Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

New *trans*-dipyridylporphyrins as building blocks for metal-mediated self-assembling of 4+4 Re(I)-porphyrin metallacycles

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Supplementary Informations

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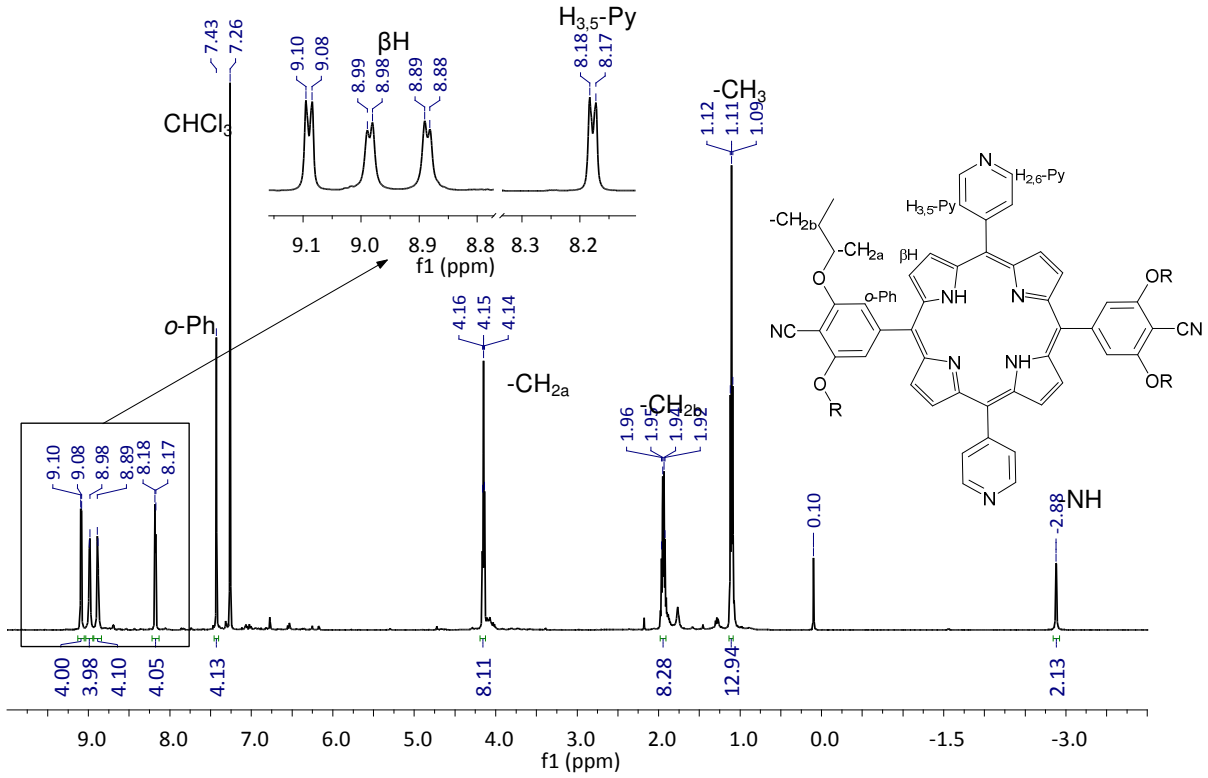

Fig S1. ^{1}H-NMR spectrum (500 MHz, $CDCl_3$) of porphyrin **P4**, with labeling scheme.

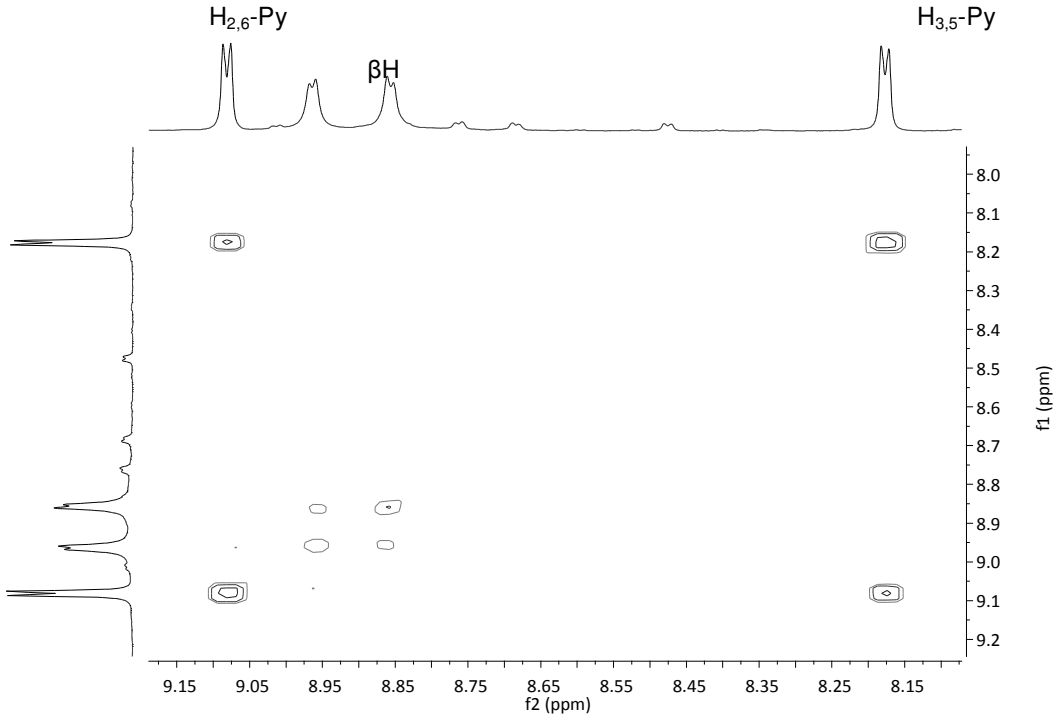

Fig. S2. Selected region of the HH-COSY spectrum (500 MHz, $CDCl_3$) of **P4**, see Figure S1 for labeling scheme.

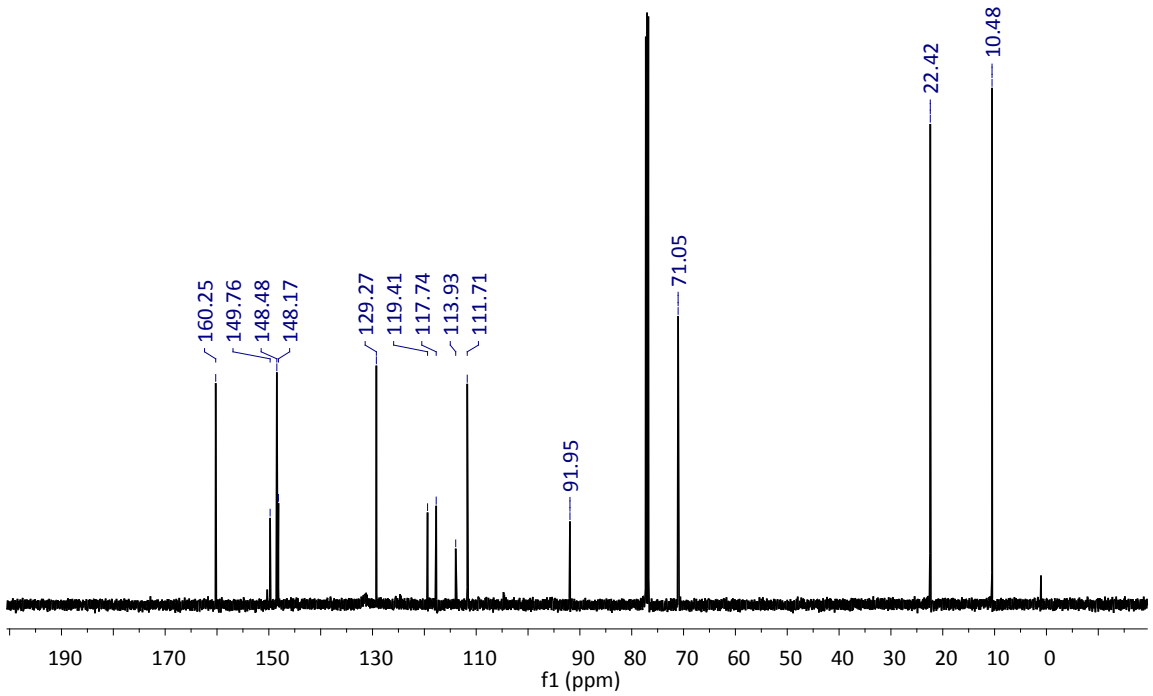

Fig. S3. ^{13}C-NMR spectrum (500 MHz, $CDCl_3$) of porphyrin **P4**.

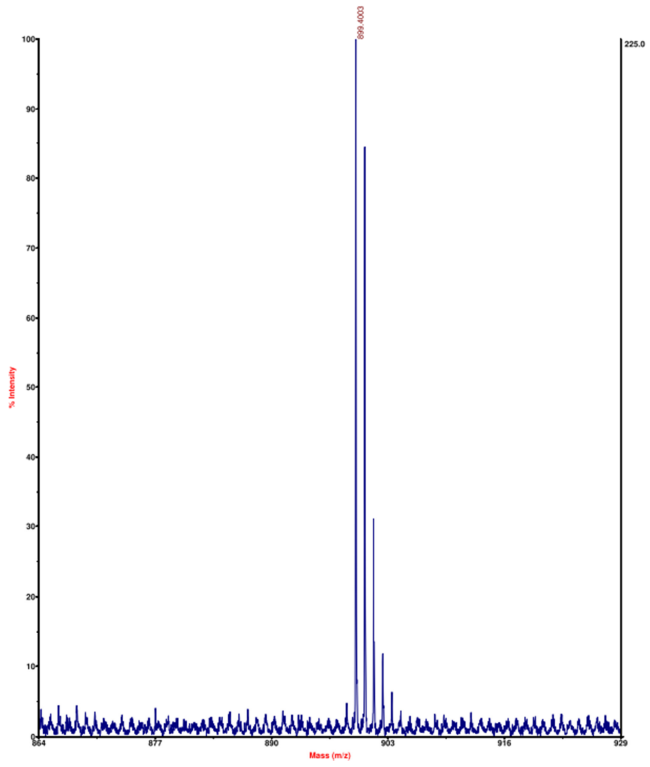

Fig. S4. HRMALDI-MS of porphyrin **P4**: m/z 899.4003 [M+H$^+$] (calcd for $C_{56}H_{51}N_8O_4$ 899.4033).

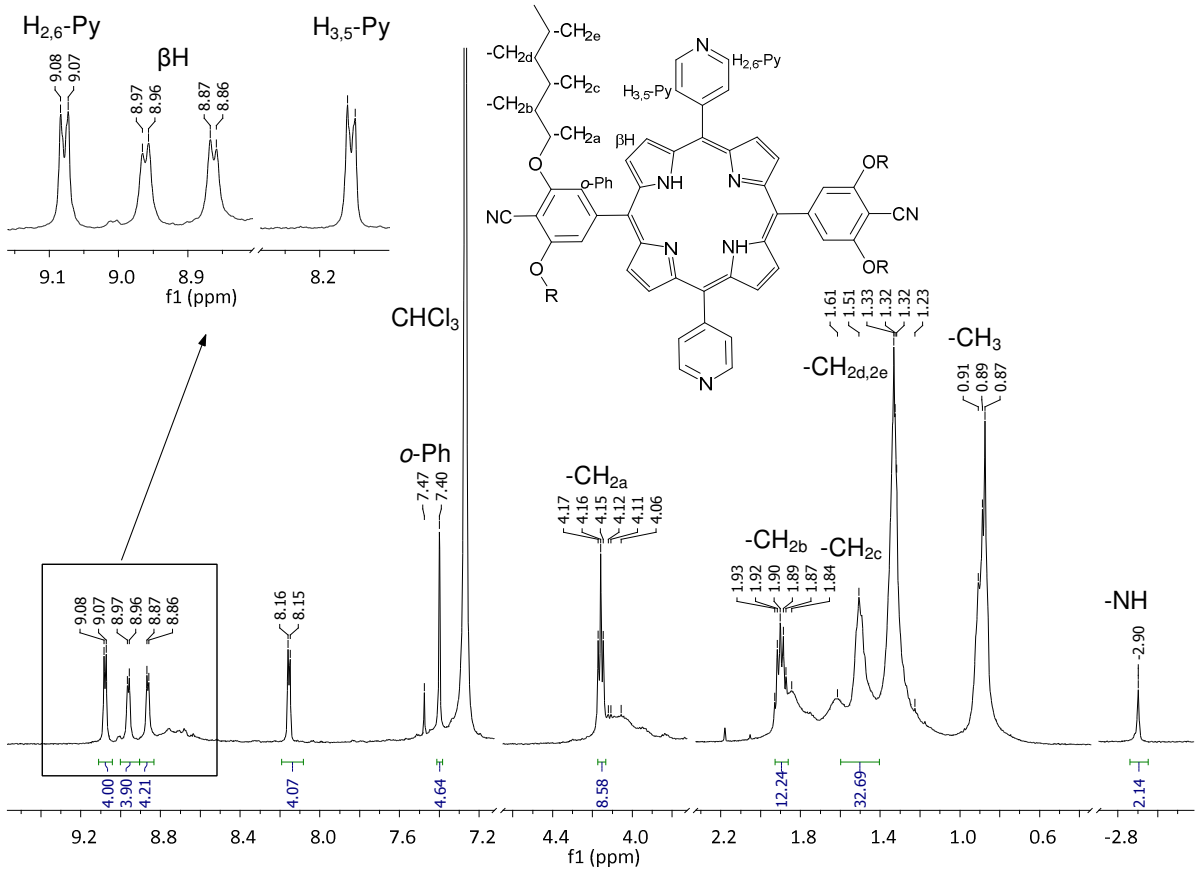

Fig. S5. ^{1}H-NMR spectrum (500 MHz, $CDCl_3$) of porphyrin **P5**, with labeling scheme.

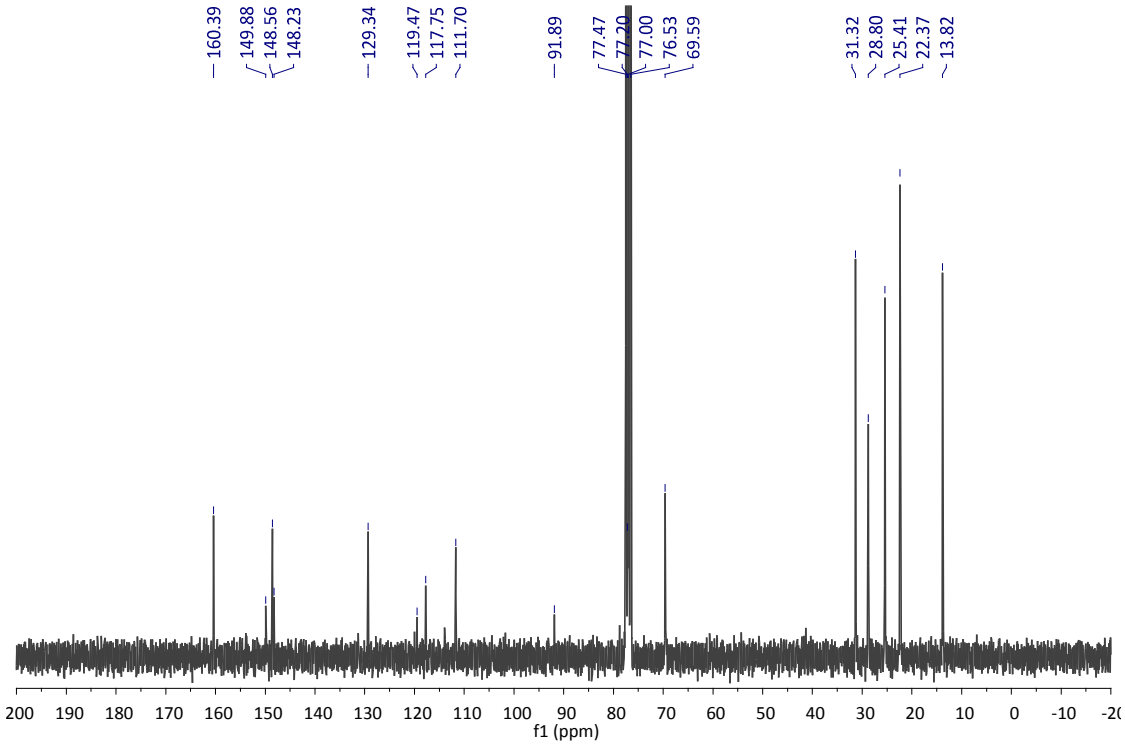

Fig. S6. ^{13}C-NMR spectrum (500 MHz, $CDCl_3$) of porphyrin **P5**.

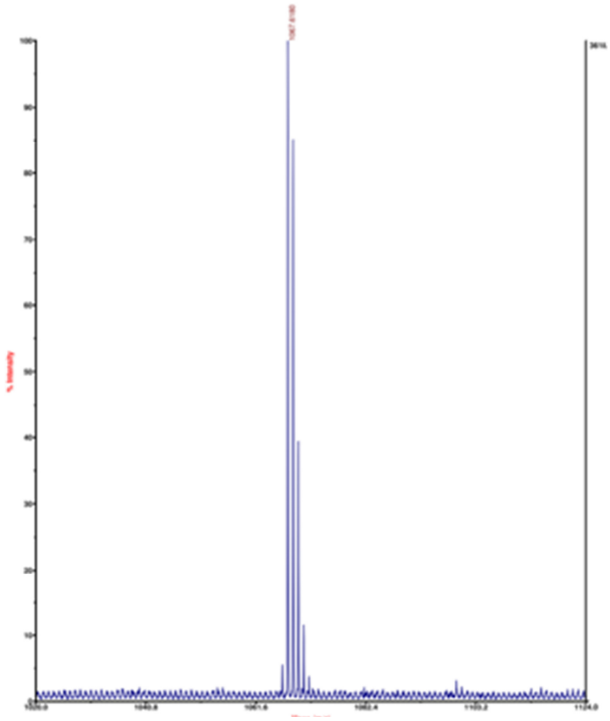

Fig. S7. HRMALDI-MS of porphyrin **P5**: m/z 1067,6180 [M+H$^+$] (calcd for $C_{68}H_{75}N_8O_4$ 1067.5911).

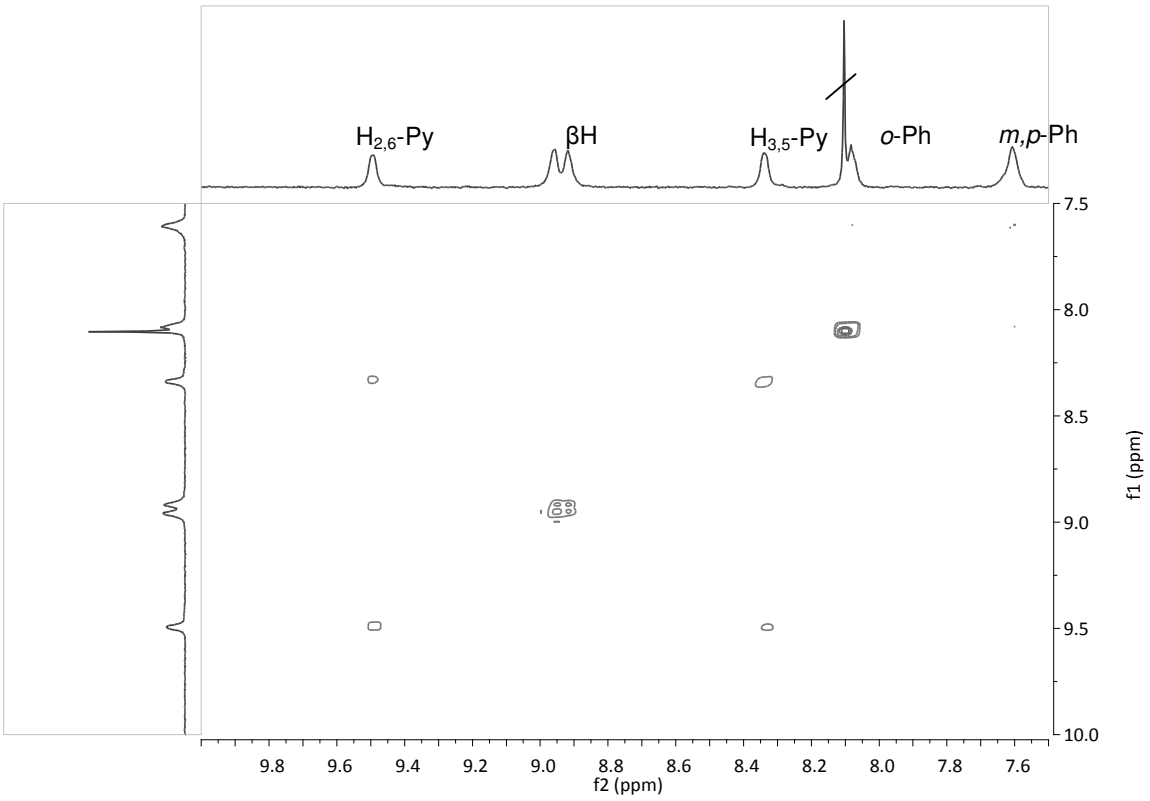

Fig S8. Selected region of the HH-COSY spectrum (500 MHz, $CDCl_3$) of $[Re(CO)_3(Zn{\cdot}P1)Br]_4$, see Scheme 5 for labeling scheme.

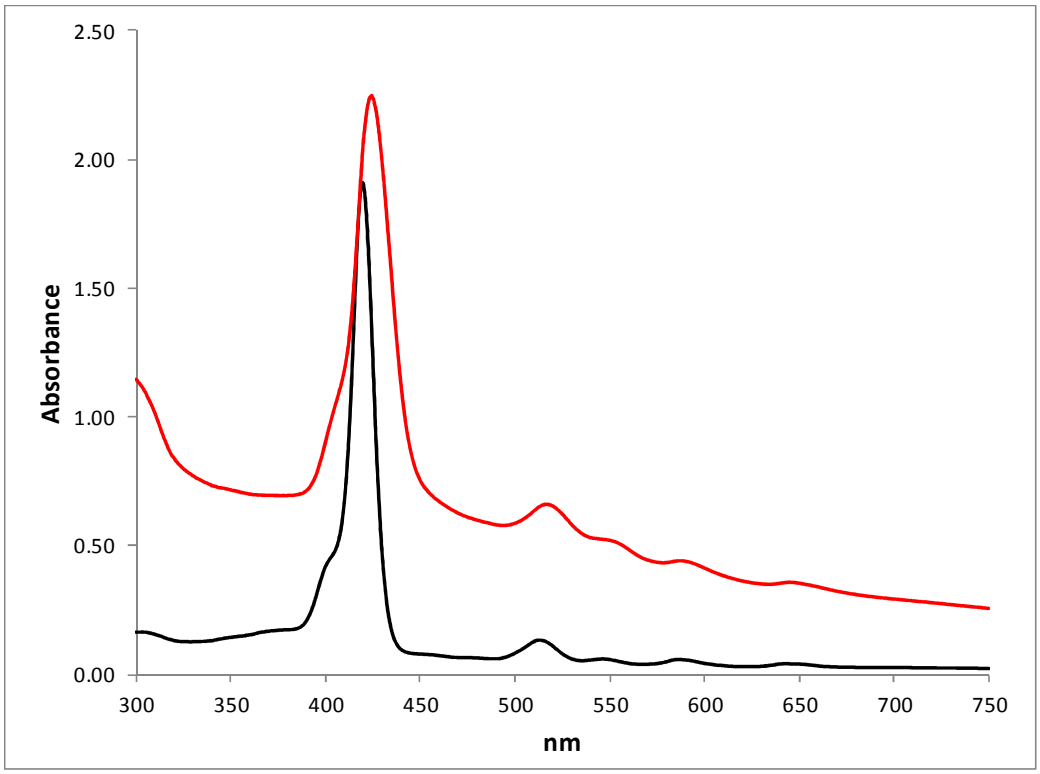

Fig S9. UV-Vis spectra of **P4** (black) and of the product obtained from reaction of **P4** and $Re(CO)_5Br$ (red) at a $2 \cdot 10^{-5}$ M concentration.

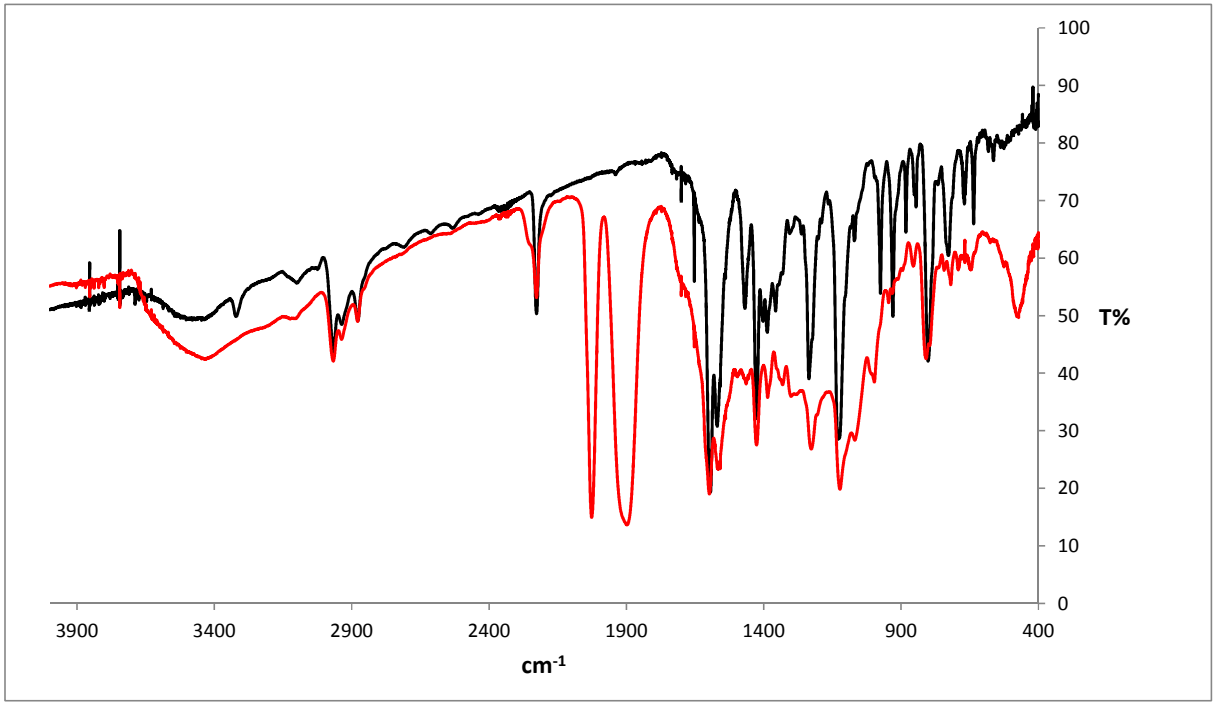

Fig S10. IR spectra in KI of **P4** (black) and of the product obtained from reaction of **P4** and $Re(CO)_5Br$ (red).

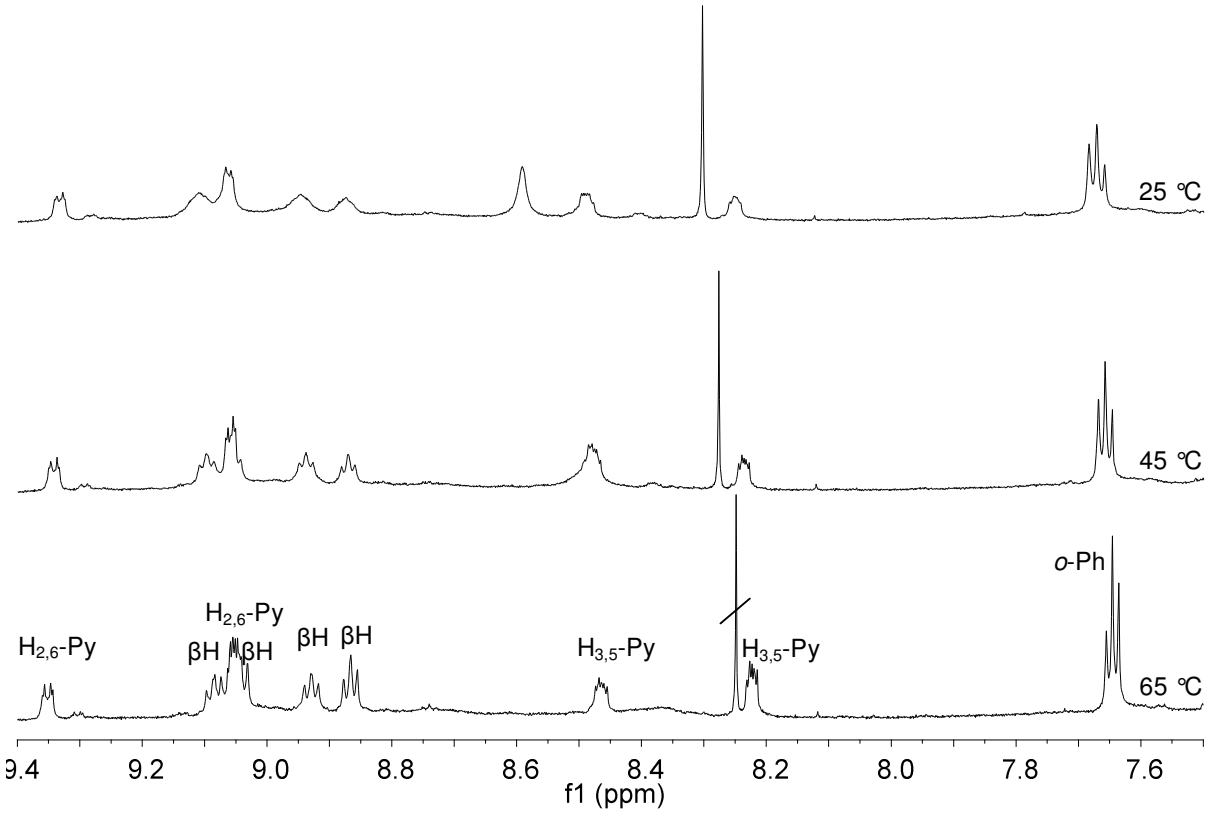

Fig S11. ^{1}H-NMR spectra (downfield region) in DMSO-d_6 of the product obtained from reaction of **P4** and $Re(CO)_5Br$, at different temperatures. From top: 25°C, 45°C, 65°C, see Figure S1 for labeling scheme.

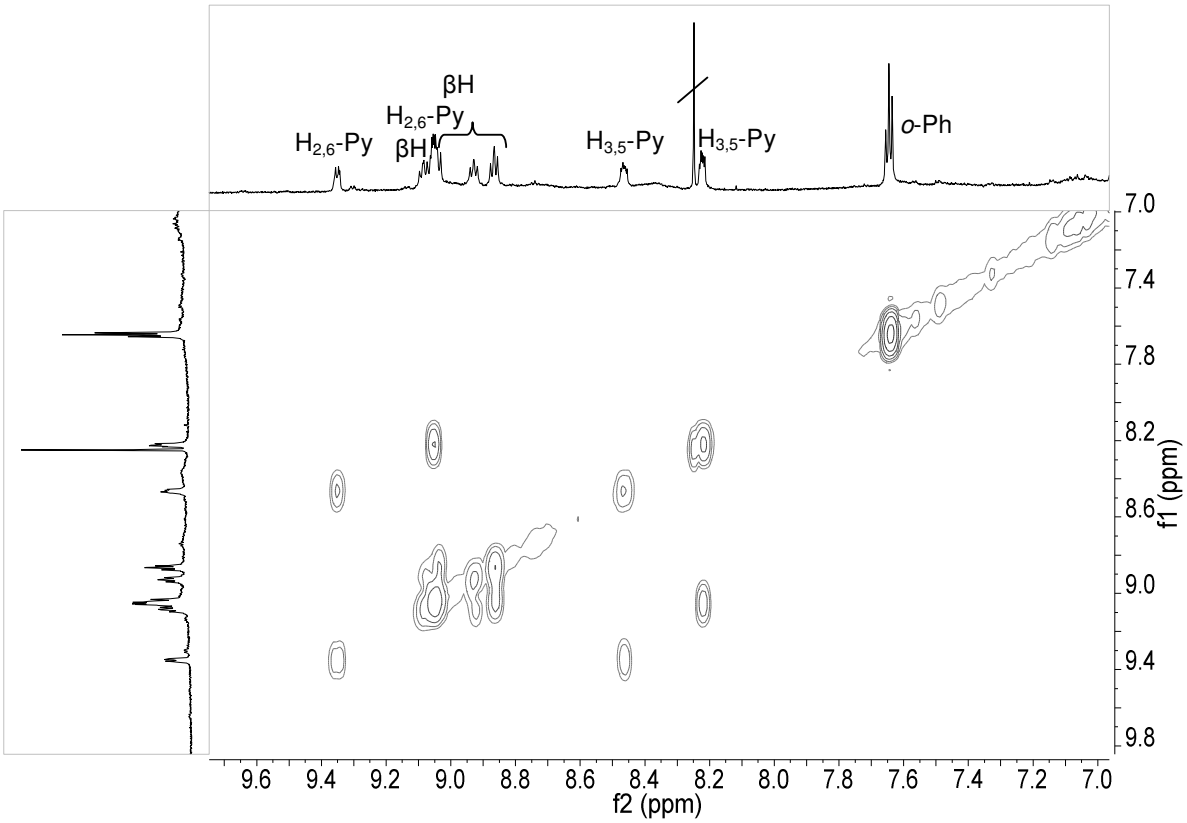

Fig S12. Selected region of the HH-COSY spectrum (500 MHz, DMSO-d_6) of the product obtained from the reaction of **P4** and $Re(CO)_5Br$, at 65 °C, see Figure S1 for labeling scheme.

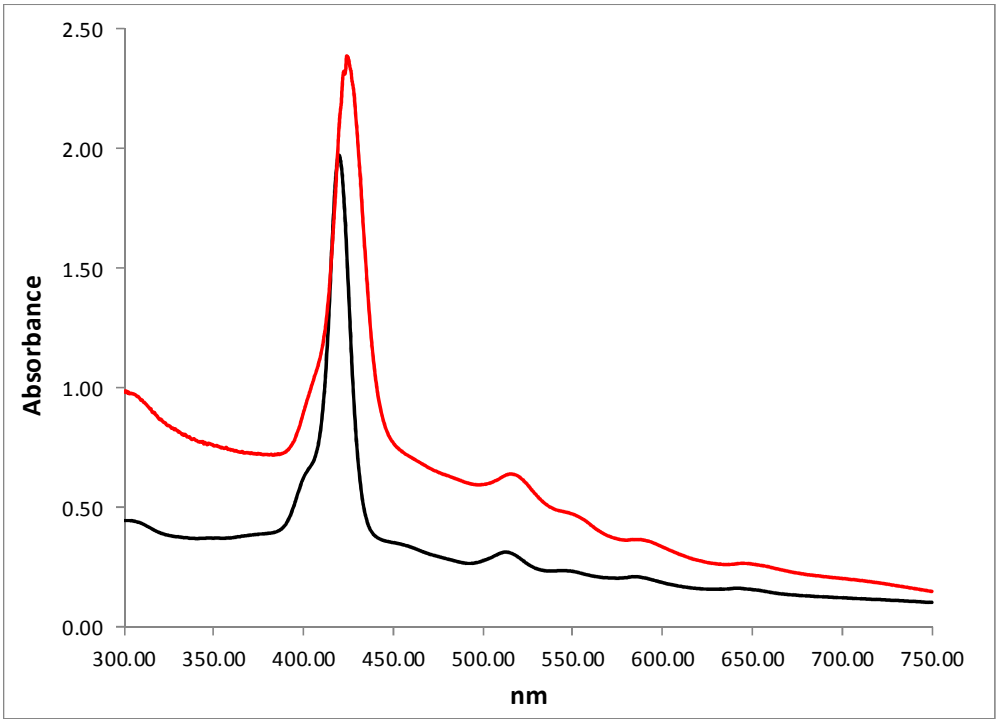

Fig S13. UV-Vis spectra of the product (red) obtained from the reaction of **P5** (black) and $Re(CO)_5Br$ in chloroform at $2 \cdot 10^{-5}$ M concentration.

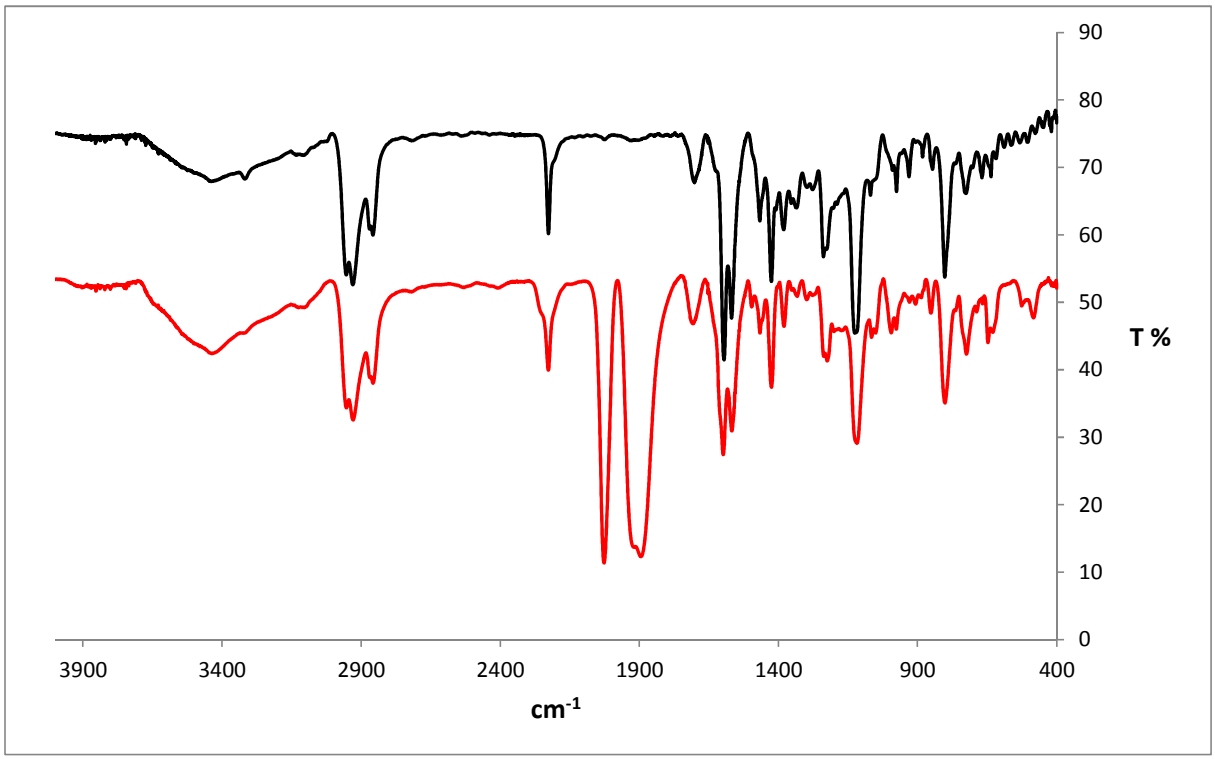

Fig S14. IR spectra in KI of the product (red) obtained from reaction of **P5** (black) and $Re(CO)_5Br$.