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Supplementary Information

Photooxidative cleavage of zinc 20-substituted chlorophyll derivatives: conformationally *P*-helix–favored formation of regioselectively 19–20 opened linear tetrapyrroles

Hitoshi Tamiaki,[*a] Yukihiro Okamoto,[a] Yuji Mikata[b] and Sunao Shoji[a]

[a]*Department of Bioscience and Biotechnology, Faculty of Science and Engineering, Ritsumeikan University, Kusatsu, Shiga 525-8577, Japan. E-mail : tamiaki@se.ritsumei.ac.jp; Fax. +81-77-561-2659; Tel. +81-77-561-2765*

[b]*KYOSEI Science Center, Nara Women's University, Nara, 630-8506, Japan*

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Table S1 Crystallographic Data for **6a**

	6a
Formula	$C_{35}H_{38}N_4NiO_5$
FW	653.41
Crystal system	triclinic
Space group	*P*1
a, Å	10.232(6)
b, Å	12.112(7)
c, Å	12.793(8)
α, deg	76.70(2)
β, deg	79.05(2)
γ, deg	81.74(2)
V, Å^3	1506(2)
Z	2
D_{calc}, g cm^{-3}	1.442
μ, cm^{-1}	6.954
$2\theta_{max}$, deg	55.0
temp, K	123
no. reflns collected	11627
no. reflns used	9082
R_{int}	0.0458
no. of params	811
final *R*1 ($I > 2\theta(I)$)	0.0579
*wR*2 (all data)	0.0660
GOF	0.991

$R1 = (\Sigma||F_o| - |F_c||)/(\Sigma|F_o|)$.

$wR2 = \{[\Sigma w(F_o^2 - F_c^2)^2]/[\Sigma w(F_o^2)^2]\}^{1/2}$.

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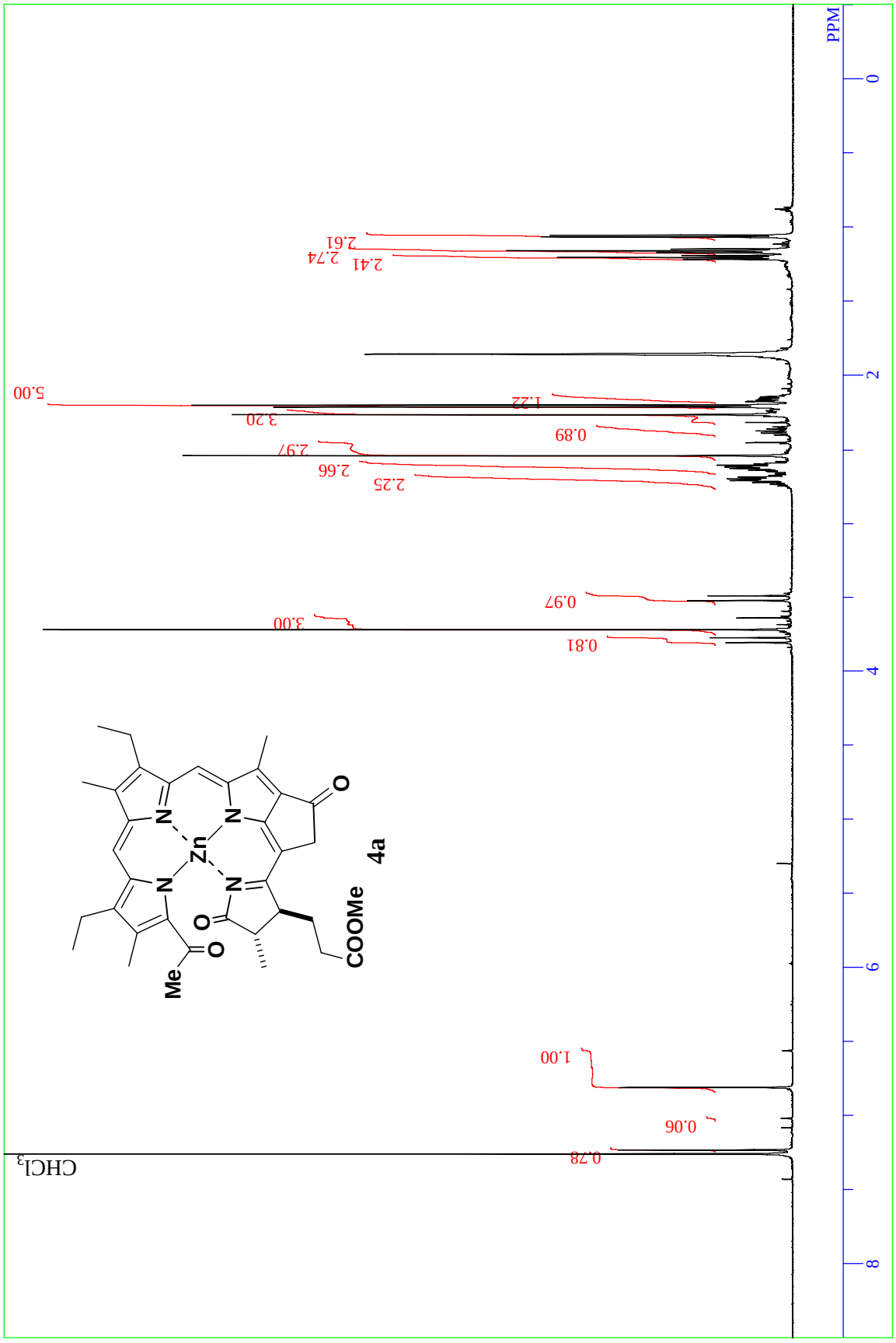

Fig. S1 ^{1}H-NMR spectrum of **4a** in $CDCl_3$.

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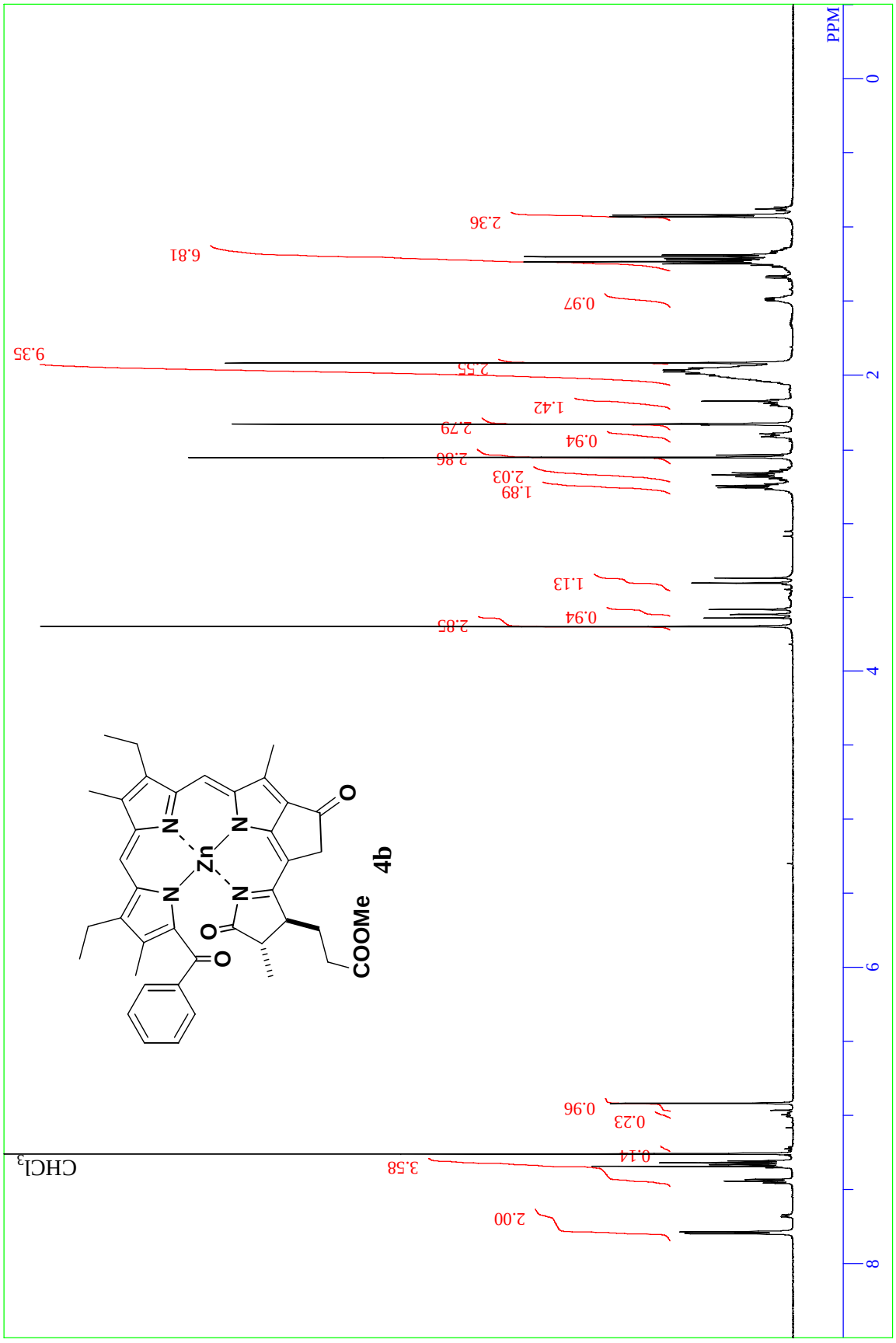

Fig. S2 ^{1}H-NMR spectrum of **4b** in $CDCl_3$.

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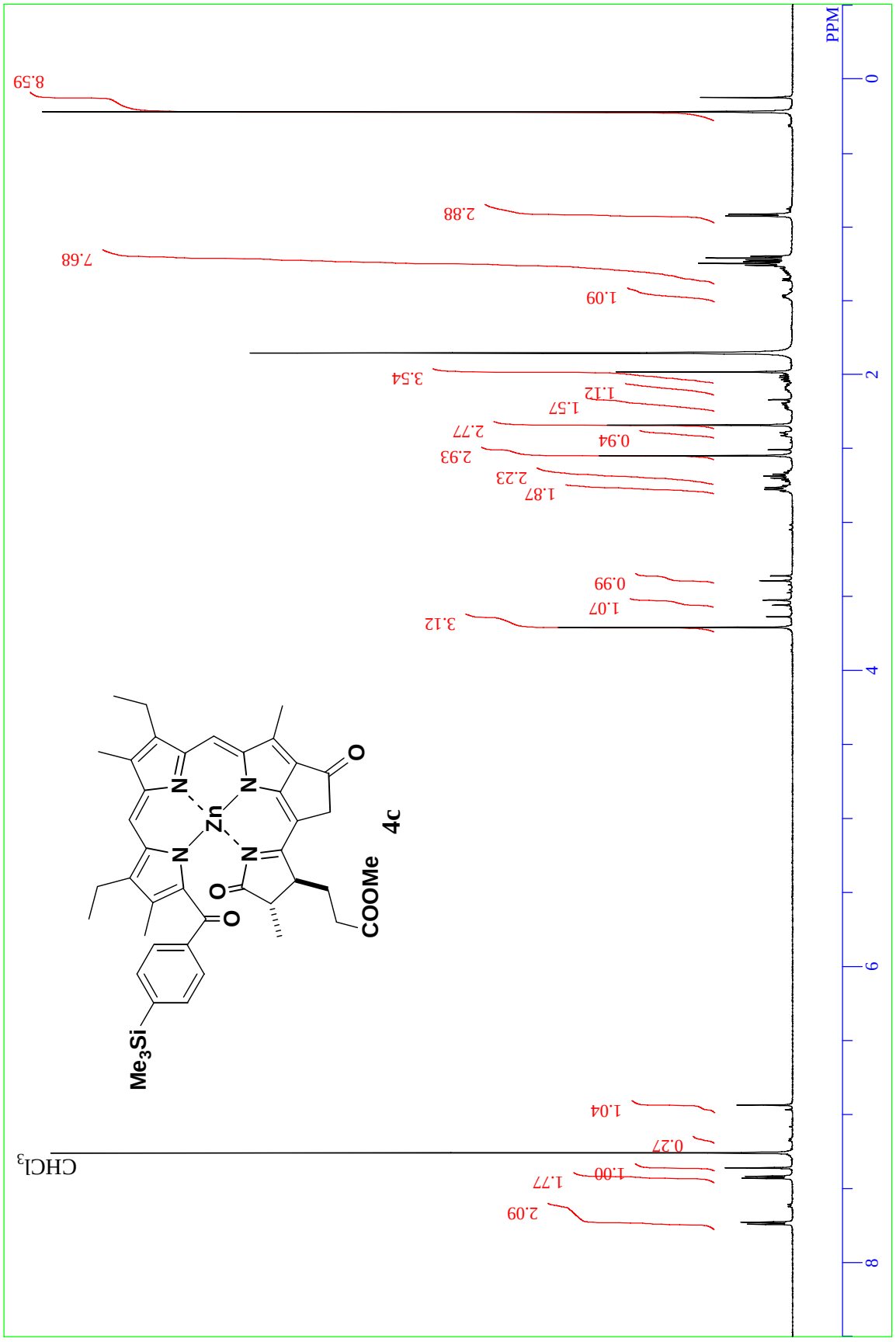

Fig. S3 ^{1}H-NMR spectrum of **4c** in $CDCl_3$.

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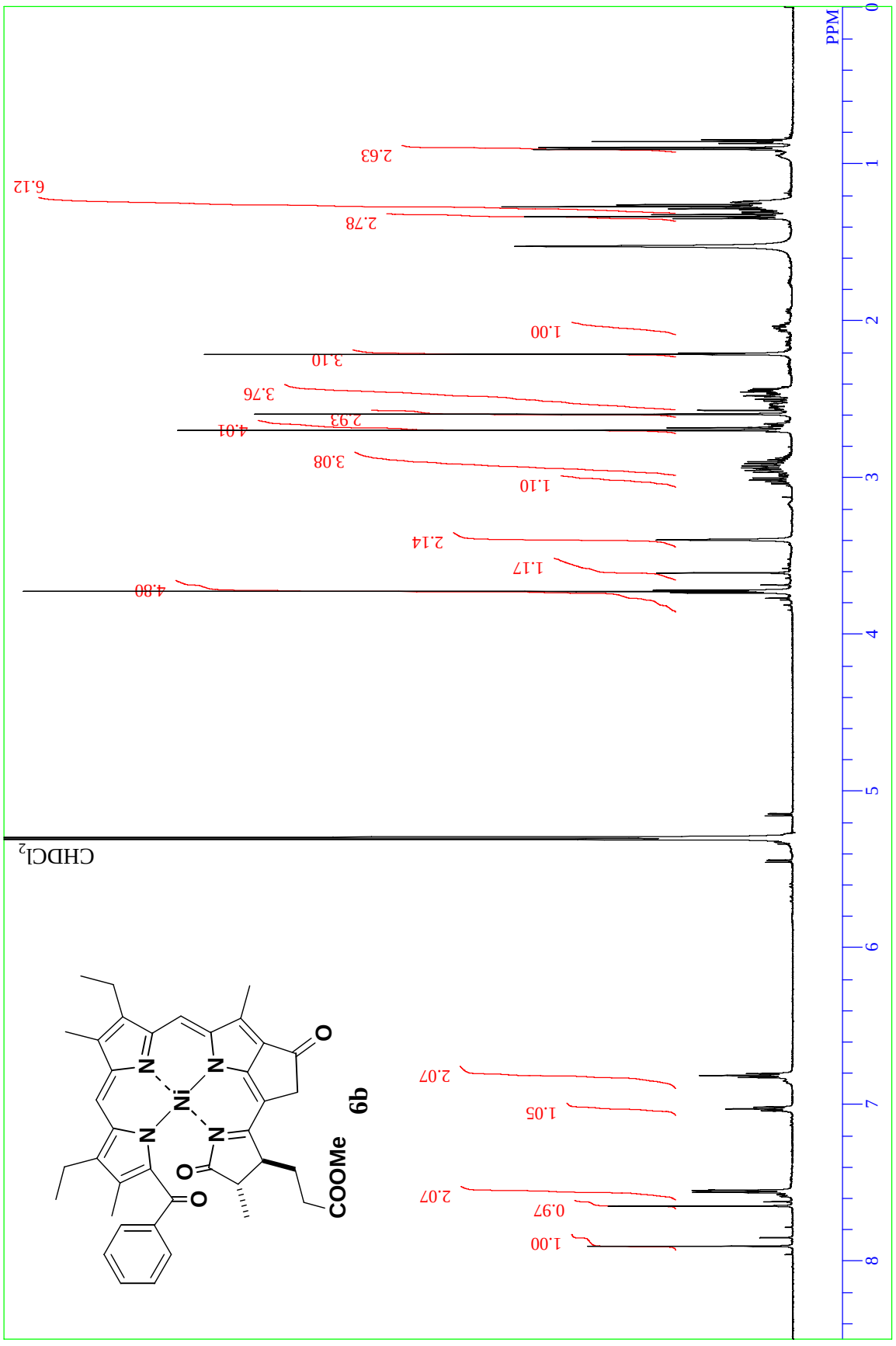

Fig. S4 ^{1}H-NMR spectrum of **6b** in CD_2Cl_2.

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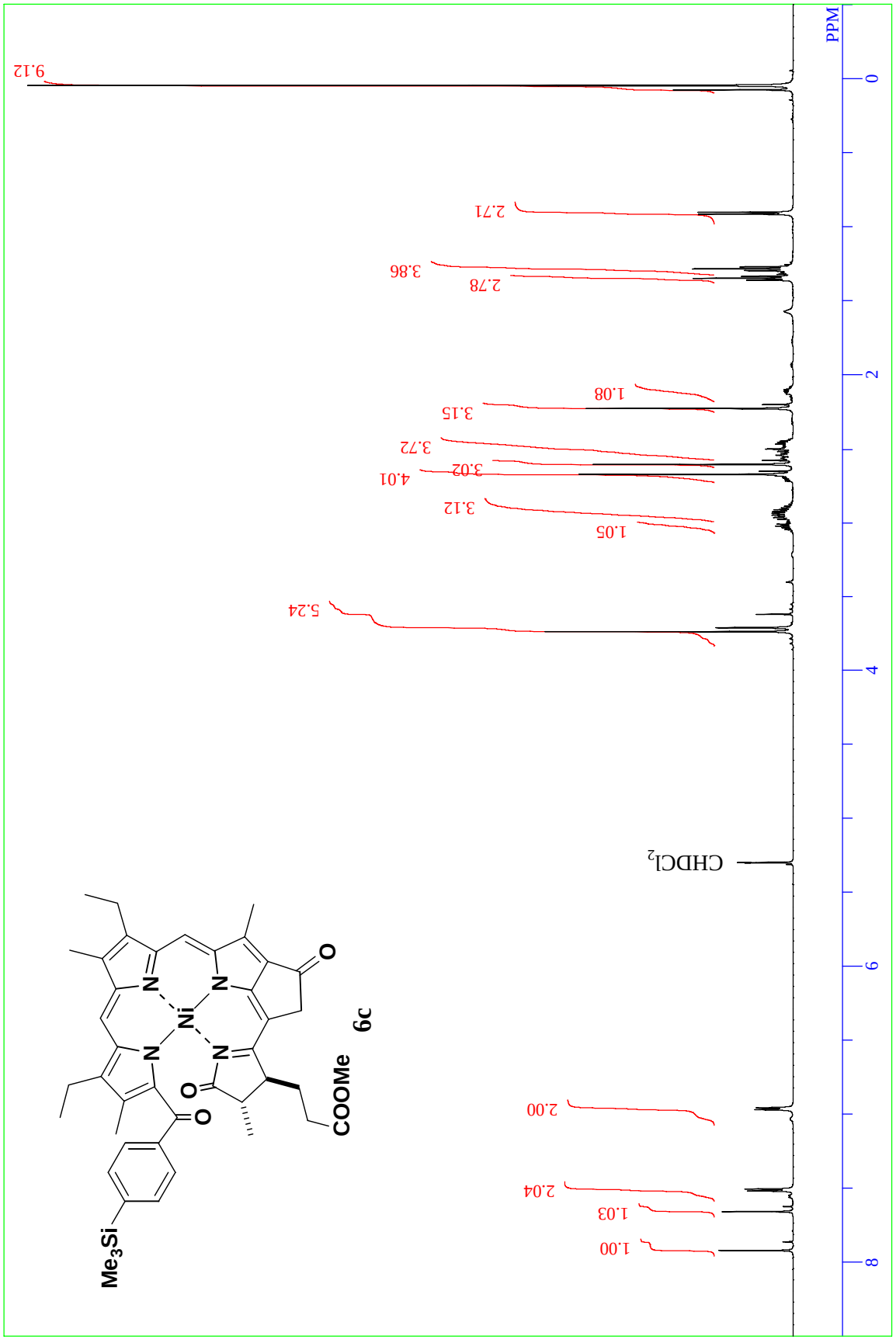

Fig. S5 ^{1}H-NMR spectrum of **6c** in CD_2Cl_2.

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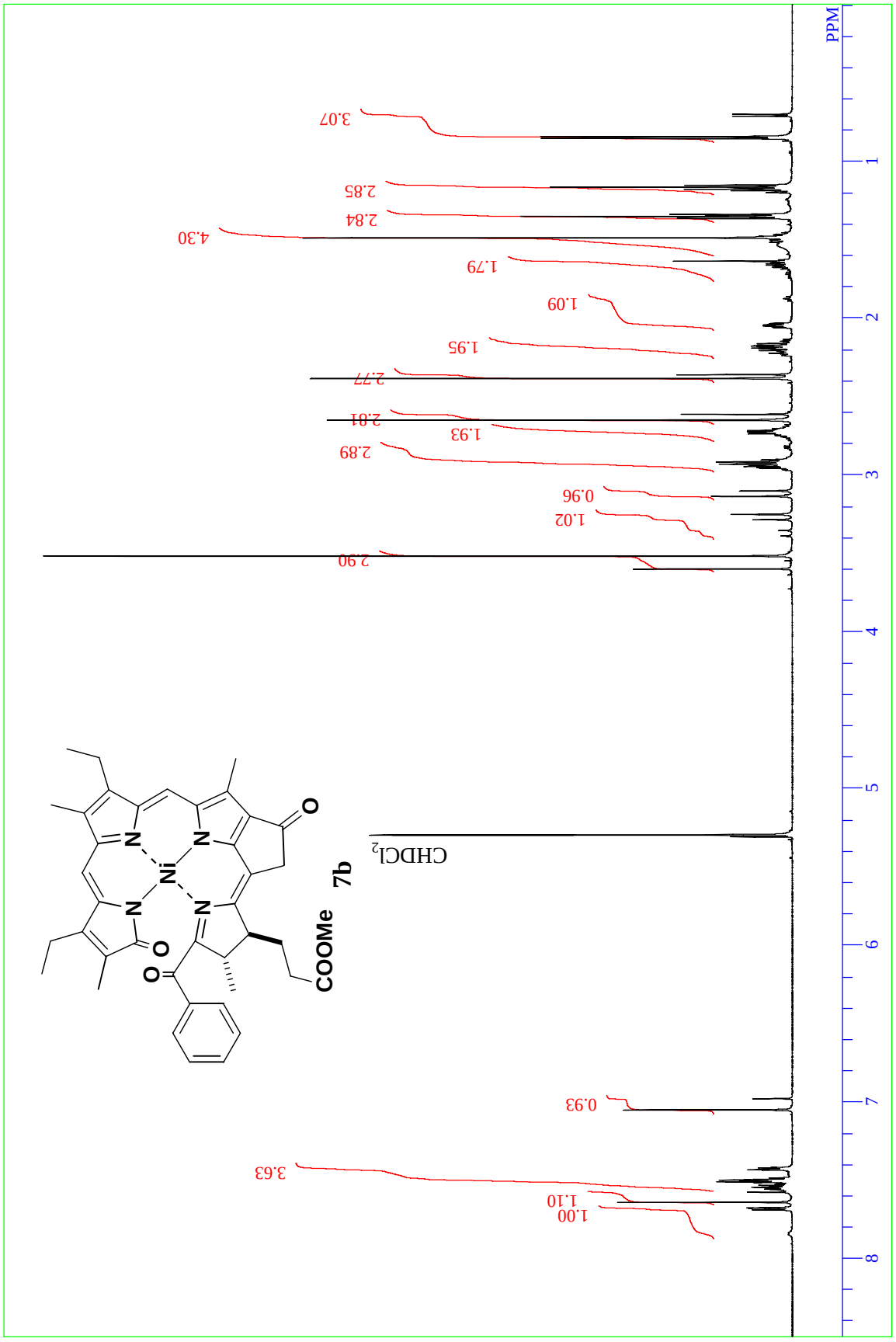

Fig. S6 ^{1}H-NMR spectrum of **7b** in CD_2Cl_2.

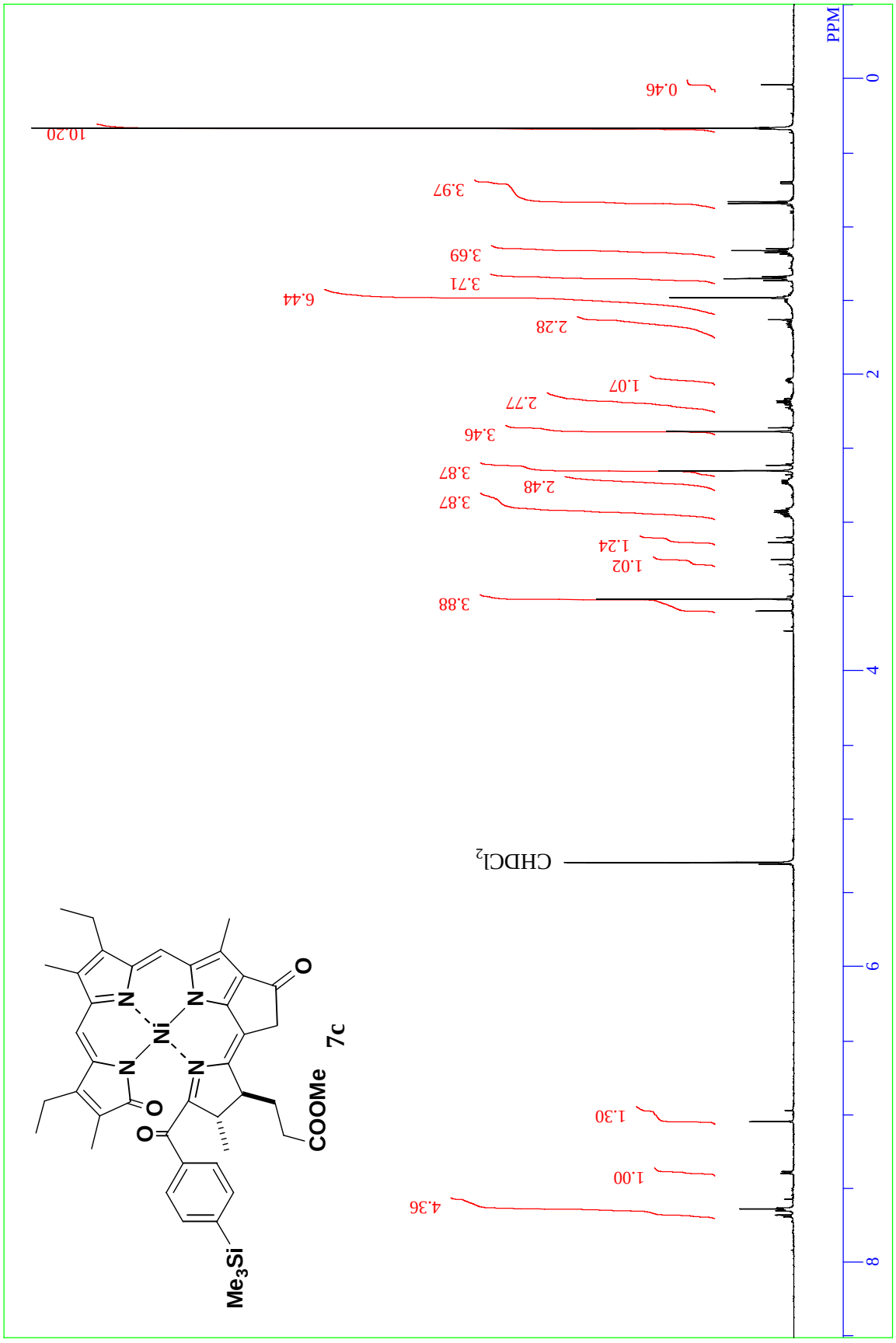

Fig. S7 ^{1}H-NMR spectrum of **7c** in CD_2Cl_2.

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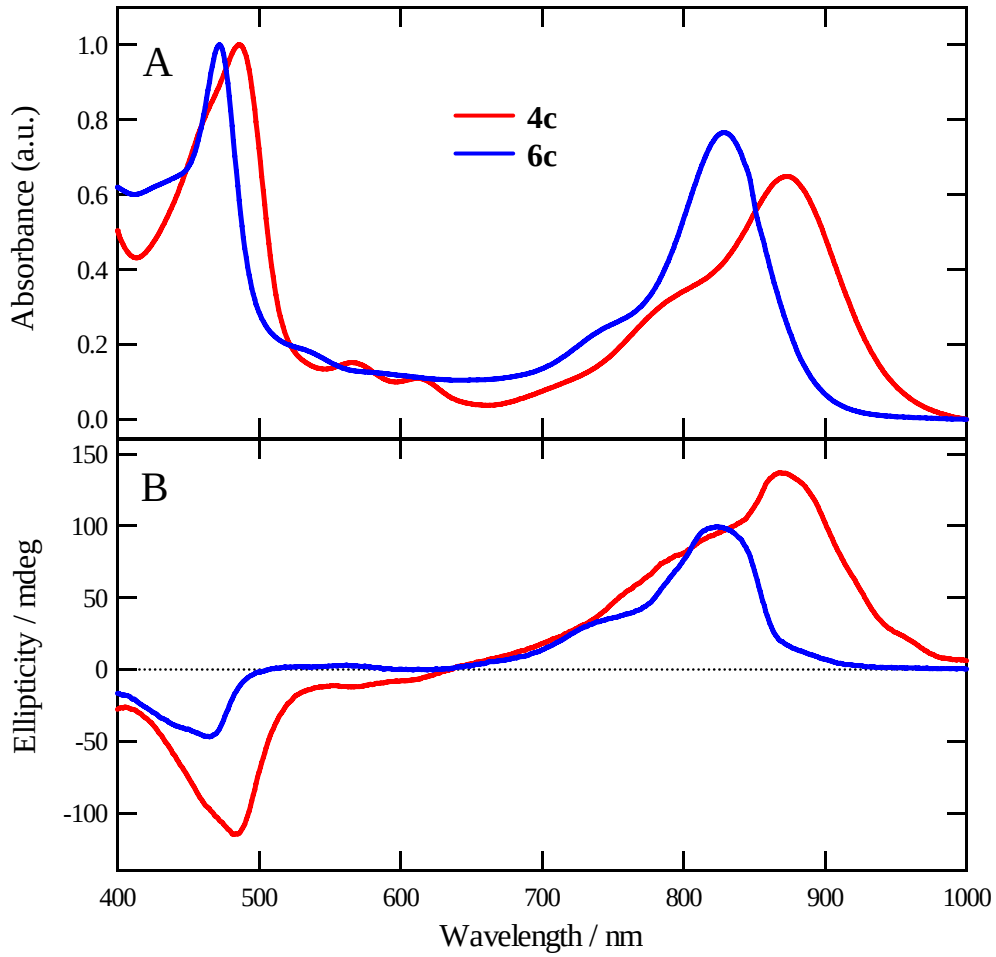

Fig. S8 Electronic absorption (A) and CD spectra (B) of zinc and nickel complexes **4c** (red) and **6c** (blue) of 1-[4-(trimethylsilyl)phenyl-carbonyl]-19-oxo-bilatriene in dichloromethane. Both the spectra in A were normalized at the Soret maxima.

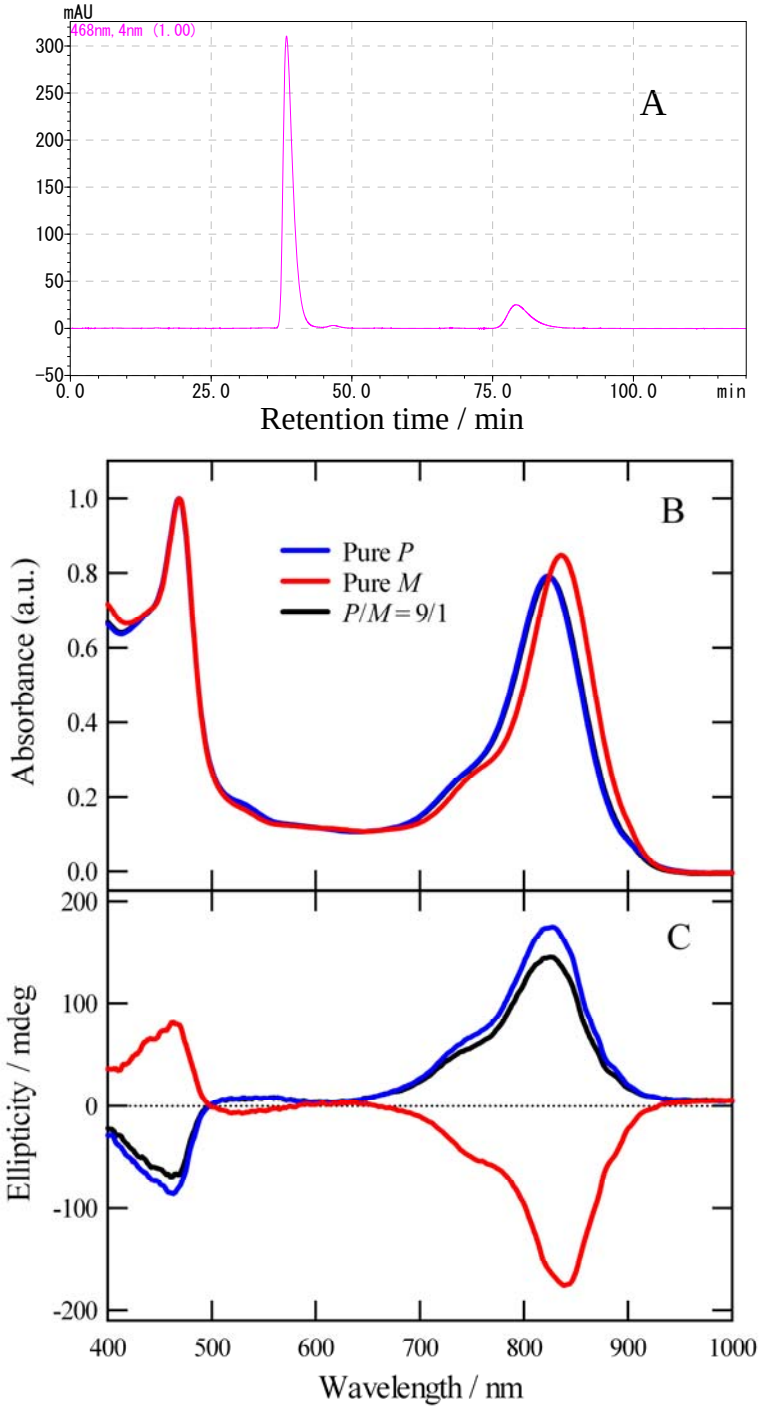

Fig. S9 Chiral HPLC (A) of nickel 1-[4-(trimethylsilyl)phenyl-carbonyl]-19-oxo-bilatriene **6c**: column, Daicel Chiralpak IC 4.6ϕ x 250 mm; eluent, methanol; flow rate, 0.8 ml min^{-1}. Electronic absorption (B) and CD spectra (C) of **6c** in methanol: *P*- (blue) and *M*-helical conformers (red) as well as their 9:1 mixture (black). All the spectra in B were normalized at the Soret maxima.

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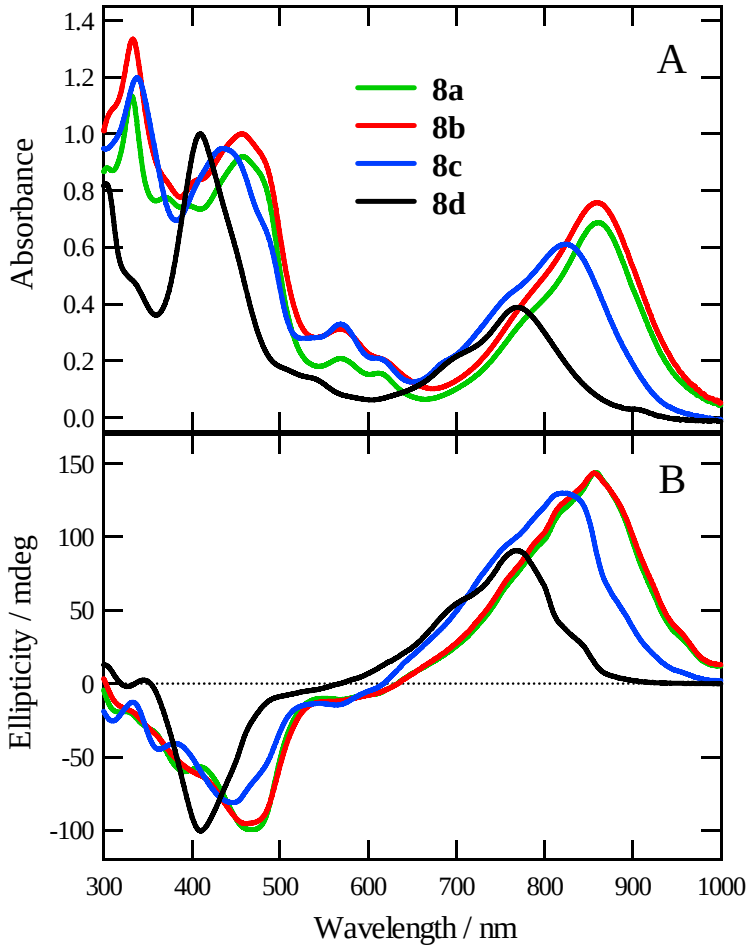

Fig. S10 Electronic absorption (A) and CD spectra (B) of zinc complexes **8a**–**d** of 1-formyl-19-oxo-bilatriene in dichloromethane. All the molecular structures are shown in Fig. 7.