Construction of building blocks for extended porphyrin arrays by nitration of porphyrin-2,3-diones and quinoxalino[2,3-b]porphyrins

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Supplementary data:

List of NOE enhancements for 7- and 12-nitro-porphyrin-diones **6a** and **6c** and 7- and 12-nitro-quinoxalinoporphyrins **10a** and **10c**.

Compound	Resonance Saturated	Resonance Enhanced (% Enhancement)
6a	δ 7.60	δ 8.31 (0.7%)
	δ7.86/7.87	δ 8.47 / 8.48 (1.7), δ 8.56 (0.9), δ 8.76 (1.2%)
	δ 8.31	δ 7.60 (3.7), δ 8.56 (4.6 %)
	δ 8.74 / 8.48	δ 7.86 / 7.87 (3.9%)
	δ 8.56	δ 7.87 (3.8), δ 8.31 (3.9%)
	δ 8.76	δ 7.86 (3.4%)
6c	δ 7.59	δ 8.27 (1.6%)
	δ 7.84 / 7.85	δ 8.50 (0.5), δ 8.59 (1.2), δ 8.70 (0.8%)
	δ 8.27	δ 7.59 (3.9), δ 8.50 (1.2), δ 8.59 (1.1%)
	δ 8.50	δ 8.27 (1.9), δ 7.85 (2.0%)
	δ 8.59	δ 7.84 (5.6), δ 8.27 (2.1%)
	δ 8.70	δ 7.85 (4.5%)
10a	δ 7.94	δ 9.00 (0.6%)
	$\delta 8.02^{a}$	δ 8.85 (2.2), δ 8.95 (0.7), δ 9.13 (1.9%)
	$\delta 8.05^{b}$	δ 8.85 (2.8), δ 8.95 (2.3), δ 9.13 (0.8%)
	δ 8.85	δ 8.02 (2.1), δ 8.05 (2.1%)
	δ 8.95	δ 8.05 (4.7%)
	δ 9.00	δ 7.94 (3.3%)
10c	δ 7.92	δ 8.96 (1.1%)
	$\delta 8.01 / 8.02$	δ 8.89 (0.7), δ 8.98 (1.1), δ 9.08 (0.9%)
	δ 8.89	δ 8.02 (3.5%)
	δ 8.96	δ 7.92 (3.5%)
	δ 8.98	δ 8.01 (3.0%)
	δ 9.08	δ 8.02 (3.5%)

^aThe resonance at δ 8.05 was also partially saturated (36%). The enhancement at δ 8.95 is due to this partial saturation. ^bThe resonance at δ 8.02 was also partially saturated (38%). The enhancement at δ 9.13 is due to this partial saturation.



Figure S1: Resonances due to the β -pyrrolic, aryl and quinoxaline protons in the ¹H NMR spectrum (400 MHz) of zinc(II) 7-nitro-quinoxalinoporphyrin **10a** in CDCl₃. The additional signals of lower intensity belong to the zinc(II) 8-nitro-quinoxalinoporphyrin **10b**. For example, the signal at δ 9.13 belongs to the 8-H β -pyrrolic position on the 7-nitro-isomer **10a** while the signal at δ 9.27 belongs to the 7-H β -pyrrolic position on the 8-nitro isomer **10b**. Integrals of these peaks were used to determine isomeric abundance.