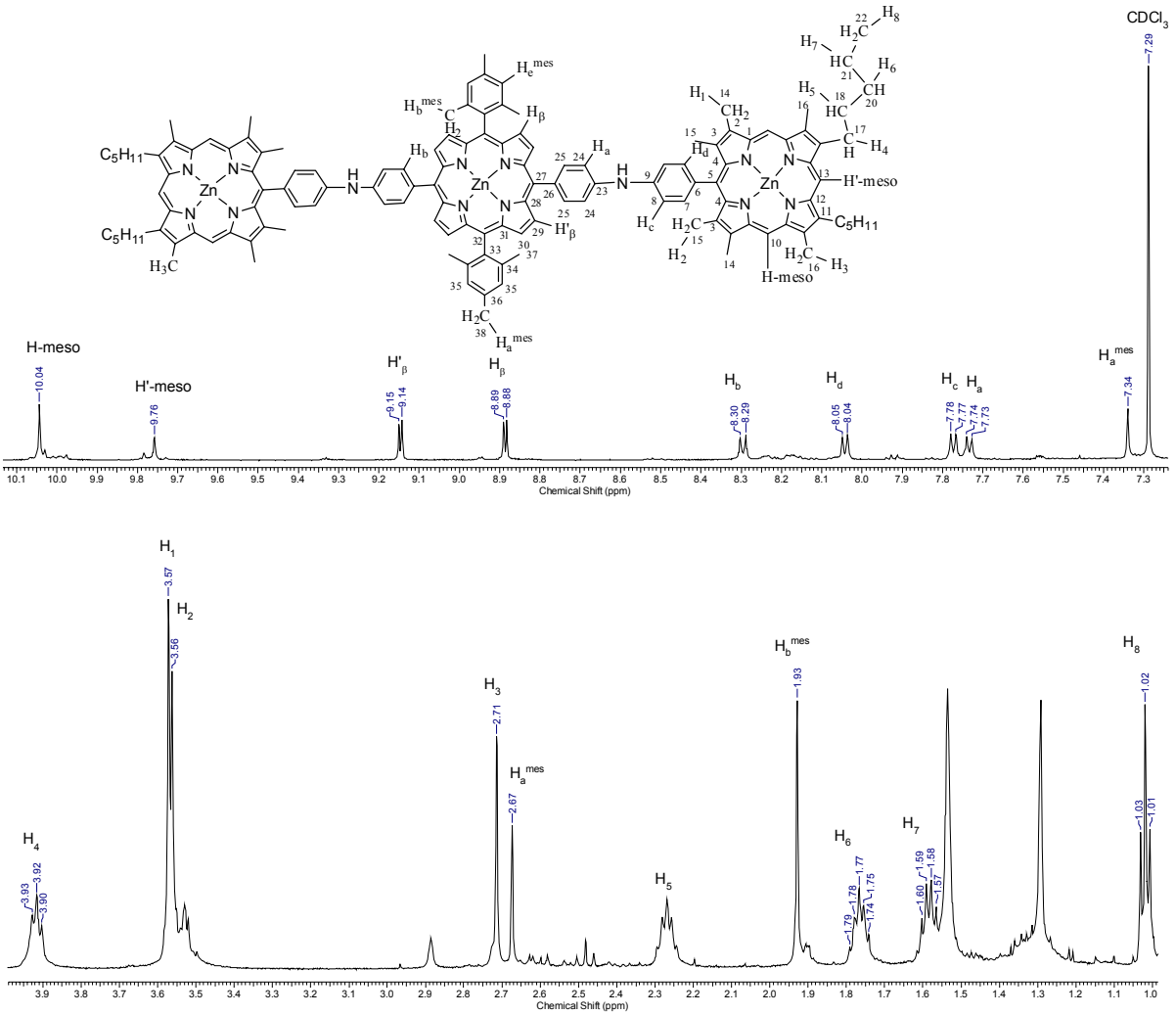
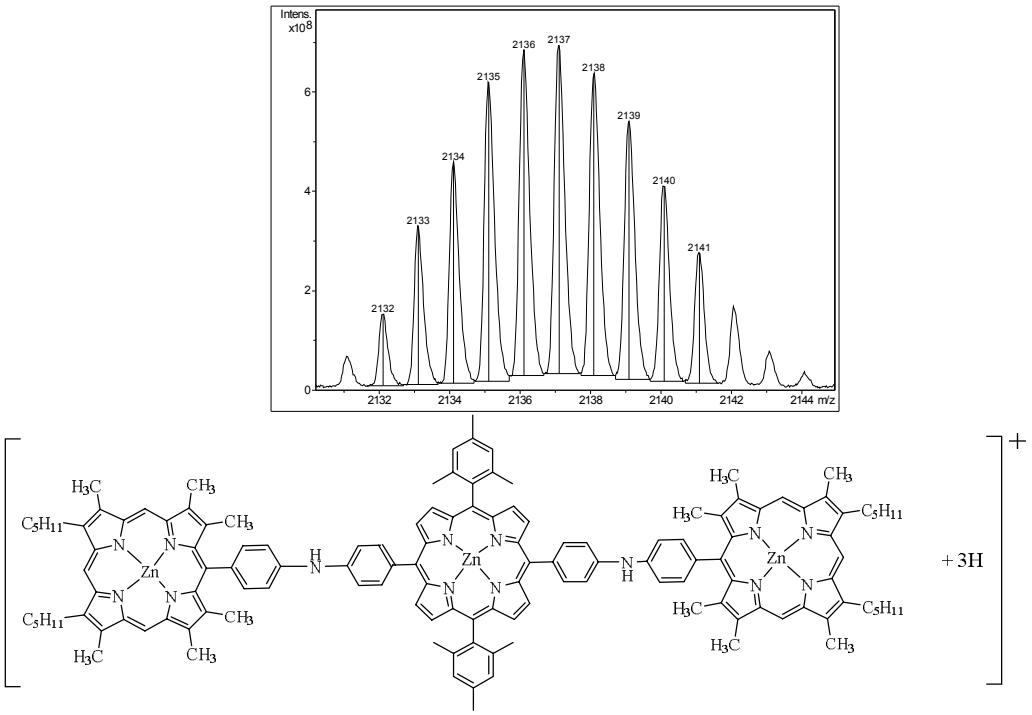


Figure 5. NMR spectra of the porphyrin trimer $ZnPMes_2(PhNH)_2$-$(ZnPPh)_2$.



Chemical Formula: $C_{134}H_{137}N_{14}Zn_3^+$ Exact Mass: 2133,9020 Molecular Weight: 2139,8075

m/z: 2136.9023 (100.0%), 2140.8980 (77.1%), 2137.9056 (71.9%), 2135.8989 (69.0%), 2138.9011 (67.2%), 2134.9054 (58.1%), 2138.8991 (57.4%), 2141.9013 (55.5%), 2139.8946 (53.2%)

Figure 6. MALDI ToF spectra of the porphyrin trimer $ZnPMes_2(PhNH)_2$-$(ZnPPh)_2$.