Chem. Eur. J. **2003**

Supporting Information

for

Design of new mimochromes with unique topology

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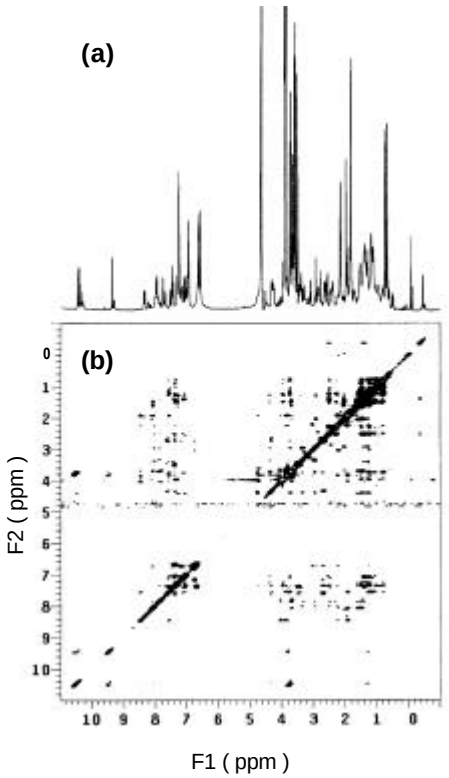
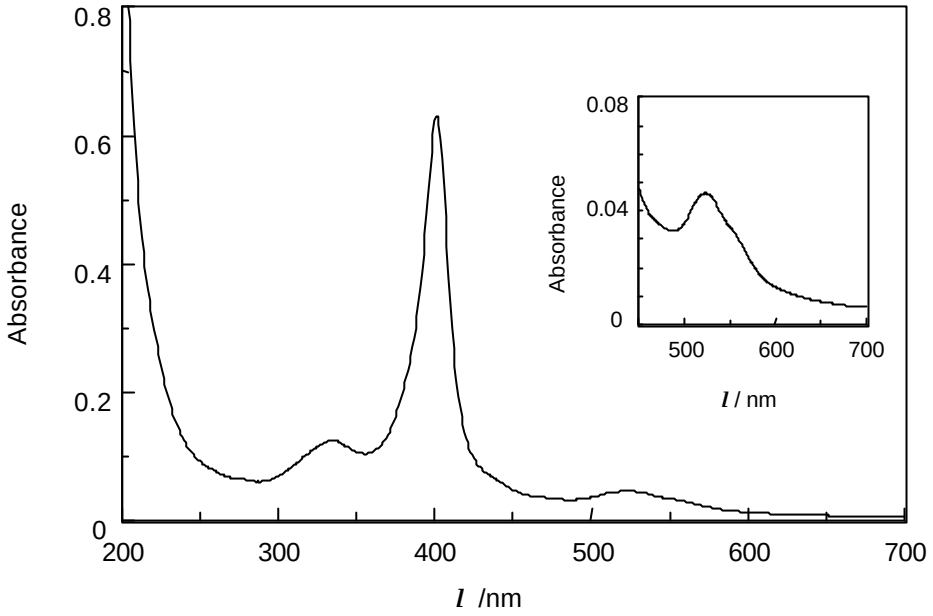
Figure S1



^{1}H NMR spectra of Co^{III}-mimochrome IV recorded at 600 MHz. **(a)** Monodimensional spectrum. **(b)** NOESY spectrum at 200 ms mixing time. Conditions: 1 mM concentration, in H_2O/CF_3CD_2OD (70:30 v/v), pH 5.5, 298 K.

Figure S2



UV-vis spectrum of Fe^{III}-mimochrome IV 1.22×10^{-5} M in water pH = 9.5

Table S1

Co^{III}-Mimochrome IV L isomer ^1H chemical shift (ppm) and $^3J_{HNaCH}$ (Hz).					
Peptide chains resonances					
Residue	**$^3J_{HN\text{-}aCH}$**		**proton**	**d (ppm) chain2a**	**d (ppm) chain18b**
Ac^0			CH_3	1.9	1.9
Glu^1	4		NH	8.05	8.08
			αCH	3.66	3.70
			β,β'CH_2	1.58, 1.48	1.6, 1.5
			γ,γ'CH_2	2.0	2.04
Ser^2	5		NH	7.80	7.86
			αCH	4.00	4.02
			β,β'CH_2	3.93-3.70	3.90-3.70
Gln^3	4		NH	8.47	8.43
			αCH	3.80	3.84
			β,β'CH_2	1.90	1.90
			γ,γ'CH_2	2.24	2.24
			$CONH_2$	6.70-7.36	6.70-7.42
Leu^4	6		NH	7.58	7.53
			αCH	3.74	3.73
			β,β'CH_2	1.28-1.15	1.20-1.05
			γ,γ'CH_2	1.20	1.20
			δ,δ'CH_3	0.75-0.80	0.75-0.80
His^5	6		NH	7.12	7.05
			αCH	2.48	2.54
			β,β'CH_2	1.36	1.37
			δCH	-0.38	-0.40
			εCH	-0.10	-0.05
			NH^{δ}	-	-
Ser^6	5		NH	7.42	7.34
			αCH	3.38	3.43
			β,β'CH_2	3.54, 348	3.53, 348
Asn^7	6		NH	7.56	7.63
			αCH	4.30	4.32
			β,β'CH_2	2.72-2.62	2.72, 2.58
			$CONH_2$	6.76-7.14	6.76-7.18
Lys^8	*		NH	7.36	7.36
			αCH	3.92	3.96
			β,β'CH_2	0.80	0.90
			γ,γ'CH_2	1.45-1.28	1.5-1.22
			δ,δ'CH_2	1.52-1.10	1.44-1.02
			ε,ε'CH_2	2.51-2.24	2.47-2.3
			NH^{ζ}	8.01	7.85
Arg^9	*		NH	7.25	7.26
			αCH	4.37	4.39
			β,β'CH_2	1.4-1.25	1.62-1.5
			γ,γ'CH_2	1.25-1.15	1.36-1.26
			δ,δ'CH_2	3.03-2.2	2.91-2.01
			$NH^{\varepsilon\eta1\eta2}$	8.12	8.04
			$CONH_2$	7.06-7.28	7.08-7.28

Deuteroporphyrin resonances					
2,18 a,a'-CH_2	4.9-4.35	**7CH_3**	3.83	**13H**	9.46
2,18 b,b'-CH_2	3.35-2.95	**8H**	9.47	**15H**	10.46
3CH_3	3.75	**10H**	10.54	**17CH_3**	3.70
5H	10.56	**12CH_3**	3.81	**20H**	10.44

Chemical shift are relative to TSP (see Matherial and methods); (-) indicates a resonance that could not be observed; (*) indicates a $^3J_{NH\text{-}\alpha CH}$ not measurable because resonance overlap.

Table S2

Intramolecular Hydrogen Bonds of CoIII mimochrome IV.

Donor	Acceptor	Chain 2a	Chain 18b
N_3	O_0	2.8	2.7
N_4	O_1	3.1	3.0
N_5	O_1	2.8	2.9
N_5^{δ}	O_1	2.8	3.1
N_6	O_2	2.9	2.7
N_7	O_3	2.8	
N_7	O_4	3.0	2.8
N_8	O_4	2.9	4.1
N_8	O_5		3.0
N_9	O_7	2.6	2.6
$N_9^{\eta 2}$	O_8		2.7
N_9^{ε}	O_8		2.6

2a and 18b refer to the peptide chain linked to the propionyl group at position 2 and 18 of the deuteroporphyrin ring, respectively.