

## A panchromatic pyrazine-fused porphyrin dimer

Inna A. Abdulaeva, Daria A. Polivanovskaia, Kirill P. Birin,  
Yulia G. Gorbunova and Aslan Yu. Tsivadze

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### Materials and methods

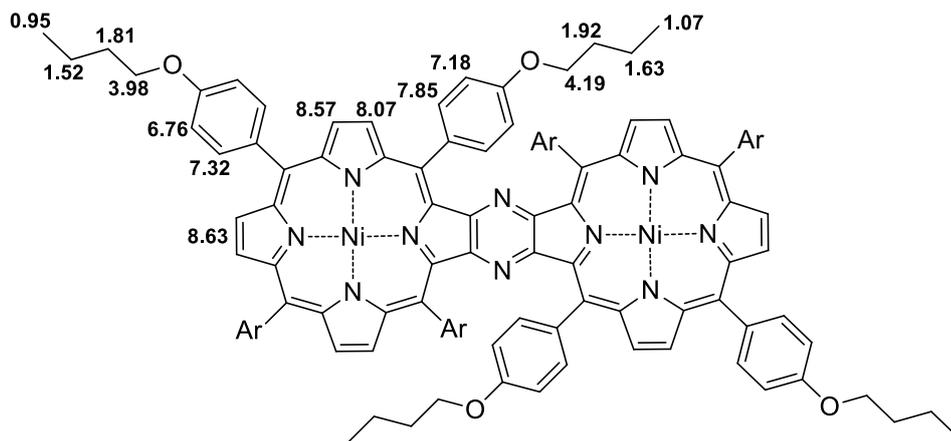
All the used chemicals were purchased from commercial suppliers, unless otherwise stated. The solvents have been purified according to the conventional methods [S1]. 3,5-Di-tertbutyl-*o*-quinone was prepared according to the published procedure [S2]. Chromatographic purification was performed with Macherey-Nagel Silica 60, 0.063-0.2 mm. Merck aluminum plates (TLC Silica 60 F254) were used for TLC analysis with hexane/dichloromethane mixtures as eluents.

MALDI-TOF mass-spectra were recorded at Bruker Daltonics Ultraflex spectrometer in positive ions mode without matrix. UV-Vis spectra were recorded at Thermo Scientific Evolution 202 spectrophotometer in rectangular quartz cells with 10 mm optical path in 250-900 nm range. <sup>1</sup>H-NMR spectra were recorded at Bruker Avance III spectrometer with 600 MHz proton frequency in CDCl<sub>3</sub> at ambient temperature with the use of the residual solvent resonance as internal reference. The measurements were made at the Shared Facility Centers of the Institute of Physical Chemistry and Electrochemistry RAS.

### References

- [S1] W. L. F. Armarego and C. L. L. Chai, *Purification of Laboratory Chemicals*, Elsevier/Butterworth-Heinemann, 2009.
- [S2] E. Rufino-Felipe, J. Caballero-Jiménez, L.-G. Guerrero-Ramírez, M. Flores-Álamo and M.-Á. Muñoz-Hernández, *Inorg. Chem. Commun.*, 2016, **63** 107.

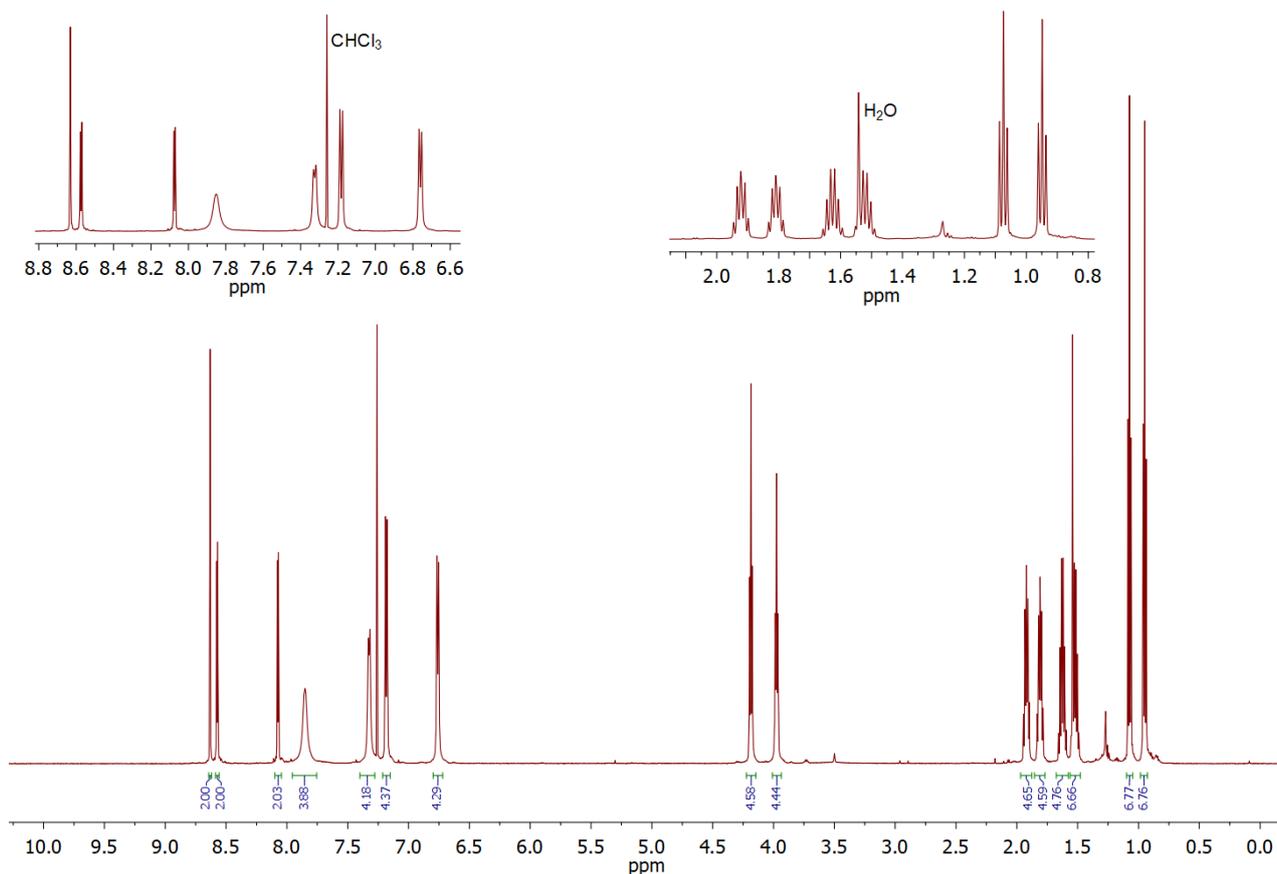
## NMR characterization of complex 5



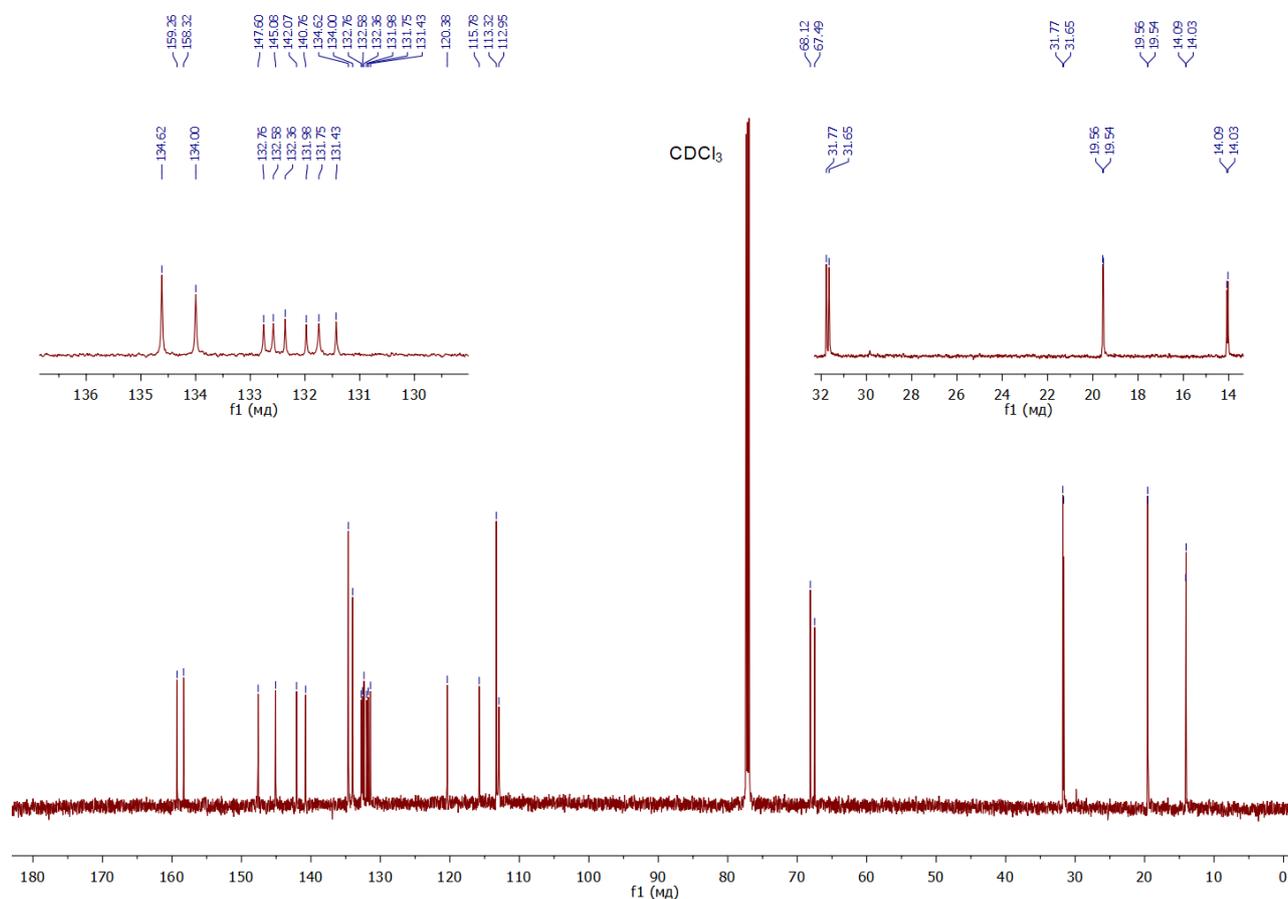
**Figure S1** Assignment of  $^1\text{H}$  NMR resonances in the spectrum of complex **5** ( $\text{CDCl}_3$ ).

**Table S1** Assignment of  $^{13}\text{C}$  NMR resonances in the spectrum of complex **5** ( $\text{CDCl}_3$ )

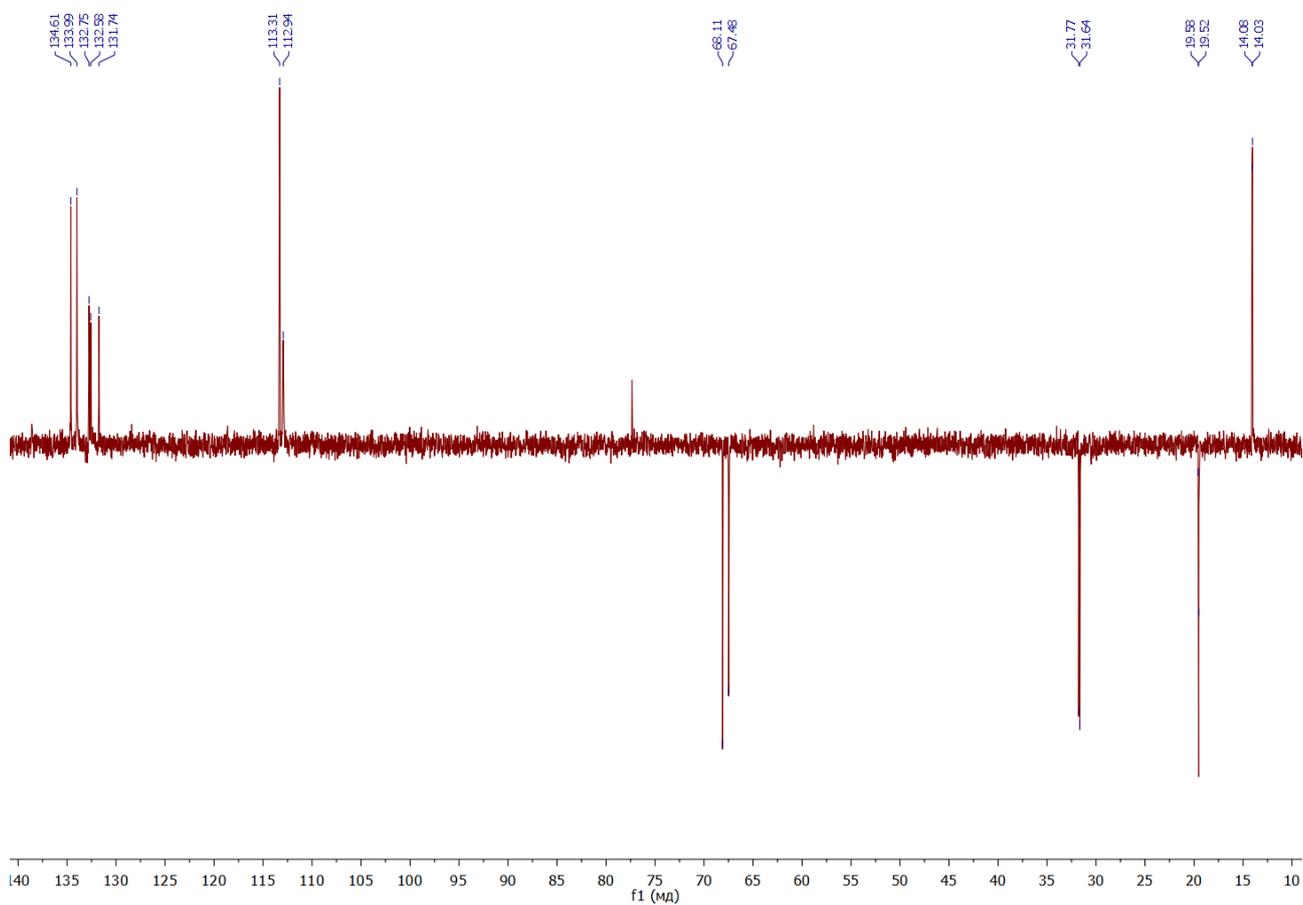
$\delta$ , ppm	Type	Assignment
131.98	C	C1
147.60	C	C2
115.78	C	C3
140.76	C	C4
132.76	CH	C5
132.58	CH	C6
145.08	C	C7
120.38	C	C8
142.07	C	C9
131.75	CH	C10
132.36	C	C11
134.62	CH	C12
113.32	CH	C13
159.26	C	C14
68.12	$\text{CH}_2$	C15
31.77	$\text{CH}_2$	C16
19.56	$\text{CH}_2$	C17
14.09	$\text{CH}_3$	C18
131.43	C	C19
134.00	CH	C20
112.95	CH	C21
158.32	C	C22
67.49	$\text{CH}_2$	C23
31.65	$\text{CH}_2$	C24
19.54	$\text{CH}_2$	C25
14.03	$\text{CH}_3$	C26



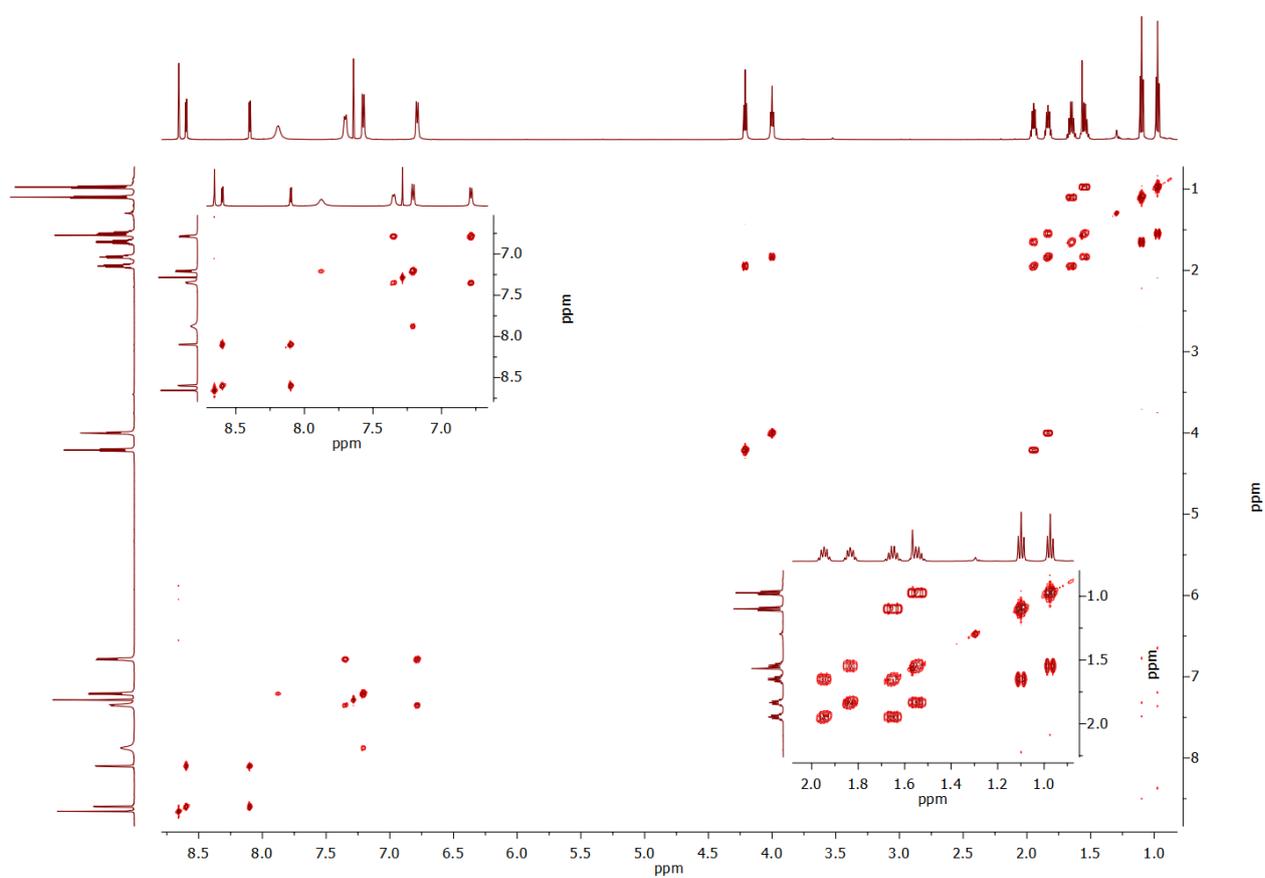
**Figure S2**  $^1\text{H}$  NMR spectrum of complex **5** ( $\text{CDCl}_3$ ).



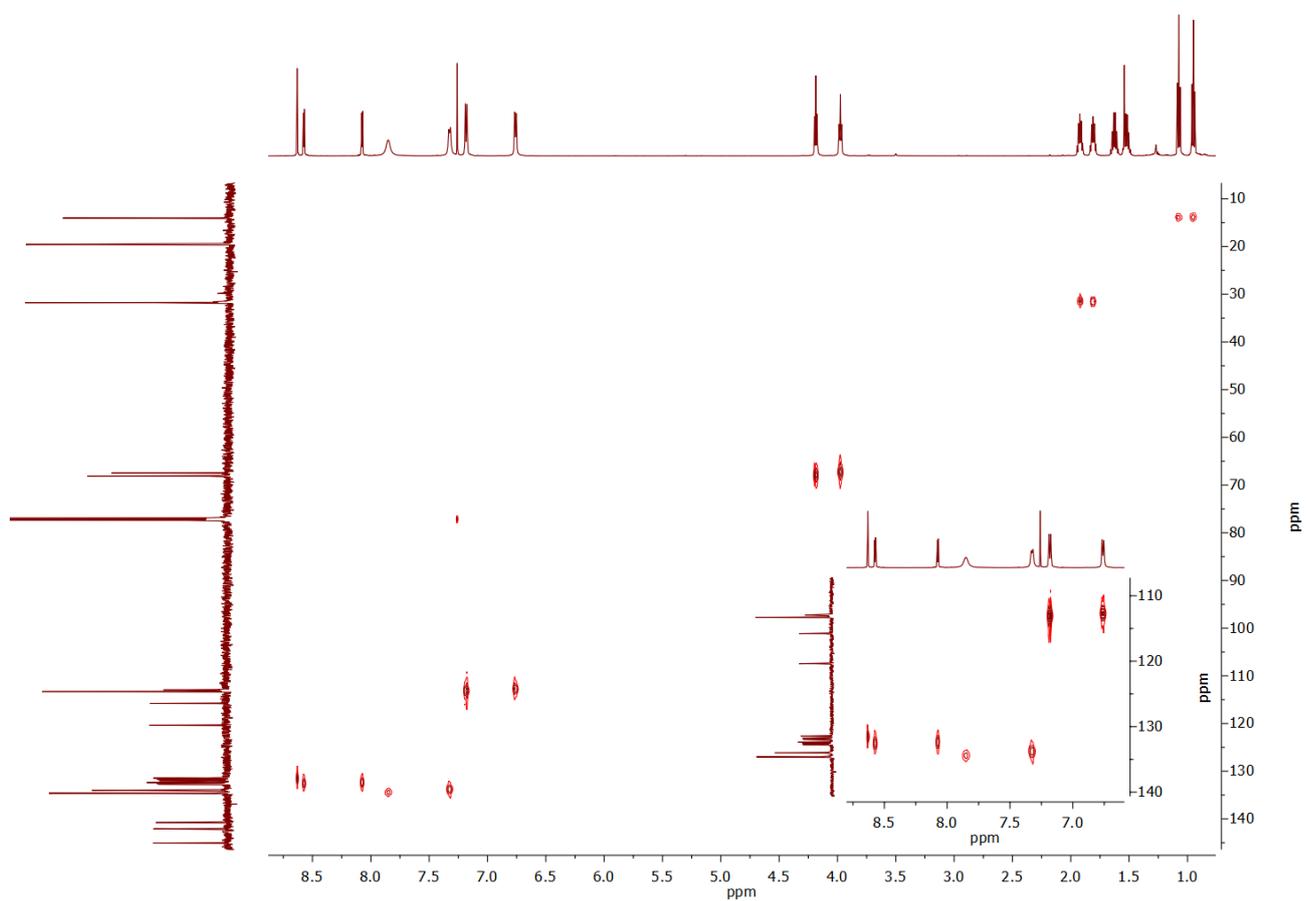
**Figure S3**  $^{13}\text{C}$  NMR spectrum of complex **5** ( $\text{CDCl}_3$ ).



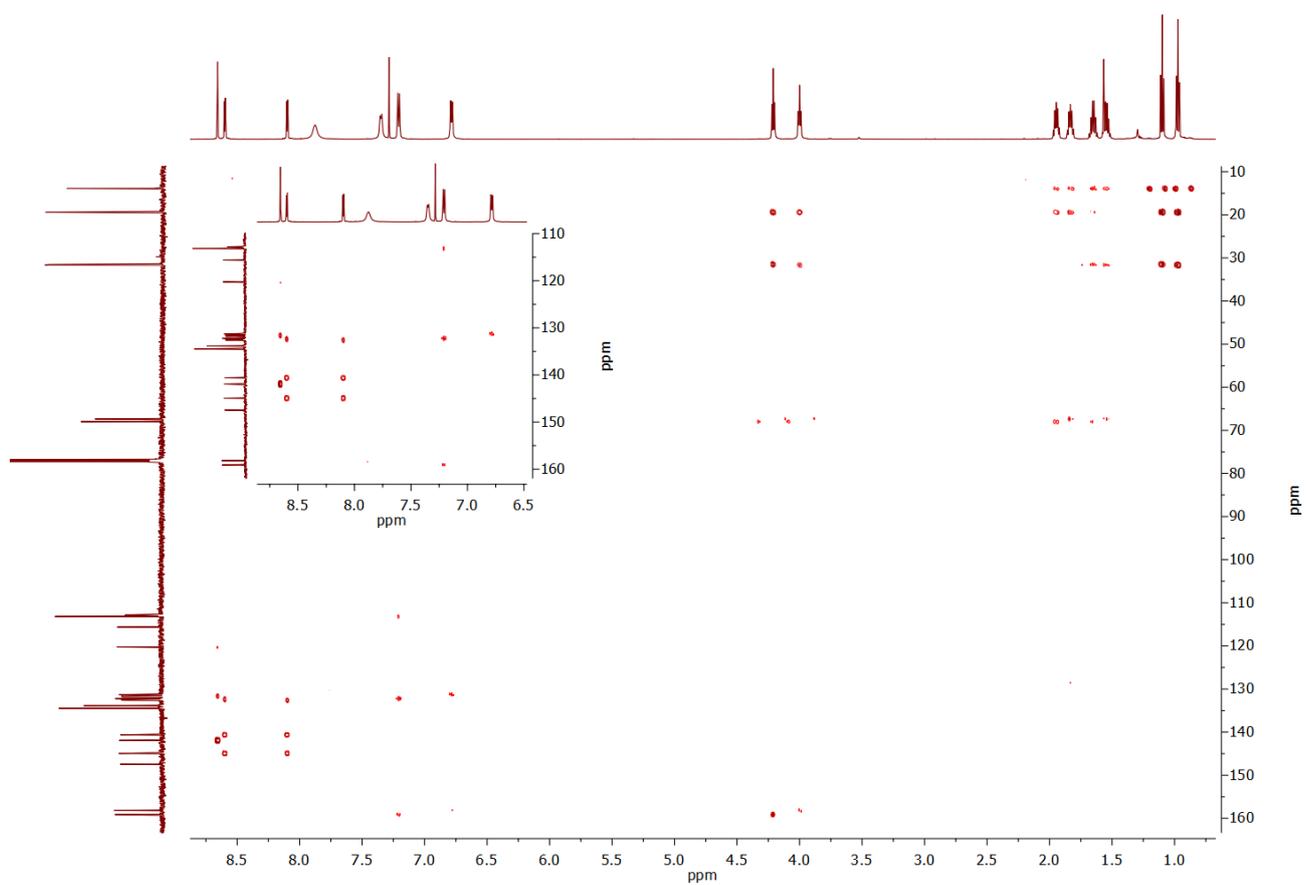
**Figure S4**  $^{13}\text{C}$ -DEPT NMR spectrum of complex **5** ( $\text{CDCl}_3$ ).



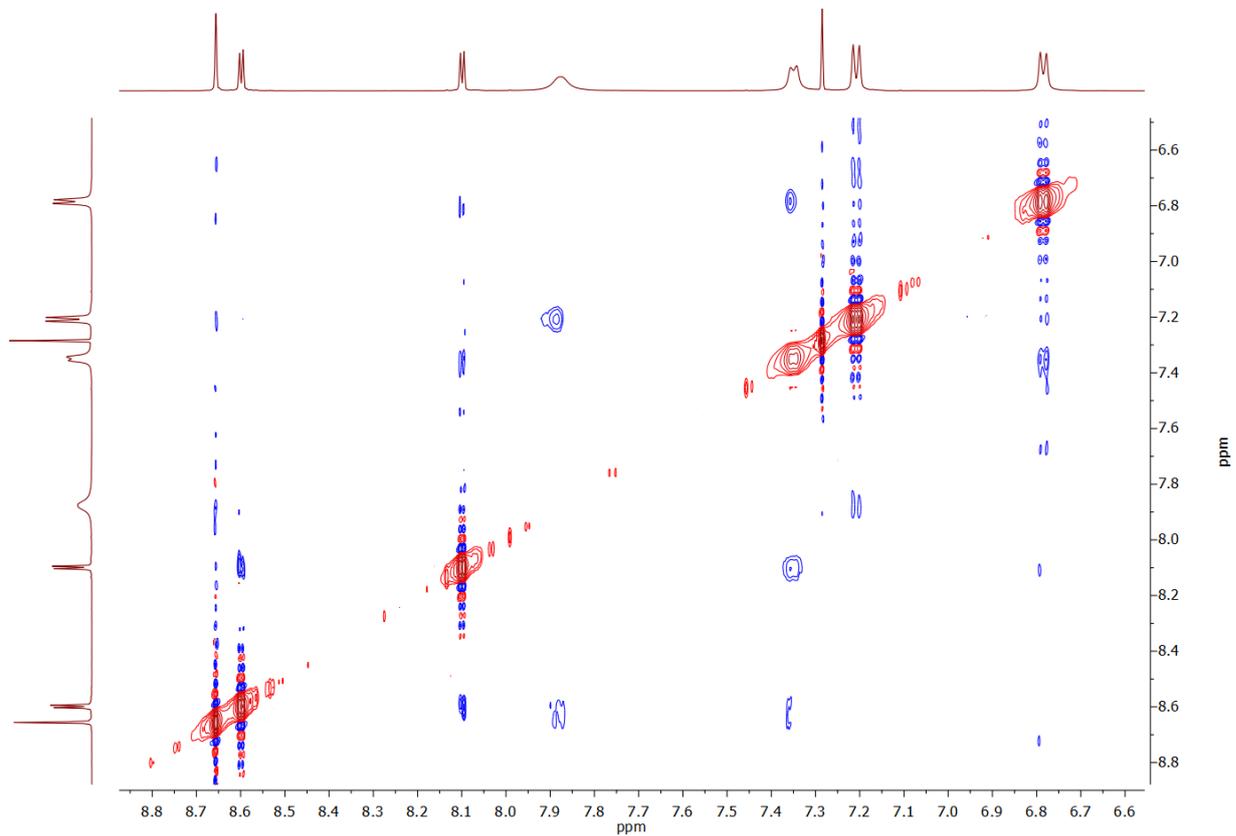
**Figure S5** COSY spectrum of complex **5** ( $\text{CDCl}_3$ ).



**Figure S6**  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of complex **5** ( $\text{CDCl}_3$ ).



**Figure S7**  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of complex **5** ( $\text{CDCl}_3$ ).



**Figure S8** ROESY spectrum of complex **5** ( $\text{CDCl}_3$ ).

### MALDI-TOF MS characterization of complex **5**

