Supporting Information

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Synthesis of chalcone-containing zinc and cobalt metallophthalocyanines; investigation of their photochemical, DPPH radical scavenging and metal chelating characters

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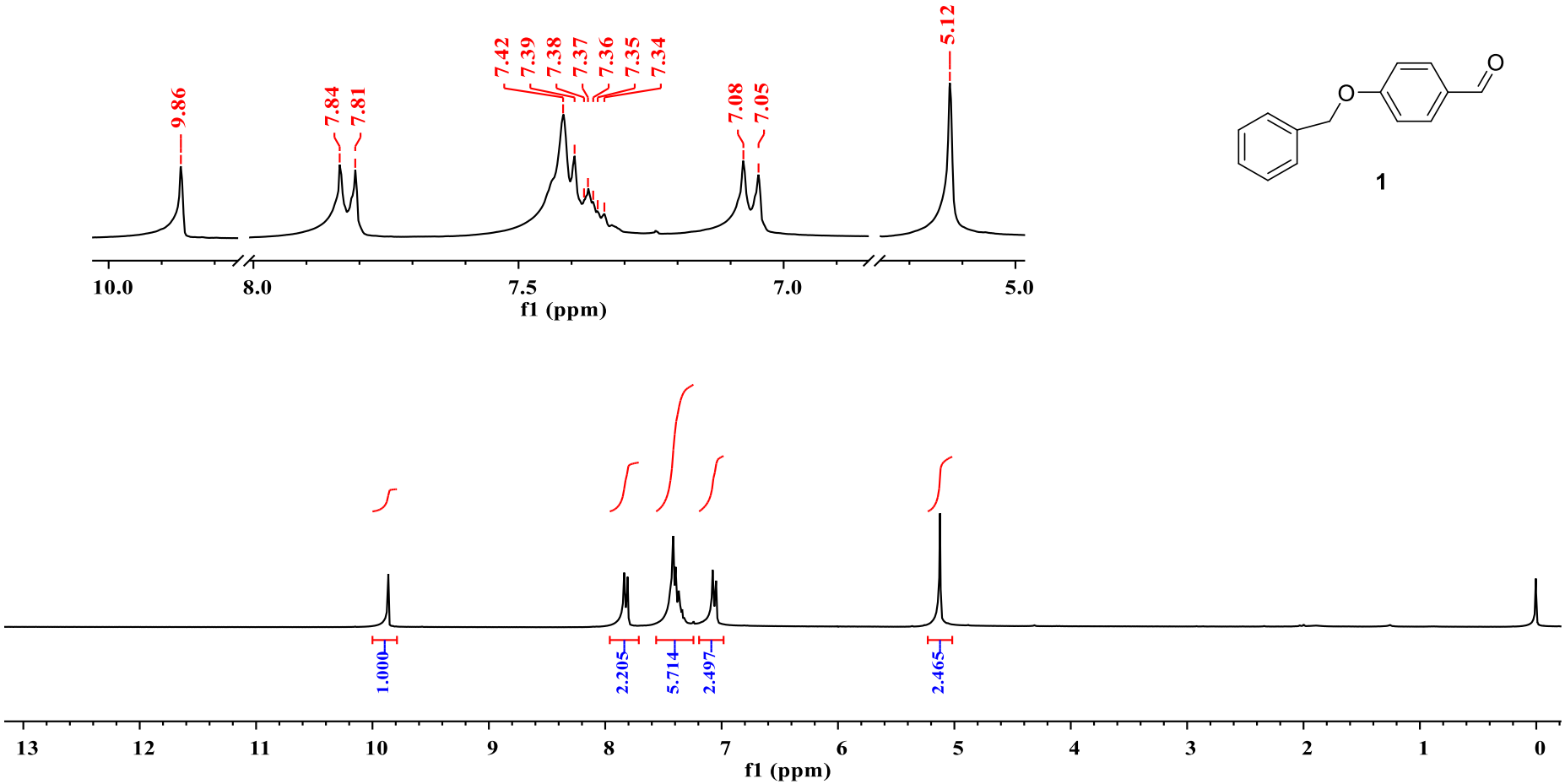


Figure S1: ^{1}H NMR spectrum of compound **1** in ($CDCl_3$)

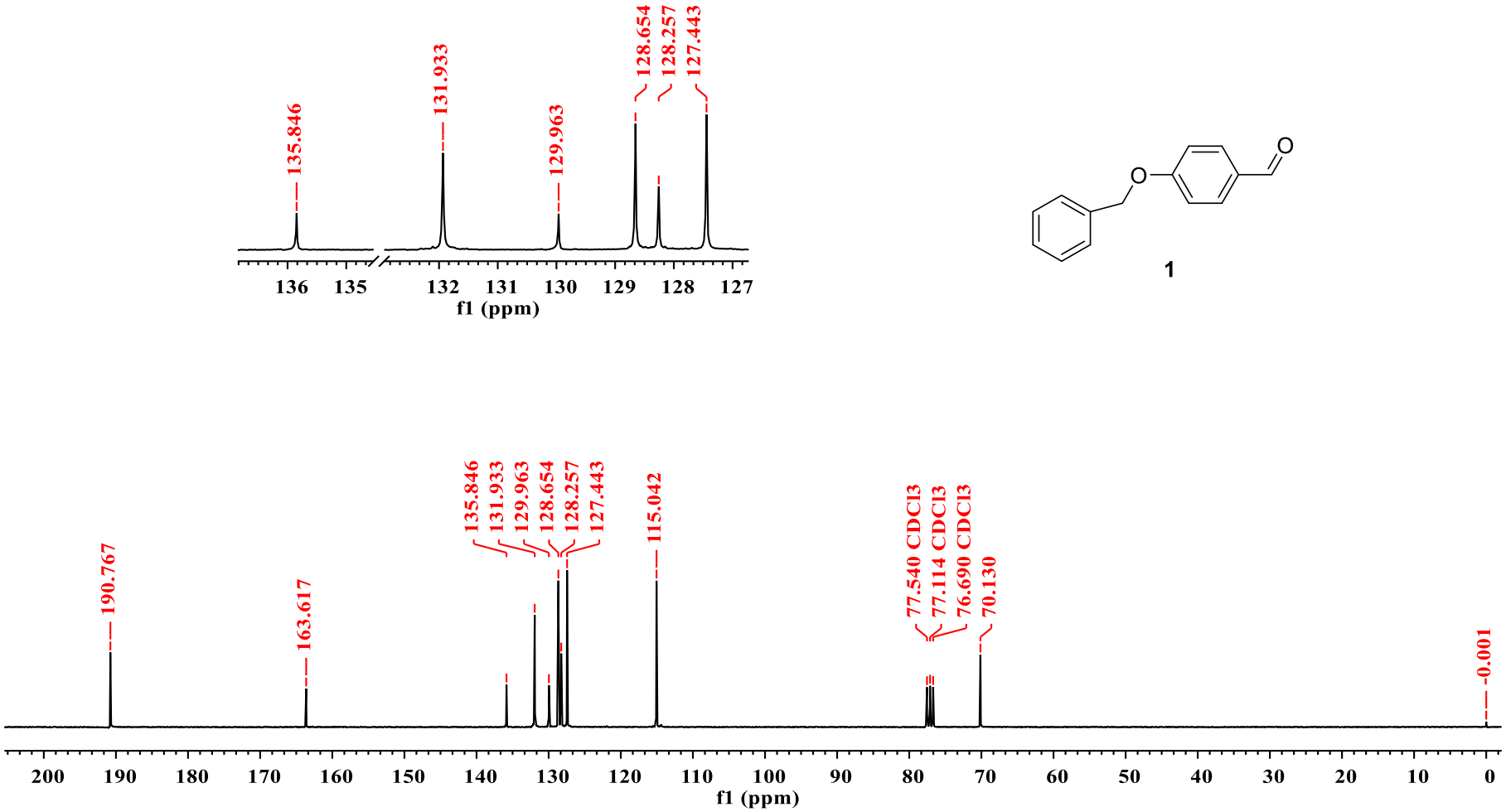


Figure S2: ^{13}C NMR spectrum of compound **1 (**in $CDCl_3$)

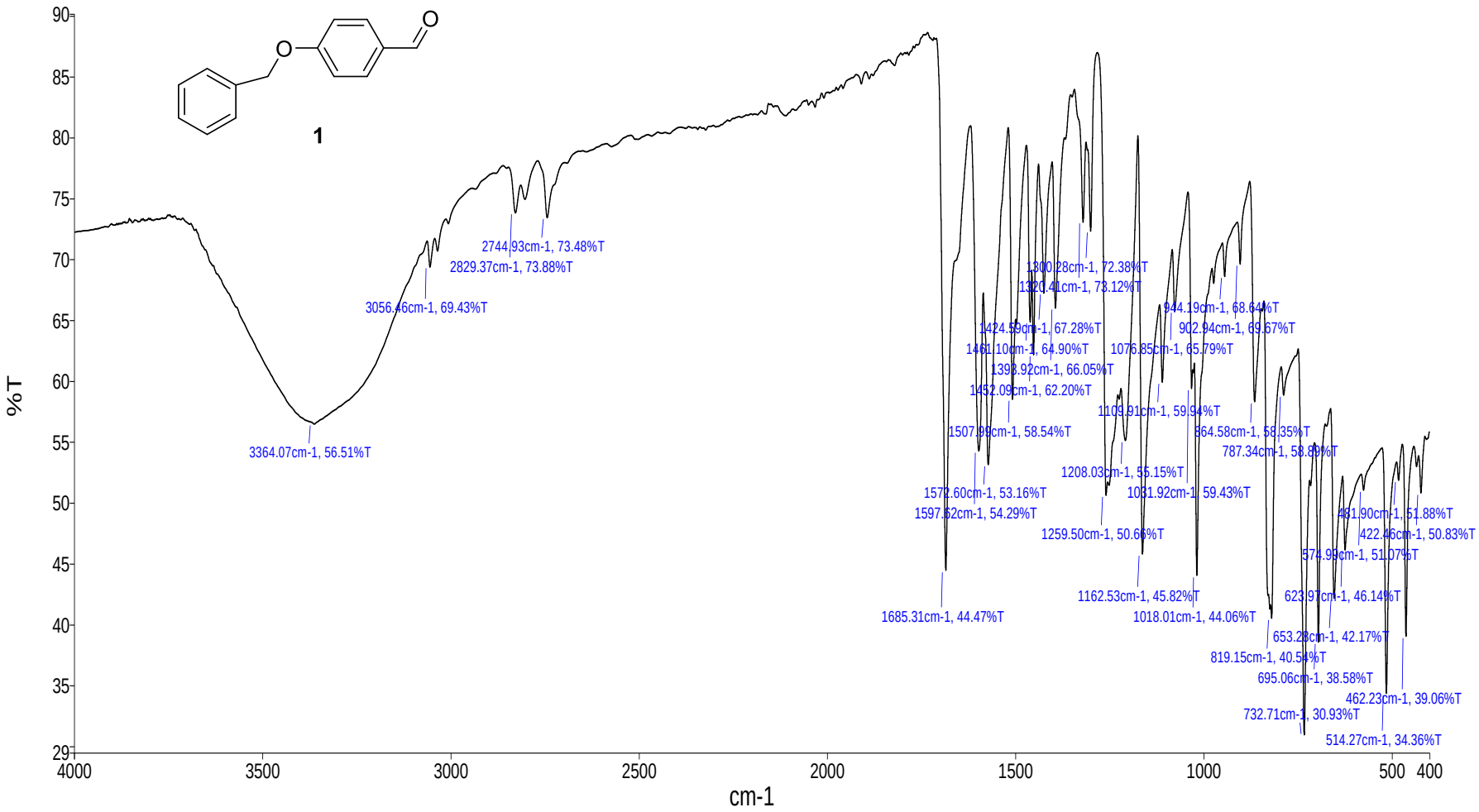


Figure S3: FT-IR spectrum of compound **1**

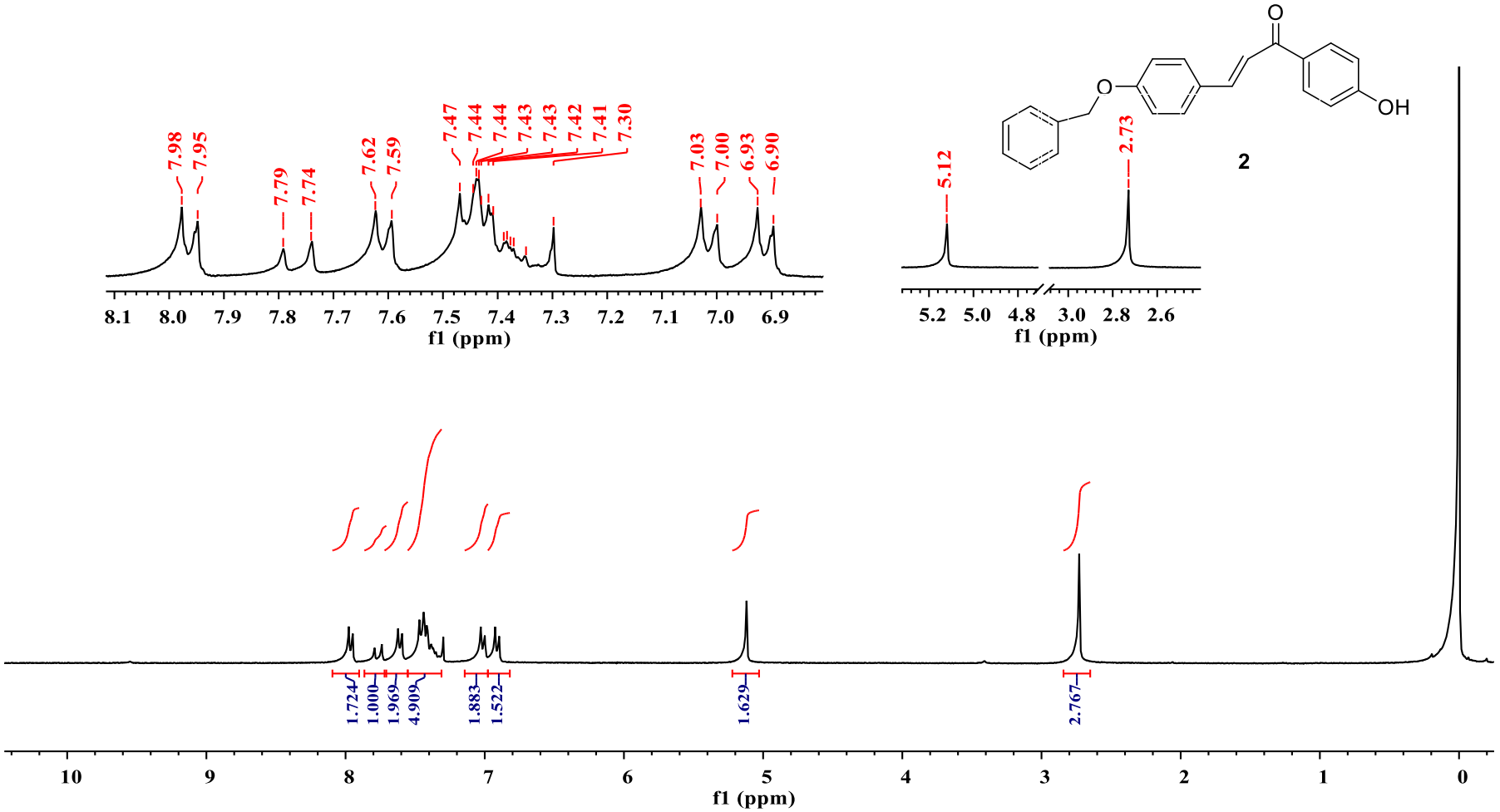


Figure S4: ^{1}H NMR spectrum of compound **2 (**in $CDCl_3$ / CD_3OD: 5/1)

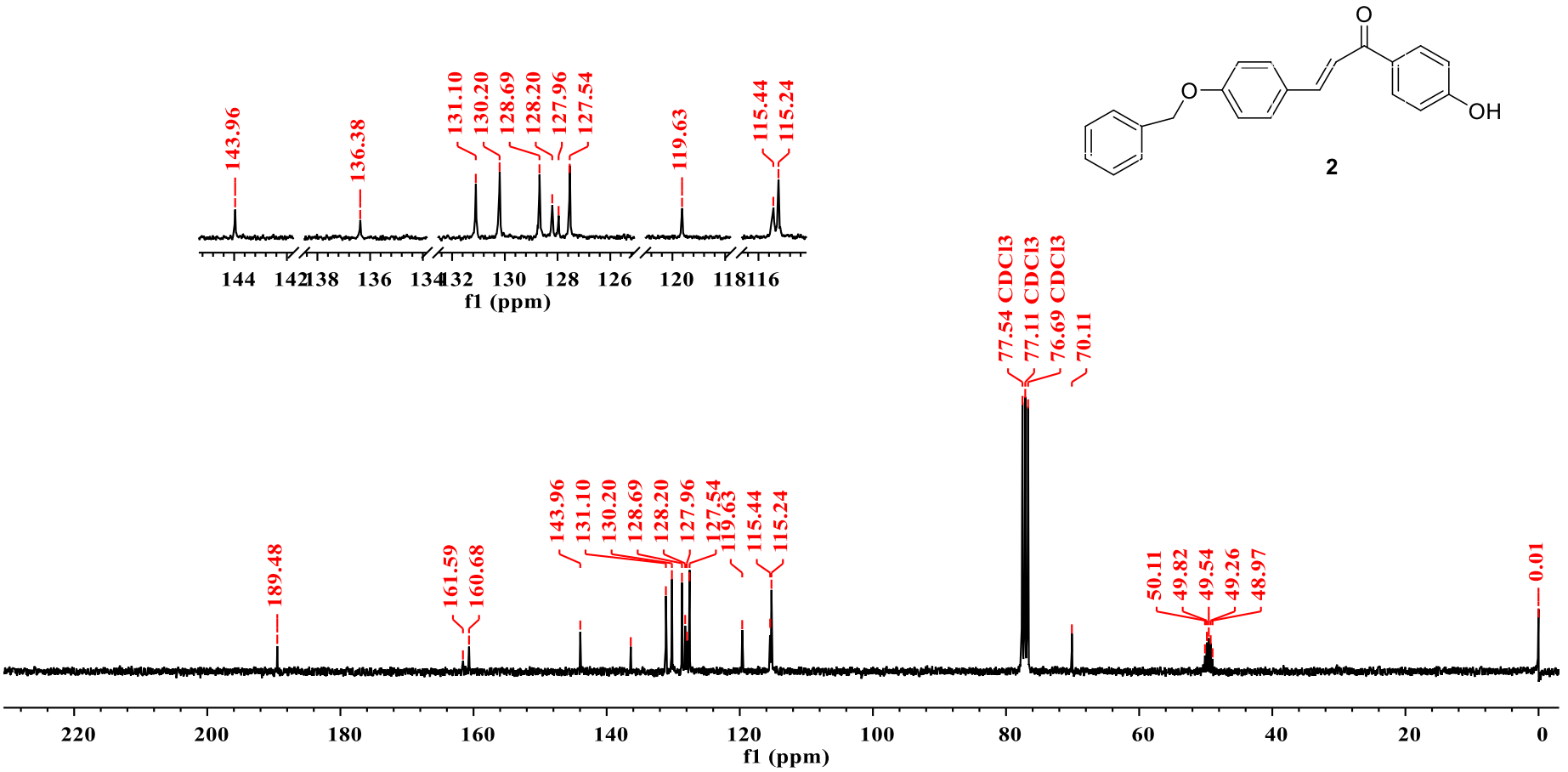


Figure S5: ^{13}C NMR of spectrum of compound **2 (**in $CDCl_3$ / CD_3OD: 5/1)

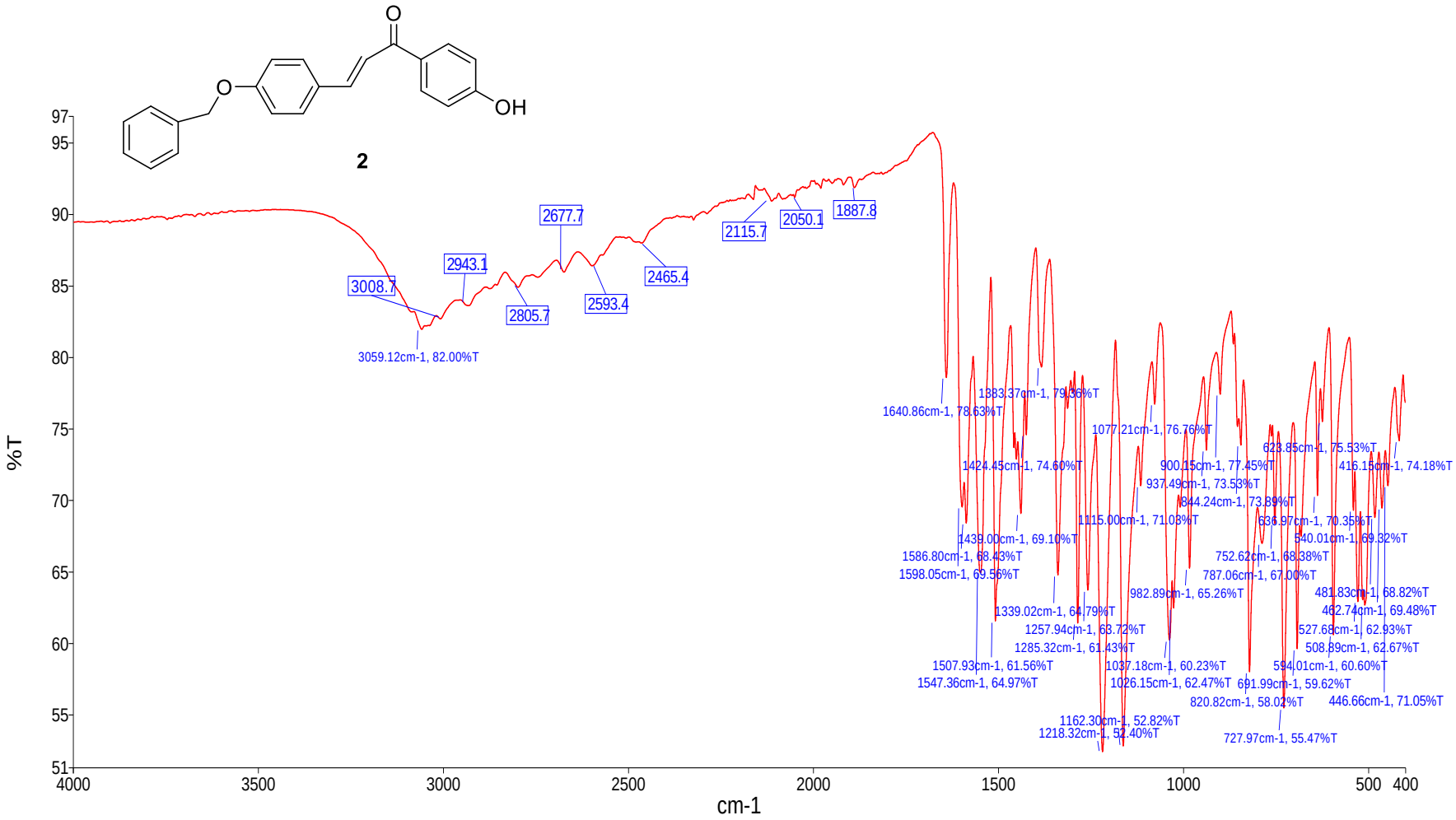


Figure S6. FT-IR spectrum of compound **2**

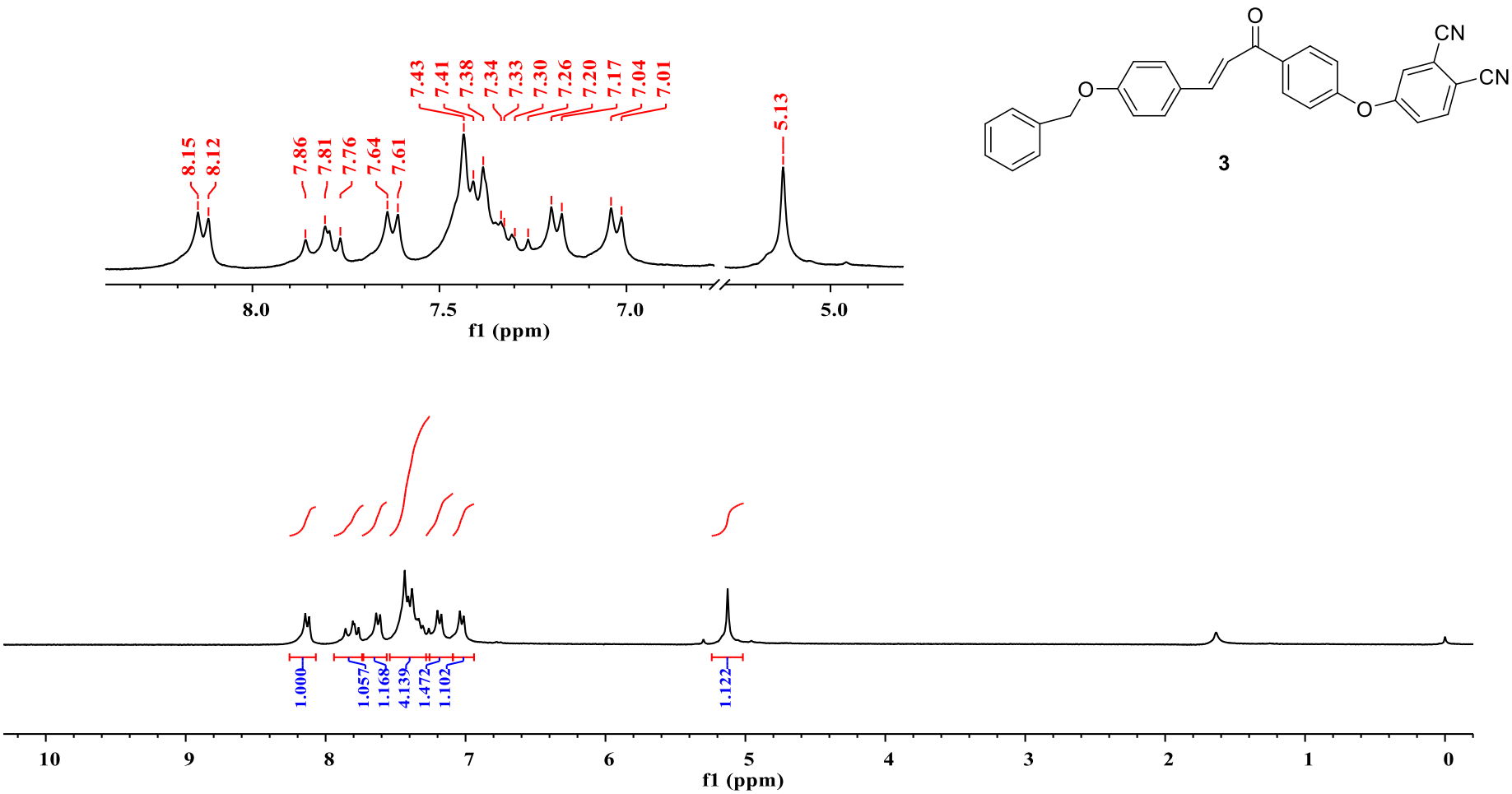


Figure S7: ^{1}H NMR spectrum of compound **3 (**in $CDCl_3$)

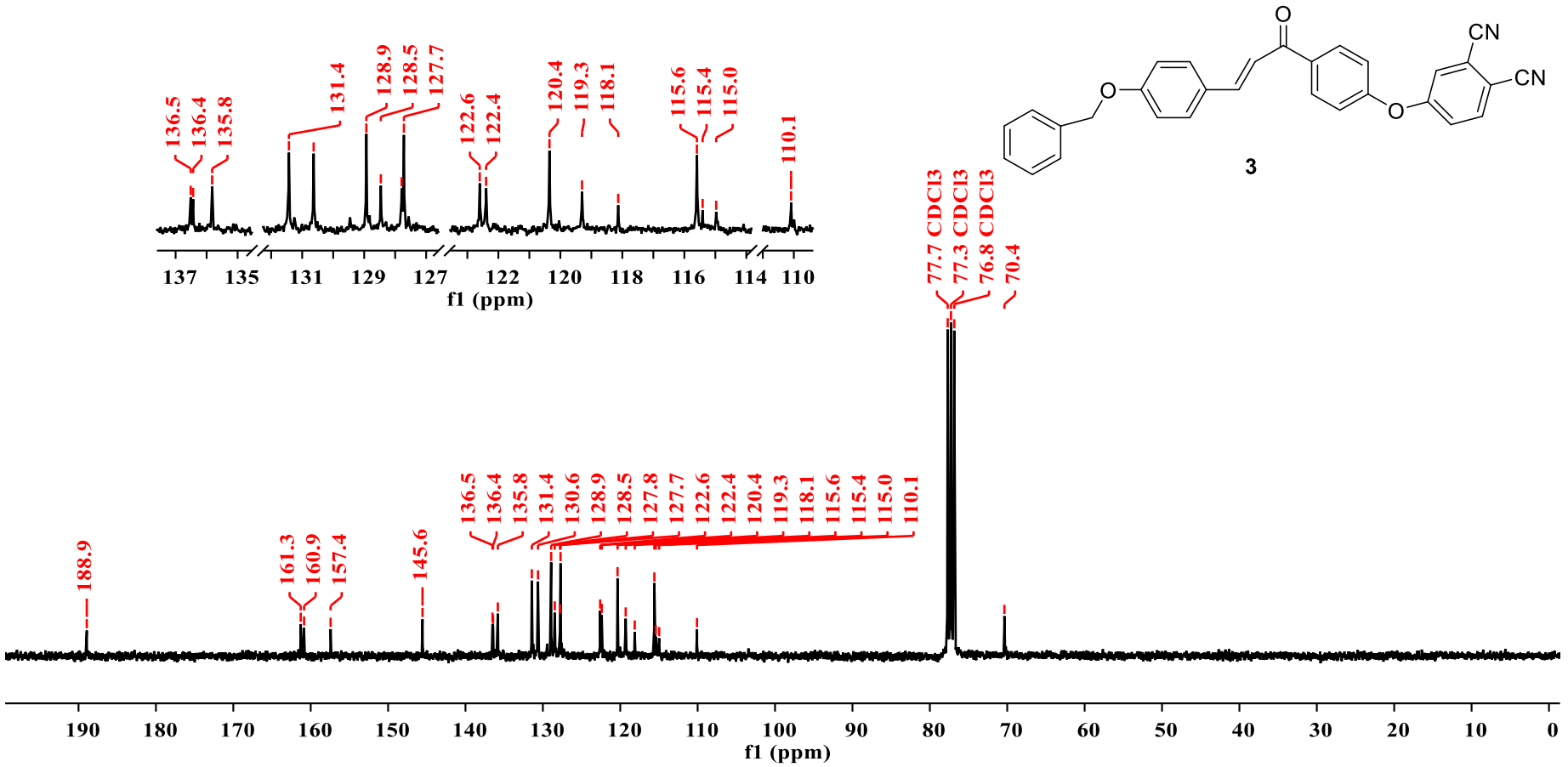


Figure S8: ^{13}C NMR of spectrum of compound **3 (**in $CDCl_3$)

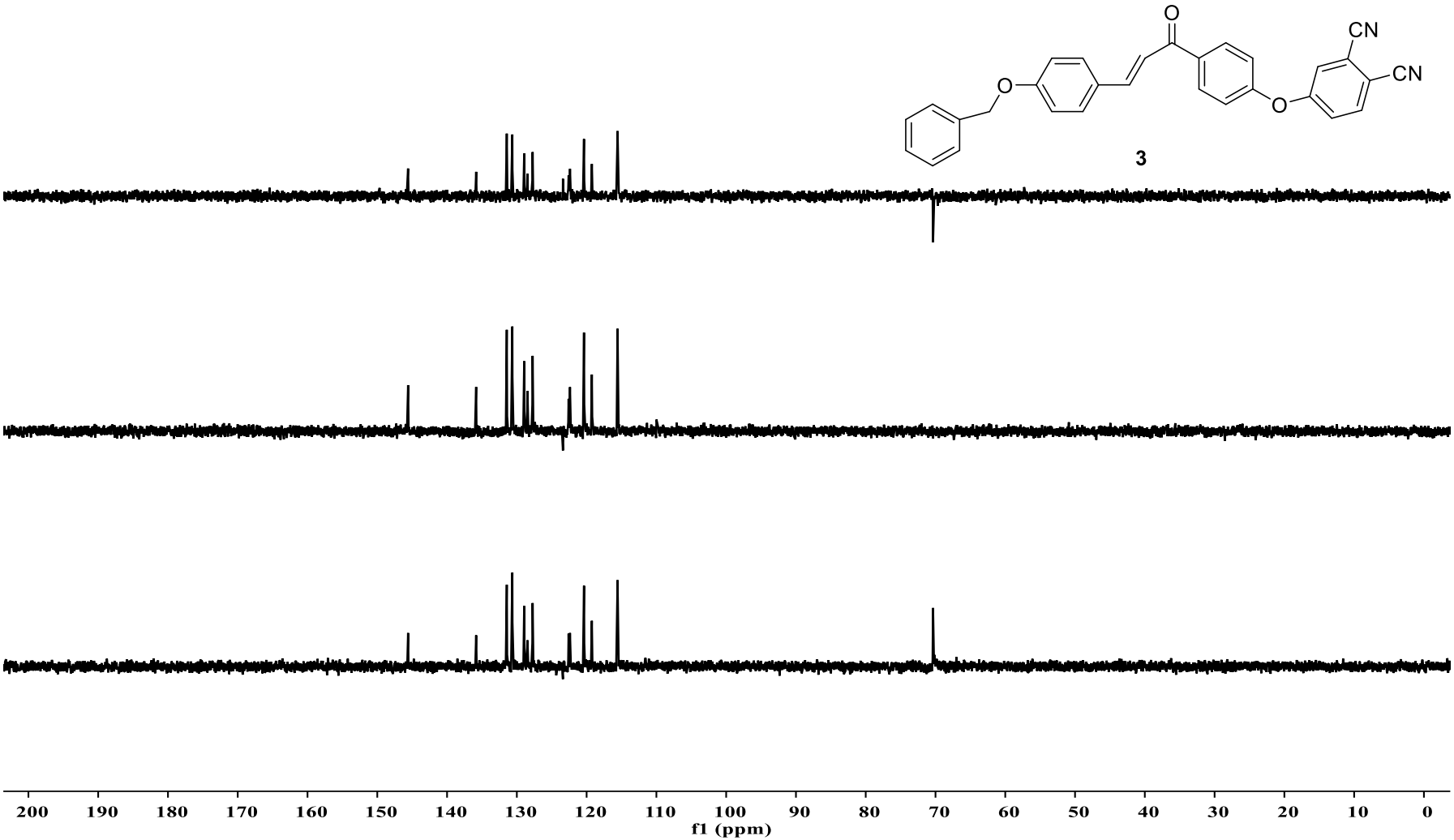


Figure S9: Dept NMR Spectrum of compound **3 (**in $CDCl_3$)

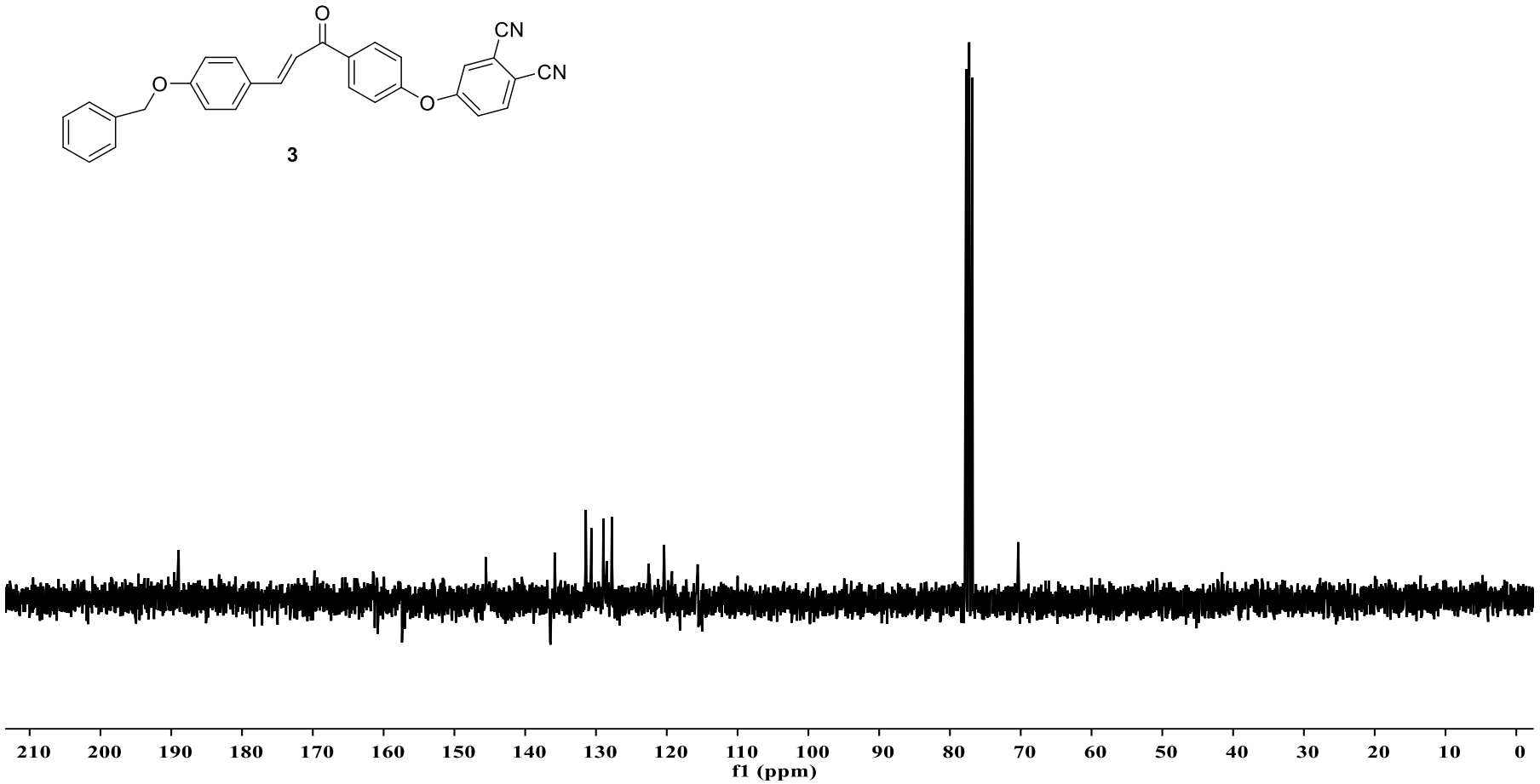


Figure S10: APT spectrum of compound **3** (in $CDCl_3$)

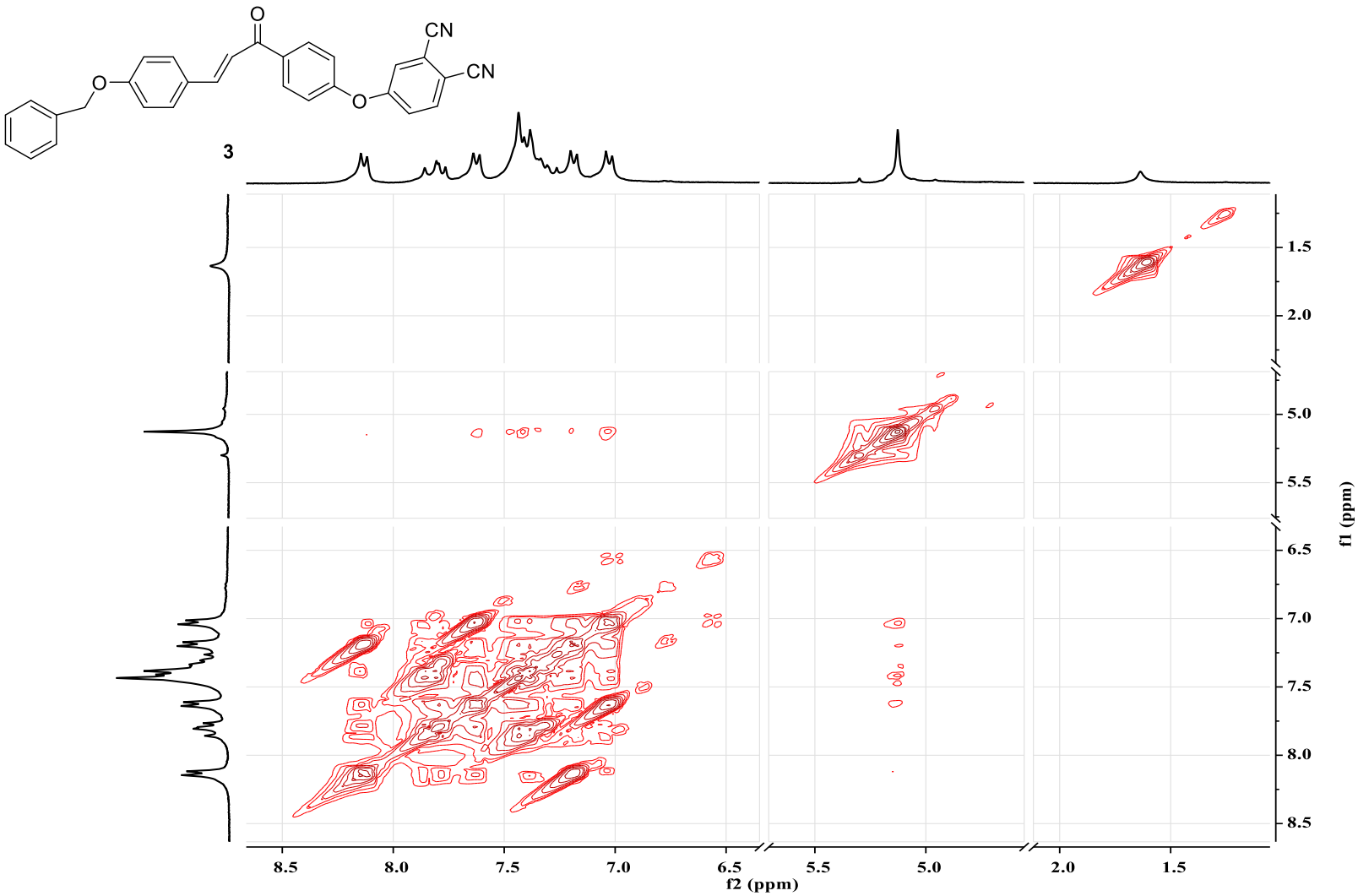


Figure S11: COSY spectrum of compound **3** (in $CDCl_3$)

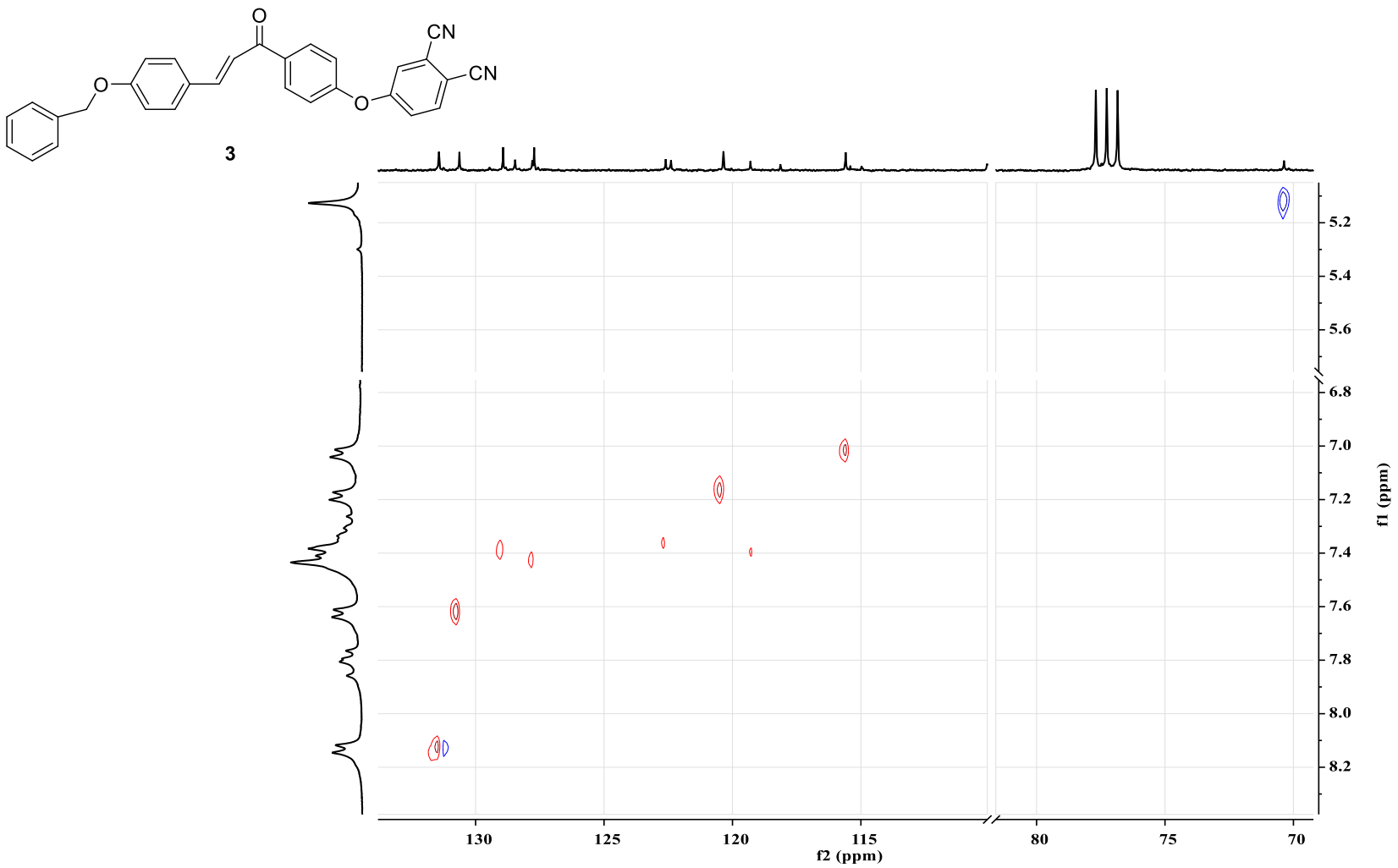


Figure S12: HETCOR spectrum of compound **3** (in CDCl3)

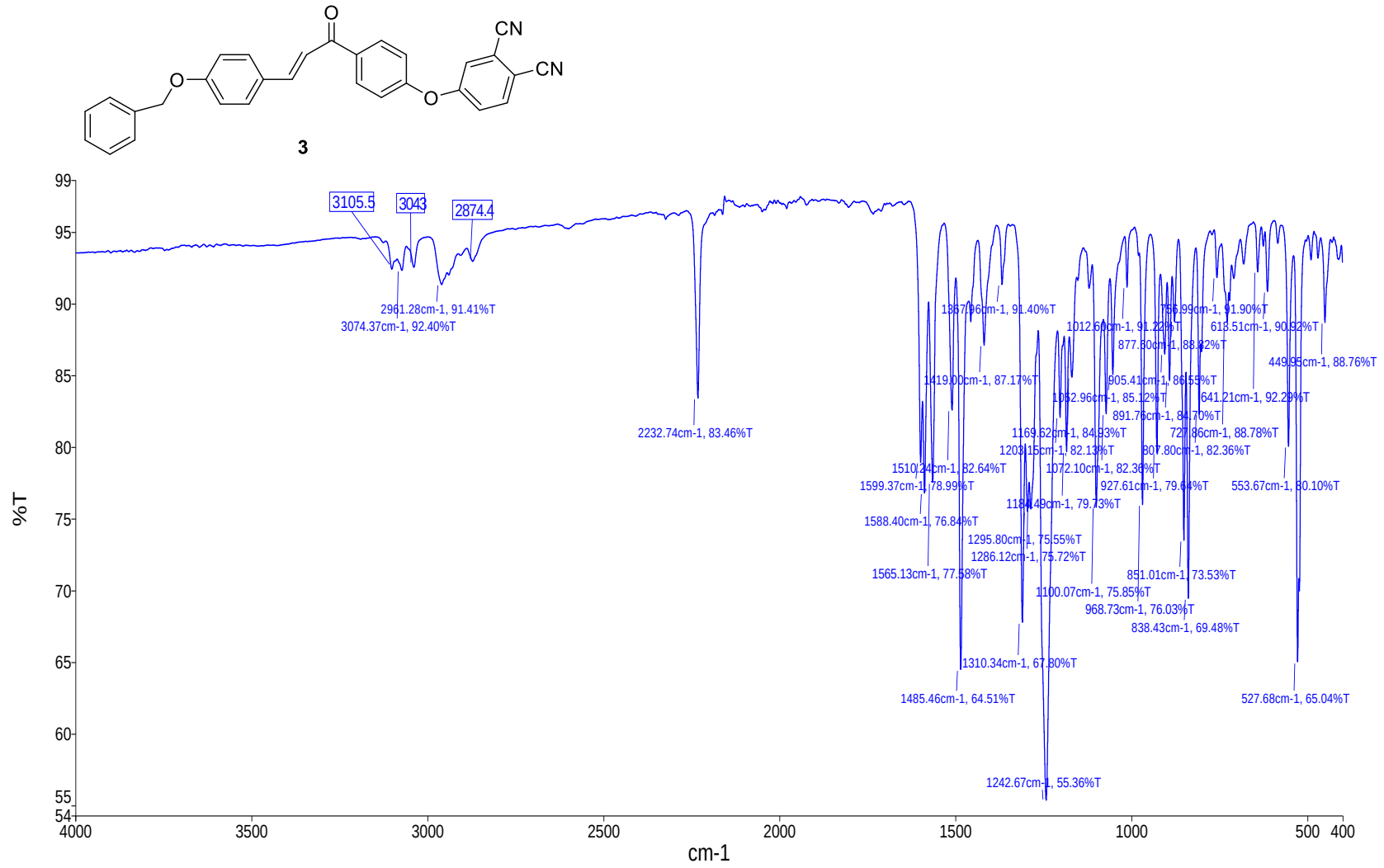


Figure S13: FT-IR spectrum of compound **3**

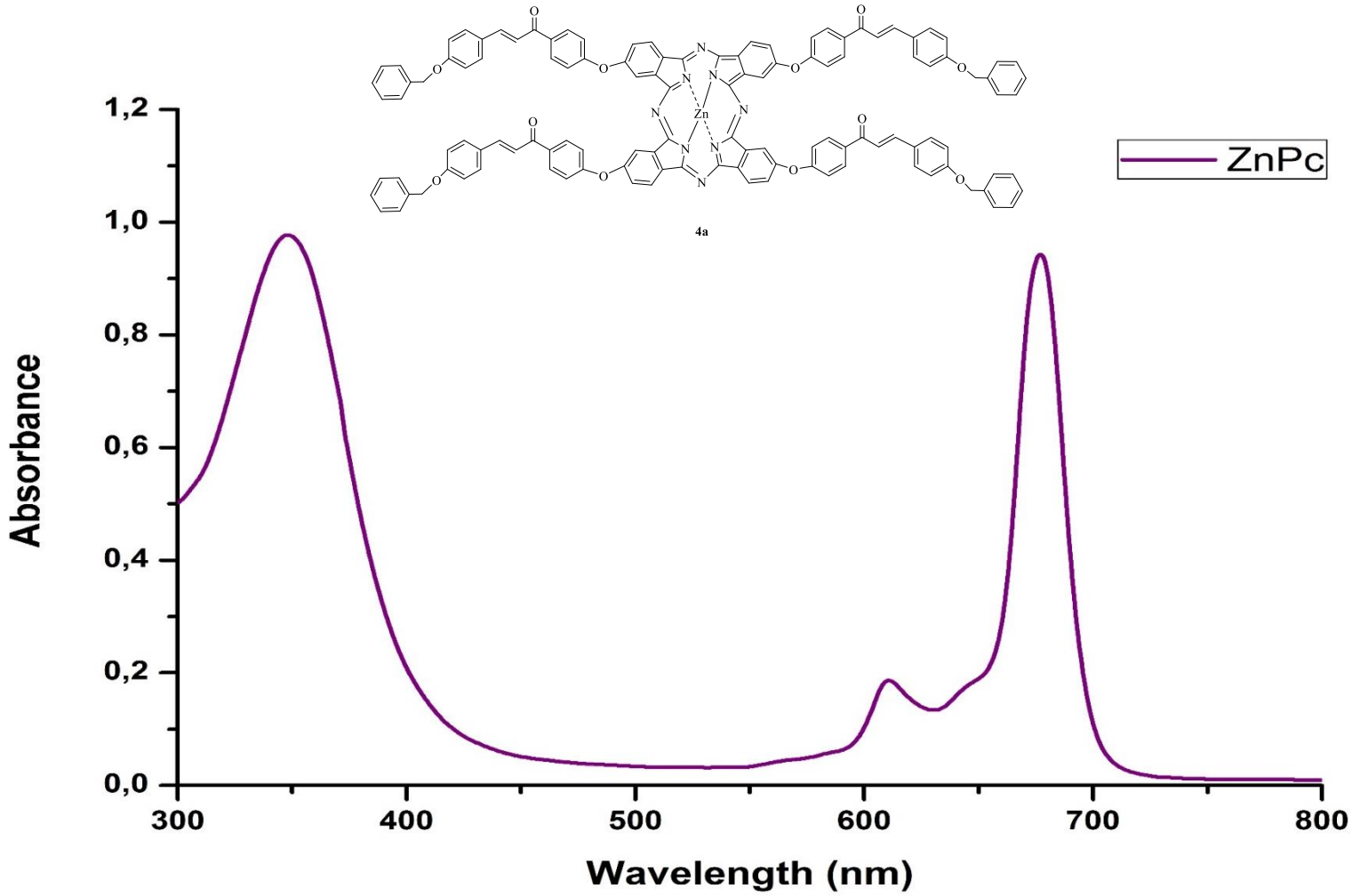


Figure S14: UV-Vis spectrum of compound **4a** (in DMF)

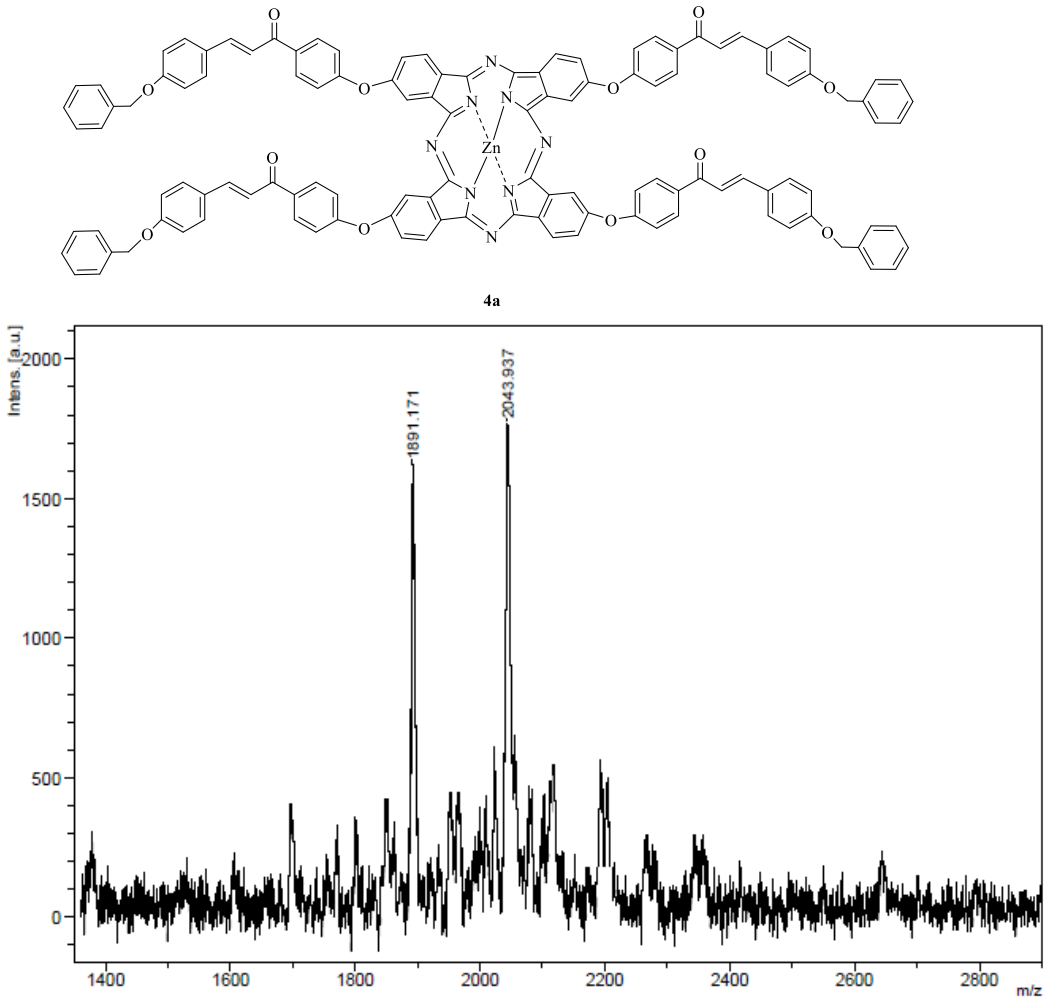


Figure S15: MALDI-TOF mass spectrum of compound **4a** in 1,8,9-anthracenetriol

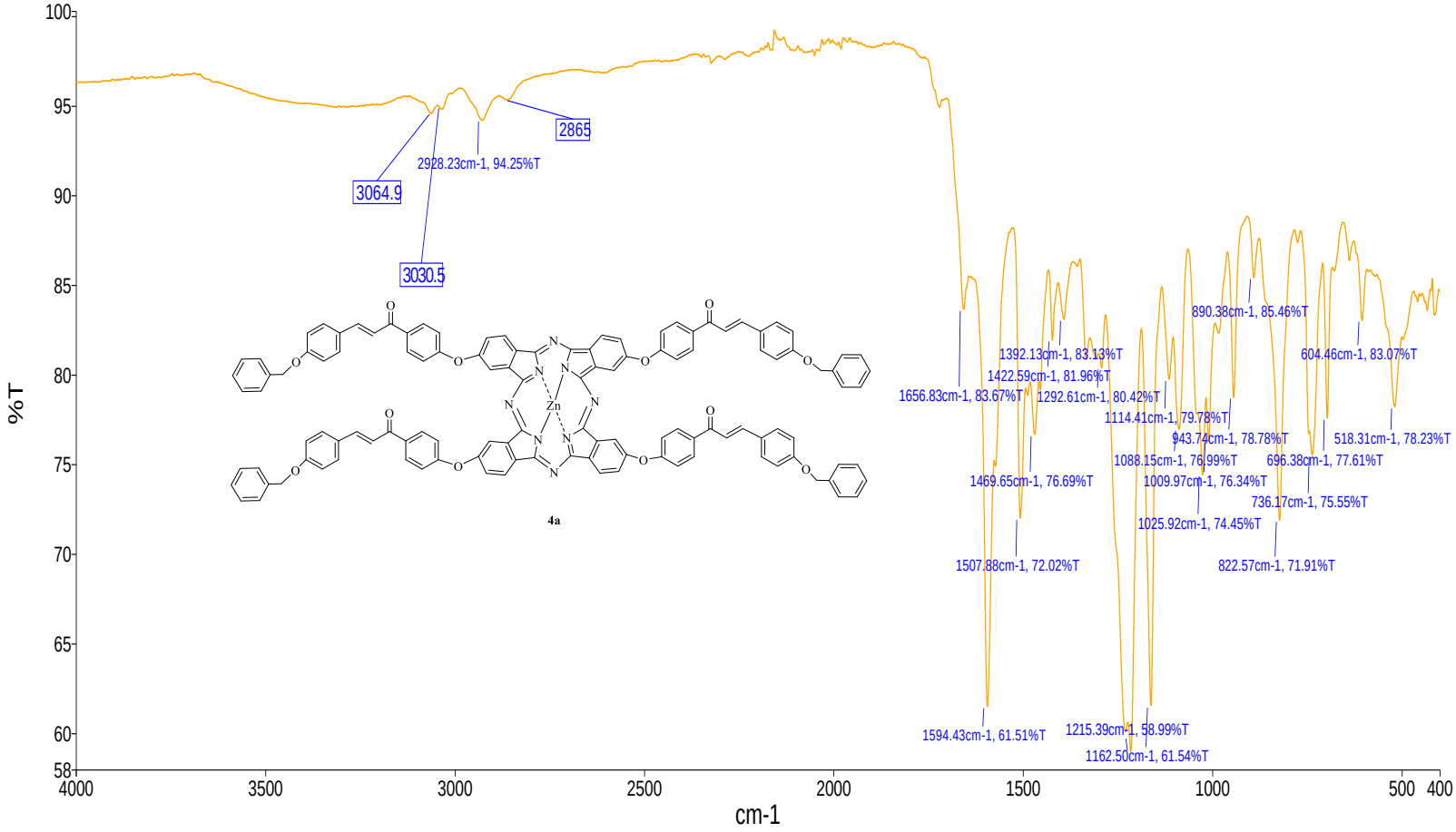


Figure S16: FT-IR spectrum of compound **4a**

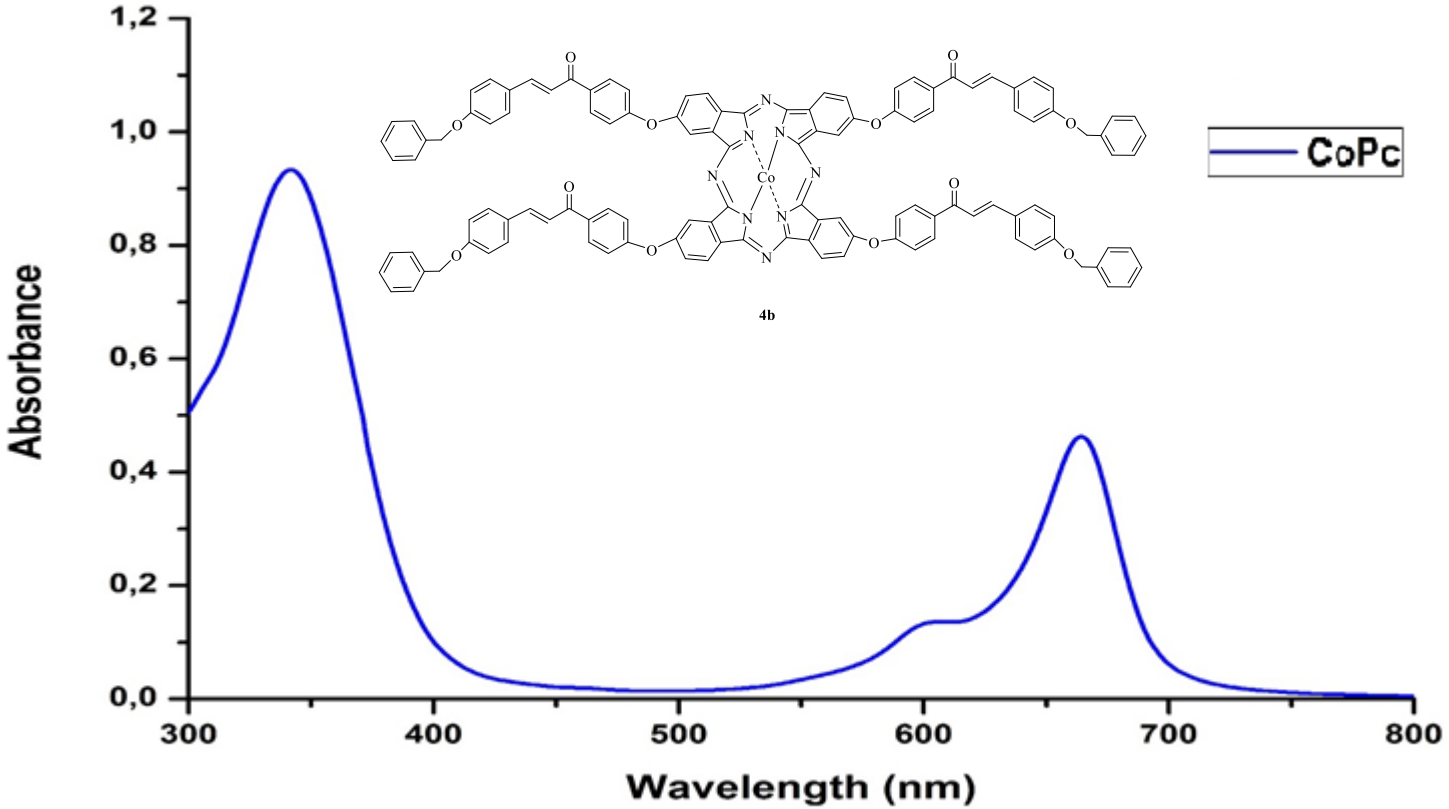


Figure S17: UV-Vis spectrum of compound **4b (**in DMF)

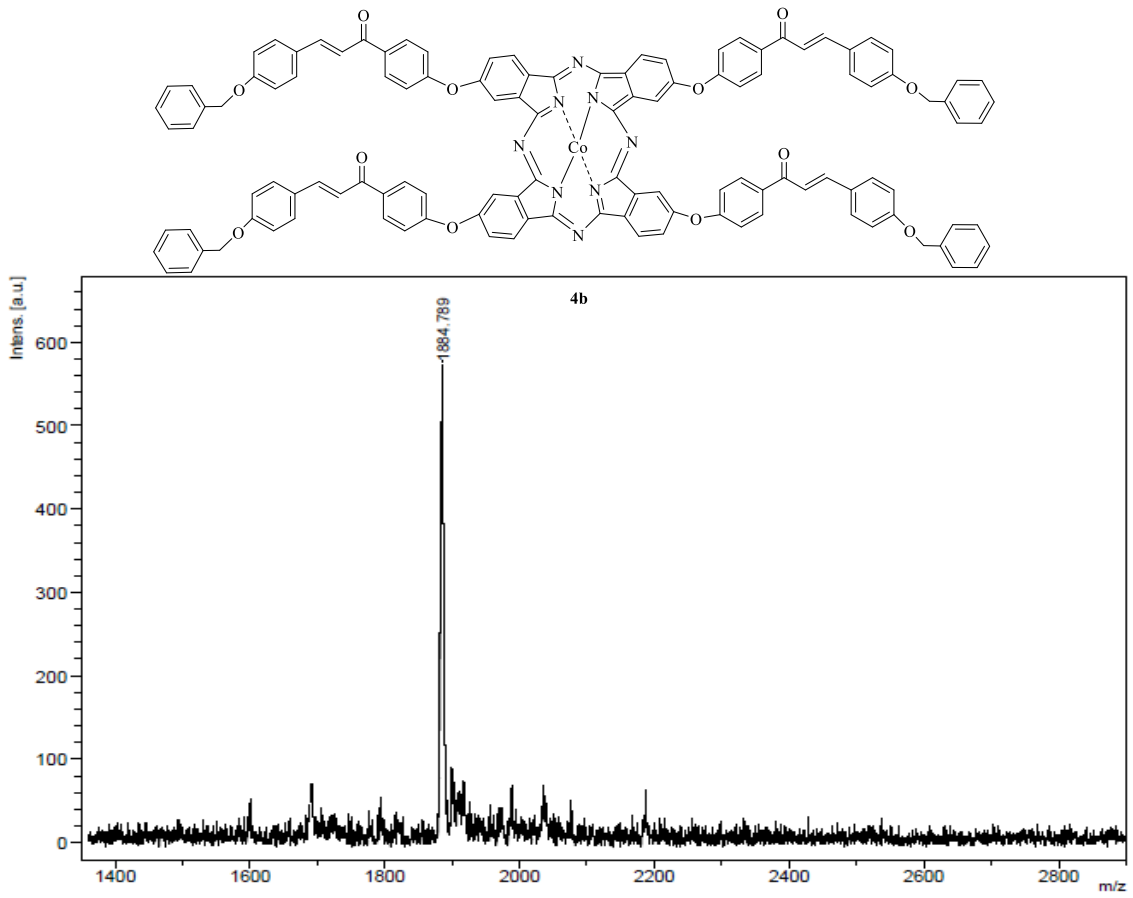


Figure S18: MALDI-TOF mass spectrum of **4b** in 1,8,9-anthracenetriol

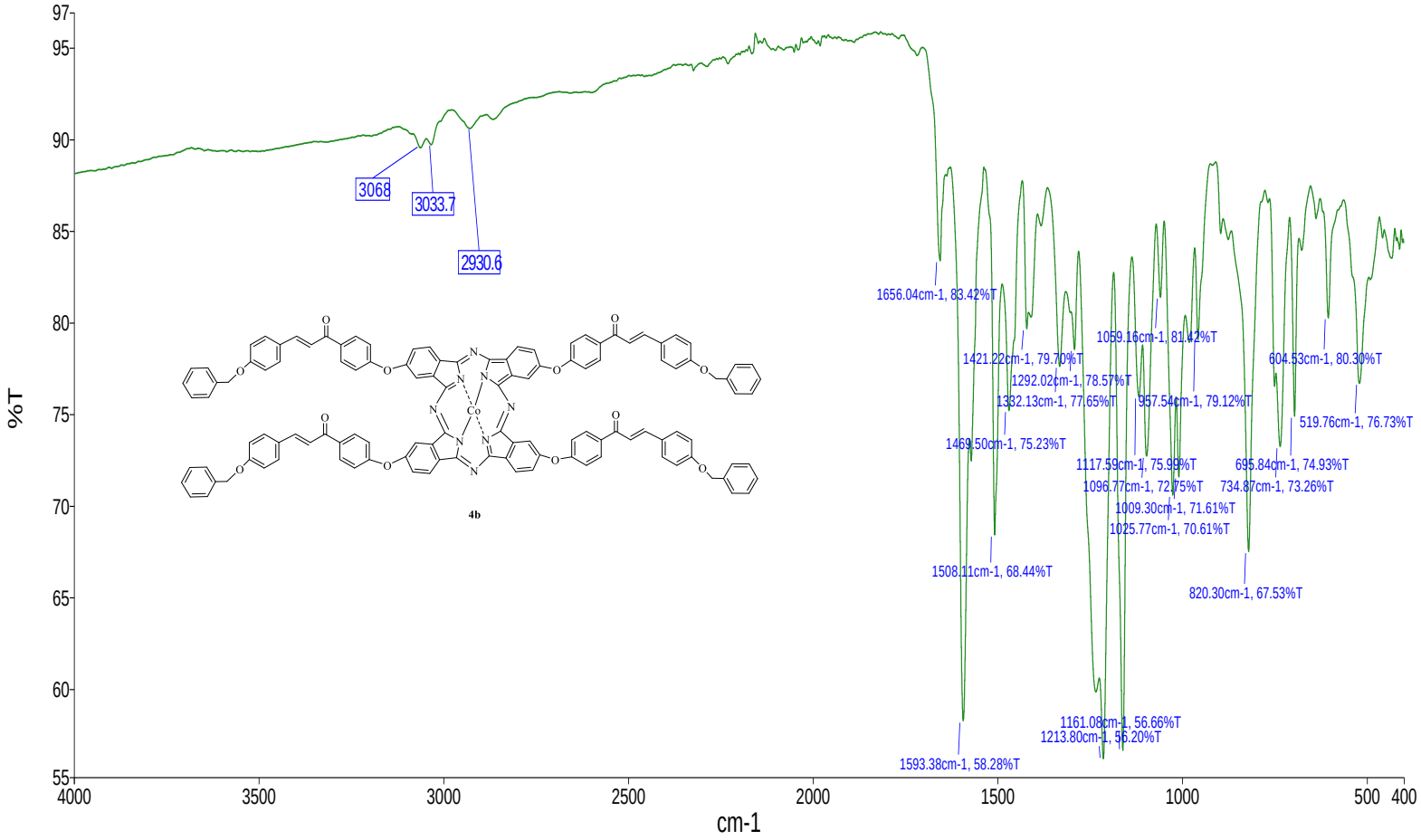
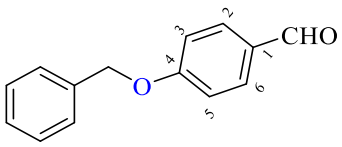


Figure S19: FT-IR spectrum of compound **4b**

S1: Structure Elucidation of Compounds 1-2

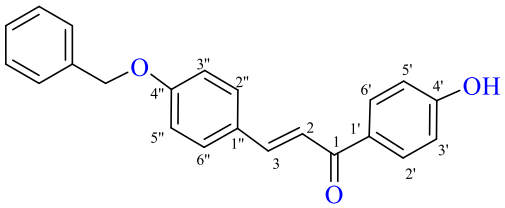
In the IR spectra of **1** (see Figure S3), Ar-H and aliphatic-H bands were observed at 3362 and 2829 cm^{-1}, respectively. In particular, the strong peak at 1685 cm^{-1} belongs to the aldehyde carbonyl group. The peaks at 1598 cm^{-1}, 1572 cm^{-1} and 1508 cm^{-1} were attributed to the carbon-carbon double bands of the aromatic ring. The most prominent peak at 1018 cm^{-1} is the C-O-C band.



benzyloxy)benzaldehyde (**1**)

^{1}H NMR spectra of compound **1** exhibited the CHO proton at 9.86 ppm as a singlet. While H_2/H_6 of the aromatic ring resonated as an AA' part of AA'BB' system giving quasi doublet at 7.82 ppm, H_3/H_5 resonated as BB' part of AA'BB' system giving doublet at 7.15 ppm. The resonance signal belongs to 5 H of phenyl appeared as multiplet between 7.48 – 7.32 ppm. The resonance signal of $PhCH_2O$ gave a broad singlet at 5.12 ppm (Figure S1) Additionally, all ^{13}C-NMR signals are in agreement with structure (Figure S2).

IR spectra of compound **2** (Figure S6) exhibited hydroxyl stretching bands at 3059 and 3049 cm^{-1}. The aliphatic C-H strength was observed at 2849 cm^{-1}. While the C = O group of the aldehyde disappeared, the new peaks belong to the C=O and C = C bonds of the new compound appeared at 1641 cm^{-1}, 1597 cm^{-1} and 1586 cm^{-1}.



(*E*)-3-(4-(benzyloxy)phenyl)-1-(4-hydroxyphenyl)prop-2-en-1-one (**2**)

The resonance signal of H_2'/H_6' appeared as an AA' part of AA'BB' system as a quasi doublet at 7.97 ppm, and H_3'/H_5' gave BB' part of AA'BB' system as a quasi doublet at 7.10 ppm. Similarly, while H_2''/H_6'' arose as an AA' part of AA' BB' system as a quasi doublet at 7.62 ppm, H_3''/H_5'' were resonated as a quasi doublet as BB' part of AA' BB' system at 6.92 ppm. H_3 appeared as a doublet at 7.76 ppm ($J_{6,7}$ = 15.0 Hz). 5 H of phenyl ring and H_2 resonated as a multiplet between 7.51-7.35 ppm and OCH_2 appeared as a singlet at 5.12 ppm (Figure S4). ^{13}C- NMR resonance frequencies of 16 carbons are fully compatible with the structure (Figure S5).