Construction of Covalent Organic Frameworks with Amide-like Isoquinolone Linkages: Ultrastable Architectures for Accelerated Photocatalytic SET Transformation

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1 General information

1.1 Reagents

Unless otherwise noted, all the chemicals and reagents were purchased in analytical purity from commercial suppliers and used directly without further purification. 3,3'-divinyl-[1,1'-biphenyl]-4,4'-dicarbaldehyde (**CHO-2**) and Am-COF-1 were synthesized following the procedures reported in our previous work.[1] Isotopically enriched ^{13}C-labeled terephthalaldehyde was synthesized according to our previous work.[2]

1.2 Characterization methods

Liquid ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra of all monomers were acquired at room temperature on Bruker Avance spectrometer operating at 600 MHz (^{1}H NMR), 151 MHz (^{13}C NMR) and 564 MHz (^{19}F NMR). Chemical shifts (δ) are reported in ppm with residual solvent peak as the reference, and peaks are reported as follows: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet or unresolved, with coupling constants in Hz. Fourier transform infrared (FT-IR) spectroscopy measurements were conducted on a Nicolet 6700 spectrometer (Thermo Scientific, USA) equipped with an ATR cell. Powder X-ray diffraction (PXRD) analysis was conducted on a Bruker D8 Advance diffractometer with Cu Kα radiation (2θ range: 2-40°; Scan step size: 0.02°; Time per step: 1 s). The specific Brunauer-Emmett-Teller (BET) surface area and pore size distribution were measured using a Micrometrics ASAP 2040 instrument at 77 K. High resolution transmission electron microscope (HR-TEM) images were obtained on a JEM-2100F instrument at an accelerating voltage of 200 kV. Scanning electron microscope (SEM) images were obtained on a Hitachi SU 8010 instrument. Solid-state ^{13}C cross polarization magic angle spinning (^{13}C-CP/MAS) NMR spectra were collected on a Bruker Avance III HD 400 spectrometer. X-ray photoelectron spectroscopy (XPS) measurements were performed on a Thermo ESCALAB 250 spectrometer with non-monochromatic Al Kα x-rays as the excitation source and C 1s (284.8 eV) as the reference line. Solid-state UV-Vis diffuse reflectance spectra (UV/Vis DRS) were collected on a Perkin-Elmer LAMBDA 650S spectrometer with $BaSO_4$ as the reference. Thermal stability was investigated on a DZ-STA200 thermogravimetric

(TG) analyzer with temperature ranging from 303 to 1073 K under N_2 atmosphere at a heating rate of 10 K min^{-1}. Photoluminescence lifetime was measured using the time-correlated single photon counting technique (FluoTime 250). The topographic images and KPFM surface potential were measured using atomic force microscope (Bruker Multimode 8 D). Ultraviolet-visible (UV-Vis) absorption spectra were acquired using a SHIMADZU UV-1800 spectrophotometer, equipped with an L6380 deuterium lamp source and a silicon photodiode array detector, in a 1 cm path length quartz cuvette. The Cu content in IQO-COF-1 was determined using an Agilent 5110 ICP-OES (Agilent, USA) with the parameters RF Power: 1150 W, Plsama flow: 12 L/min, Auxiliary flow: 0.7 L/min, Nebulizer flow: 0.5 L/min, Sample uptake delay: 10 s, Instr stabilization delay: 10 s, Replocates: 2.

The fs-TA measurements were performed employing a regenerative amplified Ti: sapphire laser system (coherent; 800nm, 85 fs, 7 mJ pulse-1, and 1 kHz repetition rate) as the laser source and a Helios spectrometer (Ultrafast Systems LLC), as described previously. As briefly described, the 800 nm output pulse from the regenerative amplifier was split into two parts using a 50% beam splitter. The transmitted portion was used to pump a TOPAS optical parametric amplifier (OPA), which generated a wavelength-tunable laser pulse from 250 nm to 2.5 um as a pump beam. A 400 nm pump beam was created by the frequency doubling of one part of the 8oo nm beam in the beta barium borate (BBO) crystal. The reflected 800 nm beam was again split into two parts. The single part exhibiting less than 10% was attenuated with a neutral density filter and focused into a 2 mm thick sapphire window to generate a white-light continuum (WLC) to be used for the probe beam. Accordingly, the probe beam was focused with an Al parabolic reflector onto the sample. Subsequently, the probe beam was collimated and then focused into a fiber-coupled spectrometer with complementary metal oxide semiconductor (CMOS) sensors and detected at a frequency of 1 kHz. In turn, a series of neutral-density filters were employed to adjust the power of the pump beam, after which the pump beam was focused at the sample with a beam waist of about 300 μm. The delay between the pump and probe pulses was controlled by a motorized delay

stage. The pump pulses were chopped by a synchronized chopper at 500 Hz and the absorbance change was calculated with two adjacent probe pulses (pump blocked and pump unblocked). Finally, the IRF of this system, determined by measuring solvent responses under the same experiment conditions (except a higher excitation power), came to $\approx$120 fs.

In situ infrared spectra were recorded on a Thermo Fisher iS50 Diffuse Reflectance Infrared Fourier Transform Spectroscopy (DRIFTS) system equipped with a liquid nitrogen-cooled MCT detector and a custom-designed reaction cell. A gold-coated silicon optical prism was used to enhance surface sensitivity. Spectra were collected over the range of 4000-400 cm^{-1} with a resolution of 4 cm^{-1} and 32 scans per spectrum. The SCD-380A automatic supercritical dryer (Shianjia Technology) was employed to perform the drying process. The procedure involved immersing the samples in anhydrous ethanol at 5 °C, followed by 10 cycles of CO_2 washing to completely displace the ethanol. Subsequently, supercritical drying was carried out at 35°C for 50 minutes. Finally, the system was vented at a rate of 200 mL/min to obtain the dried material.

The generation of phenyl ketone radicals was determined by electron paramagnetic resonance (EPR) spectra, which was recorded on a JES-FA200 spectrometer under visible light irradiation using *N*-benzylidene-2-methylpropan-2-amine (PBN) as the spin trapper.

1.3 Electrochemical measurements

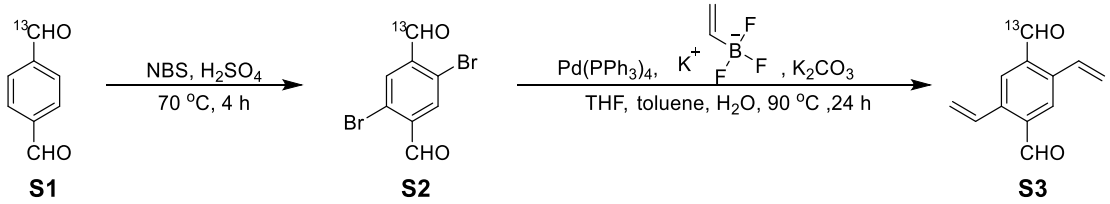
Electrochemical measurements were performed on the CHI660E workstation (Chenhua Instruments, China), and the standard three-electrode system included platinum plate as the counter electrode, Ag/AgCl electrode as the reference electrode, and a working electrode. The working electrode was prepared as follows: 15 mg of sample was thoroughly mixed with 200 μL isopropanol containing 5% Nafion, and the resulting suspension was carefully loaded on the ITO glass substrate (10 × 25 × 1.1 mm) and dried at 60 ^{o}C under vacuum for 1 h. For Mott-Schottky tests, the perturbation was 5 mV with frequencies of 1000, 2000, and 3000 Hz.

1.4 Computational methods

Conformational searches were performed with *xtb* with GFN0-xTB method.[3] To limit the number of conformers, an energy window of 5.0 kcal/mol relative to the minimum was utilized and mirror image conformations were not retained to avoid conformer duplication. Subsequent DFT optimization was performed with Gaussian 16, Rev. A03.[4] Unless specified otherwise, geometry optimizations were computed with default convergence thresholds and without symmetry constraints. All structures were optimized in the gas phase with the wB97XD[5] density functional. The def2-SVP[6,7] basis set was employed on all atoms. Frequency analysis was performed at the same level of theory with the geometry optimization to confirm that the optimized structures are local minima or transition states, and to gain the thermal correction to Gibbs free energy. Single-point energy calculations were conducted on the basis of optimized structures at the wB97XD/def2-TZVP[8] level. The solvent effects were taken into account in all calculations by employing the SMD[9] (solvent = DiMethylSulfoxide) solvation model. The HOMO orbital isosurfaces of molecules are drawn with Multiwfn[10] and VMD software.[11]

2 Synthesis of the building blocks

2.1 Synthesis of ^{13}C-labeled 2,5-divinylterephthalaldehyde

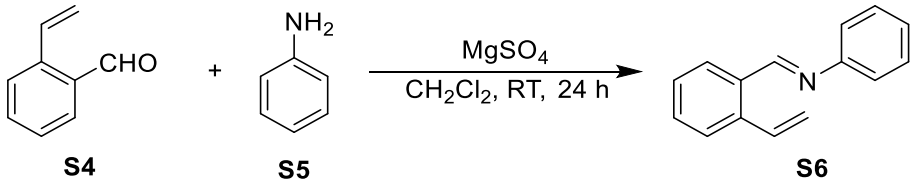


Compound S2: Similar to the reported procedure,[12] the isotopically enriched ^{13}C-labeled terephthalaldehyde (**S1**, 250 mg, 1.85 mmol) was dissolved in concentrated H_2SO_4 (3 mL), and then *N*-bromosuccinimide (NBS, 717 mg, 4.03 mmol) was added in portions to the solution over a 40-minute period at 70 ºC. The mixture was stirred at 70 ºC for an additional 4 hours. Upon cooling to room temperature, the solution was slowly poured into ice water. The suspension was filtered to afford the white solid, which was then dissolved in CH_2Cl_2. The resulting solution was extracted with sat. $NaHCO_3$, brine and dried with anhydrous Na_2SO_4, and the removal of the organic solvent under reduced pressure to afford the final product **S2** (300 mg, 1.02 mmol, yield: 55%) as a white solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 10.35 (s, 1H), 10.34 (d, J = 187.9 Hz, 1H), 8.16 (d, J = 1.7 Hz, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 189.8, 137.3 (t, J = 26.9 Hz), 135.0, 125.5 (d, J = 4.3 Hz).

Compound S3: In a 50 mL round bottom flask, **S2** (291 mg, 1.00 mmol), potassium vinyltrifluoroborate (327 mg, 2.44 mmol), K_2CO_3 (807 mg, 5.85 mmol), and $Pd(PPh_3)_4$ (32 mg, 0.03 mmol) were dissolved in a mixed solvent consisting of toluene (5 mL), THF (5 mL), and H_2O (1 mL). The resulting mixture was stirred at 90 °C under an N_2 atmosphere for 24 hours. Upon cooling to room temperature, water was added to the reaction mixture until the solid dissolved. The organic layer was then extracted with EtOAc, and the organic phase was dried with anhydrous Na_2SO_4. Removal of the solvent under reduced pressure followed, and the residue was purified by flash chromatography on silica gel using PE/EtOAc (5/1) as the eluent, yielding the final product **S3** (80 mg, 0.43 mmol, yield: 43%) as a yellow solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 10.37 (s, 1H), 10.37 (d, J = 178.1 Hz, 1H), 8.03-8.01 (m, 2H), 7.47 (dd, J=17.9, 11.1 Hz, 2H), 5.82 (d, J = 17.9 Hz, 2H), 5.61 (d, J = 11.1 Hz, 2H). ^{13}C NMR

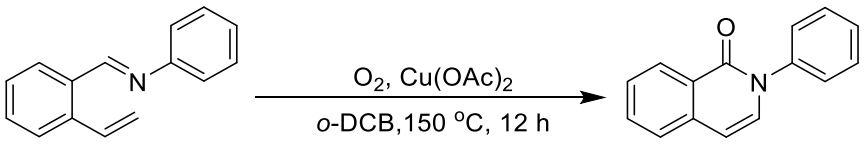
(151 MHz, $CDCl_3$) δ191.6, 139.4 (d, J = 3.9 Hz, 2H), 135.7 (t, J = 26.0 Hz), 131.8, 130.1 (d, J = 3.4 Hz, 2H), 120.8.

2.2 Model reaction



S4 **S5** **S6**

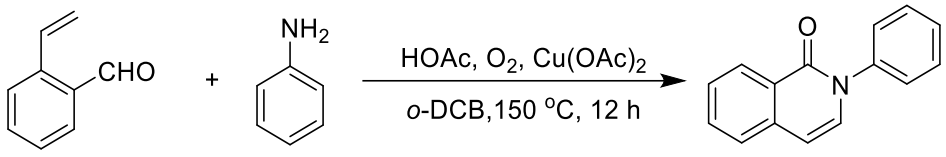
Compound S6: In a 25 mL round bottom flask, 2-vinylbenzaldehyde (**S4**, 120 mg, 0.91 mmol), aniline (**S5**, 90 mg, 0.97 mmol), and $MgSO_4$ (20 mg) were combined in CH_2Cl_2 (5 mL). The mixture was stirred at room temperature for 24 hours. The solid was then removed by filtration, and the filtrate was concentrated to yield a residue. This residue was further purified by flash chromatography on silica gel using PE/EA (20/1) as the eluent, resulting in the products **S6** (170 mg, 0.82 mmol, yield: 91%) as a yellow oil. ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.79 (s, 1H), 8.09 (d, J = 7.7 Hz, 1H), 7.51 (d, J = 7.7 Hz, 1H), 7.46-7.35 (m, 4H), 7.34-7.18 (m, 4H), 5.66 (d, J = 17.4 Hz, 1H), 5.44 (dd, J = 11.0, 0.8 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$): δ 158.9, 152.5, 139.2, 133.9, 133.1, 131.1, 129.2, 128.0, 127.1, 126.0, 121.0, 118.6.[13]



S6 **S7**

Compound S7 synthesized using a post synthetic modification method: A 10 mL Schlenk tube was charged with **S6** (31 mg, 0.15 mol), $Cu(OAc)_2$ (2.8 mg, 0.015 mol) and *o*-Dichlorobenzene (2 mL). After sonication for 5 minutes, the resulting mixture was stirred at 150 °C for 12 hours in an oxygen atmosphere. Upon cooling to room temperature, water was added to the reaction mixture until the solid dissolved. The organic layer was then extracted with EtOAc, and the organic phase was dried with anhydrous Na_2SO_4. Subsequent removal of the solvent under reduced pressure was carried out, and the residue was purified by flash chromatography on silica gel using PE/EtOAc (20/1) as the eluent, resulting in the final product **S7** (30 mg, 0.14 mmol,

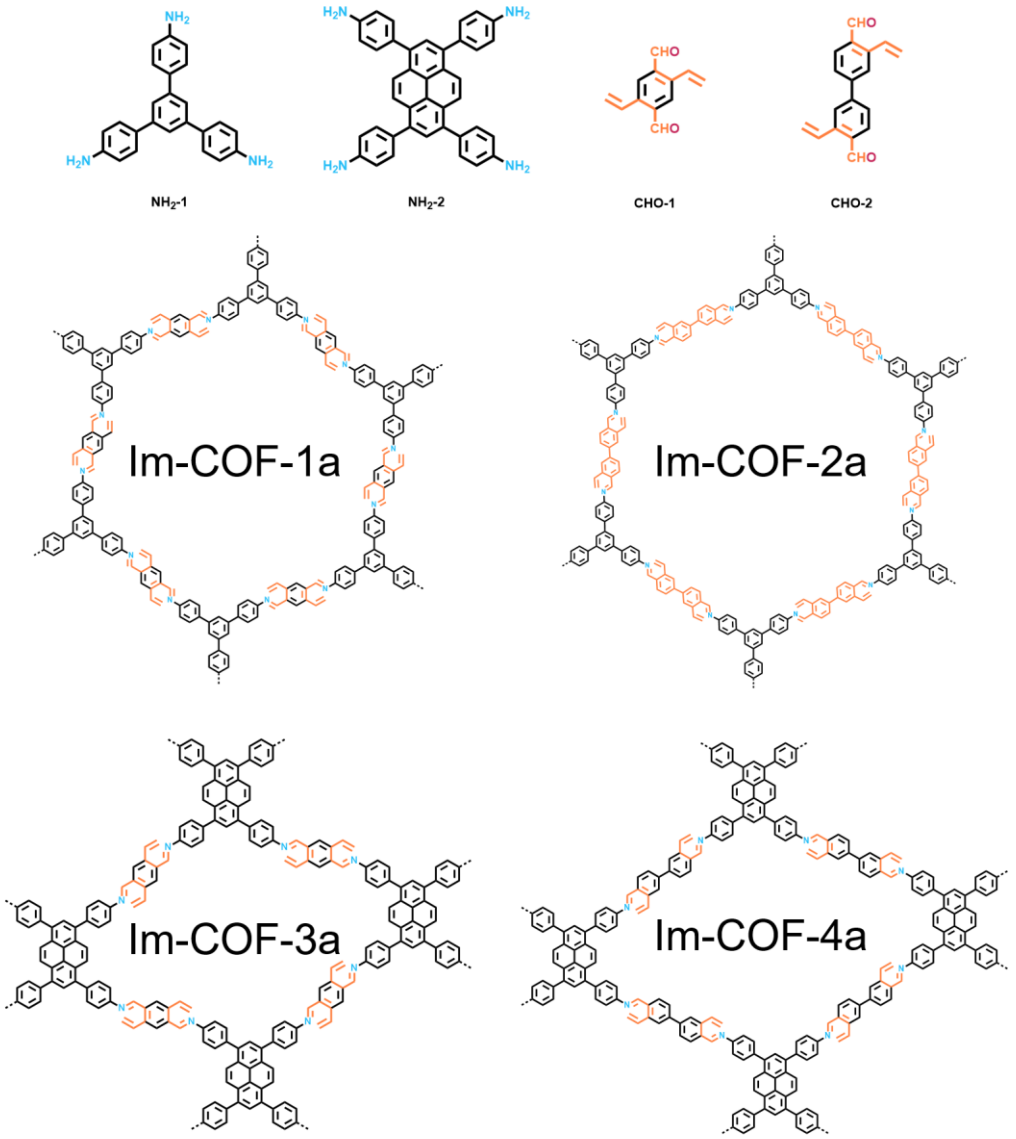
yield: 93%) as a white solid. ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.48 (d, *J* = 8.0 Hz, 1H), 7.70-7.66 (m, 1H), 7.58-7.48 (m, 4H), 7.46-7.40 (m, 3H), 7.19 (d, *J* = 7.4 Hz, 1H), 6.57 (d, *J* = 7.4 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 162.1, 141.4, 137.1, 132.6, 132.2, 129.3, 128.3, 128.1, 127.2, 126.9, 126.6, 126.0, 106.2.



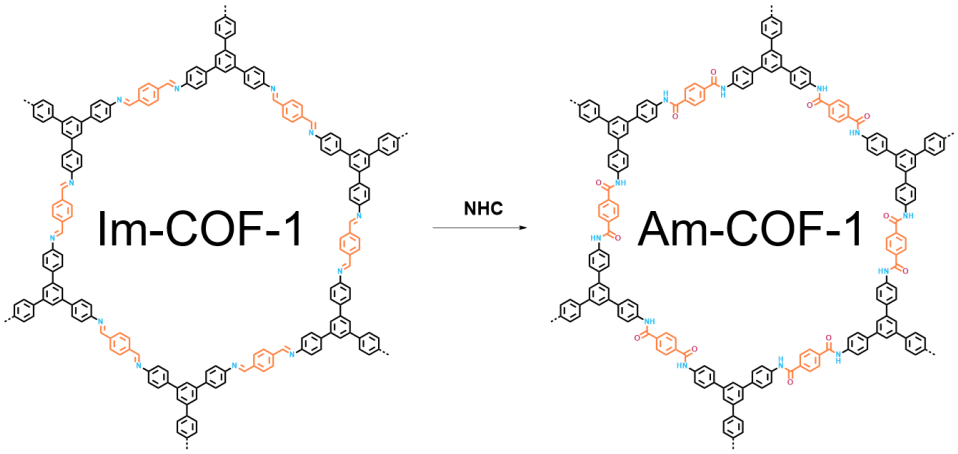
S4 **S5** **S7**

Compound S7 synthesized in one pot tandem reaction: A 10 mL Schlenk tube was charged with 2-vinylbenzaldehyde (**S4**, 28 mg, 0.21 mmol), aniline (**S5**, 21 mg, 0.22 mmol), $Cu(OAc)_2$ (7 mg, 0.004 mol), HOAc (70 μL) and *o*-Dichlorobenzene (2 mL). After sonication for 5 minutes, the resulting mixture was stirred at 150 °C for 12 hours in an oxygen atmosphere. Upon cooling to room temperature, water was added to the reaction mixture until the solid dissolved. The organic layer was then extracted with EtOAc, and the organic phase was dried with anhydrous Na_2SO_4. Subsequent removal of the solvent under reduced pressure was carried out, and the residue was purified by flash chromatography on silica gel using PE/EtOAc (20/1) as the eluent, resulting in the final product **S7** (43 mg, 0.19 mmol, yield: 92%) as a white solid.

3 Synthesis of 2D COFs



Scheme S1 Structures of the building blocks and imine-linked COFs.



Scheme S2 Structures of Im-COF-1 and Am-COF-1.[14]

3.1 Typical procedure for the synthesis of isoquinoline-linked IQO-COF-1

Synthesis by the postsynthetic modification: A 10 mL Schlenk tube was charged with Im-COF-1a (35 mg), $Cu(OAc)_2$ (3 mg, 0.017 mmol) and *o*-Dichlorobenzene (2 mL), After sonication for 10 minutes, the resulting mixture was stirred at 150 °C for 3 days in an oxygen atmosphere. Upon completion of the reaction, the solids were collected by centrifugation, repeated washing with THF, ammonia solution and water until the supernatant became colorless. The final product was obtained as a dark brown solid powder after being dried under vacuum at 80 ºC for 24 hours.

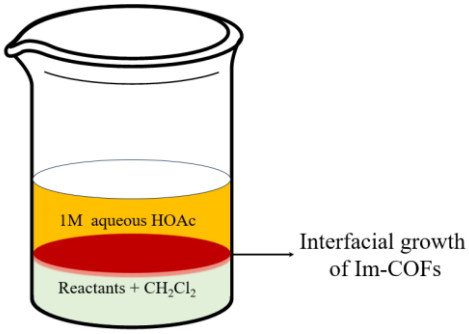
Synthesis in the one-pot tandem reaction:

Table S1. Condition optimization for the synthesis of IQO-COF-1[a]

Entry	Solvent	Catalyst	Temperature	Crystallinity
1	*o*-DCB/*n*-BuOH	HOAc	120	amorphous
2	Mesitylene/Dioxane	HOAc	120	amorphous
3	DMAC/Dioxane/Mesitylene	HOAc	120	amorphous
4	Mesitylene	HOAc	120	amorphous
5	*o*-DCB	HOAc	120	low
6	*o*-DCB	6M HOAc	120	low
7	*o*-DCB	TFA	120	amorphous
8	*o*-DCB/*n*-BuOH	HOAc	150	amorphous
9	Dioxane/Mesitylene	HOAc	150	amorphous
10	DMAC/Dioxane/Mesitylene	HOAc	150	amorphous
11	Mesitylene	HOAc	150	amorphous
12	*o*-DCB	HOAc	150	high
13	*o*-DCB	6M HOAc	150	low
14	*o*-DCB	TFA	150	low

[a] The total volume of the solvent was 2 mL, and the volume of each solvent in the mixed solvent is the same. The volume of the acid was 0.05 mL. *o*-DCB = *o*-Dichlorobenzene, DMAc = *N*, *N*-Dimethylacetamide.

3.2 Typical procedure for the synthesis of imine-linked Im-COFs



Scheme S3. Diagram of interfacial growth of Im-COFs

Table S2. Reaction conditions for the synthesis of different Im-COFs.

COFs	Aldehyde	Amine	Amount	Yield	Color
Im-COF-1a	22 mg 0.12 mmol	28 mg 0.08 mmol	43 mg	87%	Yellow
Im-COF-2a	24 mg 0.09 mmol	21 mg 0.06 mmol	39 mg	91%	Yellow
Im-COF-3a	19 mg 0.10 mmol	28 mg 0.05 mmol	41 mg	92%	Yellow
Im-COF-4a	26 mg 0.10 mmol	28 mg 0.05 mmol	48 mg	89%	Yellow

Reaction conditions: The mixed solution of CH_2Cl_2 (15 mL) and 1M aqueous HOAc solution (25 mL) containing aromatic aldehyde and aromatic amine was left to stand at room temperature for 3 days.

Table S3. Reaction conditions for the synthesis of different IQO- COFs.

COFs	Aldehyde	Amine	Amount	Yield	Color
IQO-COF-1	19 mg 0.09 mmol	21 mg 0.06 mmol	32 mg	86%	Brown
IQO-COF-3	24 mg 0.09 mmol	21 mg 0.06 mmol	37 mg	89%	dark yellow
IQO-COF-2	19 mg 0.10 mmol	28 mg 0.05 mmol	41 mg	93%	Brown
IQO-COF-4	26 mg 0.10 mmol	28 mg 0.05 mmol	49 mg	89%	dark yellow

Reaction conditions: Aromatic aldehyde, aromatic amine, HOAc (50 μL), $Cu(OAc)_2$ (5 mg, 0.03 mmol) in *o*-Dichlorobenzene were heat without stirring at 150 °C for 3 days in an oxygen atmosphere.

4 Characterization of 2D COFs

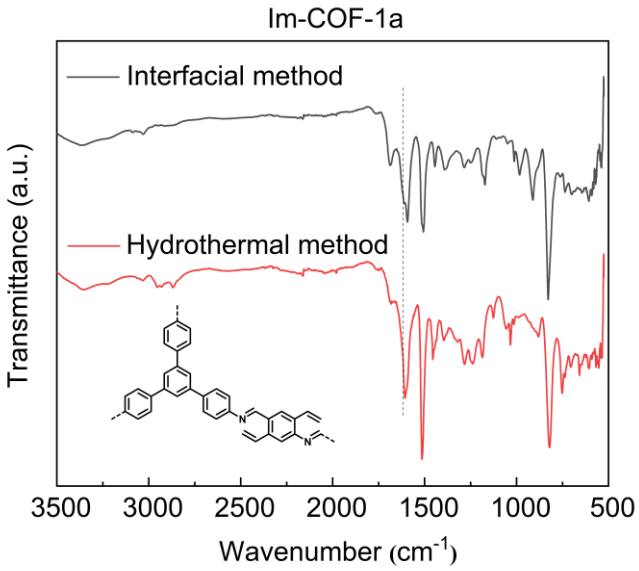


Figure S1. Preparation of Im-COF-1a by the interface method and the hydrothermal method (120 ℃). Note: We also attempted to prepare the Im-COF-1a under conventional solvothermal conditions (120 ºC). However, the resulting material exhibited neither the characteristic C=N stretching at ~1620 cm^{-1} nor satisfactory crystallinity. Based on our proposed mechanism for IQO-COF formation, we attribute this to the elevated temperature triggering *in situ* thermal 6π-electrocyclization of the *ortho*-vinyl imine linkages, prematurely consuming the C=N bonds and disrupting framework crystallization.

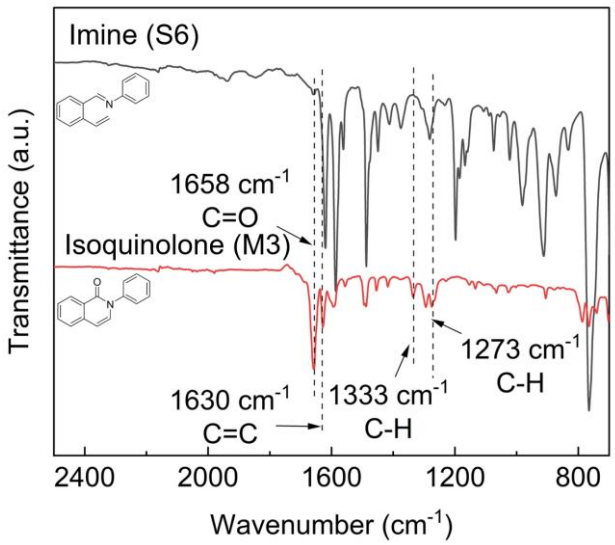


Figure S2. FT-IR spectra of Imine (S6) and Isoquinolone (M3) in the model reaction

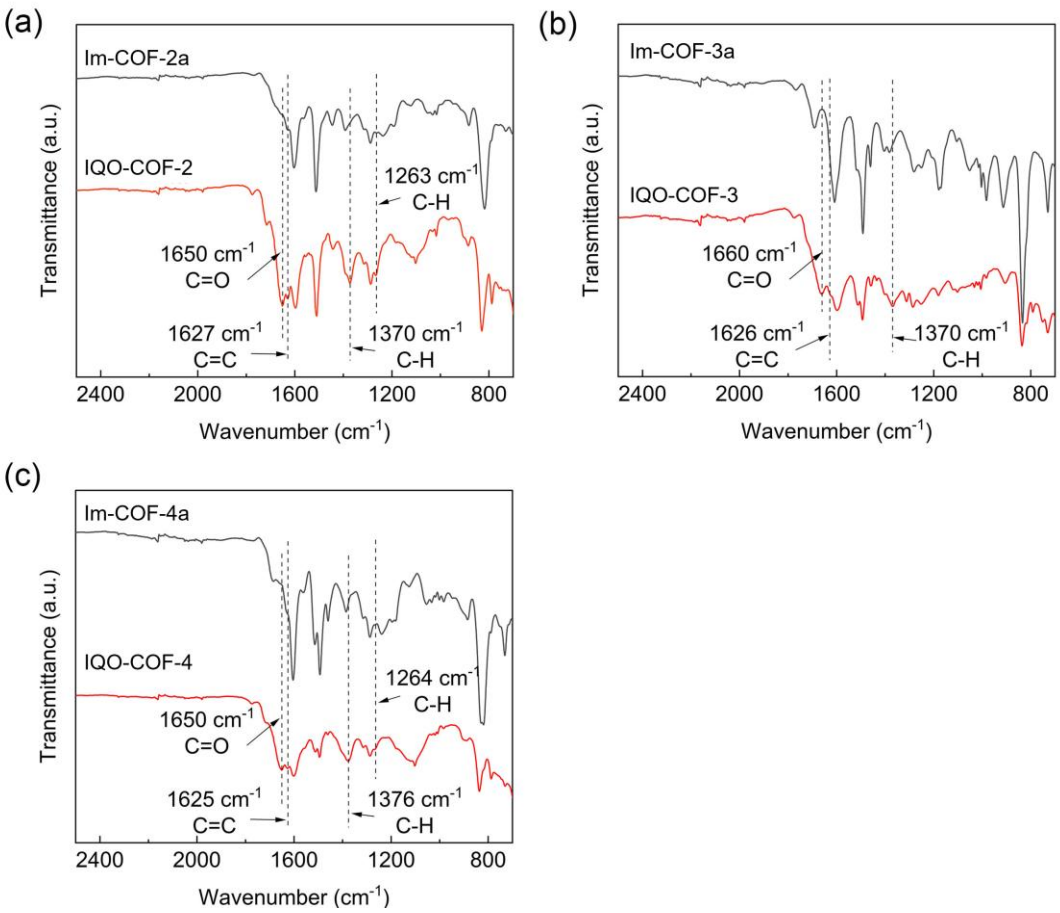


Figure S3. FT-IR spectra of Im-COF-2a and IQO-COF-2 (a), Im-COF-3a and IQO-COF-3 (b), and Im-COF-4a and IQO-COF-4 (c).

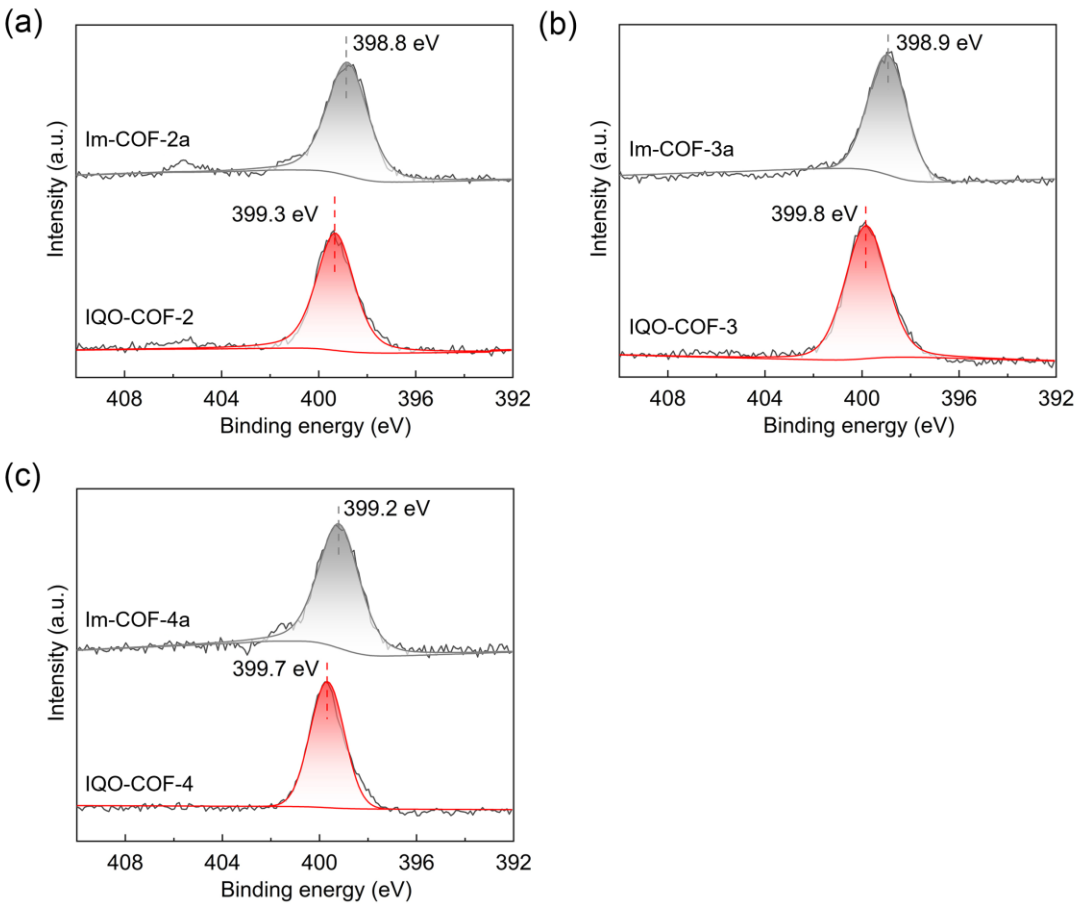


Figure S4. High resolution N 1s XPS spectra ofIm-COF-2a and IQO-COF-2 (a), Im-COF-3a and IQO-COF-3 (b), and Im-COF-4a and IQO-COF-4 (c).

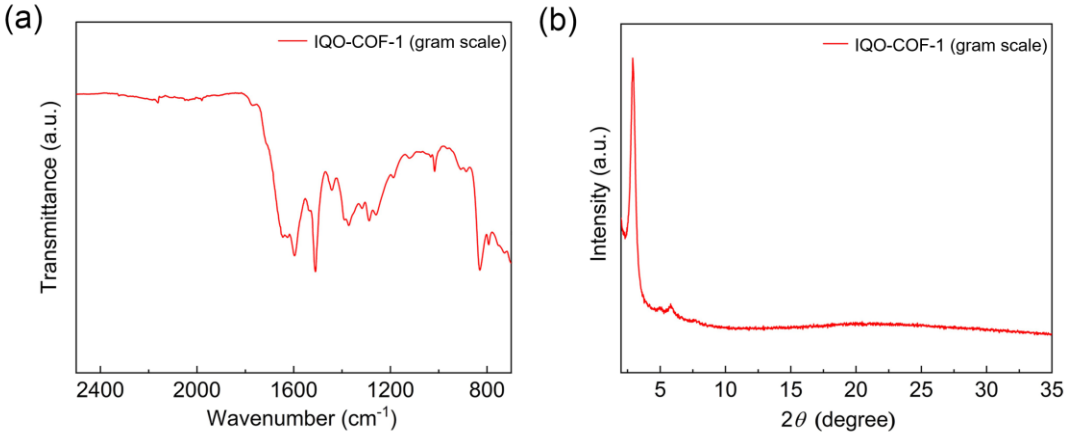


Figure S5. FT-IR spectra and experimental PXRD patterns of IQO-COF-1 afforded in the gram-scale reaction.

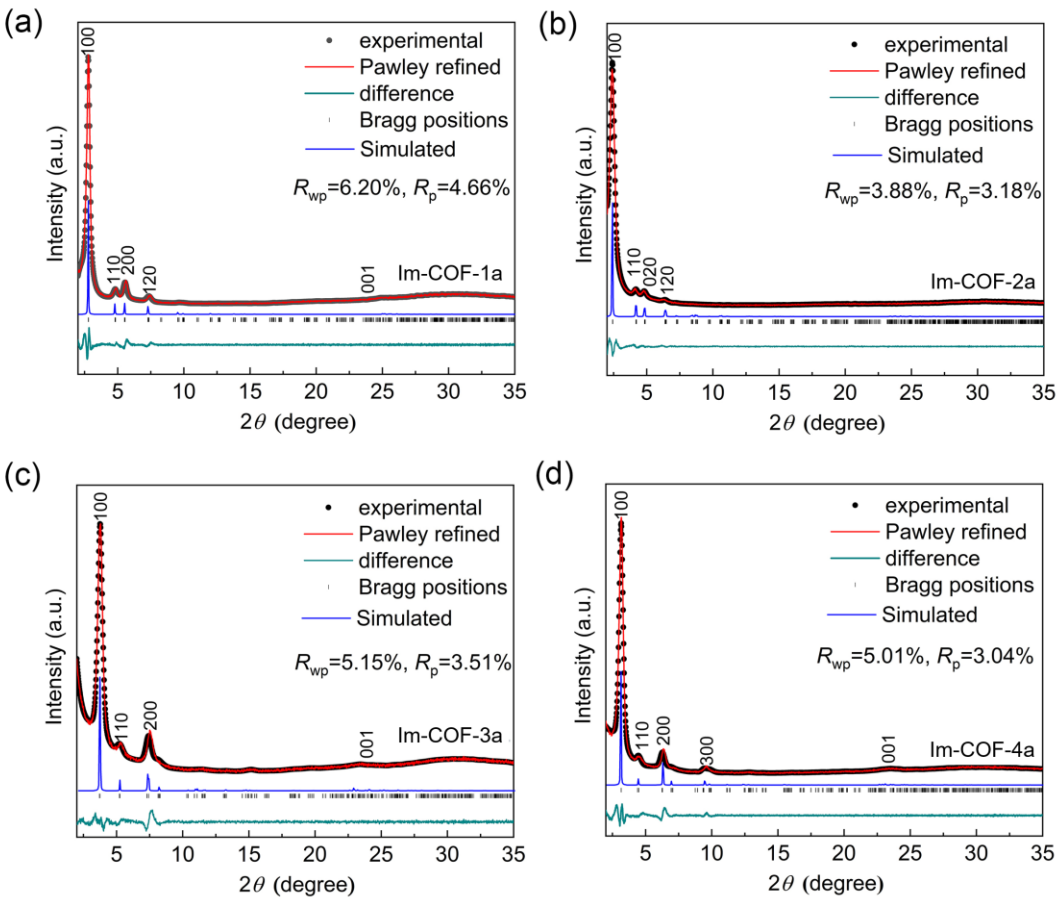


Figure S6. Experimental, Pawley-refined and simulated eclipsed AA stacking PXRD patterns of Im-COF-1a (a), Im-COF-2a (b), Im-COF-3a (c), Im-COF-4a (d).

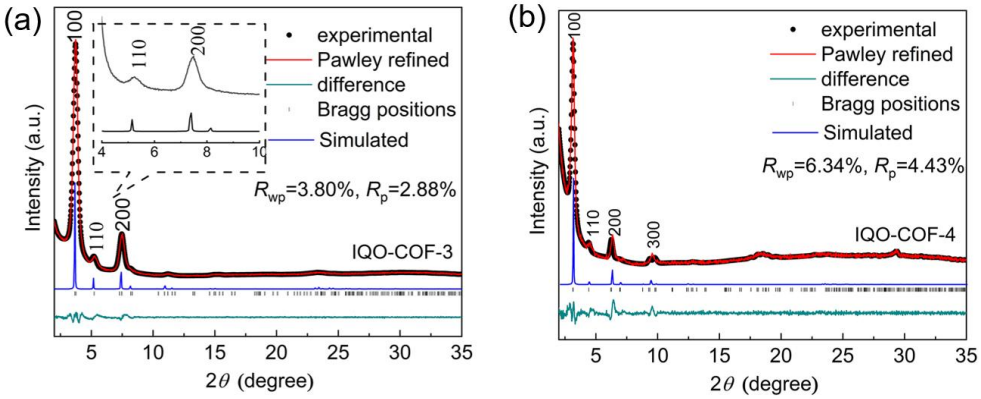


Figure S7. Experimental, Pawley-refined and simulated eclipsed AA stacking PXRD patterns of IQO-COF-3 (a) and IQO-COF-4 (b).

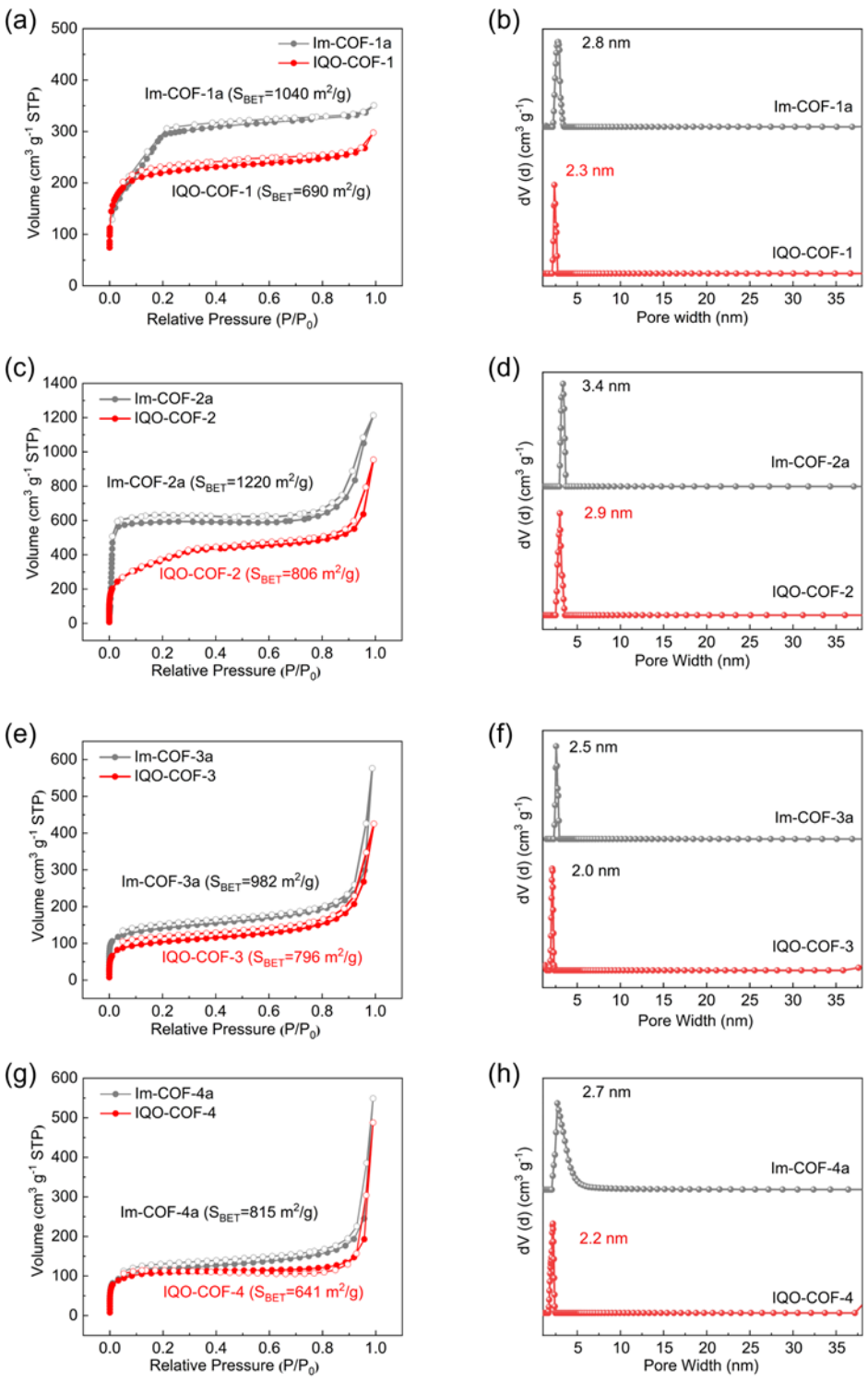


Figure S8. (a) N_2 sorption isotherms at 77 K and (b) pore size distribution of Im-COF-1a and IQO-COF-1. (c) N_2 sorption isotherms at 77 K and (d) pore size distribution of Im-COF-2a and IQO-COF-2. (e) N_2 sorption isotherms at 77 K and (f) pore size distribution of Im-COF-3a and IQO-COF-3. (g) N_2 sorption isotherms at 77 K and (h) pore size distribution of Im-COF-4a and IQO-COF-4.

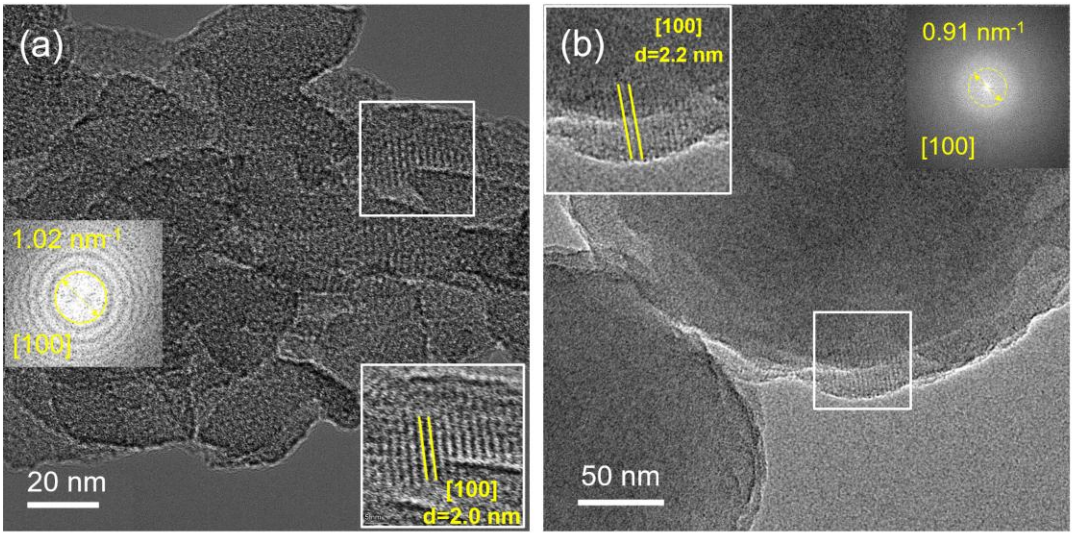


Figure S9. HRTEM images of IQO-COF-3 (a) and IQO-COF-4 (b).

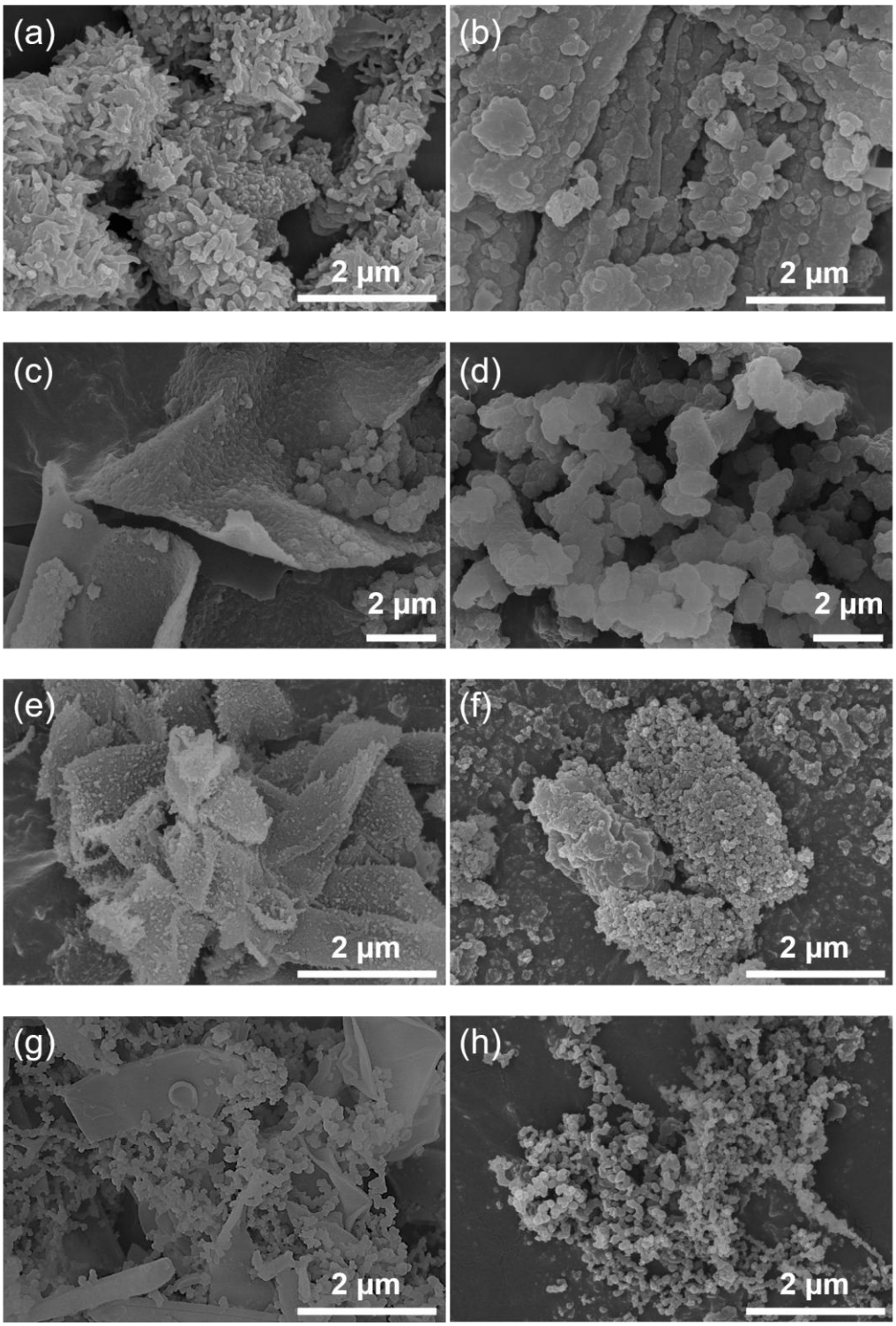


Figure S10. SEM images of Im-COF-1a (a), IQO-COF-1 (b), Im-COF-2a (c), IQO-COF-2 (d), Im-COF-3a (e), IQO-COF-3 (f), Im-COF-4a (g), IQO-COF-4 (h).

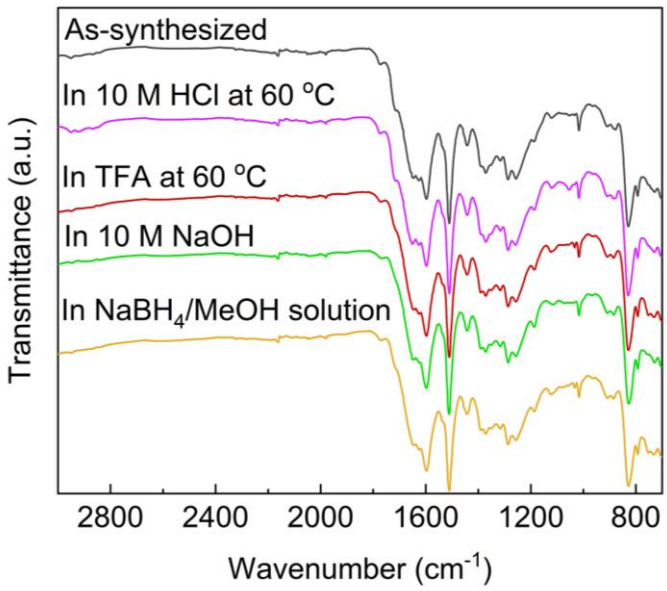


Figure S11. FT-IR of as-prepared IQO-COF-1 after being subjected to different harsh chemical conditions.

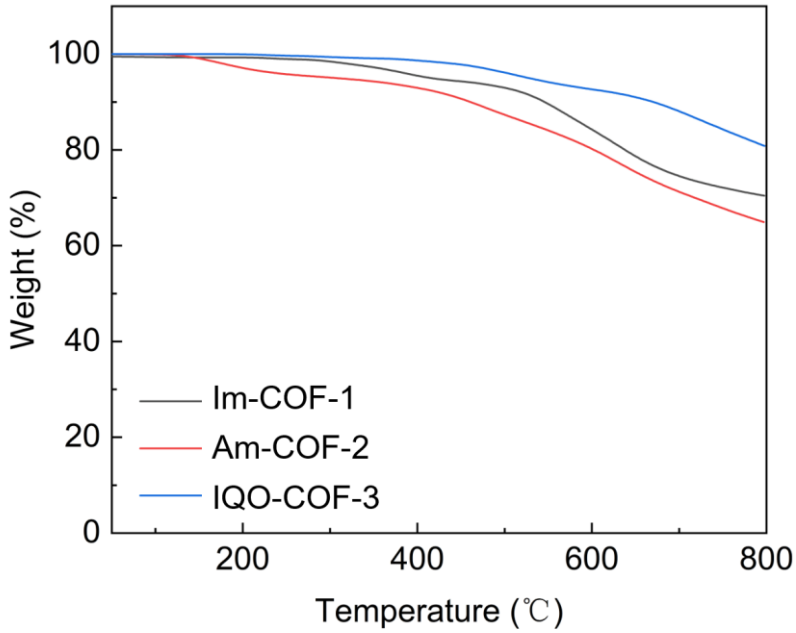


Figure S12. Thermal stability of Im-COF-1, Am-COF-1, and IQO-COF-1 evaluated by TGA measurement.

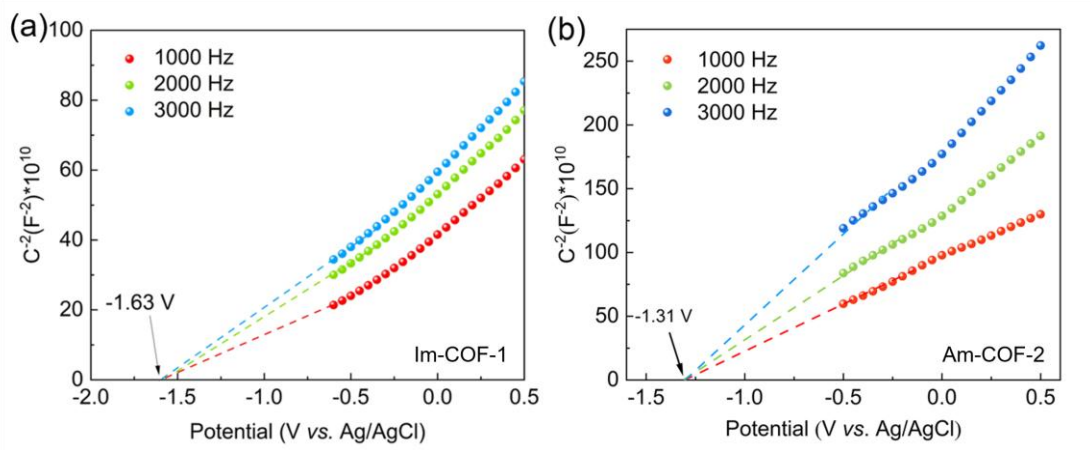


Figure S13. Mott–Schottky plots of Im-COF-1 (a) and Am-COF-1 (b).

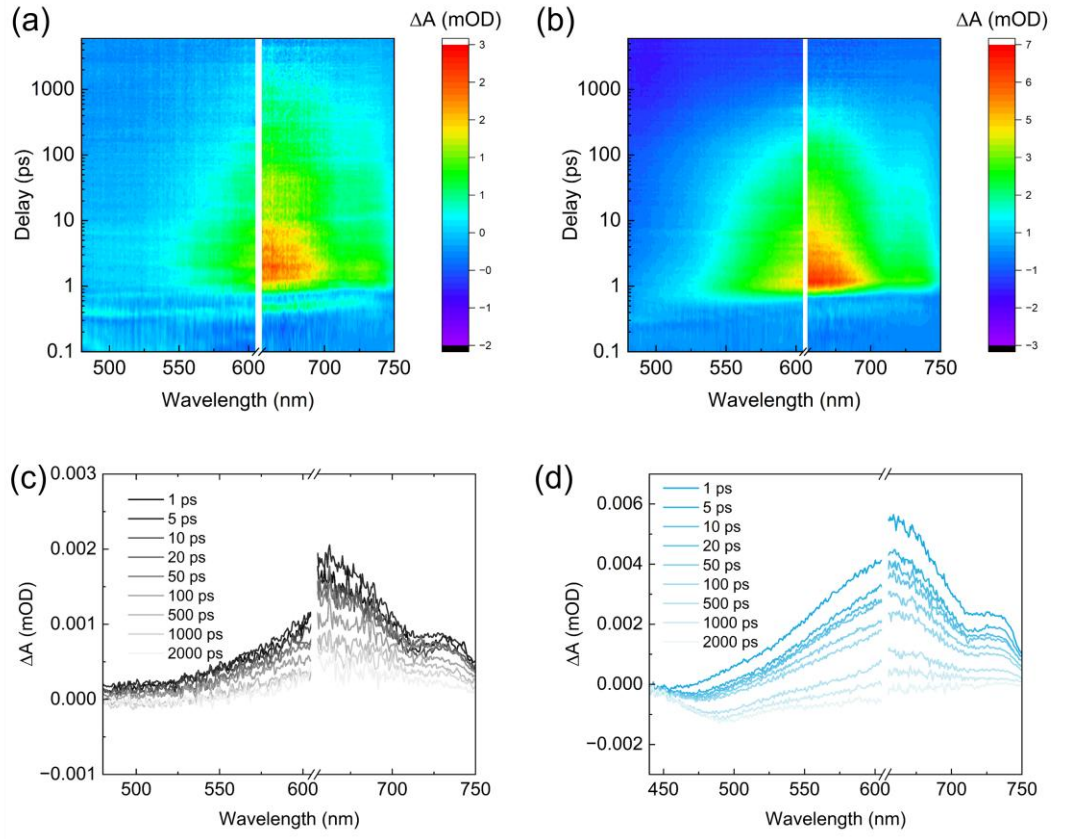


Figure S14. 2D transient absorption surface plots of Im-COF-1 (a) and Am-COF-1 (b). fs-TA spectra of Im-COF-1 (c) and Am-COF-1 (d).

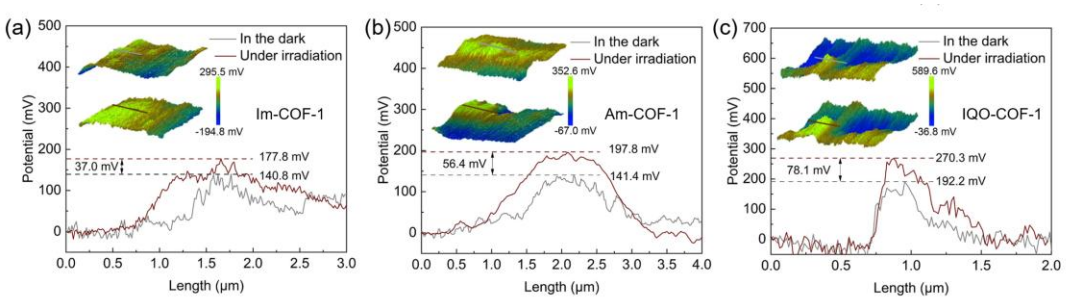
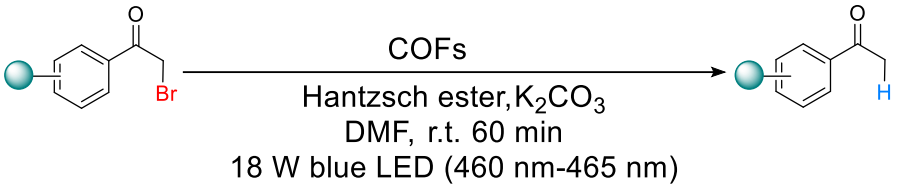


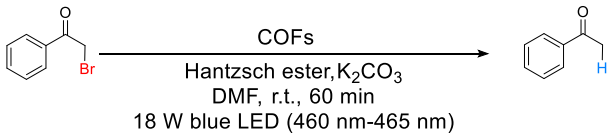
Figure S15. The comparison topographic images (inset) before and after light illumination and the comparative KPFM surface potential curves of Im-COF-1 (a), Am-COF-1 (b), and IQO-COF-1 (c).

5 Photocatalytic reductive dehalogenation of α-bromoacetophenone derivatives



General Procedure 1: A 10 mL Pyrex glass tube equipped with a stir bar was charged with α-bromoacetophenone (0.4 mmol, 1 equiv.), Hantzsch easter (0.44 mmol, 1.1 equiv.), K_2CO_3 (0.8 mmol, 2 equiv.), COF (5 mg), and DMF (1.0 mL), and the reaction mixture was irradiated in the photoreactor (18 W blue LEDs, 460-465 nm) with cooling fan for 1 h under argon atmosphere. After the reaction ended, the solid was collected by filtration, and washed with EtOAc. The filtrate was concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel with PE/ EtOAc as the eluent to afford the products.

Table S4. Photocatalytic activity of IQO-COFs compared with Im-COFs.



Entry	Catalyst	Yield
1	Im-COF-1a	62%
2	IQO-COF-1	96%
3	Im-COF-2a	57%
4	IQO-COF-2	77%
5	Im-COF-3a	56%
6	IQO-COF-3	72%
7	Im-COF-4a	53%
8	IQO-COF-4	69%

Reaction conditions: α-bromoacetophenone (0.4 mmol), Hantzsch ester (0.44 mmol), K_2CO_3 (0.8 mmol), COFs (5 mg), DMF (1 mL), 18 W blue LED (460-465 nm), 1 h under nitrogen atmosphere.

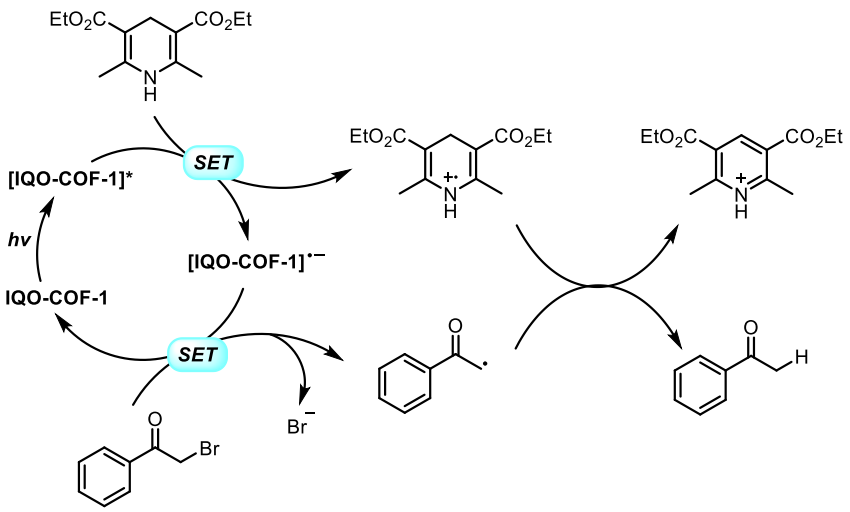


Figure S16. Plausible mechanism of photocatalytic debromination.

Recycling test: The conversion of α-bromoacetophenone to **1** was selected as the model reaction to evaluate the stability of IQO-COF-1. After the reaction ended, IQO-COF-1 was recovered by filtration, washed repeatedly with H_2O, THF and CH_3OH (20 mL), and the dried catalyst was directly used for the next run.

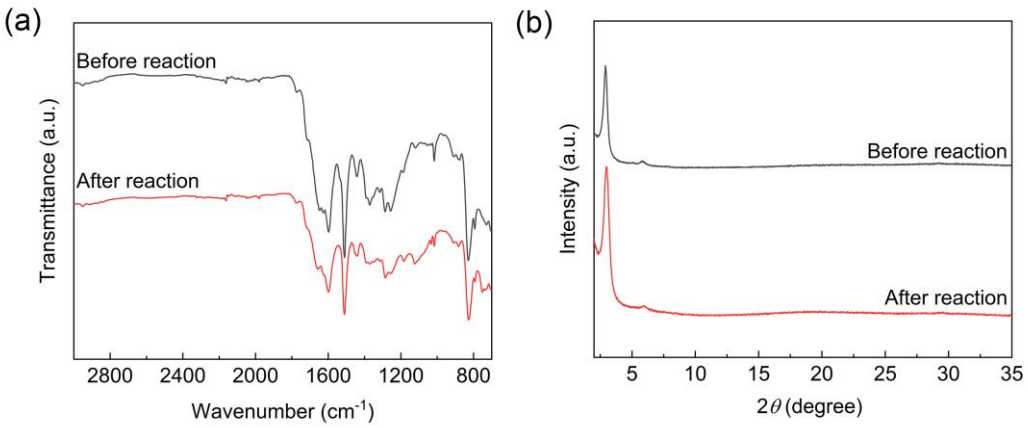
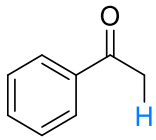


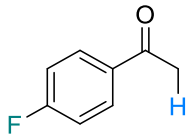
Figure S17. FT-IR spectra (a) and PXRD patterns (b) of IQO-COF-1 before and after five runs of the photocatalytic reaction.

Supplementary explanation of Fig. S17: Initially, under light irradiation, IQO-COF-1 acts as a photosensitizer and is excited to form the [IQO-COF-1]* species, which exists in a charge-separated state with photogenerated electrons and holes. Subsequently, the Hantzsch ester donates an electron to the hole of [IQO-COF-1]*, leading to its oxidation and the formation of a radical cation. Concurrently, the photogenerated electron reduces α-bromoacetophenone via a single-electron transfer

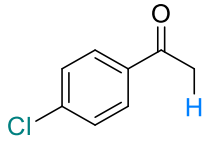
(SET) process, generating an acetophenone radical intermediate and restoring IQO-COF-1 to its ground state. Finally, the acetophenone radical abstracts a hydrogen atom from the radical cation of the Hantzsch ester, yielding the desired product. Notably, potassium carbonate serves as a base catalyst to neutralize the protonated pyridinium byproduct derived from the Hantzsch ester.



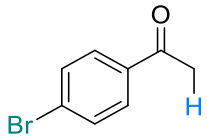
acetophenone (**1**): 46 mg, 0.38 mmol, 96% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.94 (d, J = 7.1 Hz, 2H), 7.54 (t, J = 7.3 Hz, 1H), 7.44 (d, J = 7.9 Hz, 2H), 2.60 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 198.2, 137.1, 133.1, 128.6, 128.3, 26.6.[14]



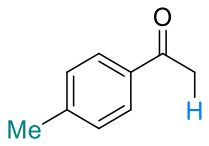
1-(4-fluorophenyl)ethan-1-one (**2**): 48 mg, 0.35 mmol, 88% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.98-7.96 (m, 2H), 7.11 (t, J = 8.5 Hz, 2H), 2.57 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 196.5, 165.8 (d, J = 254.8 Hz), 133.6 (d, $J_{C\text{-}F}$ = 2.4 Hz), 130.9 (d, $J_{C\text{-}F}$ = 9.7 Hz,), 115.6 (d, $J_{C\text{-}F}$ = 21.9 Hz), 26.5. ^{19}F NMR (564 MHz, $CDCl_3$) δ -105.4 (s).[14,15]



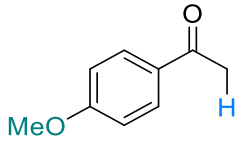
1-(4-chlorophenyl)ethan-1-one (**3**): 57 mg, 0.37 mmol, 92% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.88 (d, J = 8.6 Hz, 2H), 7.42 (d, J = 8.6 Hz, 2H), 2.58 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 196.8, 139.6, 135.4, 129.7, 128.9, 26.5.[14]



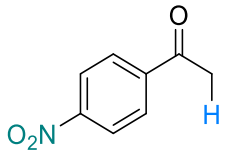
1-(4-bromophenyl)ethan-1-one (**4**): 76 mg, 0.38 mmol, 94% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.81 (d, J = 8.7 Hz, 2H), 7.60 (d, J = 8.7 Hz, 2H), 2.58 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$): δ 197.0, 135.8, 131.9, 129.9, 128.3, 26.5.[14]



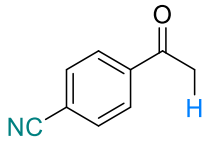
1-(*p*-tolyl)ethan-1-one (**5**): 51 mg, 0.38 mmol, 96% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.2 Hz, 2H), 7.25 (d, *J* = 8.2 Hz, 2H), 2.57 (s, 3H), 2.40 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 197.9, 143.9, 134.7, 129.2, 128.4, 26.5, 21.6.[14]



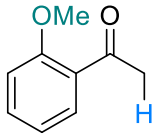
1-(4-methoxyphenyl)ethan-1-one (**6**): 55 mg, 0.37 mmol, 92% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.93 (d, *J* = 8.9 Hz, 2H), 6.92 (d, *J* = 8.9 Hz, 2H), 3.86 (s, 3H), 2.54 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 196.8, 163.5, 130.6, 130.3, 113.7, 55.5, 26.3.[14]



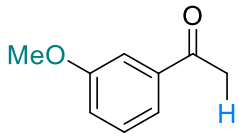
1-(4-nitrophenyl)ethan-1-one (**7**): 61 mg, 0.37 mmol, 93% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.29 (d, *J* = 8.6 Hz, 2H), 8.10 (d, *J* = 8.6 Hz, 2H), 2.67 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 196.3, 150.4, 141.4, 129.3, 123.9, 27.0.[14]



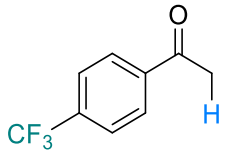
4-acetylbenzonitrile (**8**): 55 mg, 0.38 mmol, 95% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.04 (d, *J* = 8.4 Hz, 2H), 7.77 (d, *J* = 8.4 Hz, 2H), 2.64 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 196.5, 139.9, 132.5, 128.7, 117.9, 116.4, 26.8.[14]



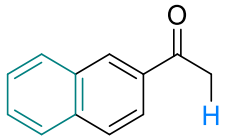
2'-Methoxyacetophenone (**9**): 57 mg, 0.38 mmol, 95% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.71 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.46-7.41 (m, 1H), 6.98-6.92 (m, 2H), 3.87 (s, 3H), 2.59 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 199.9, 158.9, 133.7, 130.3, 128.2, 120.5, 111.6, 55.5, 31.9.[16]



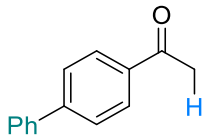
1-(3-methoxyphenyl)ethan-1-one (**10**): 57 mg, 0.38 mmol, 96% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.53-7.49 (m, 1H), 7.47-7.45 (m, 1H), 7.36-7.32 (m, 1H), 7.10-7.07 (m, 1H), 3.83 (s, 3H), 2.57 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 198.0, 159.8, 138.5, 129.6, 121.1, 119.6, 112.4, 55.4, 26.7.[16]



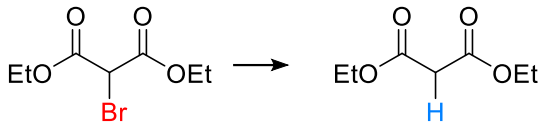
1-(4-(trifluoromethyl)phenyl)ethan-1-one (**11**): 73 mg, 0.39 mmol, 98% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.04 (d, J = 8.2 Hz, 2H), 7.72 (d, J = 8.2 Hz, 2H), 2.63 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 197.0, 139.7, 134.4 (q, $J_{C\text{-}F}$ = 32.6 Hz), 128.6, 125.7 (q, $J_{C\text{-}F}$ = 3.6 Hz), 123.6 (q, $J_{C\text{-}F}$ = 272.8 Hz), 26.8. ^{19}F NMR (564 MHz, $CDCl_3$): δ -63.2.[16]



1-(naphthalen-2-yl)ethan-1-one (**12**): 66 mg, 0.39 mmol, 98% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.46 (s, 1H), 8.04 (dd, J = 8.6, 1.6 Hz, 1H), 7.96 (d, J = 8.1 Hz, 1H), 7.88 (m, 2H), 7.61-7.54 (m, 2H), 2.72 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 198.1, 135.6, 134.5, 132.5, 130.2, 129.6, 128.5, 128.4, 127.8, 126.8, 123.9, 26.7.[16]

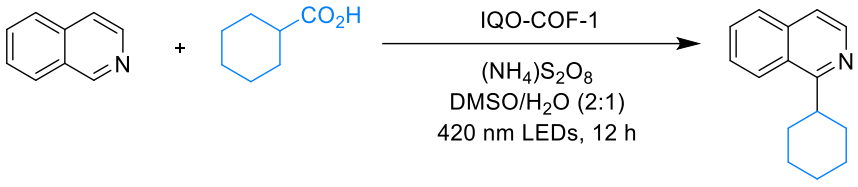


1-([1,1'-biphenyl]-4-yl)ethan-1-one (**13**): 74 mg, 0.38 mmol, 94% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.04 (d, J = 8.4 Hz, 2H), 7.69 (d, J = 8.4 Hz, 2H), 7.63 (d, J = 7.2 Hz, 2H), 7.48 (t, J = 7.6 Hz, 2H), 7.41 (t, J = 7.4 Hz, 1H), 2.64 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 197.8, 145.8, 139.9, 135.9, 129.0, 128.9, 128.3, 127.3, 127.2, 26.7.[16]



diethyl malonate (**14**): 60 mg, 0.38 mmol, 96% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 4.16 (q, *J* = 7.1 Hz, 4H), 3.32 (s, 2H), 1.25 (t, *J* = 7.1 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 166.6, 61.4, 41.6, 14.0.[16]

6 Photocatalytic decarboxylative Minisci reaction

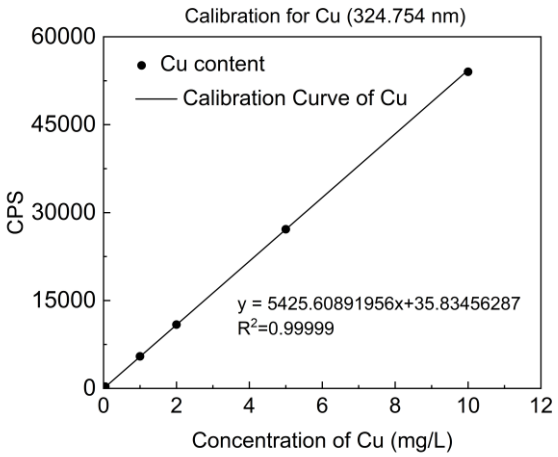


15

General Procedure 2: A 10 mL Schlenk flask equipped with a stir bar was charged with ammonium persulfate ($(NH_4)_2S_2O_8$) (0.4 mmol, 2 equiv.) and IQO-COF-1 (5 mg). After sealing with glass plug, the tube was evacuated and refilled with argon (repeated for three times). Then the liquid samples isoquinoline (0.2 mmol, 1 equiv.), cyclohexanecarboxylic acid (CyCOOH) (0.6 mmol, 3 equiv.) and DMSO/H_2O (2 mL/1 mL) were added sequentially. The reaction mixture was irradiated in the photoreactor (6 W blue LEDs, 420-425 nm) with cooling fan for 12 h under argon atmosphere. After the reaction ended, the solid was collected by filtration, and washed with H_2O and EtOAc. The resulting filtrate was treated with triethylamine (0.2 mL), and extracted with EtOAc. The organic phase was dried with anhydrous Na_2SO_4, and concentrated under rotary evaporator. The residue was purified by flash chromatography on silica gel with PE/EtOAc (10:1) as the eluent to afford the final product (**15**, 40.1 mg, 0.19 mmol, yield: 95%) as yellow oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.48 (d, *J* = 5.6 Hz, 1H), 8.22 (d, *J* = 8.5 Hz, 1H), 7.80 (d, *J* = 8.1 Hz, 1H), 7.65-7.62 (m, 1H), 7.59-7.56 (m, 1H), 7.47 (d, *J* = 5.6 Hz, 1H), 3.59-3.54 (m, 1H), 1.90-1.80 (m, 7H), 1.57-1.36 (m, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.4, 141.6, 136.1, 129.2, 127.2, 126.5, 126.0, 124.4, 118.6, 41.2, 32.3, 26.6, 26.0.[17]

Table S5. The detected signals of Cu content in IQO-COF-1 measured by ICP-OES directly.

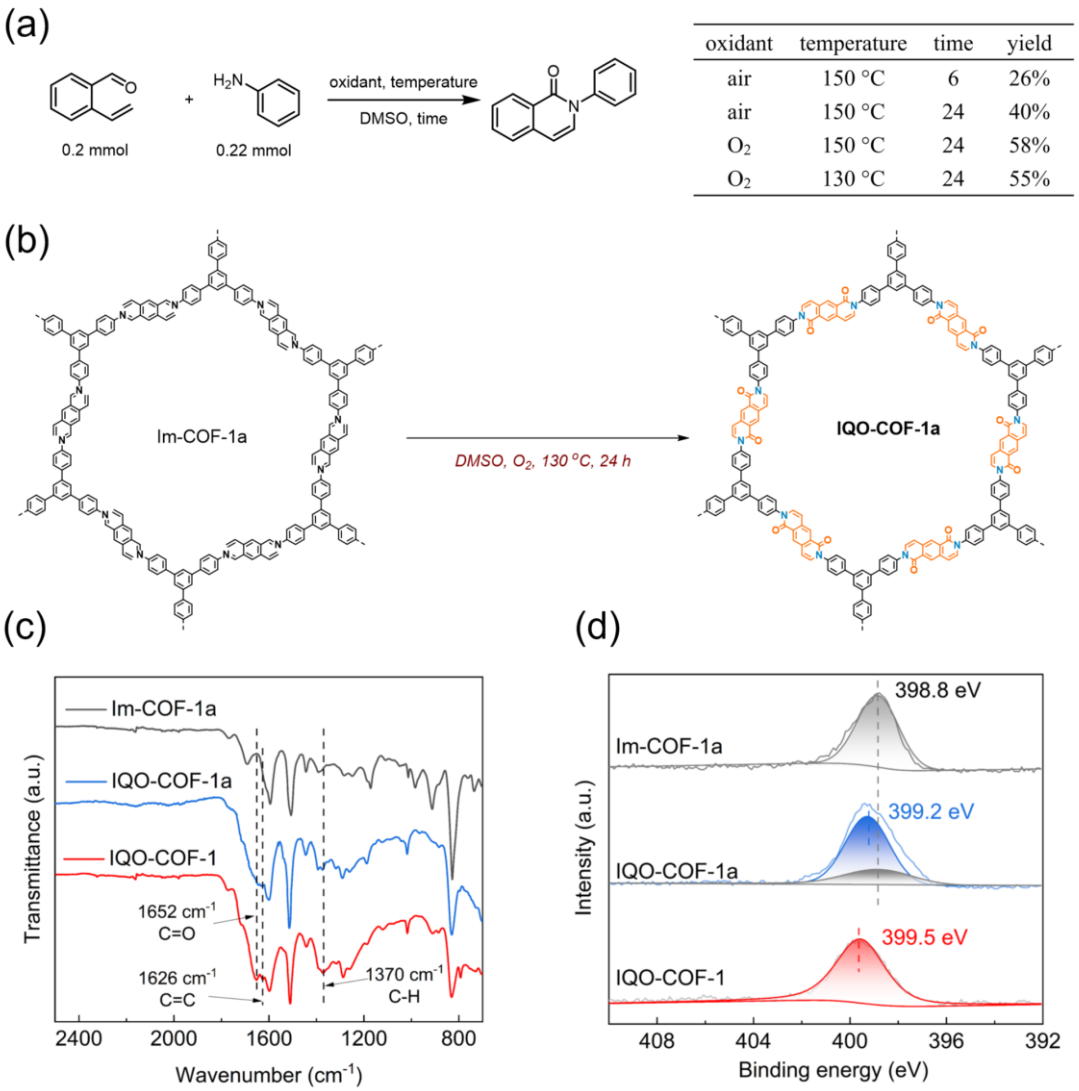
Sample Weight (g)	Final Volume (mL)	Concentration of Cu (mg/L)	Cu Content of the Sample (mg/kg)	Cu Content of the Sample (wt%)
0.0412	25	7.0535	4280.05	0.43



Negligible Effect of Copper Residue on Catalytic Efficiency: ICP-OES analysis measured a residual copper content of 0.43 wt% in IQO-COF-1 (Table S5). To rule out any contribution of this residual copper to the material's enhanced catalytic activity, we successfully synthesized two isoquinolone-linked COFs from the original *o*-vinyl functionalized imine-bridged Im-COF-1a, denoted as IQO-COF-1a (partially converted) and IQO-COF-1b (fully converted), via entirely metal-free postsynthetic strategies (Fig. S18 and S19). Although these samples lack long-range crystallinity, their structures were unambiguously verified by FT-IR and XPS analyses.

Both IQO-COF-1a and IQO-COF-1b exhibited photocatalytic activity in the decarboxylative Minisci reaction comparable to that of the original $Cu(OAc)_2$-synthesized IQO-COF-1, and significantly higher than that of imine- or amide-linked COFs (Table S6). Control reactions showed that adding extra $Cu(OAc)_2$ to IQO-COFs decreased rather than enhanced activity. These results demonstrate that the superior photocatalytic performance of IQO-COF-1 originates from the intrinsic isoquinolone framework, rather than from any trace copper species.

The details of the control experiments are as follows:



oxidant	temperature	time	yield
air	150 °C	6	26%
air	150 °C	24	40%
O_2	150 °C	24	58%
O_2	130 °C	24	55%

Figure S18. Synthesis of IQO-COF-1a via metal-free direct oxidative. Screening of oxidation conditions (a). Metal-free transformation (b). FT-IR spectra (c) and high resolution N1s XPS spectra (d) of Im-COF-1a, IQO-COF-1a and IQO-COF-1.

Based on the optimization of copper-catalyzed oxidative synthesis of isoquinolones reported by Lee *et al.*,[18] it was observed that even under metal-free conditions, the in situ generated imine could undergo 6π-electrocyclization and be oxidized by air, yielding the target compound with an efficiency of 26% (Fig. S18a). Building on this finding, the yield was successfully increased to 58% by extending the reaction time to 24 hours and employing oxygen as the oxidant. A comparable yield was also achieved when the reaction temperature was reduced to 130 °C. However, when the solvent was changed to *o*-DCB, as used in the one-pot synthesis of IQO-COFs,

the desired product was not obtained, making it impossible to synthesize IQO-COFs via the metal-free one-pot strategy.

Based on these results, direct oxidation of Im-COF-1a under metal-free conditions was attempted to synthesize IQO-COF-1a (Fig. S18b). FT-IR analysis revealed that the spectrum of IQO-COF-1a obtained without metal catalysts was largely consistent with that of IQO-COF-1 synthesized using $Cu(OAc)_2$, with new characteristic peaks emerging at 1652, 1626, and 1370 cm^{-1}. It is worth noting that the C=O stretching vibration at 1652 cm^{-1} in IQO-COF-1a appeared relatively weaker, which could be attributed to incomplete oxidation under the metal-free reaction conditions. This observation was further corroborated by subsequent XPS analysis.

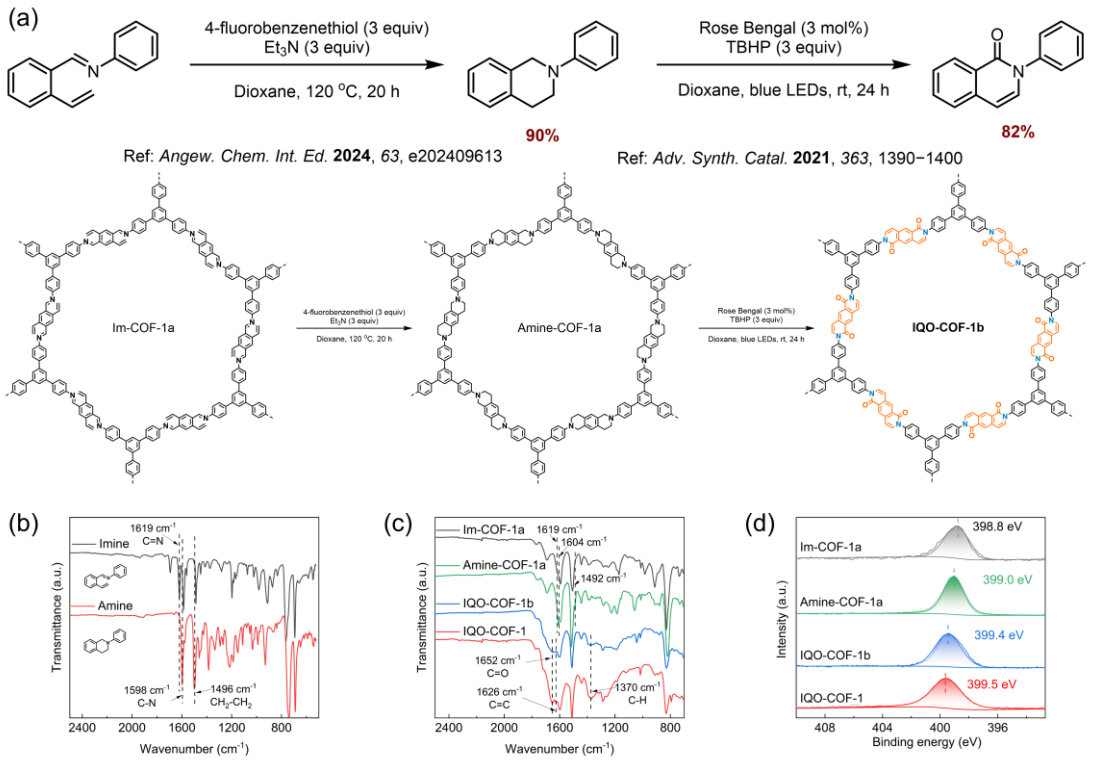


Figure S19. Synthesis of IQO-COF-1b *via* a two-step post-modification. Synthetic route (a). FT-IR spectra of model compounds (Imine and Amine) (b). FT-IR spectra (c) and high resolution N1s XPS spectra (d) of Im-COF-1a, Amine-COF-1a, IQO-COF-1b and IQO-COF-1.

A two-step metal-free post-modification route was also designed. This approach involves thermal cyclization and reduction of the *o*-vinyl imine to yield the

tetrahydroisoquinoline intermediate,[19] followed by photocatalytic oxidation to furnish the isoquinolone product (Fig. S19a).[20]

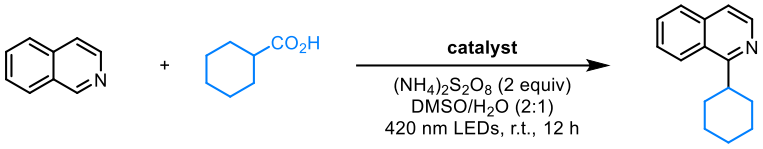
Under argon atmosphere, add *N*-phenyl-1-(2-vinylphenyl)methanimine (0.5 mmol), 4-fluorothiophenol (1.5 mmol), and triethylamine (1.5 mmol) sequentially into a 10 mL Schlenk tube. Then, dissolve the mixture in 3 mL of anhydrous 1,4-dioxane. Seal the tube tightly and place it in an oil bath at 120 °C with stirring for 20 hours. After completion, cool the reaction mixture to room temperature and remove the solvent under reduced pressure to afford the crude product. Purify the crude product by flash column chromatography over silica gel pretreated with petroleum ether/triethylamine (50:1), using petroleum ether and ethyl acetate (20:1) as the eluent. 2-Phenyl-1,2,3,4-tetrahydroisoquinoline was obtained as a white solid (94.2 mg, 90% yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.32-7.30 (m, 2H), 7.21-7.17 (m, 4H), 7.00 (d, J = 8.0 Hz, 2H), 6.85 (t, J = 7.3 Hz, 1H), 4.43 (s, 2H), 3.58 (t, J = 5.8 Hz, 2H), 3.01 (t, J = 5.8 Hz, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 150.5, 134.8, 134.4, 129.1, 128.4, 126.5, 126.2, 125.9, 118.6, 115.1, 50.7, 46.4, 29.0.[19]

To a screw-cap Schlenk tube equipped with a magnetic stir bar, 2-phenyl-1,2,3,4-tetrahydroisoquinoline (0.3 mmol) and rose bengal (3 mol%) were dissolved in 1,4-dioxane (3 mL). Then, TBHP (0.9 mmol, 5–6 M in decane) was added via syringe. The resulting mixture was stirred and irradiated with 24 W blue LEDs at room temperature for 24 h. Upon completion, the reaction mixture was diluted with water (10 mL) and extracted with EtOAc (3 × 10 mL). The combined organic layers were washed with brine, dried over Na_2SO_4, and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel using ethyl acetate/petroleum ether to afford the 2-phenylisoquinolin-1(2*H*)-one (**S7**, 54.4 mg, 82% yield) as a white solid.

Subsequently, this methodology was applied to Im-COF-1a, successfully yielding Amine-COF-1a and IQO-COF-1b. FT-IR and XPS analyses indicated efficient conversion for both steps. The FT-IR spectral changes observed during the transformation from Im-COF-1a to Amine-COF-1a were consistent with those seen in

the model reactions (Fig. S19b and S19c). Furthermore, the FT-IR and XPS data for IQO-COF-1b obtained via this route showed high consistency with those of IQO-COF-1 synthesized using $Cu(OAc)_2$ catalysis. However, PXRD analysis revealed that IQO-COF-1b lacks long-range structural order.

Table S6. Control experiments for copper residue effects



entry	catalyst	yield
1	Im-COF-1	62%
2	Am-COF-1	72%
3	IQO-COF-1	95%
4	IQO-COF-1a	88%
5	IQO-COF-1b	94%
6	IQO-COF-1+ $Cu(OAc)_2$	72%
7	IQO-COF-1a+ $Cu(OAc)_2$	70%
8	IQO-COF-1b+ $Cu(OAc)_2$	72%

Reaction conditions: isoquinoline (0.2 mmol), cyclohexylcarboxylic acid (0.6 mmol), $(NH_4)_2S_2O_8$ (0.4 mmol), COFs (5 mg), DMSO/H_2O (2 mL/1 mL), 6 W 420 nm LEDs, 12 h under nitrogen atmosphere.

To directly address the concern regarding copper contamination, we conducted a series of control experiments (Table S6). The results demonstrate that both metal-free IQO-COF-1a and IQO-COF-1b exhibit high catalytic activity (entries 4 and 5), significantly outperforming Im-COF-1 and Am-COF-1. Notably, the catalytic efficiency of IQO-COF-1b is comparable to that of $Cu(OAc)_2$-synthesized IQO-COF-1, whereas IQO-COF-1a shows slightly lower activity, likely due to incomplete conversion from Im-COF-1a to IQO-COF-1a. This observation further suggests a positive correlation between the degree of isoquinolone linkage formation and catalytic performance. Moreover, the addition of extra $Cu(OAc)_2$ to these IQO-COFs did not enhance their activity but instead led to a decrease in yield (entries 6–8). These results collectively confirm that the superior catalytic performance of IQO-COFs in the

decarboxylative Minisci reaction originates from the intrinsic properties of the isoquinolone structure, rather than any residual copper.

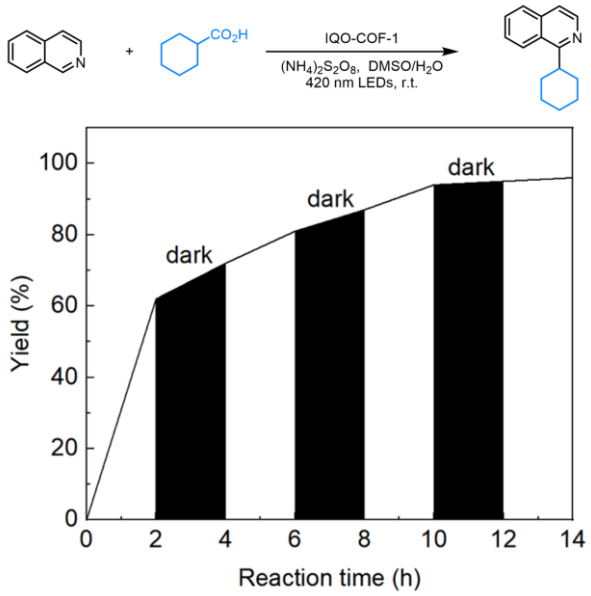
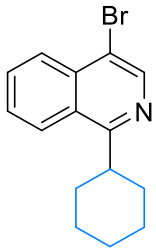


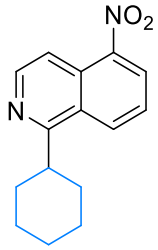
Figure S20. Light on/off experiments of the decarboxylative Minisci reaction.

Light on/off experiments: To elucidate the underlying mechanism, we performed a series of light on/off cycles, each comprising 2 hours of irradiation and 2 hours of darkness, repeated three times. The critical finding is the persistent rise in product yield under dark conditions. This demonstrates that the propagation steps of the reaction continue without a photochemical driving force, strongly supporting the existence of a radical chain mechanism.

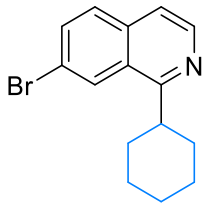


4-bromo-1-cyclohexylisoquinoline (16): Following **GP2** with 4-bromoisoquinoline (0.2 mmol), $(NH_4)_2S_2O_8$ (0.4 mmol), IQO-COF-1 (5 mg), CyCOOH (0.6 mmol), DMSO/H_2O (2 mL/1 mL), obtained as white solid in 89% yield (51.6 mg) after purification by column chromatography on silica gel eluting with PE/EtOAc (10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.65 (s, 1H), 8.19 (m, 2H), 7.77-7.74 (m, 1H), 7.65-7.62 (m, 1H), 3.53-3.48 (m, 1H), 1.96-1.90 (m, 4H), 1.82-1.75 (m, 3H), 1.56-1.48 (m, 2H),

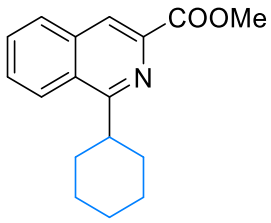
1.41-1.34 (m, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.4, 143.6, 134.9, 130.8, 127.7, 127.6, 126.9, 125.1, 117.5, 41.5, 32.6, 26.8, 26.2.[17]



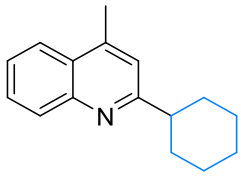
1-cyclohexyl-5-nitro-isoquinoline (17): Following **GP2** with 5-nitroisoquinoline (0.2 mmol), $(NH_4)_2S_2O_8$ (0.4 mmol), IQO-COF-1 (5 mg), CyCOOH (0.6 mmol), DMSO/H_2O (2 mL/1 mL), obtained as yellow oil in 92% yield (47.1 mg) after purification by column chromatography on silica gel eluting with PE/EtOAc (10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.68 (d, J = 6.1 Hz, 1H), 8.58 (d, J = 8.6 Hz, 1H), 8.42 (dd, J = 7.6, 0.9 Hz, 1H), 8.22 (d, J = 6.1 Hz, 1H), 7.69 (t, J = 8.0 Hz, 1H), 3.59-3.54 (m, 1H), 1.97-1.93 (m, 4H), 1.87-1.80 (m, 3H), 1.57-1.49 (m, 2H), 1.42-1.34 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 166.4, 145.9, 145.1, 131.3, 128.8, 127.2, 126.8, 125.1, 113.4, 42.1, 32.6, 26.7, 26.0.[17]



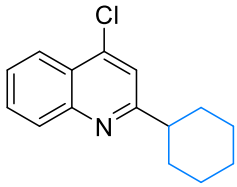
7-bromo-1-cyclohexylnaphthalene (18): Following **GP2** with CyCOOH (1.0 mmol), 7-bromoisoquinoline (0.2 mmol), $(NH_4)_2S_2O_8$ (0.4 mmol), IQO-COF-1 (5 mg) and DMSO/H_2O (2 mL/1 mL), obtained as colorless oil in 95% yield (55.2 mg) after purification by column chromatography on silica gel eluting with PE/EtOAc (10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.48 (d, J = 5.7 Hz, 1H), 8.07 (d, J = 9.1 Hz, 1H), 7.96 (d, J = 2.0 Hz, 1H), 7.63 (dd, J = 9.0, 2.0 Hz, 1H), 7.37 (d, J = 5.7 Hz, 1H), 3.59-3.42 (m, 1H), 2.07-1.89 (m, 4H), 1.89-1.71 (m, 3H), 1.61-1.46 (m, 2H), 1.44-1.33 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 166.0, 143.0, 137.6, 130.3, 129.6, 126.6, 124.7, 124.3, 117.9, 41.6, 32.6, 26.8, 26.2.[21]



3-isoquinolinecarboxylic acid (19): Following **GP2** with methyl isoquinoline-3-carboxylate (0.2 mmol), $(NH_4)_2S_2O_8$ (0.4 mmol), IQO-COF-1 (5 mg), CyCOOH (0.6 mmol), DMSO/H_2O (2 mL/1 mL), obtained as colorless oil in 41% yield (22.0 mg) after purification by column chromatography on silica gel eluting with PE/EtOAc (10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.38 (s, 1H), 8.27-8.26 (m, 1H), 7.93 (d, J = 7.3 Hz, 1H), 7.72-7.68 (m, 2H), 4.02 (s, 3H), 3.58-3.55 (m, 1H), 2.01-1.91 (m, 6H), 1.81 (d, J = 12.5 Hz, 1H), 1.57-1.50 (m, 2H), 1.45-1.41 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 167.0, 166.2, 140.8, 136.1, 130.2, 129.1, 127.9, 125.1, 122.5, 52.8, 42.2, 32.4, 26.9, 26.2.[17]

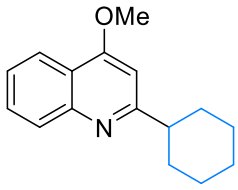


2-cyclohexyl-4-methylquinoline (20): Following **GP2** with lepidine (0.2 mmol), $(NH_4)_2S_2O_8$ (0.4 mmol), IQO-COF-1 (5 mg), CyCOOH (0.6 mmol), DMSO/H_2O (2 mL/1 mL), obtained as colorless oil in 93% yield (42.0 mg) after purification by column chromatography on silica gel eluting with PE/EtOAc (10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.05 (d, J = 8.1 Hz, 1H), 7.92 (dd, J = 8.3, 0.9 Hz, 1H), 7.67-7.64 (m, 1H), 7.49-7.46 (m, 1H), 7.16 (s, 1H), 2.90-2.85 (m, 1H), 2.67 (d, J = 0.8 Hz, 3H), 2.03-1.99 (m, 2H),1.91-1.87 (m, 2H), 1.80-1.78 (m, 1H), 1.63 (m, 2H), 1.51-1.43 (m, 2H), 1.37-1.32 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 166.4, 147.5, 144.1, 129.4, 128.8, 126.9, 125.2, 123.4, 120.1, 47.5, 32.7, 26.5, 26.0, 18.7.[17]

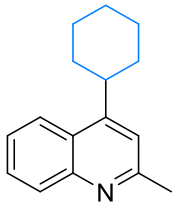


4-chloro-2-cyclohexylquinoline (21): Following **GP2** with 4-chloroquinoline (0.2

mmol), $(NH_4)_2S_2O_8$ (0.4 mmol), IQO-COF-1 (5 mg), CyCOOH (0.6 mmol), DMSO/H_2O (2 mL/1 mL), obtained as colorless oil in 49% yield (24.1 mg) after purification by column chromatography on silica gel eluting with PE/EtOAc (10:1).[1]H NMR (600 MHz, $CDCl_3$) δ 8.17 (dd, *J* = 8.3, 0.6 Hz, 1H), 8.05 (d, *J* = 8.4 Hz, 1H), 7.74-7.71 (m, 1H), 7.58-7.55 (m, 1H), 7.42 (s, 1H), 2.90-2.86 (m, 1H), 2.02 (dd, *J* = 13.4, 1.54 Hz, 2H), 1.91-1.88 (m, 2H), 1.80-1.78 (m, 1H), 1.64-1.58 (m, 2H), 1.50-1.42 (m, 2H), 1.37-1.31 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$): δ 166.7, 148.6, 142.5, 130.1, 129.2, 126.5, 125.1, 123.8, 119.7, 47.3, 32.6, 26.4, 25.9.[17]

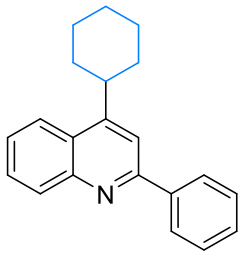


2-cyclohexyl-4-methoxyquinoline (22): Following **GP2** with CyCOOH (1.0 mmol) to the reaction mixture, 4-methoxyquinoline (0.2 mmol), $(NH_4)_2S_2O_8$ (0.4 mmol), IQO-COF-1 (5 mg) and DMSO/H_2O (2 mL/1 mL), obtained as colorless oil in 74% yield (35.6 mg) after purification by column chromatography on silica gel eluting with PE/EtOAc (10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.13 (d, *J* = 8.3 Hz, 1H), 7.99 (d, *J* = 8.4 Hz, 1H), 7.69-7.61 (m, 1H), 7.47-7.39 (m, 1H), 6.65 (s, 1H), 4.04 (s, 3H), 2.89 (tt, *J* = 12.0, 3.3 Hz, 1H), 2.09-1.97 (m, 2H), 1.95-1.84 (m, 2H), 1.83-1.74 (m, 1H), 1.69-1.55 (m, 2H), 1.54-1.41 (m, 2H), 1.41-1.30 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 168.1, 162.4, 148.7, 129.5, 128.4, 124.7, 121.5, 120.2, 97.9, 55.4, 48.2, 32.9, 26.5, 26.1.[17]

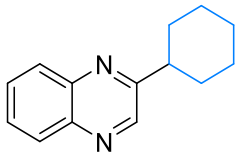


4-cyclohexyl-2-methylquinoline (23): Following **GP2** with quinaldine (0.2 mmol), $(NH_4)_2S_2O_8$ (0.4 mmol), IQO-COF-1 (5 mg), CyCOOH (0.6 mmol), DMSO/H_2O (2 mL/1 mL), obtained as yellow oil in 92% yield (41.6 mg) after purification by column chromatography on silica gel eluting with PE/EtOAc (10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.5 Hz, 2H), 7.66-7.63 (m, 1H), 7.49-7.47 (m, 1H), 7.16 (s, 1H),

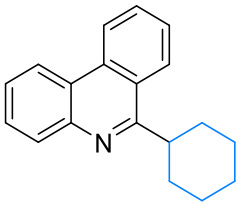
3.31-3.27 (m, 1H), 2.72 (s, 3H), 2.01-1.92 (m, 4H), 1.85 (d, J = 13.0 Hz, 1H), 1.58-1.50 (m, 4H), 1.37-1.32 (m, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 158.7, 153.2, 148.1, 129.5, 128.7, 125.2, 125.1, 122.7, 118.2, 38.7, 33.5, 26.9, 26.2, 25.5.[17]



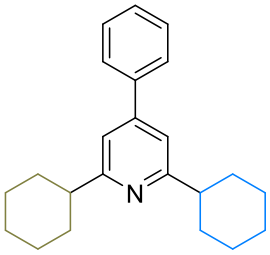
4-cyclohexyl-2-phenylquinoline (24): Following **GP2** with CyCOOH (1.0 mmol) to the reaction mixture, 2-phenylquinoline (0.2 mmol), $(NH_4)_2S_2O_8$ (0.4 mmol), IQO-COF-1 (5 mg) and DMSO/H_2O (2 mL/1 mL), obtained as colorless oil in 72% yield (41.3 mg) after purification by column chromatography on silica gel eluting with PE/EtOAc (10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.22 (d, J = 8.2 Hz, 1H), 8.17 (d, J = 7.2 Hz, 2H), 8.10 (d, J = 8.4 Hz, 1H), 7.77 (s, 1H), 7.72-7.70 (m, 1H), 7.54 (t, J = 7.3 Hz, 3H), 7.47 (t, J = 7.3 Hz, 1H), 3.40-3.36 (m, 1H), 2.09 (d, J = 12.0 Hz, 2H), 1.97 (d, J = 12.8 Hz, 2H), 1.89 (d, J = 13.4 Hz, 1H), 1.68-1.55 (m, 4H), 1.43-1.36 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 157.4, 154.0, 148.6, 140.3, 130.7, 129.2, 129.1, 128.8, 127.7, 125.9, 122.9, 115.5, 39.1, 33.7, 27.0, 26.4.[17]



2-cyclohexylquinoxaline (25): Following **GP2** with quinoxaline (0.2 mmol), $(NH_4)_2S_2O_8$ (0.4 mmol), IQO-COF-1 (5 mg), CyCOOH (0.6 mmol), TFA (0.2 mmol), and DMSO/H_2O (2 mL/1 mL), obtained as yellow oil in 91% yield (38.6 mg) after purification by column chromatography on silica gel eluting with PE/EtOAc (10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.77 (s, 1H), 8.22 (dd, J = 12.4, 8.4 Hz, 2H), 7.74-7.68 (m, 2H), 2.99-2.94 (m, 1H), 2.04 (d, J = 12.1 Hz, 2H), 1.94-1.91 (m, 2H), 1.81 (d, J = 13.0 Hz, 1H), 1.75-1.68 (m, 2H), 1.52-1.44 (m, 2H), 1.39-1.32 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$): δ 161.1, 145.0, 142.2, 141.4, 129.7, 129.1, 129.0, 128.8, 45.0, 32.3, 26.3, 25.8.[17]

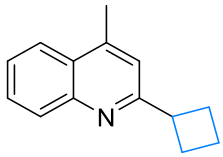


6-cyclohexylphenanthridine (26): Following **GP2** with CyCOOH (1.0 mmol) to the reaction mixture, phenanthridine (0.2 mmol), $(NH_4)_2S_2O_8$ (0.4 mmol), IQO-COF-1 (5 mg) and DMSO/H_2O (2 mL/1 mL), obtained as white solid in 99% yield (51.7 mg) after purification by column chromatography on silica gel eluting with PE/EtOAc (10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.65 (d, *J* = 8.2 Hz, 1H), 8.53 (d, *J* = 7.9 Hz, 1H), 8.22 (d, *J* = 8.2 Hz, 1H), 8.16 (d, *J* = 8.1 Hz, 1H), 7.82-7.79 (m, 1H), 7.72-7.67 (m, 2H), 7.62-7.59 (m, 1H), 3.65-3.60 (m, 1H), 2.10 (d, *J* = 12.0 Hz, 2H), 2.00-1.96 (m, 4H), 1.87 (d, *J* = 12.9 Hz, 1H), 1.63-1.56 (m, 2H), 1.49-1.44 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$): δ 165.3, 144.0, 133.1, 130.0, 130.9, 128.4, 127.1, 126.2, 125.7, 124.8, 123.4, 122.6, 121.9, 42.1, 32.4, 27.0, 26.4.[22]

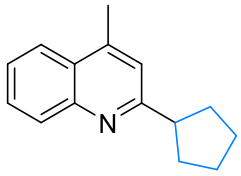


2-cyclohexyl-4-phenylpyridine (27): Following **GP2** with CyCOOH (1.0 mmol), TFA (0.2 mmol), 4-phenylpyridine (0.2 mmol), $(NH_4)_2S_2O_8$ (0.4 mmol), IQO-COF-1 (5 mg) and DMSO/H_2O (2 mL/1 mL), obtained as white solid in 47% yield (22.1 mg) after purification by column chromatography on silica gel eluting with PE/EtOAc (10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.57 (d, *J* = 4.9 Hz, 1H), 7.63-7.62 (m, 2H), 7.48-7.46 (m, 2H), 7.43-7.41 (m, 1H), 7.36 (s, 1H), 7.31 (dd, *J* = 5.1, 1.6 Hz, 1H), 2.79-2.74 (m, 1H), 2.02-1.99 (m, 2H), 1.90-1.86 (m, 2H), 1.78-1.76 (m, 1H), 1.63-1.56 (m, 2H), 1.48-1.40 (m, 2H), 1.35-1.28 (m, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 166.9, 149.4, 148.7, 138.7, 128.9, 128.7, 127.0, 119.1, 119.0, 46.6, 32.9, 26.5, 26.0. **27-di** (17.7 mg, 28%), **2,6-Dicyclohexyl-4-phenylpyridine:** ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.63-7.62 (m, 2H), 7.48-7.45 (m, 2H), 42-7.39 (m, 1H), 7.17 (s, 2H), 2.78-2.74 (m, 2H), 2.02 (d, *J* = 11.7 Hz, 4H), 1.88-1.85 (m, 4H), 1.78-1.75 (m, 2H), 1.58-1.51 (m, 4H), 1.49-1.41 (m, 4H),

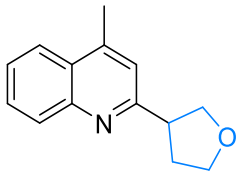
1.34-1.26 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$): δ 166.2, 148.9, 139.6, 128.8, 128.4, 127.1, 115.9, 46.7, 33.1, 26.6, 26.1.[17]



4-methyl-2-(3-methylcyclobutyl)quinoline (28): Following **GP2** with lepidine (0.2 mmol), $(NH_4)_2S_2O_8$ (0.4 mmol), IQO-COF-1 (5 mg), cyclo-butyl formic acid (0.6 mmol), DMSO/H_2O (2 mL/1 mL), obtained as yellow oil in 67% yield (26.4 mg) after purification by column chromatography on silica gel eluting with PE/EtOAc (10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.06 (d, *J* = 8.4 Hz, 1H), 7.94 (d, *J* = 8.3 Hz, 1H), 7.68-7.65 (m, 1H), 7.50-7.48 (m, 1H), 7.19 (s, 1H), 3.86-3.80 (m, 1H), 2.68 (s, 3H), 2.47-2.42 (m, 4H), 2.16-2.08 (m, 1H), 1.98-1.93 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 161.9, 144.8, 141.3, 126.7, 126.1, 124.1, 122.6, 120.7, 117.4, 39.8, 25.4, 15.9, 15.5.[20]

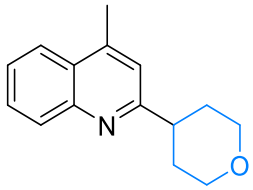


2-cyclopentyl-4-methylquinoline (29): Following **GP2** with TFA (0.2 mmol), lepidine (0.2 mmol), $(NH_4)_2S_2O_8$ (0.4 mmol), IQO-COF-1 (5 mg), cyclopentanecarboxylic acid (0.6 mmol) and DMSO/H_2O (2 mL/1 mL), obtained as yellow oil in 93% yield (39.3 mg) after purification by column chromatography on silica gel eluting with PE/EtOAc (10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.3 Hz, 1H), 7.96 (dd, *J* = 8.3, 0.8 Hz, 1H), 7.70-7.67 (m, 1H), 7.53-7.50 (m, 1H), 7.16 (s, 1H), 3.00-2.95 (m, 1H), 2.69 (d, *J* = 0.8 Hz, 3H), 2.30-2.24 (m, 2H), 2.11-1.87 (m, 6H). ^{13}C NMR (151 MHz, $CDCl_3$): δ 166.0, 147.5, 144.2, 129.5, 129.0, 127.0, 125.4, 123.6, 120.7, 48.9, 33.7, 26.1, 18.9.[17]

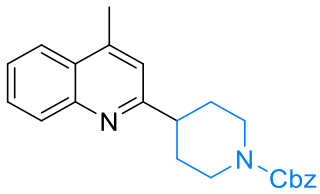


4-methyl-2-(tetrahydro-3-furanyl)-quinoline (30): Following **GP2** with 4-chloroquinoline (0.2 mmol), $(NH_4)_2S_2O_8$ (0.4 mmol), IQO-COF-1 (5 mg), CyCOOH

(0.6 mmol), DMSO/H_2O (2 mL/1 mL), obtained as yellow oil in 57% yield (24.3 mg) after purification by column chromatography on silica gel eluting with PE/EtOAc (10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8.2 Hz, 1H), 7.95 (dd, *J* = 8.3, 0.8 Hz, 1H), 7.69-7.67 (m, 1H), 7.53-7.50 (m, 1H), 7.20 (s, 1H), 4.23 (t, *J* = 8.3 Hz, 1H), 4.17-4.13 (m, 1H), 4.05 (dd, *J* = 8.6, 6.7 Hz, 1H), 2.95 (dd, *J* = 15.8, 7.6 Hz, 1H), 3.77-3.72 (m, 1H), 2.69 (d, *J* = 0.8 Hz, 3H), 2.49-2.43-2.51 (m, 1H), 2.33-2.27 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 162.5, 147.4, 144.8, 129.5, 129.1, 127.0, 125.7, 123.5, 120.5, 73.5, 68.7, 47.6, 33.4, 18.7.[21]

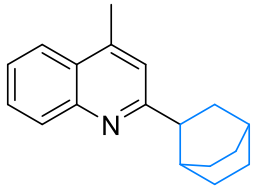


4-methyl-2-(tetrahydro-2H-pyran-4-yl)quinoline (31): Following **GP2** with lepidine (0.2 mmol), $(NH_4)_2S_2O_8$ (0.4 mmol), IQO-COF-1 (5 mg), tetrahydro-2H-pyran-4-carboxylic acid (0.6 mmol), DMSO/H_2O (2 mL/1 mL), obtained as yellow oil in 96% yield (43.6 mg) after purification by column chromatography on silica gel eluting with PE/EtOAc (10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.04 (d, *J* = 8.3 Hz, 1H), 7.95 (d, *J* = 8.3 Hz, 1H), 7.68 (t, *J* = 7.2 Hz, 1H), 7.51 (dd, *J* = 8.2, 7.1 Hz, 1H), 7.17 (s, 1H), 4.13 (dd, *J* = 11.0, 6.7 Hz, 2H), 3.61-3.57 (m, 2H), 3.14-3.10 (m, 1H), 2.69 (s, 3H), 2.05-1.90 (m, 4H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.2, 147.6, 144.6, 129.5, 129.1, 127.1, 125.6, 123.6, 119.9, 68.1, 44.4, 32.3, 18.8.[21]

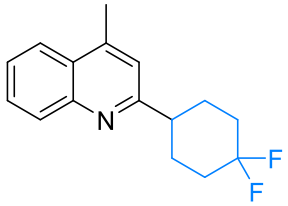


benzyl-4-(4-methylquinolin-2-yl)piperidine-1-carboxylate (32): Following **GP2** with TFA (0.2 mmol), lepidine (0.2 mmol), $(NH_4)_2S_2O_8$ (0.4 mmol), IQO-COF-1 (5 mg), N-Cbz-4-Piperidinecarboxylic acid (0.6 mmol) and DMSO/H_2O (2 mL/1 mL), obtained as white solid in 98% yield (70.6 mg) after purification by column chromatography on silica gel eluting with PE/EtOAc (5:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.3 Hz, 1H), 7.95 (d, *J* = 8.3 Hz, 1H), 7.69-7.66 (m, 1H), 7.53-7.50 (m,

1H), 7.40-7.31 (m, 5H), 7.13 (s, 1H), 5.18 (s, 2H), 4.39-4.36 (m, 2H), 3.06-2.97 (m, 3H), 2.68 (s, 3H), 2.00-1.86 (m, 4H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.0, 155.4, 147.6, 144.8, 126.9, 129.5, 129.2, 128.5, 128.0, 127.9, 127.1, 125.8, 123.7, 120.0, 67.1, 45.3, 44.4, 18.9.[25]

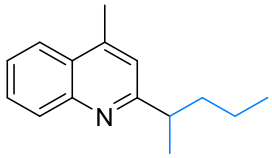


(bicyclo[2.2.1]heptan-2-yl)-4-methylquinoline (33): Following **GP2** with TFA (0.2 mmol), lepidine (0.2 mmol), $(NH_4)_2S_2O_8$ (0.4 mmol), IQO-COF-1 (5 mg), bicyclo[2.2.2]octane-2-carboxylicacid (0.6 mmol) and DMSO/H_2O (2 mL/1 mL), obtained as colorless oil in 97% yield (48.7 mg) after purification by column chromatography on silica gel eluting with PE/EtOAc (10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.05 (d, *J* = 8.4 Hz, 1H), 7.93 (dd, *J* = 8.2, 0.7 Hz, 1H), 7.67-7.64 (m, 1H), 7.49-7.47 (m, 1H), 7.18 (s, 1H), 3.01 (dd, *J* = 8.8, 5.5 Hz, 1H), 2.67 (d, *J* = 0.6 Hz, 3H), 2.58 (d, *J* = 3.4 Hz, 1H), 2.42 (s, 1H), 2.27-2.24 (m, 1H), 1.76-1.29 (m, 8H), 1.20-1.18 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.6, 147.5, 143.7, 129.7, 128.8, 126.8, 125.3, 123.5, 121.6, 50.1, 43.1, 36.8, 36.3, 36.1, 30.5, 29.8, 29.2, 18.8.[23]

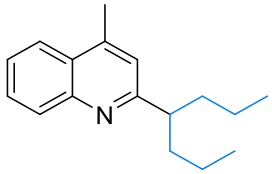


2-(4,4-difluorocyclohexyl)-4-methylquinoline (34): Following **GP2** with TFA (0.2 mmol), lepidine (0.2 mmol), $(NH_4)_2S_2O_8$ (0.4 mmol), IQO-COF-1 (5 mg), 4,4-difluorocyclohexanecarboxylic acid (0.6 mmol) and DMSO/H_2O (2 mL/1 mL), obtained as yellow solid in 93% yield (48.6 mg) after purification by column chromatography on silica gel eluting with PE/EtOAc (10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.3 Hz, 1H), 7.96 (dd, *J* = 8.3, 0.8 Hz, 1H), 7.70-7.67 (m, 1H), 7.53-7.50 (m, 1H), 7.16 (s, 1H), 3.00-2.95 (m, 1H), 2.69 (d, *J* = 0.8 Hz, 3H), 2.30-2.24 (m, 2H), 2.11-1.87 (m, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 163.8, 147.5, 144.7, 129.5, 129.2, 127.1, 125.7, 123.6, 119.7, 45.1, 33.7 (dd, *J* = 26.4, 22.8 Hz), 28.7 (d, *J* = 9.7

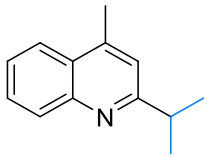
Hz), 18.8. ^{19}F NMR (564 MHz, $CDCl_3$) δ -91.66 (d, J = 235.8 Hz), -101.49 (d, J = 235.8 Hz).[23]



4-methyl-2-(pentan-2-yl)quinoline (35): Following **GP2** with TFA (0.2 mmol), lepidine (0.2 mmol), $(NH_4)_2S_2O_8$ (0.4 mmol), IQO-COF-1 (5 mg), 2-methylpentanoic acid (0.6 mmol) and DMSO/H_2O (2 mL/1 mL), obtained as colorless oil in 96% yield (40.9 mg) after purification by column chromatography on silica gel eluting with PE/EtOAc (10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.06 (d, J = 8.2 Hz, 1H), 7.94 (dd, J = 8.2, 0.6 Hz, 1H), 7.67-7.65 (m, 1H), 7.50-7.48 (m, 1H), 7.13 (s, 1H), 3.08-3.04 (m, 1H), 2.68 (s, 3H), 1.81-1.77 (m, 1H), 1.67-1.63 (m, 1H), 1.39-1.33 (m, 4H), 1.5-1.21 (m, 1H), 0.90 (t, J = 7.3 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 167.0, 147.7, 144.3, 129.6, 129.0, 127.1, 125.4, 123.6, 120.2, 42.8, 39.4, 21.0, 20.8, 18.9, 14.3.[17]

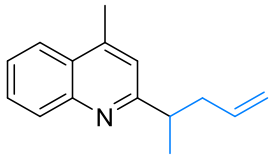


2-(heptan-4-yl)-4-methylquinoline (36): Following **GP2** with TFA (0.2 mmol), lepidine (0.2 mmol), $(NH_4)_2S_2O_8$ (0.4 mmol), IQO-COF-1 (5 mg), valproic acid (0.6 mmol) and DMSO/H_2O (2 mL/1 mL), obtained as colorless oil in 85% yield (41.0 mg) after purification by column chromatography on silica gel eluting with PE/EtOAc (10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.07 (d, J = 8.4 Hz, 1H), 7.94 (dd, J = 8.3, 0.9 Hz, 1H), 7.67-7.64 (m, 1H), 7.50-7.48 (m, 1H), 7.10 (s, 1H), 2.95-2.90 (m, 1H), 2.68 (d, J = 0.7 Hz, 3H), 1.78-1.67 (m, 4H), 1.32-1.27 (m, 2H), 1.19-1.12 (m, 2H), 0.86 (t, J = 7.4 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 166.1,147.8, 144.0, 129.7, 128.9, 127.1, 125.4, 123.6, 120.8, 48.5, 38.1, 20.9, 18.9, 14.3.[17]

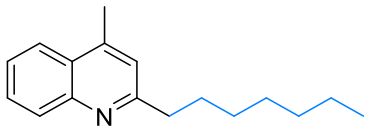


2-isopropyl-4-methylquinoline (37): Following **GP2** with TFA (0.2 mmol), lepidine

(0.2 mmol), $(NH_4)_2S_2O_8$ (0.4 mmol), IQO-COF-1 (5 mg), isobutyric acid (0.6 mmol) and DMSO/H_2O (2 mL/1 mL), obtained as colorless oil in 68% yield (25.2 mg) after purification by column chromatography on silica gel eluting with PE/EtOAc (10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.05 (d, J = 8.4 Hz, 1H), 7.94 (d, J = 8.3 Hz, 1H), 7.68-7.65 (m, 1H), 7.51-7.48 (m, 1H), 7.17 (s, 1H), 3.25-3.18 (m, 1H), 2.68 (s, 3H), 1.39 (d, J = 7.0 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 167.4, 147.6, 144.4, 129.6, 129.0, 127.1, 125.5, 123.6, 119.8, 37.3, 22.6, 18.9.[23]

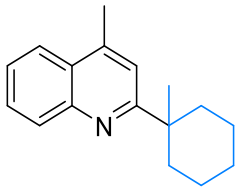


4-methyl-2-(pent-4-en-2-yl)quinoline (38): Following **GP2** with TFA (0.2 mmol), lepidine (0.2 mmol), $(NH_4)_2S_2O_8$ (0.4 mmol), IQO-COF-1 (5 mg), 2-methyl-4-pentenoic acid (0.6 mmol) and DMSO/H_2O (2 mL/1 mL), obtained as colorless oil in 95% yield (40.1 mg) after purification by column chromatography on silica gel eluting with PE/EtOAc (10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.06 (d, J = 8.4 Hz, 1H), 7.95 (d, J = 7.8 Hz, 1H), 7.68-7.66 (m, 1H), 7.52-7.49 (m, 1H), 7.14 (s, 1H), 5.82-5.76 (m, 1H), 5.04 (dd, J = 17.1, 1.6 Hz, 1H), 4.96 (dd, J = 17.0, 0.9 Hz, 1H), 3.17-3.11 (m, 1H), 2.69 (s, 3H), 2.65-2.61 (m, 1H), 2.44-2.39 (m, 1H), 1.27 (d, J = 7.0 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.9, 147.6, 144.3, 136.9, 129.6, 128.9, 127.1, 125.5, 123.6, 120.4, 116.2, 42.5, 41.1, 20.1, 18.9.[23]

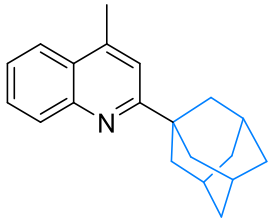


2-heptyl-4-methylquinoline (39): Following **GP2** with TFA (0.2 mmol) to the reaction mixture, lepidine (0.2 mmol), $(NH_4)_2S_2O_8$ (0.4 mmol), IQO-COF-1 (5 mg), octanoic acid (0.6 mmol) and DMSO/H_2O (2 mL/1 mL), obtained as yellow oil in 40% yield (19.3 mg) after purification by column chromatography on silica gel eluting with PE/EtOAc (10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.05 (d, J = 8.4 Hz, 1H), 7.94 (d, J = 8.3 Hz, 1H), 7.68-7.65 (m, 1H), 7.51-7.48 (m, 1H), 7.14 (s, 1H), 2.91 (t, J = 8.4 Hz, 2H), 2.67 (s, 3H), 1.82-1.77 (m, 2H), 1.42-1.27 (m, 8H), 0.87 (t, J = 6.8 Hz, 3H). ^{13}C

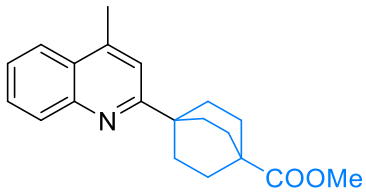
NMR (151 MHz, $CDCl_3$) δ 162.7, 147.5, 144.2, 129.2, 129.0, 126.7, 125.3, 123.5, 122.0, 39.2, 31.7, 30.1, 29.5, 29.1, 22.6, 18.7, 14.0.[27]



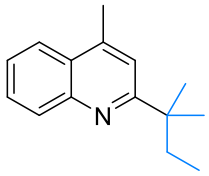
4-methyl-2-(1-methylcyclohexyl)quinoline (40): Following **GP2** with TFA (0.2 mmol) to the reaction mixture, lepidine (0.2 mmol), $(NH_4)_2S_2O_8$ (0.4 mmol), IQO-COF-1 (5 mg), 1-methylcyclohexanecarboxylic acid (0.6 mmol) and DMSO/H_2O (2 mL/1 mL), obtained as yellow oil in 96% yield (46.0 mg) after purification by column chromatography on silica gel eluting with PE/EtOAc (10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.07 (d, J = 8.4 Hz, 1H), 7.95 (dd, J = 8.3, 0.9 Hz, 1H), 7.67-7.65 (m, 1H), 7.51-7.48 (m, 1H), 7.33 (s, 1H), 2.70 (d, J = 0.7 Hz, 3H), 2.39-2.35 (m, 2H), 1.65-1.59 (m, 4H), 1.50-1.45 (m, 4H), 1.30 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$): δ 168.3, 147.7, 143.6, 130.1, 128.7, 126.6, 125.4, 123.5, 119.4, 41.4, 37.3, 29.8, 26.5, 23.0, 19.1.[26]



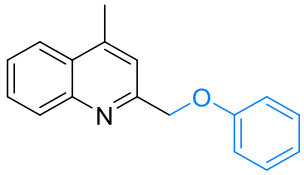
2-(adamantan-1-yl)-4-methylquinoline (41): Following **GP2** with lepidine (0.2 mmol), $(NH_4)_2S_2O_8$ (0.4 mmol), IQO-COF-1 (5 mg), adamantane-1-carboxylic acid (0.6 mmol), DMSO/H_2O (2 mL/1 mL), obtained as white solid in 94% yield (50.1 mg) after purification by column chromatography on silica gel eluting with PE/EtOAc (5:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.08 (d, J = 8.4 Hz, 1H), 7.94 (d, J = 8.2 Hz, 1H), 7.66 (t, J = 7.0 Hz, 1H), 7.49 (t, J = 7.1 Hz, 1H), 7.34 (s, 1H), 2.69 (s, 3H), 2.18-2.12 (m, 9H), 1.84 (s, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 168.8, 147.7, 143.7, 130.1, 128.7, 126.8, 125.4, 123.5, 118.6, 41.9, 39.7, 37.0, 29.0, 19.1.[24]



4-(4-methyl-2-quinolinyl)bicyclo[2.2.2]octane-1-carboxylatemethyl (42): Following **GP2** with lepidine (0.2 mmol), $(NH_4)_2S_2O_8$ (0.4 mmol), IQO-COF-1 (5 mg), phenoxyacetic acid (0.6 mmol), DMSO/H_2O (2 mL/1 mL), obtained as white solid in 52% yield (32.2 mg) after purification by column chromatography on silica gel eluting with PE/EtOAc (5:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.03 (d, *J*=8.3 Hz, 1H), 7.92 (d, *J*=8.2 Hz, 1H), 7.66 (t, *J* = 7.6 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 1H), 7.27 (s, 1H), 3.69 (s, 3H), 2.67 (s, 3H), 2.07-2.05 (m, 6H), 1.97-1.95 (m, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 178.6, 167.2, 147.4, 143.8, 129.8, 128.9, 126.7, 125.5, 123.5, 119.1, 51.7, 39.4, 38.1, 30.5, 28.7, 19.0.[20]

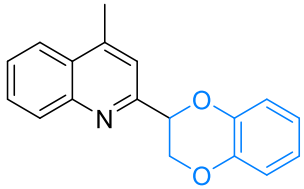


4-methyl-2-(tert-pentyl)quinoline (43): Following **GP2** with lepidine (0.2 mmol), $(NH_4)_2S_2O_8$ (0.4 mmol), IQO-COF-1 (5 mg), 2,2-dimethylbutanoic acid (0.6 mmol), DMSO/H_2O (2 mL/1 mL), obtained as colorless oil in 35% yield (14.9 mg) after purification by column chromatography on silica gel eluting with PE/EtOAc (5:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.08 (d, *J* = 8.2 Hz, 1H), 7.95 (dd, *J* = 8.3, 0.7 Hz, 1H), 7.66 (ddd, *J* = 8.4, 6.8, 1.2 Hz, 1H), 7.50 (ddd, *J* = 8.2, 6.8, 1.2 Hz, 1H), 7.31 (s, 1H), 2.69 (s, 3H), 1.85 (q, *J* = 7.6 Hz, 2H), 1.43 (s, 6H), 0.74 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 168.2, 147.5, 143.5, 130.1, 128.8, 126.6, 125.5, 123.5, 119.5, 41.3, 36.0, 27.5, 19.1, 9.4.[28]



4-methyl-2-(phenoxymethyl)quinoline (44): Following **GP2** with lepidine (0.2 mmol), $(NH_4)_2S_2O_8$ (0.4 mmol), IQO-COF-1 (5 mg), phenoxyacetic acid (0.6 mmol), DMSO/H_2O (2 mL/1 mL), obtained as colorless oil in 83% yield (41.4 mg) after purification by column chromatography on silica gel eluting with PE/EtOAc (5:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.09 (d, *J* = 8.3 Hz, 1H), 8.00 (d, *J* = 8.3 Hz, 1H), 7.74-7.71

(m, 1H), 7.58-7.55 (m, 1H), 7.53 (s, 1H), 7.31-7.28 (m, 2H), 7.04 (d, J = 7.9 Hz, 2H), 6.97 (t, J = 7.3 Hz, 1H), 5.35 (s, 2H), 2.72 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 158.9, 157.6, 147.4, 145.4, 129.6, 129.5, 129.4, 127.7, 126.3, 123.8, 121.2, 119.8, 114.9, 71.3, 18.9.[26]



2-(2,3-dihydrobenzo[b][1,4]dioxin-2-yl)-4-methylquinoline (45): Following **GP2** with lepidine (0.2 mmol), $(NH_4)_2S_2O_8$ (0.4 mmol), IQO-COF-1 (5 mg), 1,4-benzodioxan-2-carboxylic acid (0.6 mmol), DMSO/H_2O (2 mL/1 mL), obtained as colorless oil in 49% yield (27.2 mg) after purification by column chromatography on silica gel eluting with PE/EtOAc (5:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.08 (d, J = 8.3 Hz, 1H), 8.01 (dd, J = 8.3, 0.7 Hz, 1H), 7.75-7.73 (m, 1H), 7.60-7.57 (m, 1H), 7.54 (s, 1H), 7.09-7.07 (m, 1H), 6.96-6.89 (m, 3H), 5.42 (dd, J = 8.0, 2.6 Hz, 1H), 4.71 (dd, J = 11.4, 2.6 Hz, 1H), 4.30 (dd, J = 11.4, 8.1 Hz, 1H), 2.75 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 156.3, 147.3, 145.7, 143.4, 143.3, 129.7, 129.5, 127.7, 126.5, 123.8, 123.7, 121.6, 119.0, 117.4, 117.3, 75.9, 67.9, 19.0.[26]

7 Theoretical results

7.1 Marcus theory calculations for the single electron transfer.

We used the Marcus theory to estimate the barriers for the single electron transfer (SET) processes.

The SET pathway is shown as:

$$\mathbf{COF^{*}} + \mathbf{(NH_4)_2S_2O_8} \rightarrow \mathbf{COF^{+}} + \mathbf{(NH_4)_2SO_4 \cdot OSO_3^{\cdot -}} \qquad (1)$$

The following equation was used to calculate the activation free energy of activation in the SET pathway:

$$\Delta G_{SET}^{\neq} = \Delta G_0^{\neq}[1 + \frac{\Delta_r G^{\theta}}{4\Delta G_0^{\neq}}]^2 \qquad (2)$$

Here, $\Delta_r G^{\theta}$ is the reaction energy of eq. 1 obtained from DFT calculations. The intrinsic barrier is determined using $\Delta G_0^{\neq} = \lambda_0/4$, where λ_0 is the solvent reorganization energy that can be calculated as follows:

$$\lambda_0 = \sqrt{\lambda_1 \lambda_2} \qquad (3)$$

Where λ_1 and λ_2 are the reorganization energies of electron donor and acceptor, respectively. Here we follow the suggestion in the Amador-Bedolla's study.[29]

We proceed to compute λ_1 through:

$$G_2(x_1) - G_1(x_1) = \lambda_1 + \Delta G_1 \qquad (4)$$

and to compute λ_2 we use

$$G_1(x_2) - G_2(x_2) = \lambda_2 + \Delta G_2 \qquad (5)$$

leading to

$$\Delta G_0^{\neq} = \frac{\lambda_0}{4} \qquad (6)$$

Thus,

for **Im-COF-1(p)**, $\Delta G_{SET}^{\neq} = \frac{128.6}{4} * \left[1 + \frac{-59.9}{128.6}\right]^2 = 9.2$ kcal/mol

for **Am-COF-1(p)**, $\Delta G_{SET}^{\neq} = \frac{123.2}{4} * \left[1 + \frac{-53.5}{123.2}\right]^2 = 9.9$ kcal/mol

for **IQO-COF-1(p)**, $\Delta G_{SET}^{\neq} = \frac{114.0}{4} * \left[1 + \frac{-62.3}{114.0}\right]^2 = 5.9$ kcal/mol

for **IQO-COF-2(p)**, $\Delta G_{SET}^{\neq} = \frac{121.0}{4} * \left[1 + \frac{-63.2}{114.0}\right]^2 = 6.9$ kcal/mol

for **IQO-COF-3(p)**, $\Delta G_{SET}^{\neq} = \frac{113.4}{4} * \left[1 + \frac{-53.4}{114.0}\right]^2 = 7.3$ kcal/mol

for **IQO-COF-4(p)**, $\Delta G_{SET}^{\neq} = \frac{113.1}{4} * \left[1 + \frac{-56.5}{114.0}\right]^2 = 7.1$ kcal/mol

7.2 UV-vis spectral simulation

The UV-vis spectral simulation is mainly achieved by the following steps: 1. Molecular dynamics simulation; 2. Conformational de-emphasis; 3. Calculation of spectra for conformations with Boltzmann distributions; and 4. Plotting of the UV-vis spectra.

The contents of the file md.inp, which is set up to perform the MD task, are as follows:

```
$md
    temp= 400 //temperature (K)
    time= 100.0 //total time of simulation (ps)
    dump= 50.0 //write to the trace file every few fs
    step= 1.0 //step size (fs)
    hmass=1 //H atom mass is how many times the actual mass
    shake=1 //H-related bond distances are bounded by the SHAKE algorithm
$end
```

Molclus[30] is used to perform conformational de-duplication, with the *iprog* parameter in settings.ini set to 4 to invoke *xtb*, and the *xtb_arg* parameter set to '--gfn 0 --chrg 0 --uhf 0' to indicate that this is a neutral, singlet state system and calculated with GFN0-xTB. The structures in the .xyz file were deduplication and energy-ordered with the incidental *isostat* script, and the Boltzmann distribution ratios were calculated. The spectra considering conformational weights could be plotted in *Multiwfn*[10]. UV-vis images are plotted with full width at half maximum (FWHM) set to 0.5eV and gaussian function is used as spreading function.

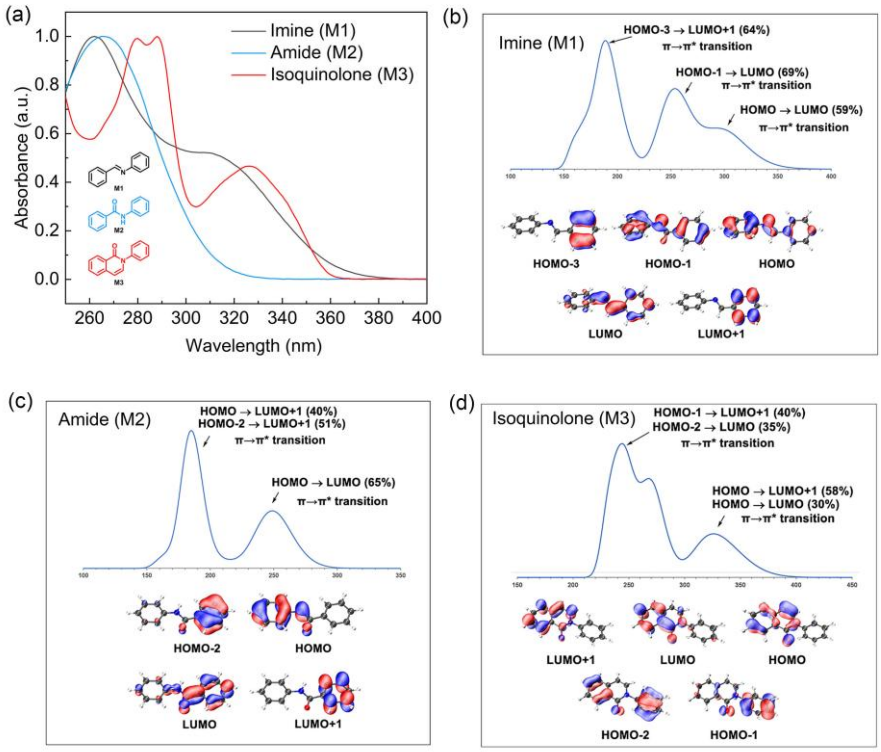


Figure S21. UV spectra of model compounds (ethanol as solvent) (a). UV-vis spectral simulation of Imine (M1) (b), Amide (M2) (c), and Isoquinolone (M3) (d).

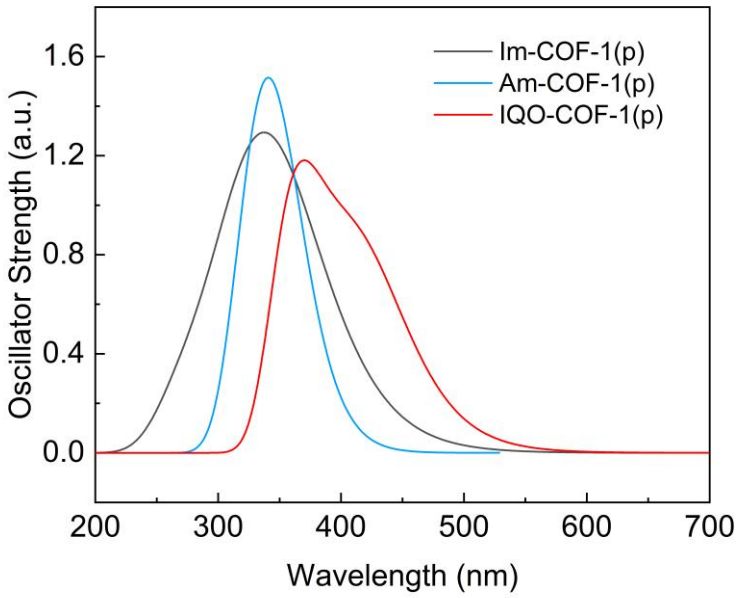


Figure S22. UV-vis spectral simulation of different COFs

7.3 Calculated energies

$G_{sol} = E_{sol} + G_{corr}$

E_{sol} refers to the single point energy involved solvent effects by wB97XD/def2-TZVP /SMD(DMSO).

G_{corr} refers to the thermal correction to the Gibbs free energy calculated at wB97XD/def2-SVP /SMD(DMSO) level of theory.

G_{sol} refers to the sum of the solvation single point energy and the thermal correction to the Gibbs free energy.

Table S7. The G_{corr}, E_{sol} and G_{sol} of Optimized Structures

File Name	Functional	G_{corr}(Hartree)	charge◇spin	E_{sol}(Hartree)
Im-COF-1(p)$^+$	UwB97XD	0.7075	(1 ◇ 2)	-2267.4137
Im-COF-1(p)	RwB97XD	0.7105	(0 ◇ 1)	-2267.4890
Am-COF-1(p)$^+$	UwB97XD	0.7200	(1 ◇ 2)	-2417.9618
Am-COF-1(p)	RwB97XD	0.7193	(0 ◇ 1)	-2418.0438
IQO-COF-1(p)$^+$	UwB97XD	0.7442	(1 ◇ 2)	-2570.3904
IQO-COF-1(p)	RwB97XD	0.7443	(0 ◇ 1)	-2570.4591
IQO-COF-2$^+$	UwB97XD	0.8185	(1 ◇ 2)	-2801.4446
IQO-COF-2	RwB97XD	0.8193	(0 ◇ 1)	-2801.5126
IQO-COF-3$^+$	UwB97XD	1.0944	(1 ◇ 2)	-3799.5246
IQO-COF-3	RwB97XD	1.0950	(0 ◇ 1)	-3799.6079
IQO-COF-4$^+$	UwB97XD	1.1722	(1 ◇ 2)	-4030.5940
IQO-COF-4	RwB97XD	1.1705	(0 ◇ 1)	-4030.6701
S_2O_8-2NH_4	RwB97XD	0.0958	(0 ◇ 1)	-1511.3512
SO_4+SO_4^--2NH_4	UwB97XD	0.0851	(-1 ◇ 2)	-1511.5084

7.4 Coordinates

Im-COF-1(p)$^+$			Im-COF-1(p)		
C	-14.050002	-4.135388 -1.017215	C	-13.740959	-4.794619 -0.671281
C	-13.123875	-4.154400 0.025980	C	-12.511145	-4.813041 -0.012821

C -14.083838 -3.045919 -1.887977	C -14.231516 -3.590684 -1.177501
C -12.237070 -3.092609 0.196780	C -11.777464 -3.637371 0.137558
H -13.094305 -4.999839 0.717479	H -12.120800 -5.749153 0.393659
C -13.198629 -1.983017 -1.716840	C -13.498491 -2.414712 -1.026434
H -14.800843 -3.024540 -2.712149	H -15.190295 -3.566113 -1.700995
C -12.262399 -1.991340 -0.672008	C -12.259850 -2.420167 -0.367135
H -11.528645 -3.111843 1.028742	H -10.824324 -3.663442 0.671459
H -13.224473 -1.143508 -2.416015	H -13.886855 -1.482351 -1.443515
C -11.317476 -0.855435 -0.489126	C -11.476465 -1.163871 -0.207305
C -11.738904 0.463865 -0.699209	C -12.121659 0.047382 0.069285
C -9.992373 -1.084883 -0.109322	C -10.082073 -1.172641 -0.331130
C -10.866867 1.546789 -0.529534	C -11.397828 1.235924 0.222607
H -12.770884 0.652211 -1.003584	H -13.209470 0.065307 0.167571
C -9.098412 -0.018563 0.078062	C -9.332843 0.001280 -0.184182
H -9.655930 -2.110570 0.052294	H -9.569270 -2.112990 -0.546060
C -9.551342 1.293626 -0.132175	C -10.004316 1.198482 0.092925
C -11.332768 2.941176 -0.764471	C -12.098350 2.516463 0.517860
H -8.867085 2.133285 0.002067	H -9.430616 2.120743 0.209475
C -12.618897 3.343142 -0.373980	C -13.206766 2.546576 1.377911
C -10.494915 3.881980 -1.381863	C -11.666734 3.721538 -0.057123
C -13.053679 4.649103 -0.593583	C -13.863366 3.744711 1.654305
H -13.282528 2.632355 0.124619	H -13.550130 1.623982 1.852296
C -10.930974 5.187315 -1.602358	C -12.323788 4.919517 0.219117
H -9.495763 3.585940 -1.711123	H -10.817311 3.721312 -0.744647
C -12.211760 5.575893 -1.208835	C -13.424496 4.936155 1.076119
H -14.056197 4.945373 -0.275803	H -14.720445 3.747235 2.332070
H -10.266434 5.903783 -2.091055	H -11.975840 5.845704 -0.244592
H -12.553188 6.599285 -1.381275	H -13.939313 5.875212 1.292628
C -7.705676 -0.272073 0.484081	C -7.851362 -0.024406 -0.319732

C	-7.044741	-1.471239	0.102961	C	-7.227020	-0.840460	-1.276720
C	-6.988777	0.678401	1.260794	C	-7.037029	0.774637	0.495790
C	-5.743926	-1.715176	0.456337	C	-5.844230	-0.855662	-1.413852
H	-7.568369	-2.207062	-0.508909	H	-7.833448	-1.455655	-1.945802
C	-5.690201	0.460836	1.638047	C	-5.650719	0.751267	0.376153
H	-7.483217	1.591982	1.593808	H	-7.491051	1.420164	1.251486
C	-5.032564	-0.752640	1.246741	C	-5.034999	-0.076159	-0.575002
H	-5.229173	-2.625946	0.147386	H	-5.369400	-1.478896	-2.174846
H	-5.142488	1.184157	2.243598	H	-5.040580	1.394043	1.014962
N	-3.781334	-0.953780	1.563719	N	-3.645545	-0.128405	-0.757775
C	-2.795186	-1.322258	2.250191	C	-2.864426	-0.119154	0.248616
C	-1.402523	-1.124367	1.850271	C	-1.398430	-0.119559	0.106081
C	-1.073838	-0.509160	0.633242	C	-0.786571	-0.119176	-1.155497
C	-0.389253	-1.563015	2.716491	C	-0.598335	-0.120139	1.258715
C	0.259232	-0.337131	0.290230	C	0.598348	-0.120352	-1.258540
C	0.942444	-1.384705	2.370201	C	0.786584	-0.119024	1.155671
H	-0.653860	-2.042666	3.661752	H	-1.073170	-0.120676	2.243384
C	1.276349	-0.770696	1.154701	C	1.398443	-0.119621	-0.105906
H	0.522098	0.140242	-0.656801	H	1.073183	-0.121057	-2.243209
C	2.683708	-0.566795	0.761586	C	2.864442	-0.119282	-0.248441
N	3.649798	-0.920623	1.511157	N	3.645562	-0.128360	0.757950
H	-14.744819	-4.967857	-1.150841	H	-14.315571	-5.716302	-0.789667
C	13.631553	-4.236126	-2.098270	C	13.740987	-4.794601	0.671171
C	12.296571	-4.127449	-2.488607	C	12.511157	-4.813028	0.012740
C	14.185490	-3.263678	-1.265266	C	14.231549	-3.590666	1.177386
C	11.521462	-3.055381	-2.049263	C	11.777467	-3.637361	-0.137617
H	11.854742	-4.879870	-3.146332	H	12.120809	-5.749140	-0.393736
C	13.410979	-2.190911	-0.826730	C	13.498515	-2.414698	1.026341
H	15.228039	-3.342771	-0.947869	H	15.190341	-3.566094	1.700857

C	12.067022	-2.070434	-1.211928	C	12.259858	-2.420157	0.367070
H	10.482314	-2.973839	-2.377297	H	10.824315	-3.663433	-0.671497
H	13.852543	-1.445986	-0.160171	H	13.886882	-1.482335	1.443416
C	11.239989	-0.924595	-0.742194	C	11.476466	-1.163864	0.207257
C	11.790854	0.358793	-0.644936	C	12.121650	0.047390	-0.069355
C	9.898242	-1.111394	-0.389142	C	10.082078	-1.172637	0.331117
C	11.025747	1.444226	-0.201852	C	11.397811	1.235929	-0.222669
H	12.836444	0.516291	-0.919412	H	13.209458	0.065317	-0.167672
C	9.109595	-0.043916	0.057655	C	9.332842	0.001281	0.184181
H	9.459356	-2.108894	-0.463972	H	9.569281	-2.112985	0.546068
C	9.687474	1.228554	0.147620	C	10.004303	1.198485	-0.092951
C	11.625156	2.803957	-0.104839	C	12.098325	2.516468	-0.517948
H	9.084006	2.069500	0.496651	H	9.430595	2.120742	-0.209494
C	12.524651	3.262266	-1.079437	C	13.206723	2.546576	-1.378023
C	11.304214	3.657292	0.961823	C	11.666717	3.721546	0.057033
C	13.085345	4.535356	-0.990625	C	13.863316	3.744711	-1.654438
H	12.775935	2.622427	-1.928882	H	13.550078	1.623979	-1.852408
C	11.866202	4.929849	1.051127	C	12.323765	4.919524	-0.219228
H	10.620466	3.315824	1.742958	H	10.817307	3.721323	0.744572
C	12.758598	5.374284	0.075126	C	13.424456	4.936158	-1.076251
H	13.777878	4.876019	-1.764105	H	14.720382	3.747231	-2.332220
H	11.608868	5.576017	1.893845	H	11.975825	5.845715	0.244480
H	13.198283	6.372012	0.145108	H	13.939268	5.875213	-1.292776
C	7.684536	-0.258654	0.428255	C	7.851365	-0.024405	0.319774
C	7.275292	-1.433876	1.078387	C	7.227054	-0.840453	1.276787
C	6.711417	0.712480	0.149700	C	7.037007	0.774630	-0.495728
C	5.946773	-1.629835	1.436415	C	5.844269	-0.855651	1.413976
H	8.011691	-2.198892	1.335360	H	7.833506	-1.455654	1.945844
C	5.376747	0.515845	0.489596	C	5.650699	0.751261	-0.376039

H	6.994985	1.638045	-0.356762	H	7.491005	1.420144	-1.251451
C	4.975428	-0.667535	1.127241	C	5.035015	-0.076150	0.575152
H	5.641743	-2.538538	1.959965	H	5.369476	-1.478887	2.174991
H	4.643390	1.296145	0.273945	H	5.040529	1.394017	-1.014839
H	14.238792	-5.076767	-2.442214	H	14.315609	-5.716281	0.789538
H	1.739845	-1.720298	3.035306	H	1.411578	-0.119288	2.050786
H	-1.865075	-0.169537	-0.039215	H	-1.411565	-0.119552	-2.050612
H	-2.991251	-1.825204	3.212404	H	-3.245351	-0.122080	1.286123
H	2.842657	-0.098254	-0.225978	H	3.245371	-0.122385	-1.285946
Am-COF-1(p)$^{+}$				Am-COF-1			
C	13.295664	-4.547125	2.794317	C	13.325026	-4.759609	2.400424
C	12.120090	-4.754524	2.072243	C	12.143814	-4.906160	1.672660
C	13.849859	-3.268115	2.852450	C	13.887059	-3.491515	2.550295
C	11.503589	-3.691699	1.413850	C	11.529230	-3.793783	1.099940
H	11.681311	-5.753559	2.014389	H	11.698786	-5.895683	1.543249
C	13.234231	-2.205287	2.193208	C	13.273228	-2.379091	1.976841
H	14.766543	-3.092926	3.420745	H	14.808460	-3.364384	3.123703
C	12.051762	-2.400860	1.463355	C	12.084495	-2.512972	1.243220
H	10.592839	-3.872339	0.837527	H	10.613928	-3.926045	0.517784
H	13.670190	-1.205595	2.262404	H	13.715247	-1.389625	2.117612
C	11.394568	-1.266793	0.756326	C	11.427427	-1.324197	0.632366
C	12.160848	-0.296247	0.099768	C	12.193125	-0.306483	0.050817
C	9.999273	-1.154026	0.733528	C	10.032566	-1.204819	0.629092
C	11.555886	0.773309	-0.571352	C	11.587270	0.816645	-0.525124
H	13.250337	-0.375087	0.110877	H	13.282355	-0.390229	0.046349
C	9.367427	-0.095286	0.069691	C	9.399502	-0.092128	0.061365
H	9.392627	-1.906738	1.242407	H	9.427127	-1.995225	1.078449
C	10.158728	0.861279	-0.578184	C	10.190683	0.911788	-0.510869
C	12.383996	1.798735	-1.264638	C	12.413697	1.890808	-1.142429

H	9.675773	1.691799	-1.098118	H	9.709150	1.785796	-0.955222
C	13.548895	1.433225	-1.956388	C	13.563161	1.575934	-1.883217
C	12.018812	3.153513	-1.241861	C	12.061305	3.241522	-0.998856
C	14.323669	2.392500	-2.606482	C	14.335766	2.580797	-2.463244
H	13.844729	0.382341	-2.003055	H	13.847954	0.530375	-2.024279
C	12.794185	4.112716	-1.891301	C	12.834587	4.246212	-1.578265
H	11.126601	3.465793	-0.693655	H	11.180831	3.513068	-0.411289
C	13.949578	3.736207	-2.576574	C	13.974771	3.920023	-2.313080
H	15.223143	2.085776	-3.145751	H	15.223090	2.313774	-3.042308
H	12.495790	5.163229	-1.855309	H	12.546543	5.292236	-1.448620
H	14.556985	4.488141	-3.085853	H	14.580463	4.707539	-2.767685
C	7.883985	0.012820	0.052567	C	7.916225	0.020991	0.065568
C	7.117764	-0.324947	1.178691	C	7.155002	-0.440141	1.150834
C	7.201424	0.457005	-1.086779	C	7.227138	0.590451	-1.012635
C	5.733857	-0.217694	1.163745	C	5.771143	-0.333007	1.154894
H	7.610108	-0.659553	2.094796	H	7.650917	-0.875104	2.021678
C	5.812996	0.565731	-1.118909	C	5.838669	0.702659	-1.024791
H	7.762359	0.710967	-1.989521	H	7.781930	0.943214	-1.885427
C	5.061802	0.229203	0.015434	C	5.092330	0.239404	0.067582
H	5.159699	-0.474997	2.057881	H	5.201785	-0.689880	2.017321
H	5.309067	0.901747	-2.021514	H	5.329539	1.139030	-1.880306
N	3.663161	0.320170	0.083952	N	3.694342	0.313964	0.150819
C	2.781894	0.677660	-0.893209	C	2.808657	0.810988	-0.760431
C	1.339719	0.727652	-0.454961	C	1.364920	0.781451	-0.328334
O	3.092164	0.934311	-2.043354	O	3.123617	1.243601	-1.855947
C	0.951906	1.041533	0.852943	C	0.959111	0.789512	1.011728
C	0.361086	0.499506	-1.426877	C	0.393820	0.796980	-1.334352
C	-0.396011	1.108840	1.183410	C	-0.393699	0.798350	1.333170
C	-0.987741	0.543401	-1.094557	C	-0.958991	0.788248	-1.012895

H	0.666428	0.287339	-2.452577	H	0.710900	0.821731	-2.378084
C	-1.374530	0.843420	0.218573	C	-1.364816	0.781558	0.327174
H	-0.699037	1.367123	2.199224	H	-0.710805	0.824173	2.376867
C	-2.799995	0.950419	0.651835	C	-2.808535	0.811280	0.759376
O	-3.145672	1.593458	1.613412	O	-3.123383	1.244476	1.854693
N	-3.713484	0.223862	-0.133225	N	-3.694339	0.313707	-0.151463
H	13.778907	-5.380183	3.310230	H	13.806320	-5.631455	2.849787
C	-13.345359	-4.630817	-2.535228	C	-13.325537	-4.759497	-2.399841
C	-12.162890	-4.824115	-1.820715	C	-12.144283	-4.906113	-1.672159
C	-13.890417	-3.350309	-2.632579	C	-13.887511	-3.491372	-2.549671
C	-11.528726	-3.744448	-1.208660	C	-11.529597	-3.793770	-1.099481
H	-11.732662	-5.824475	-1.732445	H	-11.699302	-5.895660	-1.542774
C	-13.258460	-2.270070	-2.019231	C	-13.273575	-2.378982	-1.976261
H	-14.812787	-3.187945	-3.195144	H	-14.808944	-3.364189	-3.123015
C	-12.068059	-2.452809	-1.300086	C	-12.084796	-2.512928	-1.242727
H	-10.612591	-3.912011	-0.636851	H	-10.614267	-3.926091	-0.517383
H	-13.687229	-1.269711	-2.118276	H	-13.715551	-1.389494	-2.117007
C	-11.389107	-1.299794	-0.648044	C	-11.427608	-1.324176	-0.631954
C	-12.136086	-0.296158	-0.012466	C	-12.193189	-0.306401	-0.050362
C	-10.000771	-1.191777	-0.660389	C	-10.032742	-1.204889	-0.628812
C	-11.520523	0.799039	0.612602	C	-11.587201	0.816706	0.525475
H	-13.225938	-0.369574	-0.004182	H	-13.282423	-0.390082	-0.045777
C	-9.344205	-0.109290	-0.032924	C	-9.399530	-0.092213	-0.061213
H	-9.421936	-1.968086	-1.160204	H	-9.427422	-1.995377	-1.078179
C	-10.130094	0.876918	0.604635	C	-10.190609	0.911766	0.511062
C	-12.338251	1.850725	1.276553	C	-12.413489	1.890945	1.142839
H	-9.652935	1.724913	1.095099	H	-9.709009	1.785783	0.955318
C	-13.490299	1.509556	2.000371	C	-13.562887	1.576165	1.883775
C	-11.971869	3.202238	1.193296	C	-12.061037	3.241635	0.999188

C -14.252976 2.493563 2.626865	C -14.335362 2.581089 2.463864
H -13.785448 0.461455 2.092196	H -13.847730 0.530629 2.024907
C -12.736475 4.185427 1.818733	C -12.834190 4.246387 1.578662
H -11.089714 3.492822 0.617429	H -11.180624 3.513123 0.411503
C -13.879079 3.834648 2.538126	C -13.974305 3.920290 2.313622
H -15.142812 2.208566 3.193059	H -15.222635 2.314131 3.043037
H -12.439942 5.233754 1.737113	H -12.546099 5.292390 1.448950
H -14.477823 4.605694 3.028587	H -14.579893 4.707856 2.768278
C -7.893171 -0.012301 -0.044278	C -7.916242 0.020829 -0.065600
C -7.101300 -0.788337 -0.947532	C -7.155126 -0.440783 -1.150740
C -7.198967 0.863777 0.847245	C -7.227008 0.590719 1.012287
C -5.741186 -0.691197 -0.961626	C -5.771266 -0.333699 -1.154982
H -7.578596 -1.457168 -1.662571	H -7.651101 -0.876085 -2.021377
C -5.835500 0.964564 0.857766	C -5.838537 0.702905 1.024254
H -7.756331 1.459718 1.568737	H -7.781672 0.943861 1.885005
C -5.062905 0.185522 -0.056153	C -5.092315 0.239177 -0.068001
H -5.155030 -1.279700 -1.670351	H -5.202015 -0.690980 -2.017310
H -5.337774 1.625323 1.561349	H -5.329318 1.139644 1.879527
H -13.841948 -5.477251 -3.015311	H -13.806909 -5.631316 -2.849175
H -1.724289 0.370736 -1.882341	H -1.689784 0.816184 -1.824369
H -3.303456 -0.392450 -0.833029	H -3.301140 -0.093929 -0.993195
H 1.695030 1.261783 1.622427	H 1.689968 0.818468 1.823110
H 3.264896 0.036185 0.973161	H 3.300995 -0.093406 0.992618
IQO-COF-1(p)$^{+}$	IQO- COF-1(p)
C 13.478345 -4.831994 -1.302973	C 13.468287 4.855972 1.246257
C 12.254242 -4.526877 -1.898735	C 12.243857 4.557395 1.844655
C 14.030849 -3.948410 -0.375368	C 14.022273 3.961076 0.330463
C 11.587729 -3.347774 -1.569408	C 11.578585 3.373683 1.529691
H 11.816135 -5.208813 -2.631496	H 11.804433 5.248165 2.568298

C	13.365176	-2.768655	-0.046608	C	13.357729	2.776770	0.016025
H	14.985550	-4.181128	0.102474	H	14.977231	4.188434	-0.149469
C	12.133448	-2.450646	-0.638761	C	12.125659	2.465116	0.610935
H	10.638515	-3.112493	-2.057110	H	10.629119	3.144018	2.019545
H	13.800814	-2.094352	0.694888	H	13.794597	2.093603	-0.716572
C	11.421383	-1.190883	-0.287986	C	11.414735	1.200422	0.275575
C	12.132529	-0.002275	-0.084489	C	12.127190	0.010418	0.085002
C	10.027880	-1.173834	-0.155662	C	10.020979	1.180057	0.145711
C	11.476225	1.189512	0.245675	C	11.471239	-1.185614	-0.230269
H	13.220236	-0.004648	-0.185945	H	13.215062	0.015058	0.184713
C	9.347091	0.003892	0.174079	C	9.339991	-0.001750	-0.169261
H	9.463215	-2.095513	-0.313433	H	9.455282	2.102756	0.293548
C	10.082167	1.178539	0.372243	C	10.076905	-1.177442	-0.354849
C	12.246175	2.446544	0.456165	C	12.242032	-2.444205	-0.428446
H	9.559994	2.102985	0.629155	H	9.555311	-2.105365	-0.600309
C	13.348305	2.757338	-0.354724	C	13.345639	-2.745840	0.383942
C	11.886248	3.348446	1.469013	C	11.881497	-3.356898	-1.431418
C	14.068586	3.934494	-0.158713	C	14.066607	-3.924408	0.199037
H	13.635973	2.079624	-1.162251	H	13.633964	-2.059591	1.184006
C	12.607694	4.524884	1.665669	C	12.603552	-4.534766	-1.616956
H	11.042250	3.119230	2.124246	H	11.036382	-3.135209	-2.087796
C	13.701544	4.822744	0.852543	C	13.698833	-4.823391	-0.802429
H	14.919313	4.161625	-0.805670	H	14.918413	-4.144190	0.847130
H	12.315900	5.210309	2.465004	H	12.310997	-5.228662	-2.408676
H	14.266435	5.745145	1.006665	H	14.264200	-5.746933	-0.947761
C	7.865040	0.006624	0.311357	C	7.857570	-0.007520	-0.304012
C	7.196045	-1.081996	0.887647	C	7.185172	1.071485	-0.893795
C	7.104770	1.099799	-0.133114	C	7.097463	-1.094205	0.156077
C	5.809560	-1.085360	1.012134	C	5.797756	1.070536	-1.014366

H	7.762835	-1.938322	1.258716	H	7.750347	1.923628	-1.277556
C	5.720635	1.109500	-0.006930	C	5.712943	-1.105811	0.030077
H	7.598858	1.955259	-0.598260	H	7.593074	-1.942939	0.632467
C	5.080168	0.013035	0.566016	C	5.061931	-0.019701	-0.554356
H	5.294256	-1.937772	1.459684	H	5.283437	1.917838	-1.473125
H	5.139536	1.965475	-0.353732	H	5.133821	-1.957483	0.390500
N	3.648409	0.019401	0.717576	N	3.636465	-0.029574	-0.706474
C	3.116896	0.022415	1.960390	C	3.109971	-0.027284	-1.989744
C	2.851770	-0.011735	-0.452222	C	2.844041	-0.010245	0.439067
C	1.757497	0.006836	2.199928	C	1.783849	-0.017703	-2.232339
H	3.835844	0.045326	2.781389	H	3.851657	-0.042938	-2.789375
C	1.390659	-0.004828	-0.215193	C	1.381858	-0.012883	0.194225
O	3.362751	-0.048302	-1.547088	O	3.335994	0.015304	1.553564
C	0.866592	-0.001960	1.116678	C	0.860178	-0.013007	-1.124540
H	1.398051	0.012947	3.228415	H	1.416785	-0.023013	-3.258760
C	0.544353	-0.005705	-1.299187	C	0.528746	-0.010776	1.294958
C	-0.544382	-0.005655	1.298852	C	-0.528757	-0.011008	-1.294906
C	-0.866622	-0.001988	-1.117015	C	-0.860175	-0.012642	1.124597
H	0.952843	-0.007076	-2.311319	H	0.958009	-0.009808	2.298564
C	-1.390688	-0.004816	0.214864	C	-1.381863	-0.012757	-0.194184
H	-0.952869	-0.006973	2.310984	H	-0.957989	-0.010218	-2.298524
C	-1.757521	0.006813	-2.200256	C	-1.783844	-0.016993	2.232394
C	-2.851797	-0.011719	0.451886	C	-2.844050	-0.009980	-0.439011
H	-1.398081	0.012907	-3.228746	H	-1.416767	-0.022042	3.258812
C	-3.116942	0.022441	-1.960718	C	-3.109967	-0.026560	1.989806
O	-3.362802	-0.048294	1.546735	O	-3.336015	0.015520	-1.553505
N	-3.648446	0.019430	-0.717923	N	-3.636459	-0.029148	0.706536
H	-3.835879	0.045373	-2.781728	H	-3.851656	-0.041973	2.789436
H	14.000723	-5.756282	-1.560924	H	13.989669	5.783892	1.492965

C	-13.478154	-4.832049	1.303289	C	-13.468666	4.855688	-1.246479
C	-12.254005	-4.526922	1.898953	C	-12.244211	4.557185	-1.844864
C	-14.030746	-3.948459	0.375741	C	-14.022575	3.960791	-0.330640
C	-11.587532	-3.347810	1.569581	C	-11.578839	3.373545	-1.529844
H	-11.815830	-5.208859	2.631672	H	-11.804848	5.247956	-2.568544
C	-13.365111	-2.768696	0.046935	C	-13.357931	2.776556	-0.016146
H	-14.985486	-4.181179	-0.102020	H	-14.977553	4.188093	0.149278
C	-12.133333	-2.450682	0.638981	C	-12.125835	2.464977	-0.611042
H	-10.638283	-3.112524	2.057212	H	-10.629356	3.143933	-2.019690
H	-13.800822	-2.094390	-0.694515	H	-13.794743	2.093387	0.716483
C	-11.421318	-1.190906	0.288155	C	-11.414812	1.200353	-0.275628
C	-12.132505	-0.002314	0.084705	C	-12.127181	0.010301	-0.085027
C	-10.027827	-1.173830	0.155716	C	-10.021056	1.180101	-0.145746
C	-11.476253	1.189485	-0.245521	C	-11.471146	-1.185673	0.230274
H	-13.220204	-0.004708	0.186256	H	-13.215054	0.014864	-0.184742
C	-9.347089	0.003907	-0.174093	C	-9.339978	-0.001648	0.169257
H	-9.463129	-2.095495	0.313453	H	-9.455443	2.102847	-0.293606
C	-10.082206	1.178536	-0.372211	C	-10.076810	-1.177390	0.354853
C	-12.246241	2.446504	-0.455942	C	-12.241845	-2.444318	0.428477
H	-9.560077	2.102990	-0.629185	H	-9.555151	-2.105271	0.600329
C	-13.348309	2.757277	0.355039	C	-13.345445	-2.746038	-0.383890
C	-11.886408	3.348422	-1.468809	C	-11.881240	-3.356975	1.431457
C	-14.068622	3.934425	0.159099	C	-14.066330	-3.924652	-0.198964
H	-13.635904	2.079554	1.162585	H	-13.633832	-2.059819	-1.183958
C	-12.607885	4.524852	-1.665394	C	-12.603212	-4.534890	1.617018
H	-11.042459	3.119226	-2.124112	H	-11.036141	-3.135218	2.087833
C	-13.701674	4.822690	-0.852177	C	-13.698483	-4.823600	0.802507
H	-14.919299	4.161538	0.806127	H	-14.918132	-4.144499	-0.847039
H	-12.316162	5.210290	-2.464744	H	-12.310601	-5.228756	2.408744

H -14.266587 5.745088 -1.006242	H -14.263783 -5.747180 0.947854
C -7.865053 0.006665 -0.311498	C -7.857557 -0.007330 0.304016
C -7.196085 -1.081998 -0.887737	C -7.185234 1.071719 0.893805
C -7.104763 1.099885 0.132836	C -7.097384 -1.093993 -0.156007
C -5.809605 -1.085368 -1.012309	C -5.797822 1.070859 1.014421
H -7.762890 -1.938369 -1.258680	H -7.750474 1.923833 1.277535
C -5.720638 1.109590 0.006553	C -5.712861 -1.105517 -0.029974
H -7.598824 1.955367 0.597969	H -7.592924 -1.942777 -0.632380
C -5.080204 0.013076 -0.566337	C -5.061936 -0.019346 0.554439
H -5.294329 -1.937818 -1.459813	H -5.283548 1.918177 1.473196
H -5.139518 1.965600 0.353233	H -5.133679 -1.957174 -0.390333
H -14.000501 -5.756344 1.561275	H -13.990125 5.783553 -1.493229
S_2O_8-2NH_4	**SO_4+SO_4-2NH_4**
S 1.946988 -0.385063 0.170631	S 2.883632 -0.008124 -0.039420
O 2.808749 -0.780546 -0.928463	O 4.312369 -0.000489 0.313004
O 2.204099 -0.923301 1.492521	O 2.001958 -0.098557 1.192686
O 0.503285 -1.104436 -0.374072	O 2.553479 -1.168620 -0.948674
O 1.635652 1.076319 0.179919	O 2.510561 1.283236 -0.757071
O -0.501400 -0.988560 0.621697	O -3.190007 1.107785 0.872620
S -1.945401 -0.417220 -0.074197	S -2.950977 -0.083204 -0.035116
O -2.198992 -1.243841 -1.238527	O -3.134880 -1.369181 0.625128
O -2.808547 -0.551711 1.084823	O -4.070624 0.267471 -0.997411
O -1.637531 1.004284 -0.419029	O -1.624170 0.020848 -0.700912
N 0.324093 1.617558 -2.220802	N 0.295848 -1.873709 0.177012
H 1.056973 1.575571 -1.484773	H 1.104725 -1.820745 -0.511107
H 0.274771 2.553970 -2.631288	H 0.060014 -2.823937 0.463142
H 0.525997 0.933796 -2.955836	H 0.732382 -1.304782 0.940641
H -0.568205 1.376691 -1.732506	H -0.526402 -1.363684 -0.186857
N -0.330444 2.110915 1.775006	N 0.243193 1.967986 0.220326

H	-0.280466	3.119191	1.943641	H	-0.027361	2.948721	0.131264
H	-0.537519	1.628148	2.653704	H	0.386965	1.732642	1.205337
H	-1.058749	1.887782	1.066959	H	-0.505003	1.357299	-0.151633
H	0.563742	1.756421	1.366781	H	1.209419	1.735831	-0.274523
IQO-COF-2^{+}				IQO-COF-2			
C	-15.465074	-4.236352	-2.975737	C	-15.472199	-4.246399	-2.960451
C	-14.359369	-3.586482	-3.524826	C	-14.356040	-3.611965	-3.506465
C	-13.727078	-2.561595	-2.822748	C	-13.720804	-2.585392	-2.809488
C	-14.189456	-2.166291	-1.558197	C	-14.190419	-2.172774	-1.553123
C	-15.302189	-2.827802	-1.016845	C	-15.313621	-2.819006	-1.014847
C	-15.933652	-3.853163	-1.718818	C	-15.948126	-3.846032	-1.711661
C	-13.515358	-1.070350	-0.808954	C	-13.513159	-1.074892	-0.809480
C	-14.262723	-0.154255	-0.058998	C	-14.259311	-0.144889	-0.075587
C	-13.642671	0.872640	0.662724	C	-13.635449	0.883918	0.640062
C	-12.246968	0.973730	0.625840	C	-12.238599	0.973047	0.612392
C	-11.476080	0.071765	-0.116722	C	-11.467892	0.056660	-0.112951
C	-12.121193	-0.945274	-0.830074	C	-12.117651	-0.962374	-0.819653
C	-14.451654	1.846076	1.446742	C	-14.441624	1.872620	1.407790
C	-9.993336	0.190255	-0.144190	C	-9.983559	0.162996	-0.129785
C	-9.273573	-0.074595	-1.317707	C	-9.254267	-0.118877	-1.292835
C	-7.886438	0.028367	-1.344697	C	-7.864755	-0.025682	-1.306293
C	-7.210823	0.405173	-0.186957	C	-7.183588	0.363458	-0.154482
C	-7.898987	0.676902	0.993582	C	-7.891780	0.653653	1.011537
C	-9.283921	0.568402	1.006871	C	-9.278004	0.549145	1.020766
C	-15.680882	2.317304	0.961120	C	-15.663022	2.349867	0.908409
C	-16.436382	3.228266	1.697648	C	-16.415574	3.275339	1.629769
C	-15.978010	3.684574	2.933770	C	-15.962069	3.740632	2.864357
C	-14.757510	3.223199	3.427619	C	-14.749443	3.273401	3.371932
C	-14.001280	2.313026	2.691060	C	-13.996268	2.348680	2.650502

N	-5.776143	0.531162	-0.223875	N	-5.755846	0.486795	-0.182075
C	-4.993990	-0.351216	0.603339	C	-4.994485	-0.368966	0.617771
C	-3.534176	-0.186399	0.511338	C	-3.534092	-0.186478	0.512731
C	-2.962552	0.766209	-0.375688	C	-2.972429	0.778304	-0.349017
C	-3.823624	1.556864	-1.158538	C	-3.857662	1.596811	-1.139051
C	-5.212850	1.413128	-1.044958	C	-5.191551	1.425338	-1.028095
C	-2.703687	-0.977638	1.294899	C	-2.693001	-1.000772	1.288930
C	-1.319340	-0.830805	1.208006	C	-1.320157	-0.863442	1.215742
C	-0.726391	0.105845	0.336171	C	-0.739155	0.099067	0.359396
C	-1.556431	0.898542	-0.450209	C	-1.571255	0.906484	-0.409360
C	0.751693	0.244439	0.261701	C	0.739687	0.244453	0.282068
C	1.569263	-0.877476	0.337623	C	1.564654	-0.874179	0.341140
C	2.970805	-0.759653	0.262873	C	2.965675	-0.752937	0.266559
C	3.541143	0.521327	0.114634	C	3.534868	0.530287	0.132545
C	2.711864	1.652398	0.042850	C	2.701178	1.659406	0.076677
C	1.338418	1.520289	0.110934	C	1.328140	1.522335	0.147367
C	3.846039	-1.902315	0.328348	C	3.843325	-1.895109	0.318132
C	5.180490	-1.717508	0.248849	C	5.177358	-1.707895	0.240135
N	5.754936	-0.466859	0.106172	N	5.749681	-0.454411	0.110807
C	5.003828	0.709296	0.041038	C	4.996143	0.721399	0.058810
O	-5.553893	-1.162025	1.296189	O	-5.522531	-1.203234	1.333592
O	5.539238	1.799923	-0.058494	O	5.531460	1.813494	-0.030027
C	7.184397	-0.371989	0.067142	C	7.178647	-0.357694	0.070840
C	7.933126	-0.803072	1.160719	C	7.929385	-0.797828	1.159491
C	9.323525	-0.736758	1.119546	C	9.319764	-0.732644	1.116262
C	9.986715	-0.228000	-0.005209	C	9.981532	-0.216329	-0.005903
C	9.214098	0.204828	-1.094395	C	9.207078	0.226718	-1.089716
C	7.826278	0.130366	-1.064834	C	7.819200	0.153702	-1.057909
C	11.471968	-0.147031	-0.046945	C	11.466948	-0.139341	-0.050910

C	12.106752	0.951150	-0.639191	C	12.103862	0.958169	-0.642148
C	13.502936	1.048776	-0.674480	C	13.500258	1.051085	-0.681484
C	14.264616	0.021559	-0.104336	C	14.260227	0.020194	-0.115716
C	13.655519	-1.087933	0.494432	C	13.649085	-1.088591	0.482258
C	12.257576	-1.159278	0.516621	C	12.251000	-1.155521	0.507851
C	14.164355	2.223442	-1.306329	C	14.163768	2.224408	-1.313634
C	14.480117	-2.177831	1.085251	C	14.471578	-2.182521	1.068552
C	15.660818	-1.884235	1.784466	C	15.655107	-1.894414	1.765269
C	16.433172	-2.902992	2.339867	C	16.425389	-2.916923	2.316653
C	16.040520	-4.235039	2.205962	C	16.027793	-4.247338	2.181163
C	14.869085	-4.540067	1.512380	C	14.853512	-4.546928	1.490021
C	14.096041	-3.521422	0.957585	C	14.082557	-3.524531	0.939239
C	15.330539	2.775020	-0.754000	C	15.333727	2.771062	-0.764412
C	15.947973	3.876199	-1.344878	C	15.953350	3.870609	-1.356040
C	15.411835	4.446737	-2.499651	C	15.415649	4.444428	-2.508463
C	14.253153	3.907212	-3.058933	C	14.253153	3.909876	-3.064587
C	13.635274	2.806373	-2.468028	C	13.633109	2.810663	-2.472937
H	-15.960375	-5.039775	-3.526042	H	-15.969759	-5.051193	-3.506717
H	-13.988392	-3.874526	-4.511398	H	-13.978971	-3.913528	-4.486675
H	-12.873256	-2.049217	-3.273036	H	-12.858469	-2.085310	-3.257361
H	-15.668879	-2.550424	-0.025527	H	-15.686326	-2.528235	-0.029623
H	-16.794488	-4.360216	-1.276428	H	-16.817151	-4.340966	-1.271523
H	-15.351249	-0.243170	-0.035871	H	-15.348751	-0.224098	-0.060458
H	-11.755016	1.792385	1.155891	H	-11.743980	1.793697	1.136930
H	-11.525677	-1.676777	-1.380963	H	-11.524062	-1.705099	-1.357571
H	-9.799974	-0.354081	-2.232492	H	-9.775461	-0.404515	-2.209229
H	-7.330558	-0.185276	-2.260098	H	-7.306082	-0.251412	-2.217349
H	-7.358652	0.974865	1.893161	H	-7.355765	0.955989	1.912426
H	-9.820085	0.769512	1.936447	H	-9.819626	0.761886	1.945141

H	-16.044011	1.982537	-0.013706	H	-16.021918	2.008126	-0.065573
H	-17.387699	3.588497	1.298803	H	-17.360600	3.639995	1.220080
H	-16.570679	4.398190	3.510990	H	-16.552274	4.465826	3.429568
H	-14.392603	3.568963	4.397754	H	-14.388277	3.626145	4.340962
H	-13.055858	1.946162	3.098327	H	-13.057092	1.977659	3.068323
H	-3.433891	2.302902	-1.851883	H	-3.459522	2.354896	-1.813813
H	-5.890060	2.040401	-1.627952	H	-5.907435	2.024513	-1.592452
H	-3.135791	-1.706455	1.981931	H	-3.145290	-1.737168	1.955408
H	-0.684761	-1.448265	1.846644	H	-0.680660	-1.490251	1.840559
H	-1.139981	1.625594	-1.150005	H	-1.144732	1.645525	-1.091632
H	1.133775	-1.874605	0.437372	H	1.132423	-1.873794	0.428681
H	3.172951	2.635766	-0.062847	H	3.159230	2.645505	-0.017683
H	0.706284	2.409763	0.069909	H	0.694739	2.411403	0.119988
H	3.439755	-2.908415	0.433175	H	3.438678	-2.903053	0.411964
H	5.887628	-2.547345	0.282660	H	5.885933	-2.536881	0.264381
H	7.425773	-1.182598	2.050406	H	7.423385	-1.184232	2.046984
H	9.896090	-1.062703	1.990647	H	9.893439	-1.066214	1.983734
H	9.705869	0.584787	-1.992696	H	9.697249	0.613204	-1.986110
H	7.238823	0.455301	-1.924808	H	7.230376	0.486226	-1.914050
H	11.501761	1.763849	-1.047632	H	11.500580	1.773936	-1.046936
H	15.354609	0.069232	-0.159728	H	15.350208	0.064346	-0.174217
H	11.771222	-2.019832	0.981662	H	11.763383	-2.015934	0.971780
H	15.970868	-0.844085	1.911880	H	15.969035	-0.855597	1.894074
H	17.345397	-2.652612	2.886766	H	17.339858	-2.670744	2.861715
H	16.646133	-5.033544	2.641060	H	16.631724	-5.048795	2.613163
H	14.556202	-5.580443	1.395593	H	14.536668	-5.585972	1.372054
H	13.190759	-3.776696	0.401275	H	13.174926	-3.775603	0.384854
H	15.751373	2.349746	0.160521	H	15.755876	2.343158	0.148272
H	16.851262	4.295146	-0.894922	H	16.859621	4.285700	-0.908510

H	15.895936	5.309806	-2.962720	H	15.901465	5.306211	-2.972131
H	13.828793	4.342163	-3.967031	H	13.827456	4.347422	-3.970809
H	12.738690	2.383021	-2.927567	H	12.733503	2.391146	-2.930070
IQO-COF-3^{+}				IQO-COF-3			
C	12.025682	-5.546440	4.246806	C	12.069149	-5.582966	4.192261
C	12.485584	-4.272344	4.582505	C	12.514721	-4.306499	4.538157
C	12.169768	-3.178441	3.778538	C	12.192077	-3.210790	3.739377
C	11.389127	-3.341504	2.624612	C	11.418894	-3.374246	2.580440
C	10.925205	-4.624181	2.301534	C	10.969529	-4.659481	2.247050
C	11.243709	-5.718898	3.104757	C	11.294796	-5.755982	3.045117
C	11.015229	-2.173791	1.777196	C	11.036482	-2.204618	1.739520
C	11.979001	-1.346083	1.159263	C	11.994133	-1.359752	1.135536
C	11.550552	-0.213791	0.403968	C	11.556479	-0.225757	0.388200
C	10.158695	0.059843	0.249720	C	10.162218	0.032579	0.228212
C	9.214120	-0.821910	0.819796	C	9.223866	-0.865749	0.783398
C	9.660931	-1.902995	1.580179	C	9.680271	-1.948632	1.535824
C	12.525297	0.652886	-0.207931	C	12.524653	0.658788	-0.208659
C	7.745856	-0.645093	0.642040	C	7.754348	-0.701410	0.603202
C	7.172346	-0.618579	-0.636349	C	7.181388	-0.657228	-0.674810
C	5.794763	-0.502395	-0.796380	C	5.802542	-0.547402	-0.833782
C	4.982558	-0.406161	0.330259	C	4.979603	-0.473029	0.288552
C	5.527370	-0.431668	1.611353	C	5.531056	-0.517220	1.568045
C	6.904907	-0.554700	1.760655	C	6.908739	-0.637054	1.720127
C	13.913637	0.335568	-0.121264	C	13.916363	0.357967	-0.115493
C	14.857053	1.170978	-0.759852	C	14.853613	1.211572	-0.738922
C	14.414431	2.326262	-1.405327	C	14.400978	2.367395	-1.376417
C	13.066552	2.680167	-1.475738	C	13.049284	2.705052	-1.452887
C	12.099856	1.824320	-0.902486	C	12.089472	1.831895	-0.894387
N	3.559364	-0.271801	0.157970	N	3.563119	-0.331068	0.117767

C	2.739776	-1.372168	0.504061	C	2.740459	-1.394997	0.478611
C	1.293060	-1.175617	0.259567	C	1.292637	-1.178841	0.243697
C	0.805610	0.050823	-0.294496	C	0.814790	0.033682	-0.315890
C	1.718625	1.069857	-0.603479	C	1.768565	1.061529	-0.654648
C	3.063943	0.871015	-0.365655	C	3.080918	0.847133	-0.431998
C	0.424620	-2.196181	0.568682	C	0.409571	-2.201603	0.580663
C	-0.972901	-2.051639	0.344531	C	-0.967026	-2.055670	0.376230
C	-0.592472	0.196564	-0.515354	C	-0.562174	0.180473	-0.517913
C	-1.884956	-3.074103	0.643911	C	-1.920236	-3.086564	0.706666
C	-3.229333	-2.878485	0.398328	C	-3.231552	-2.875784	0.475498
N	-3.726757	-1.733306	-0.118824	N	-3.715309	-1.696395	-0.071433
C	-2.907864	-0.626304	-0.448407	C	-2.892801	-0.626925	-0.418473
O	3.223264	-2.384840	0.953356	O	3.198339	-2.424757	0.942030
O	-3.391517	0.392276	-0.883690	O	-3.349930	0.406810	-0.873580
C	9.768516	1.243799	-0.471749	C	9.762787	1.219567	-0.483291
C	10.686903	2.080520	-1.012272	C	10.674258	2.072510	-1.010012
C	13.390831	-1.617332	1.246138	C	13.408574	-1.614577	1.229056
C	14.305127	-0.825068	0.636280	C	14.317165	-0.805244	0.633227
C	12.702479	3.947558	-2.170213	C	12.674069	3.974166	-2.138313
C	16.316887	0.870833	-0.766261	C	16.317258	0.930400	-0.737379
C	12.008431	4.967035	-1.501904	C	11.964422	4.979662	-1.465217
C	11.706260	6.163332	-2.150238	C	11.651781	6.177896	-2.104986
C	12.093424	6.360515	-3.476421	C	12.043778	6.390977	-3.427289
C	12.788787	5.355517	-4.148749	C	12.754453	5.399961	-4.104325
C	13.093538	4.159462	-3.499628	C	13.069667	4.202005	-3.463742
C	16.807529	-0.326768	-1.307564	C	16.827587	-0.255138	-1.287001
C	18.177415	-0.581125	-1.343733	C	18.200920	-0.491203	-1.315561
C	19.079333	0.357446	-0.840559	C	19.086772	0.453931	-0.796369
C	18.602748	1.554045	-0.305241	C	18.590598	1.638691	-0.252576

C	17.232274	1.809948	-0.270981	C	17.216654	1.876263	-0.225890
C	-11.064060	6.102990	3.753109	C	-11.134737	6.106968	3.772762
C	-11.964572	5.217254	4.344813	C	-12.035503	5.216239	4.356523
C	-12.457378	4.131537	3.621530	C	-12.516274	4.128095	3.628773
C	-12.052819	3.911510	2.297523	C	-12.099330	3.910610	2.308191
C	-11.151219	4.811547	1.710446	C	-11.197571	4.815679	1.729105
C	-10.660756	5.897969	2.432938	C	-10.719097	5.904479	2.456025
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C	-11.803528	1.766902	0.948407	C	-11.826992	1.768915	0.958786
C	-12.409926	0.725617	0.184446	C	-12.421460	0.725722	0.187929
C	-13.826115	0.695322	0.013089	C	-13.836136	0.687472	0.005607
C	-14.623529	1.672662	0.649067	C	-14.644088	1.659142	0.636932
C	-14.001398	2.688153	1.376712	C	-14.033534	2.677066	1.370896
C	-11.591404	-0.296877	-0.416183	C	-11.592253	-0.290353	-0.409016
C	-16.111180	1.668725	0.565531	C	-16.130964	1.646706	0.541173
C	-16.858321	0.557631	0.984492	C	-16.875061	0.531130	0.953610
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C	-10.178400	-0.285584	-0.217174	C	-10.180804	-0.270749	-0.199841
C	-9.389036	-1.296729	-0.808523	C	-9.379653	-1.274141	-0.788611
C	-10.003679	-2.272791	-1.593106	C	-9.983139	-2.252154	-1.579626
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C	-14.389691	-0.313280	-0.846876	C	-14.387260	-0.322848	-0.860452
C	-13.617727	-1.260600	-1.431487	C	-13.605109	-1.264118	-1.441323
C	-10.373900	1.746972	1.119672	C	-10.398629	1.756321	1.141995
C	-9.605156	0.778112	0.566540	C	-9.620042	0.793355	0.592266

C	-11.945197	-3.428057	-2.611332	C	-11.909778	-3.419083	-2.612784
C	-7.913568	-1.376485	-0.617222	C	-7.904598	-1.343383	-0.588617
C	-11.491521	-3.637556	-3.921126	C	-11.444289	-3.625427	-3.918947
C	-11.983029	-4.696865	-4.683342	C	-11.922988	-4.687544	-4.685418
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C	-13.383700	-5.372545	-2.839353	C	-13.334292	-5.372521	-2.853075
C	-12.894582	-4.312368	-2.078101	C	-12.857910	-4.309590	-2.087603
C	-7.352529	-1.499877	0.660734	C	-7.348808	-1.478111	0.690232
C	-5.974638	-1.606601	0.826135	C	-5.970453	-1.579332	0.860750
C	-5.149518	-1.603650	-0.295436	C	-5.130872	-1.560743	-0.251742
C	-5.683659	-1.494350	-1.576983	C	-5.666989	-1.438537	-1.533088
C	-7.061297	-1.381367	-1.730807	C	-7.044144	-1.329037	-1.695692
C	-1.460899	-0.823956	-0.206047	C	-1.445183	-0.842601	-0.181600
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H	12.525127	-2.181957	4.052975	H	12.535698	-2.212510	4.022113
H	10.316524	-4.765817	1.404729	H	10.366618	-4.801595	1.346442
H	10.879846	-6.712972	2.834013	H	10.942053	-6.751862	2.766401
H	8.921426	-2.565370	2.037096	H	8.946192	-2.624109	1.982195
H	7.808272	-0.705932	-1.519861	H	7.819112	-0.725502	-1.558996
H	5.348471	-0.496018	-1.792952	H	5.360841	-0.526268	-1.832411
H	4.878662	-0.349875	2.485127	H	4.881312	-0.453482	2.442533
H	7.336374	-0.568065	2.763958	H	7.337687	-0.665252	2.724507
H	15.153253	2.980023	-1.875661	H	15.134722	3.034967	-1.835176
H	1.386179	2.018182	-1.024559	H	1.434279	2.006636	-1.082849
H	3.800551	1.644019	-0.591100	H	3.845232	1.590038	-0.663342
H	0.805186	-3.128817	0.989155	H	0.805697	-3.124532	1.008249
H	-0.973091	1.129370	-0.935398	H	-0.958292	1.103319	-0.945667
H	-1.552278	-4.024535	1.060039	H	-1.585983	-4.033177	1.131560

H	-3.963172	-3.657687	0.611080	H	-3.993599	-3.624269	0.695767
H	8.708550	1.477505	-0.576194	H	8.700763	1.441754	-0.591301
H	10.350206	2.965465	-1.553034	H	10.330169	2.959012	-1.543527
H	13.729036	-2.488250	1.808236	H	13.753680	-2.486842	1.784871
H	15.364765	-1.065368	0.727468	H	15.379045	-1.033434	0.729253
H	11.712345	4.824411	-0.459539	H	11.664072	4.824543	-0.425860
H	11.169288	6.948992	-1.613363	H	11.102516	6.952472	-1.564442
H	11.855267	7.298009	-3.984507	H	11.797279	7.329905	-3.928712
H	13.095489	5.501146	-5.187306	H	13.064852	5.557987	-5.139976
H	13.634449	3.373348	-4.032721	H	13.622453	3.426795	-4.000626
H	16.107875	-1.061463	-1.714023	H	16.140573	-0.994813	-1.705806
H	18.542654	-1.517245	-1.772807	H	18.581532	-1.418070	-1.751323
H	20.152971	0.156790	-0.867962	H	20.163120	0.267565	-0.817854
H	19.301712	2.294302	0.091404	H	19.276883	2.383999	0.156576
H	16.864197	2.747204	0.154201	H	16.833186	2.804247	0.205995
H	-10.678432	6.954299	4.319063	H	-10.758395	6.960086	4.342238
H	-12.285628	5.370045	5.377994	H	-12.366083	5.366892	5.387015
H	-13.159577	3.438033	4.091321	H	-13.218594	3.430611	4.092462
H	-10.839687	4.663751	0.673323	H	-10.876267	4.669830	0.694690
H	-9.962544	6.592006	1.958964	H	-10.020424	6.602236	1.988232
H	-14.624025	3.452545	1.848418	H	-14.664227	3.437343	1.838569
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H	-18.817241	-0.294245	1.269018	H	-18.831188	-0.332650	1.221027
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H	-18.703150	3.713001	-0.314968	H	-18.727503	3.675401	-0.361695
H	-16.225688	3.676076	-0.225975	H	-16.250698	3.653329	-0.251272
H	-9.384582	-3.057507	-2.035035	H	-9.355657	-3.031546	-2.019182
H	-15.460990	-0.296953	-1.049864	H	-15.457148	-0.312694	-1.071187
H	-14.080003	-1.990108	-2.097085	H	-14.058077	-1.994958	-2.111875

H	-9.900001	2.529759	1.712524	H	-9.934028	2.539734	1.741362
H	-8.525181	0.808472	0.712657	H	-8.541431	0.827784	0.747560
H	-10.751973	-2.955947	-4.349293	H	-10.705386	-2.939291	-4.340943
H	-11.623612	-4.841115	-5.705045	H	-11.554231	-4.829293	-5.704141
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IQO-COF-4^{+}				IQO-COF-4			
C	15.106542	5.511178	-4.087106	C	15.168875	5.405174	-4.124644
C	15.403198	4.185704	-4.407477	C	15.458610	4.073396	-4.424508
C	14.901362	3.146238	-3.626225	C	14.945714	3.048426	-3.631384
C	14.094438	3.415623	-2.510798	C	14.134522	3.338859	-2.524388
C	13.796803	4.750349	-2.202524	C	13.843897	4.679723	-2.236781
C	14.301189	5.790237	-2.982985	C	14.359338	5.705111	-3.029098
C	13.516684	2.310904	-1.694051	C	13.545160	2.249602	-1.695259
C	14.319304	1.345332	-1.046583	C	14.337956	1.288586	-1.029245
C	13.694715	0.281645	-0.329222	C	13.702597	0.239338	-0.300183
C	12.272228	0.215814	-0.239802	C	12.279179	0.183488	-0.218253
C	11.493413	1.230253	-0.839308	C	11.510141	1.193938	-0.836934
C	12.129449	2.239960	-1.562198	C	12.156833	2.189201	-1.570432
C	14.502110	-0.728553	0.305970	C	14.500107	-0.766249	0.354578
C	10.007095	1.260755	-0.741036	C	10.023511	1.235722	-0.748223
C	9.362710	1.322905	0.501367	C	9.371345	1.315186	0.489099
C	7.973813	1.384425	0.580964	C	7.982474	1.388592	0.558718
C	7.212002	1.397256	-0.586219	C	7.228350	1.396674	-0.613518

C	7.836667	1.346812	-1.831779	C	7.860952	1.328714	-1.854298
C	9.224050	1.277390	-1.904180	C	9.248103	1.246999	-1.916590
C	15.924797	-0.622596	0.280303	C	15.923600	-0.669256	0.335958
C	16.704976	-1.601667	0.934809	C	16.693848	-1.643184	1.009679
C	16.067764	-2.687414	1.536628	C	16.046348	-2.716158	1.623354
C	14.680171	-2.834205	1.548912	C	14.657859	-2.854462	1.629287
C	13.877259	-1.832648	0.959060	C	13.864640	-1.856792	1.020057
N	5.784262	1.488372	-0.498284	N	5.801130	1.502068	-0.535647
C	5.017238	0.408438	-0.941771	C	5.025684	0.430030	-0.983932
C	3.558873	0.576804	-0.793861	C	3.568236	0.613872	-0.846100
C	3.005907	1.746992	-0.233732	C	3.023713	1.789509	-0.289168
C	3.897784	2.792664	0.200865	C	3.923580	2.825872	0.151275
C	5.229329	2.628573	0.055340	C	5.254220	2.648018	0.014318
C	2.711758	-0.460402	-1.217543	C	2.713083	-0.414118	-1.276065
C	1.340939	-0.343564	-1.090019	C	1.342759	-0.282936	-1.157587
C	0.768442	0.822391	-0.533211	C	0.778582	0.888281	-0.603226
C	1.606490	1.850925	-0.114638	C	1.624748	1.907750	-0.178687
C	-0.707796	0.946920	-0.394084	C	-0.697179	1.027449	-0.472274
C	-1.480854	-0.152375	-0.033892	C	-1.483386	-0.065165	-0.120645
C	-2.877539	-0.046604	0.110700	C	-2.879946	0.054042	0.017011
C	-3.496571	1.198923	-0.121531	C	-3.484958	1.306971	-0.212869
C	-2.715754	2.307370	-0.488262	C	-2.690710	2.408611	-0.571318
C	-1.345928	2.186964	-0.622288	C	-1.321542	2.274871	-0.699103
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N	-5.654624	0.220194	0.387839	N	-5.655468	0.349383	0.281121
C	-4.954230	1.373455	0.021438	C	-4.941853	1.496011	-0.076372
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O	-5.529304	2.435253	-0.147383	O	-5.504304	2.564826	-0.245047

C	11.679485	-0.902978	0.446683	C	11.675637	-0.921604	0.480906
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C	15.758172	1.405624	-1.067092	C	15.777235	1.339761	-1.042268
C	16.517148	0.477920	-0.435470	C	16.526826	0.416934	-0.392546
C	14.101978	-4.044664	2.198425	C	14.068285	-4.051797	2.292619
C	18.192145	-1.527908	1.000654	C	18.180991	-1.577274	1.084300
C	13.290509	-4.934989	1.479686	C	13.254390	-4.946556	1.582187
C	12.786117	-6.084046	2.086288	C	12.738964	-6.083491	2.202220
C	13.085212	-6.362729	3.420580	C	13.029356	-6.345495	3.541808
C	13.895838	-5.487225	4.143034	C	13.842354	-5.465525	4.256126
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C	18.837789	-0.431212	1.590795	C	18.829252	-0.475213	1.661453
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C	20.995502	-1.445484	1.187056	C	20.983508	-1.508626	1.288970
C	20.363681	-2.543237	0.602881	C	20.349046	-2.611720	0.717851
C	18.972641	-2.585274	0.512890	C	18.958430	-2.646889	0.618831
C	-14.200445	-5.414923	-4.683421	C	-14.104914	-5.628066	-4.469168
C	-13.749327	-5.465567	-3.364159	C	-13.680739	-5.660996	-3.140052
C	-14.039230	-4.425785	-2.483940	C	-13.998370	-4.614208	-2.276277
C	-14.794993	-3.323261	-2.913649	C	-14.745322	-3.516213	-2.728275
C	-15.259152	-3.289080	-4.237594	C	-15.172833	-3.497277	-4.063208
C	-14.954806	-4.324447	-5.117865	C	-14.852933	-4.543739	-4.927720
C	-15.154971	-2.232607	-1.978423	C	-15.127026	-2.410835	-1.804385
C	-14.172745	-1.538682	-1.194837	C	-14.171107	-1.642263	-1.103507
C	-14.601935	-0.577248	-0.234830	C	-14.612447	-0.635564	-0.193534
C	-15.985216	-0.262986	-0.100367	C	-16.006928	-0.387020	-0.021196
C	-16.933243	-0.882720	-0.982383	C	-16.942040	-1.124416	-0.781154
C	-16.495197	-1.865156	-1.868616	C	-16.482637	-2.124502	-1.638894
C	-13.642217	0.073948	0.595615	C	-13.647943	0.131236	0.553427

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8 Copies of NMR spectra

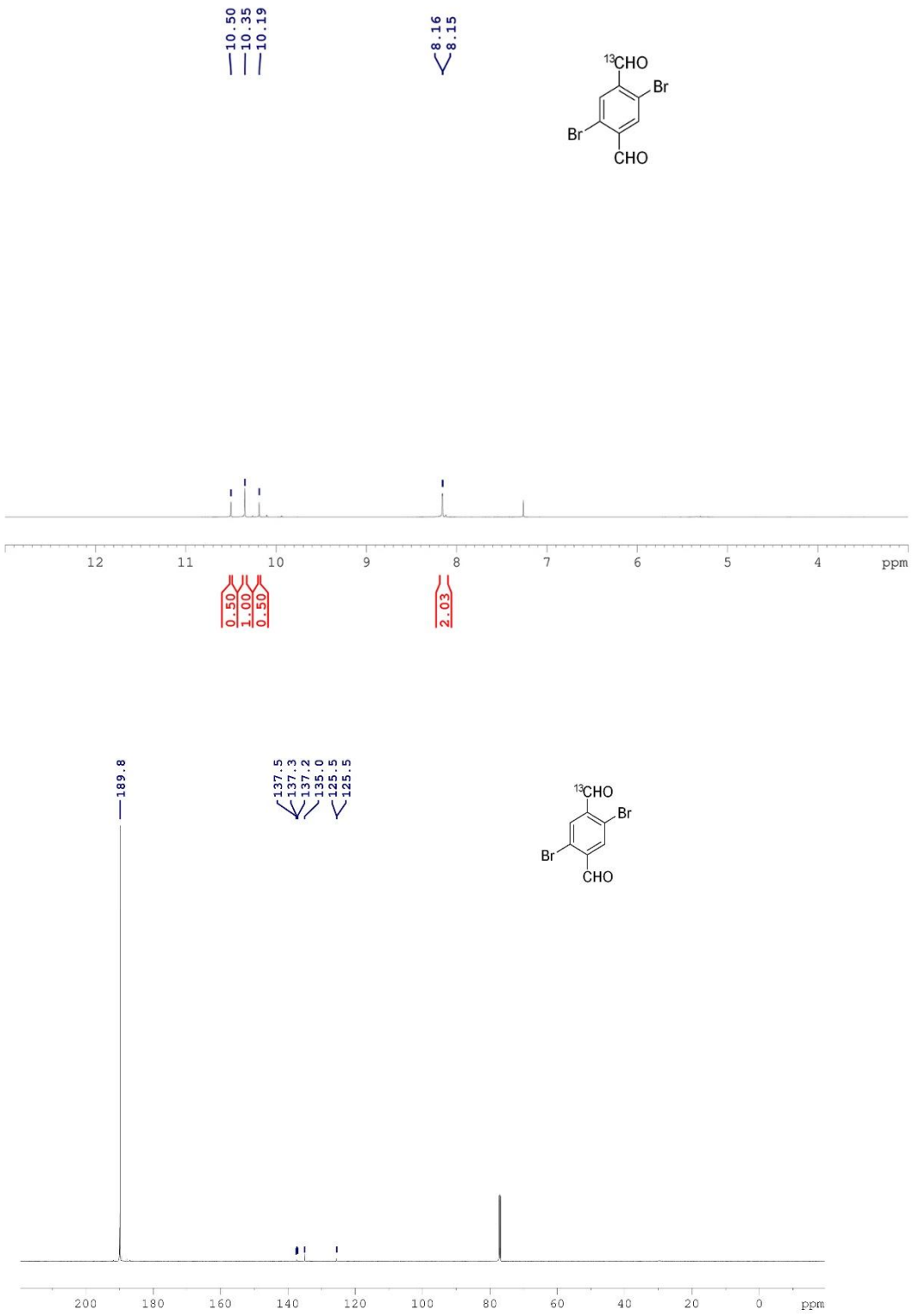


Figure S23. ^{1}H NMR and ^{13}C NMR spectra of **S2**.

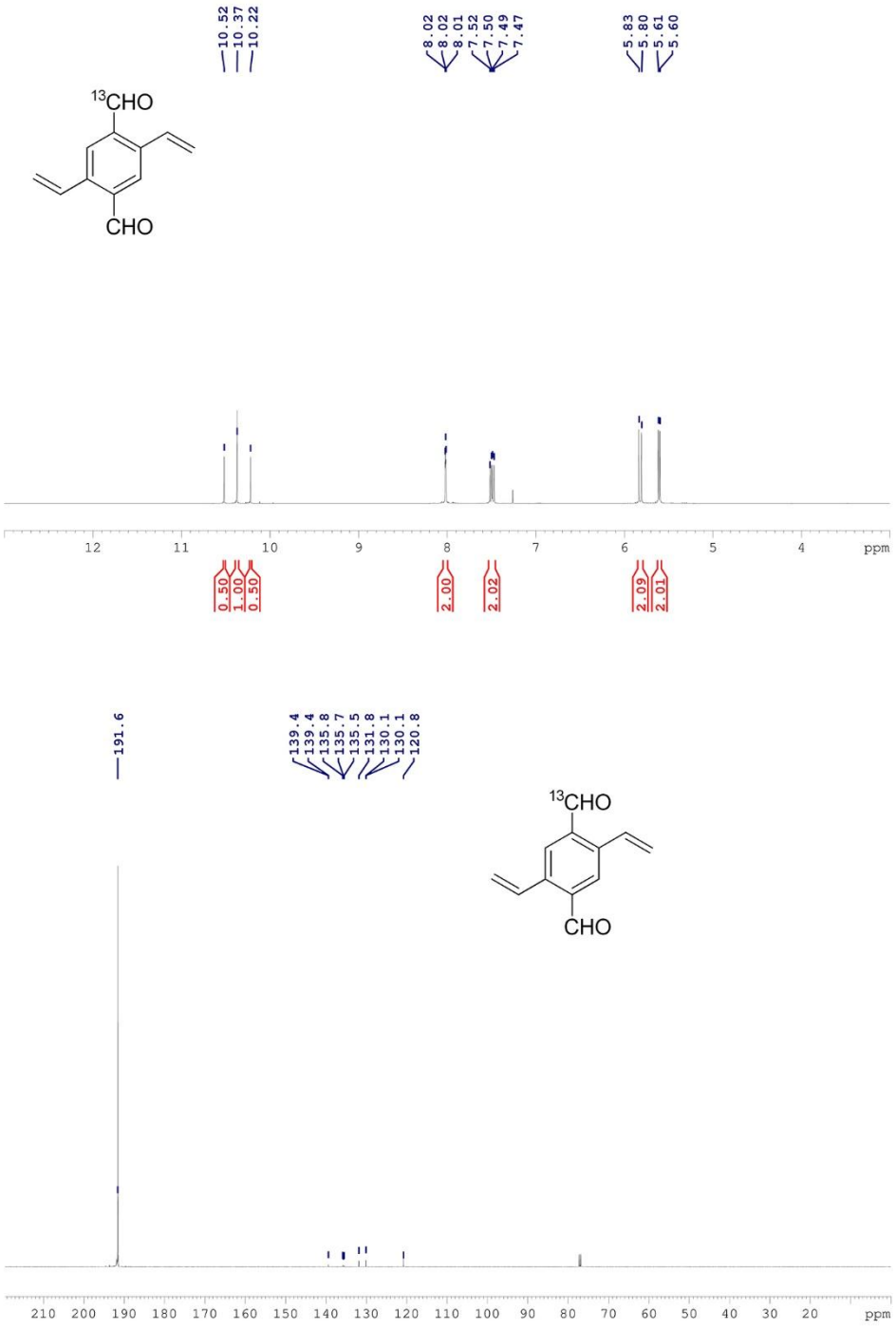


Figure S24. ^{1}H NMR and ^{13}C NMR spectra of **S3**.

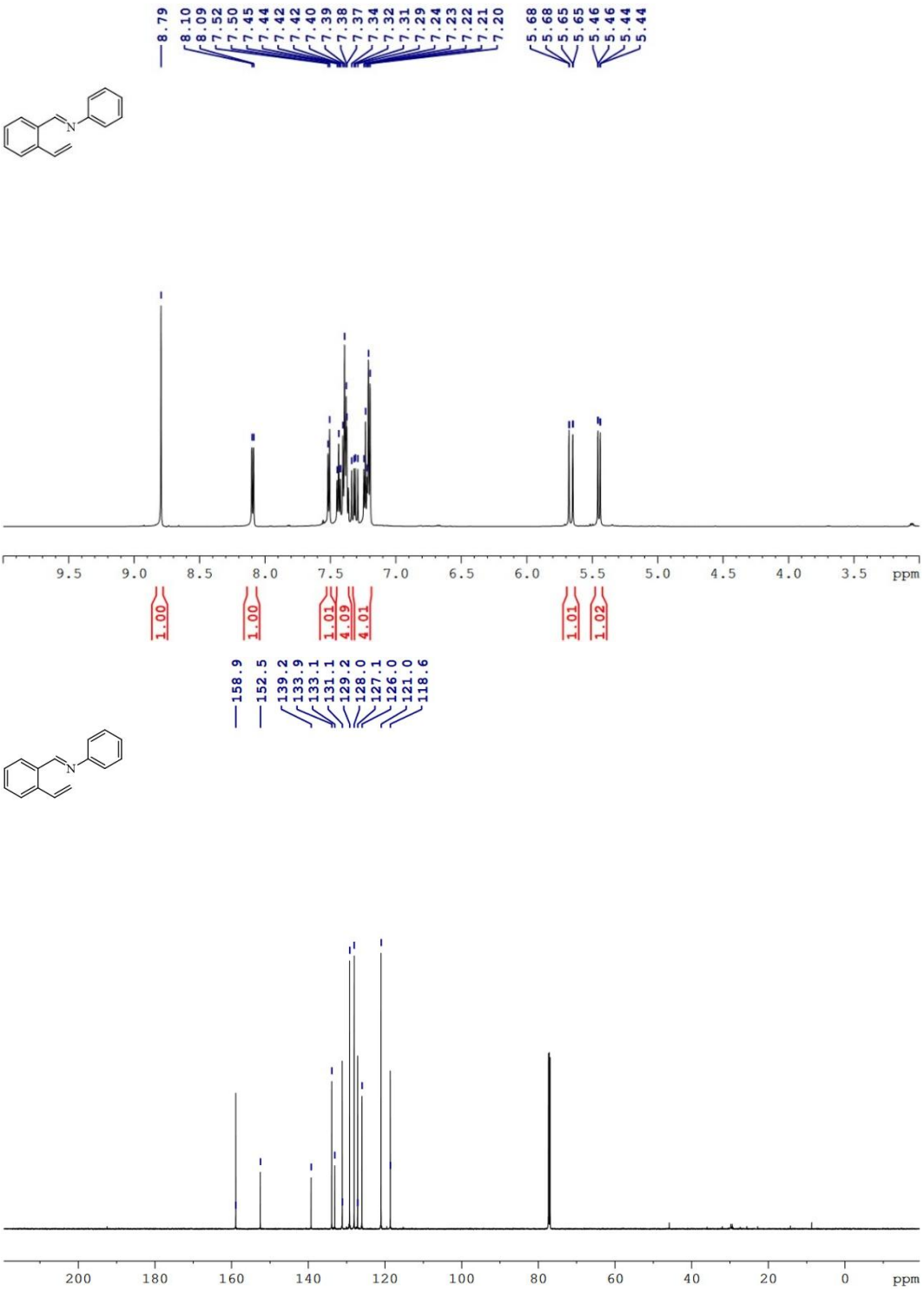


Figure S25. ^{1}H NMR and ^{13}C NMR spectra of **S6**.

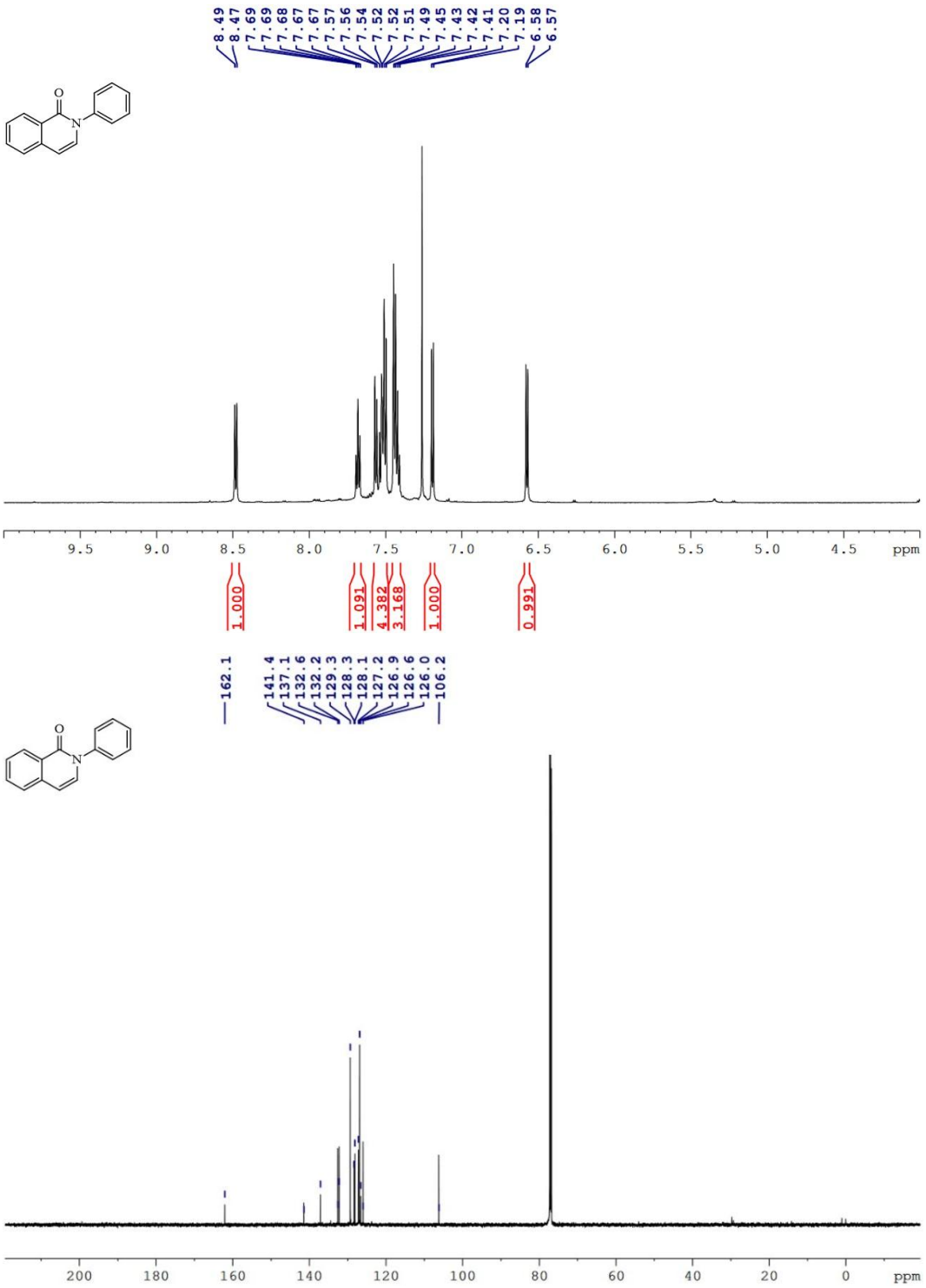


Figure S26. ^{1}H NMR and ^{13}C NMR spectra of **S7**.

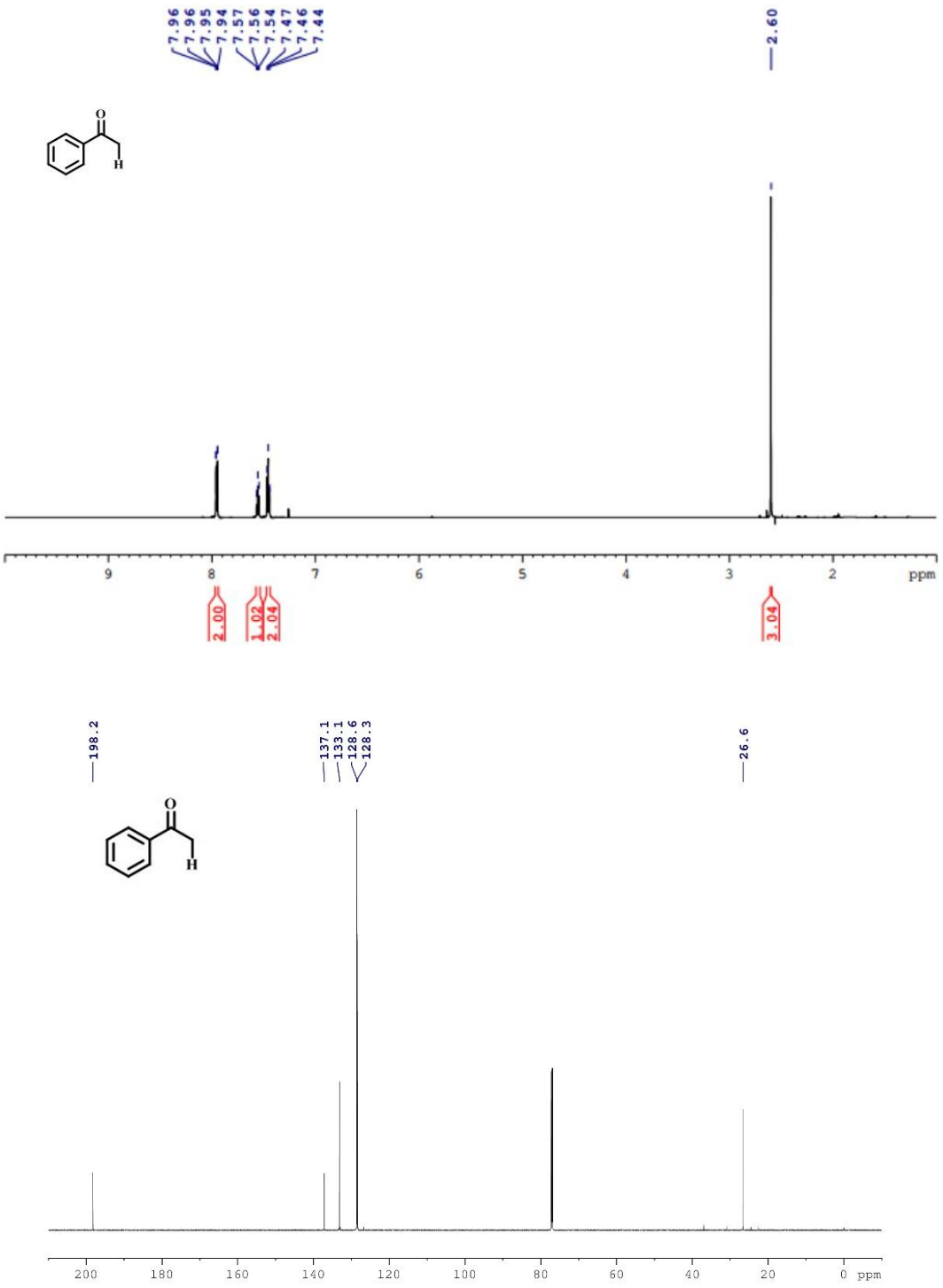


Figure S27. ^{1}H NMR and ^{13}C NMR spectra of **1**.

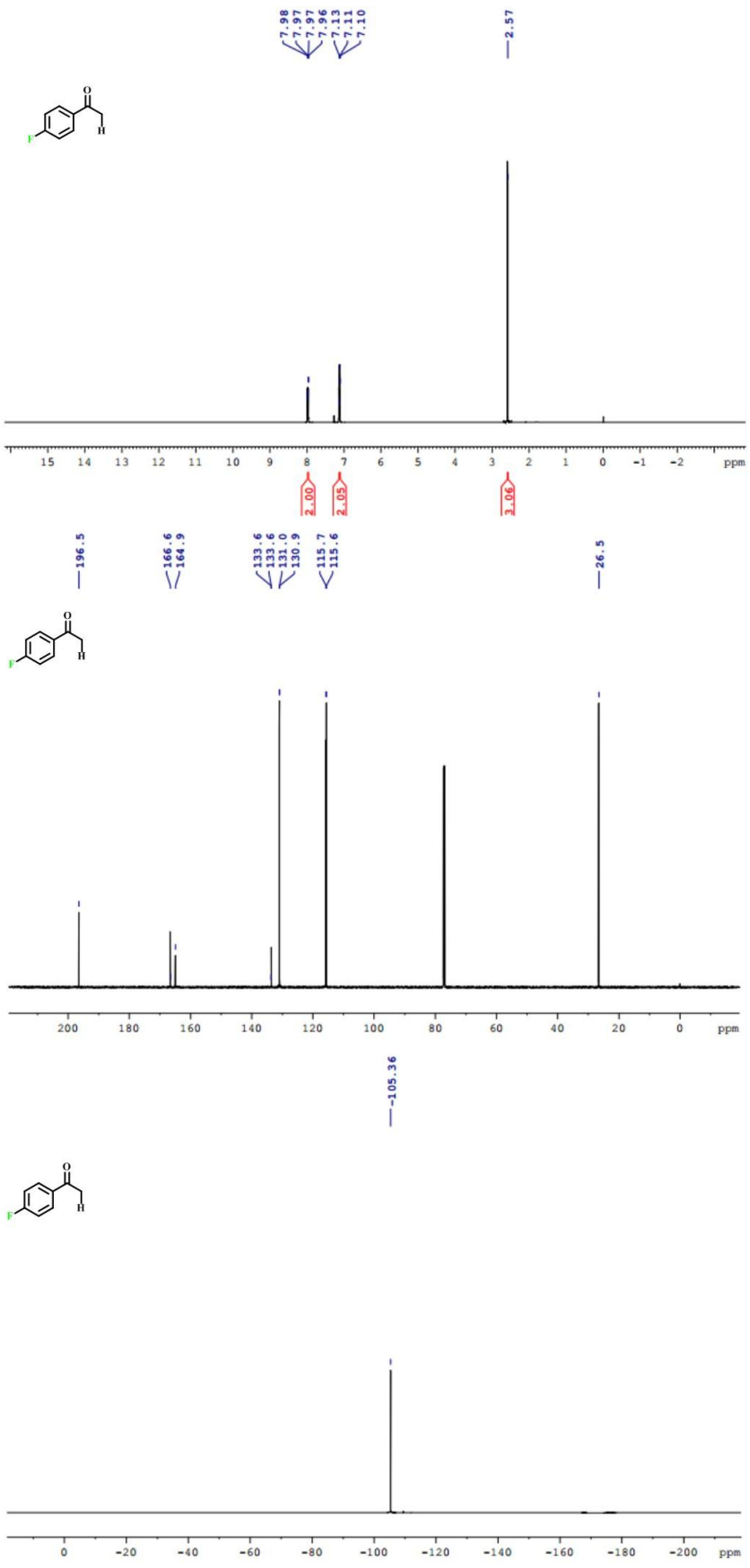


Figure S28. [1]H NMR, [13] C NMR and [19]F NMR spectra of **2**.

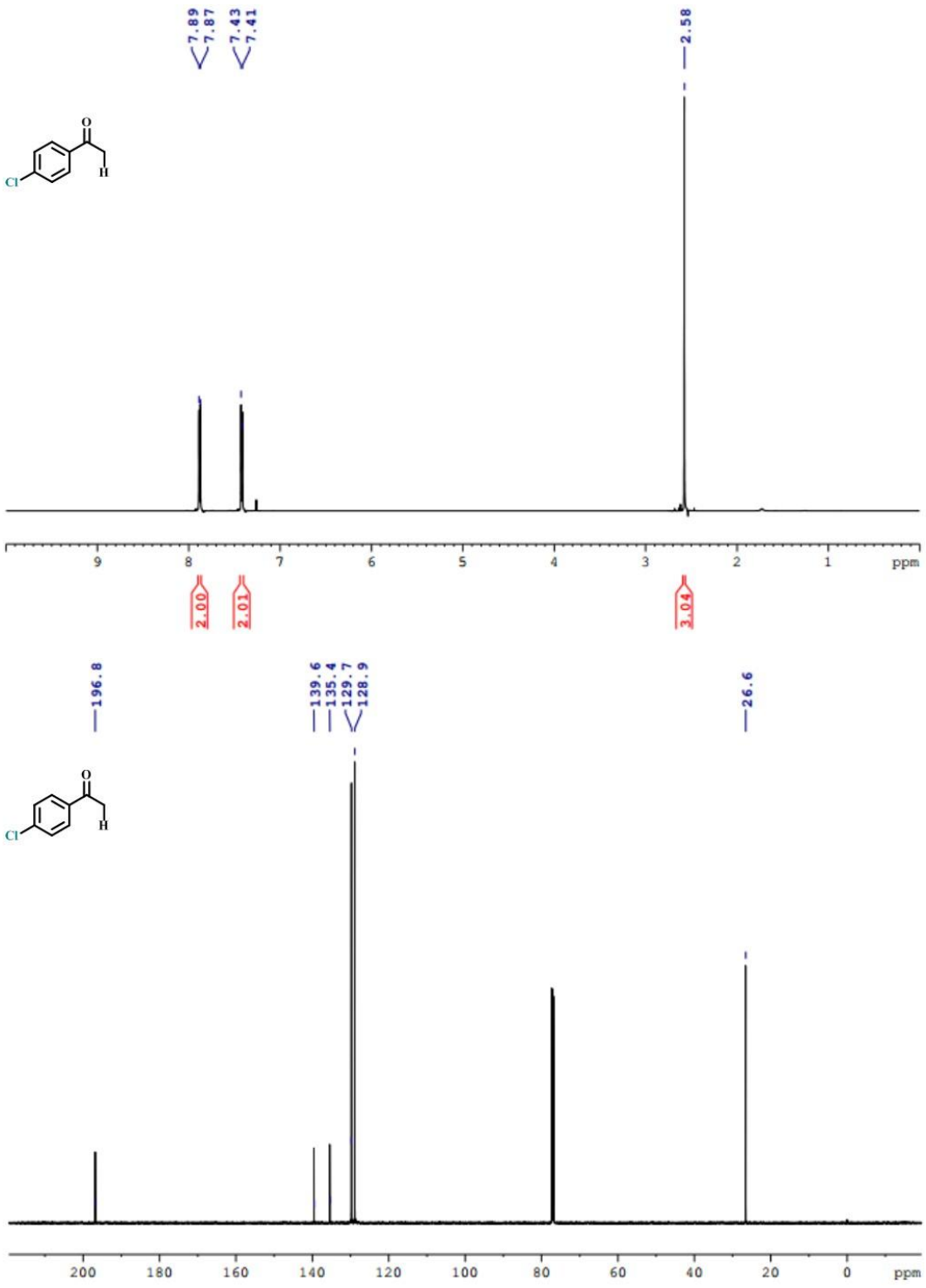


Figure S29. ^{1}H NMR and ^{13}C NMR spectra of **3**.

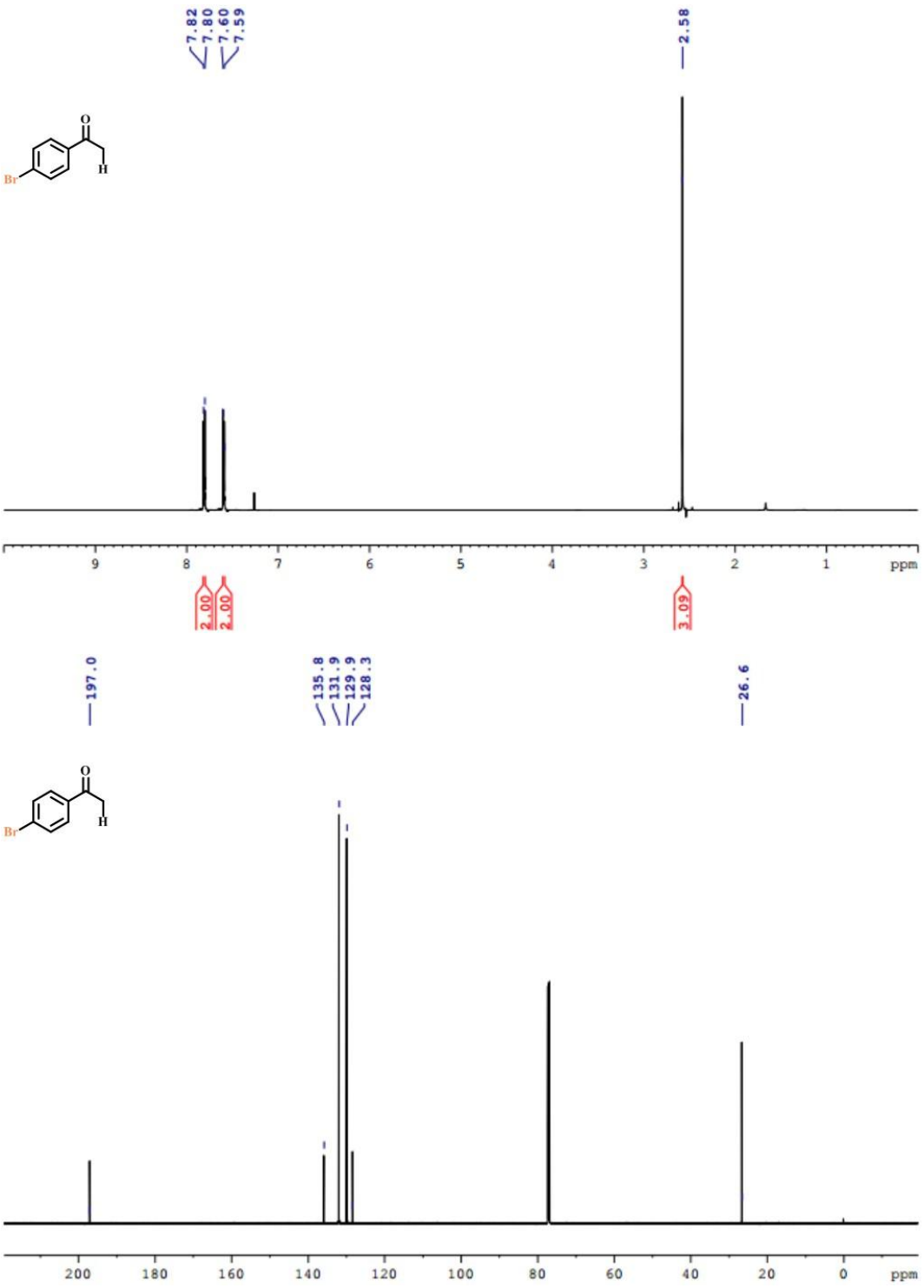


Figure S30. ^{1}H NMR and ^{13}C NMR spectra of **4**.

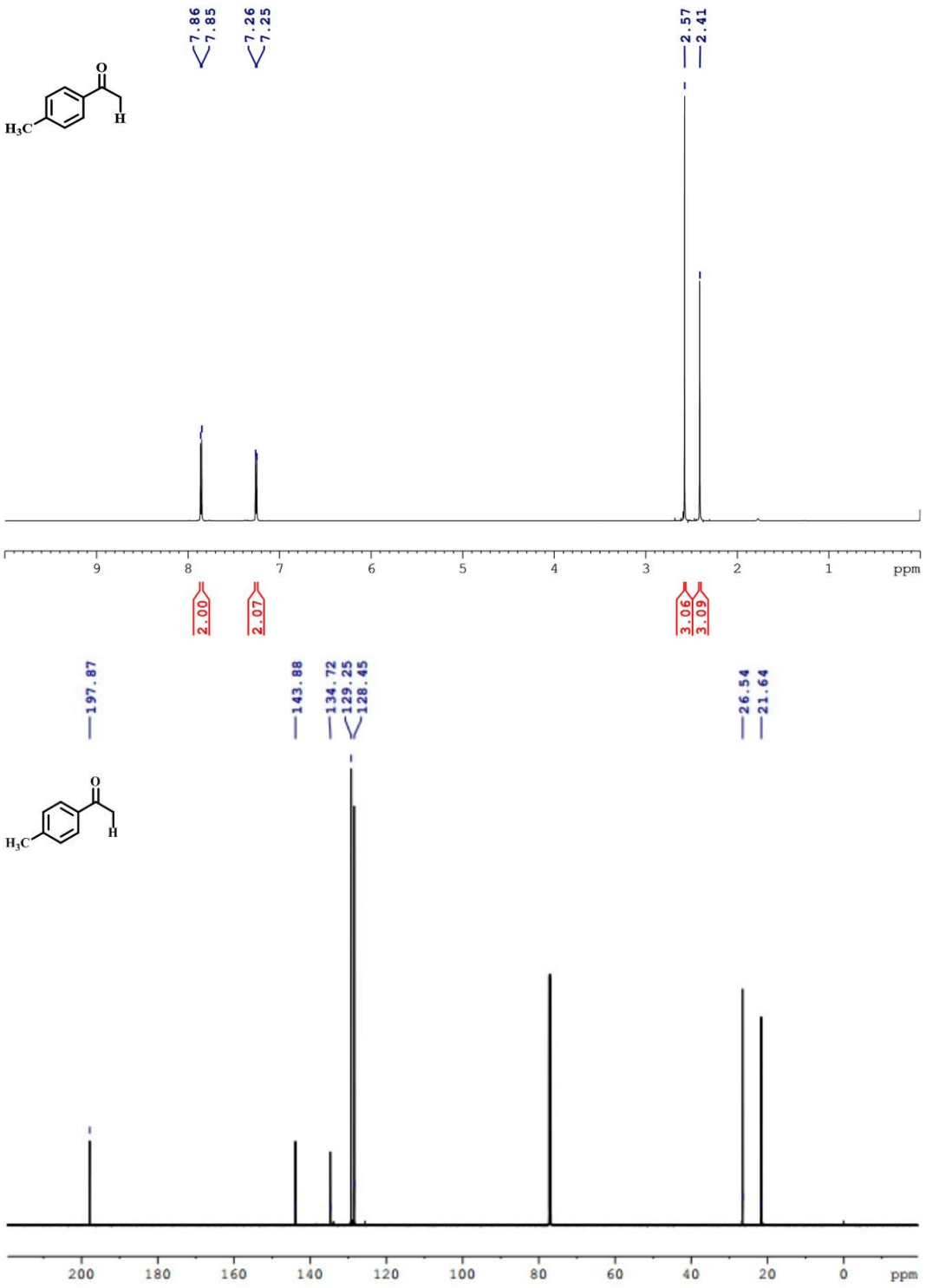


Figure S31. ^{1}H NMR and ^{13}C NMR spectra of **5**.

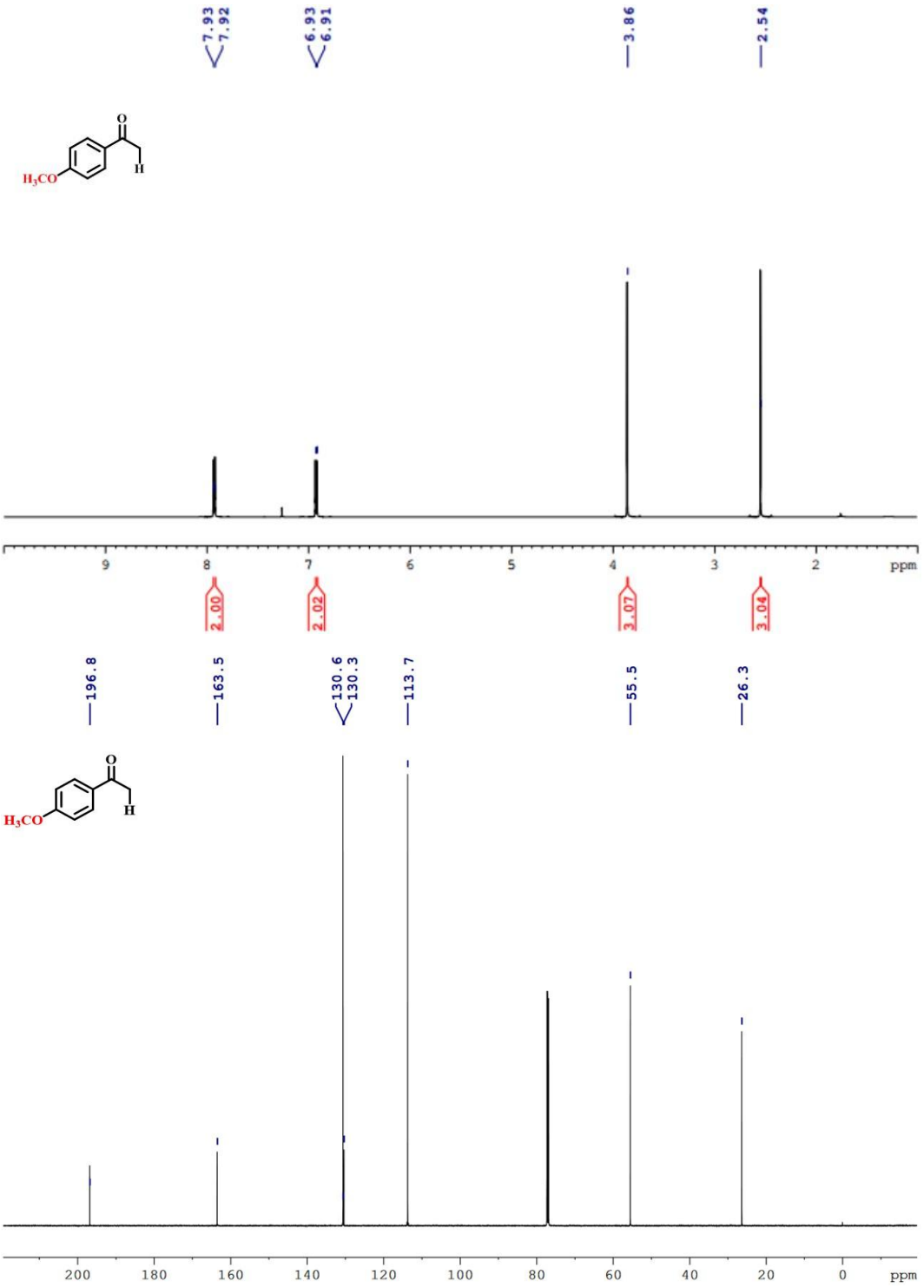


Figure S32. ^{1}H NMR and ^{13}C NMR spectra of **6**.

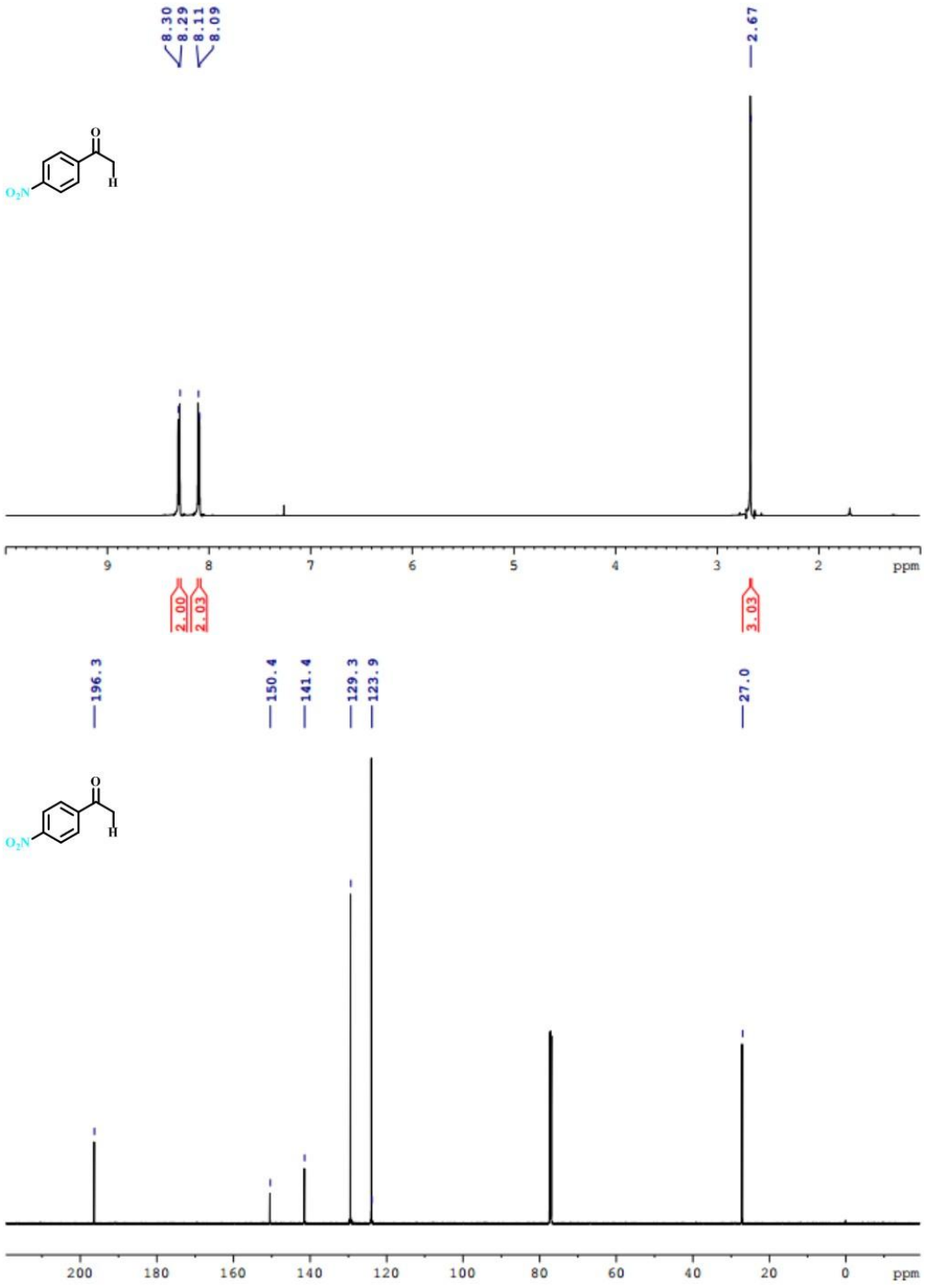


Figure S33. ^{1}H NMR and ^{13}C NMR spectra of **7**.

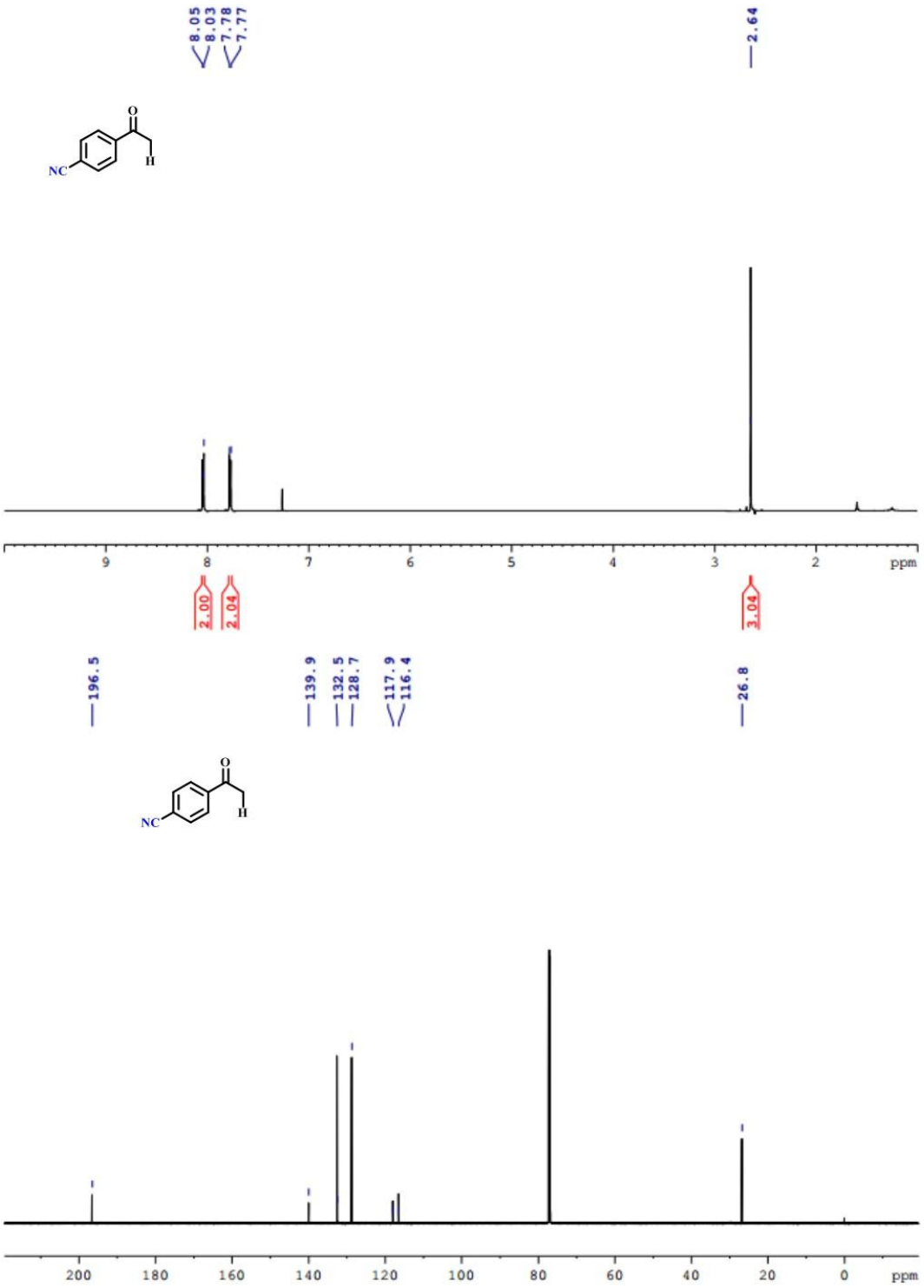


Figure S34. [1]H NMR and [13] C NMR spectra of **8**.

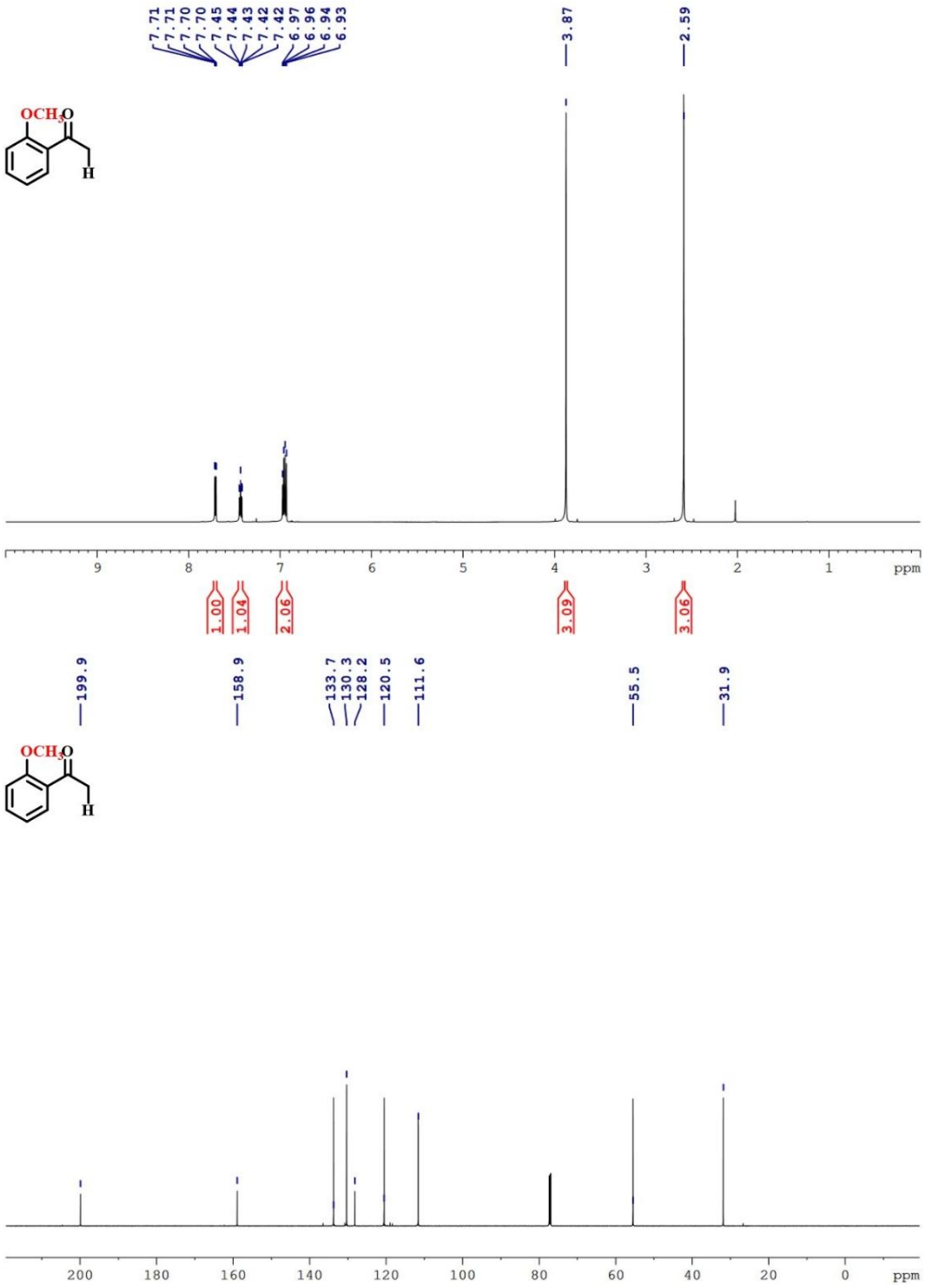


Figure S35. ^{1}H NMR and ^{13}C NMR spectra of **9**.

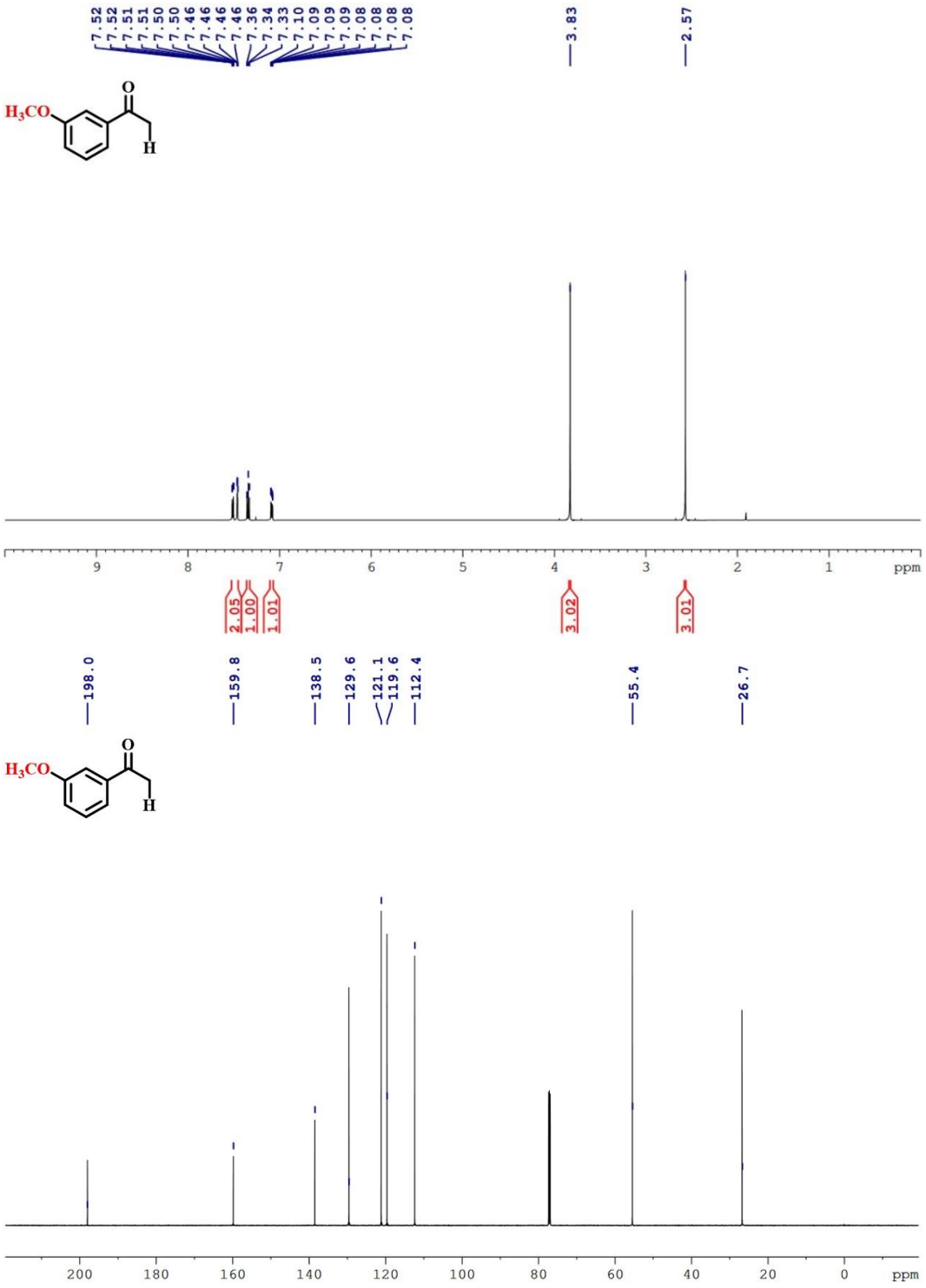


Figure S36. ^{1}H NMR and ^{13}C NMR spectra of **10**.

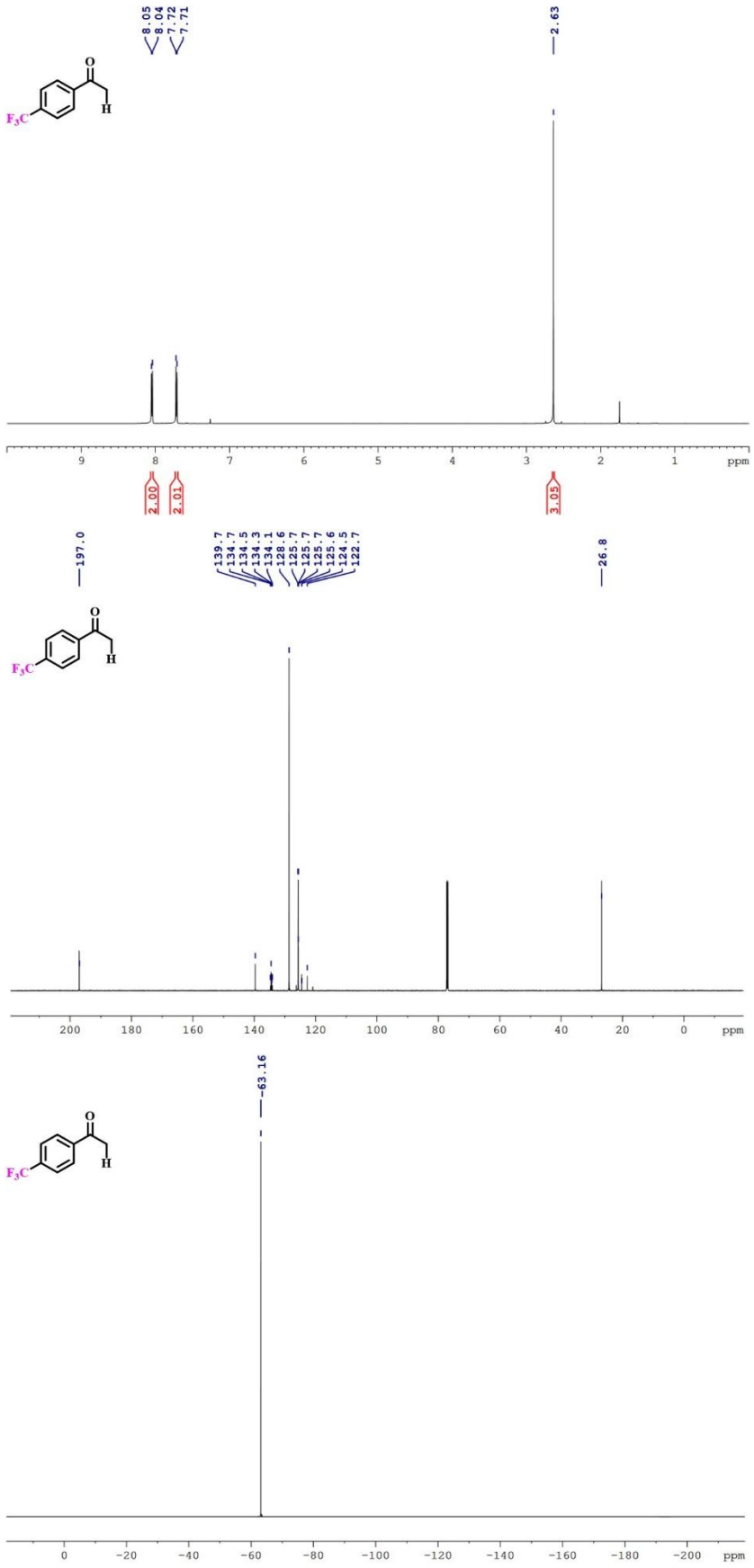


Figure S37. [1]H NMR, [13] C NMR and [19]F NMR spectra of **11**.

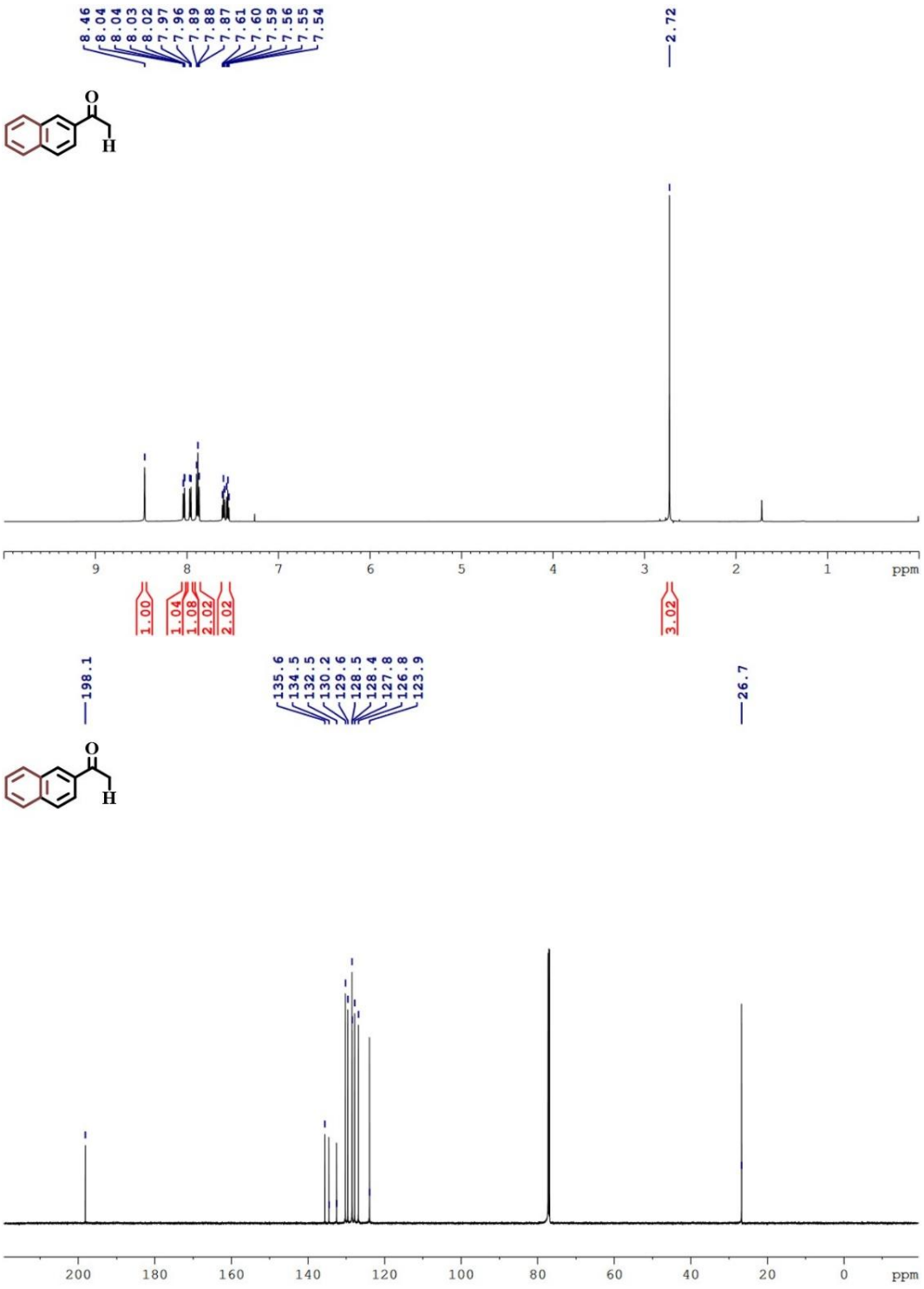


Figure S38. ^{1}H NMR and ^{13}C NMR spectra of **12**.

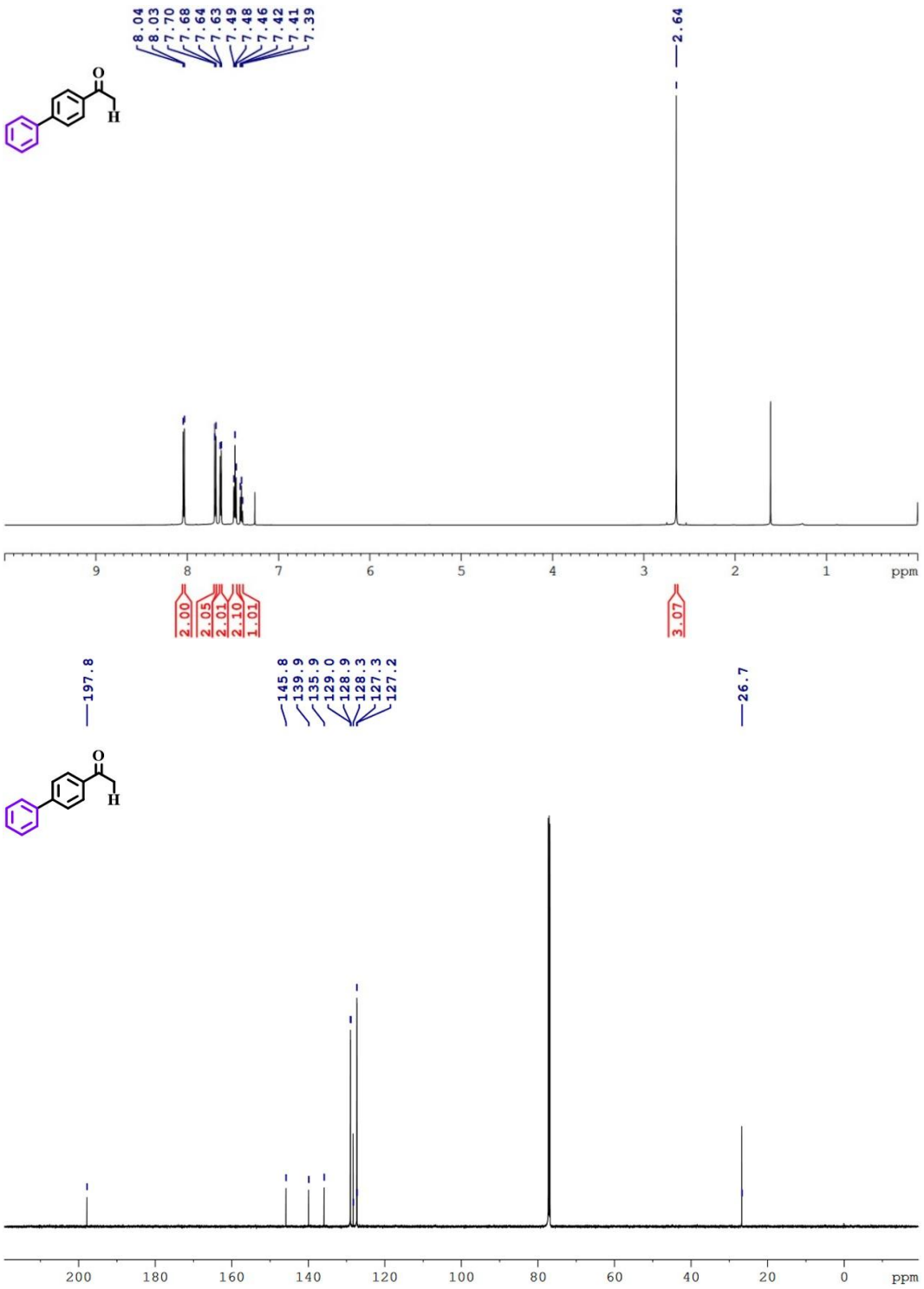


Figure S39. ^{1}H NMR and ^{13}C NMR spectra of **13**.

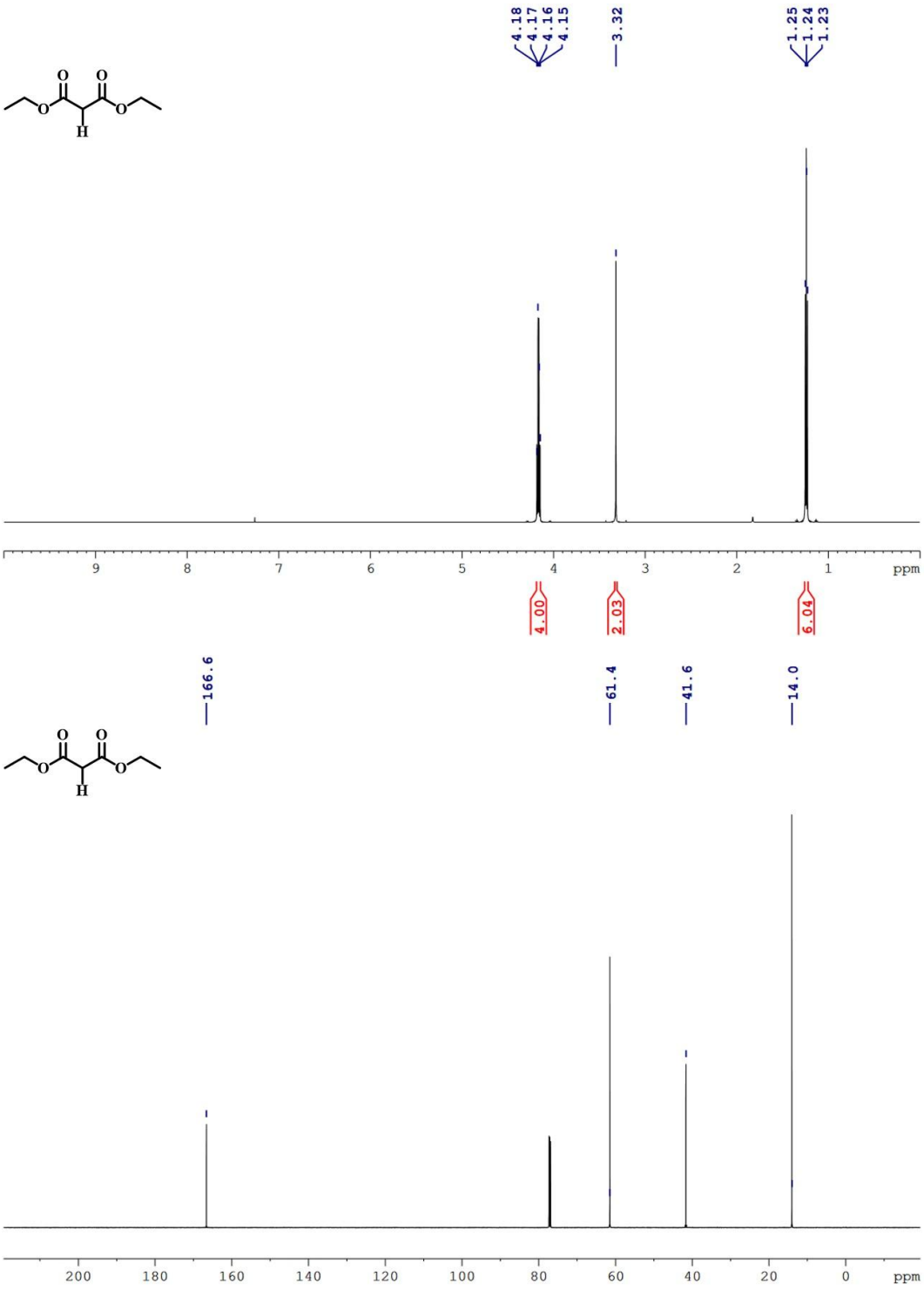


Figure S40. ^{1}H NMR and ^{13}C NMR spectra of **14**.

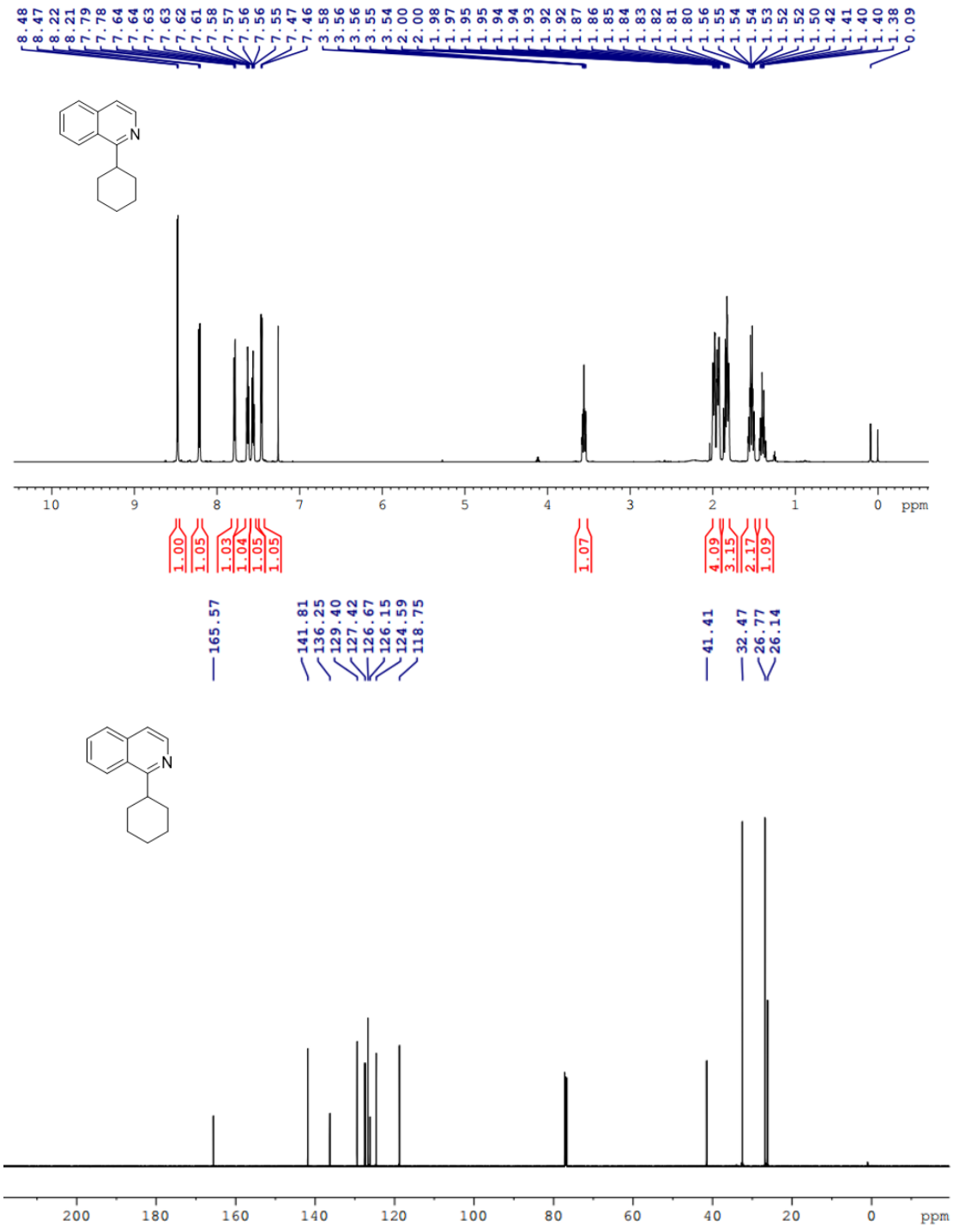


Figure S41. [1]H NMR and [13] C NMR spectra of **15**.

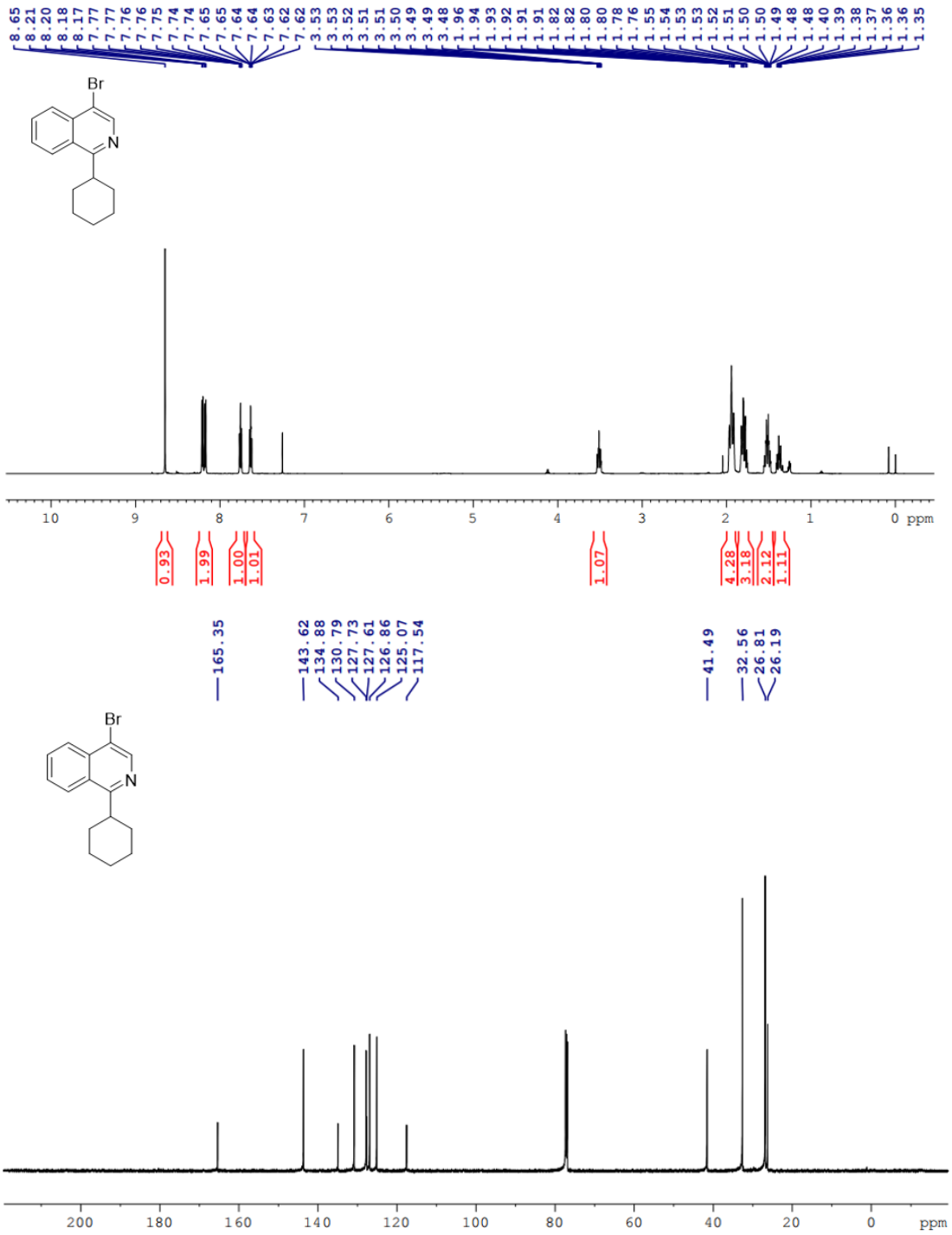


Figure S42. ^{1}H NMR and ^{13}C NMR spectra of **16**.

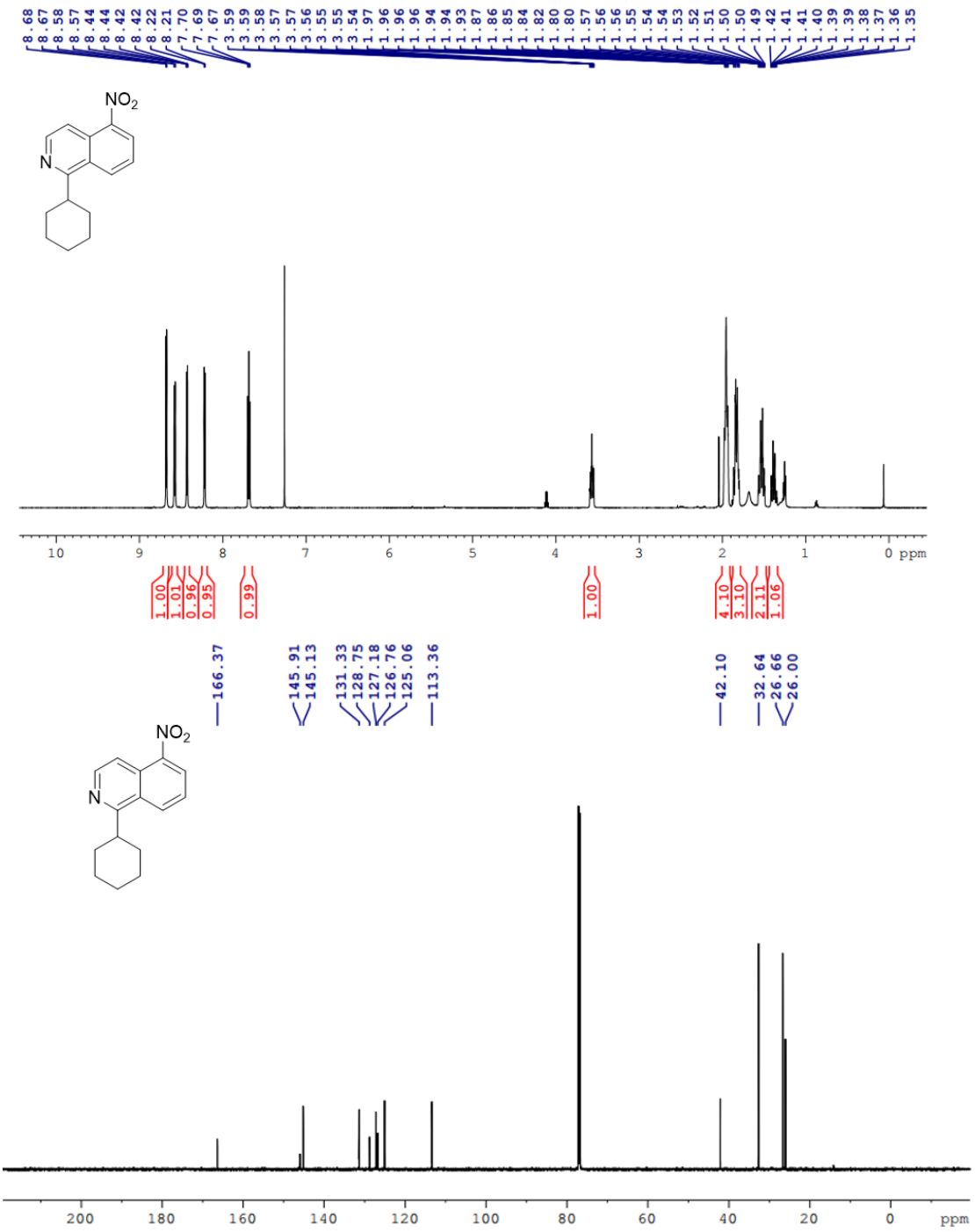


Figure S43. ^{1}H NMR and ^{13}C NMR spectra of **17**.

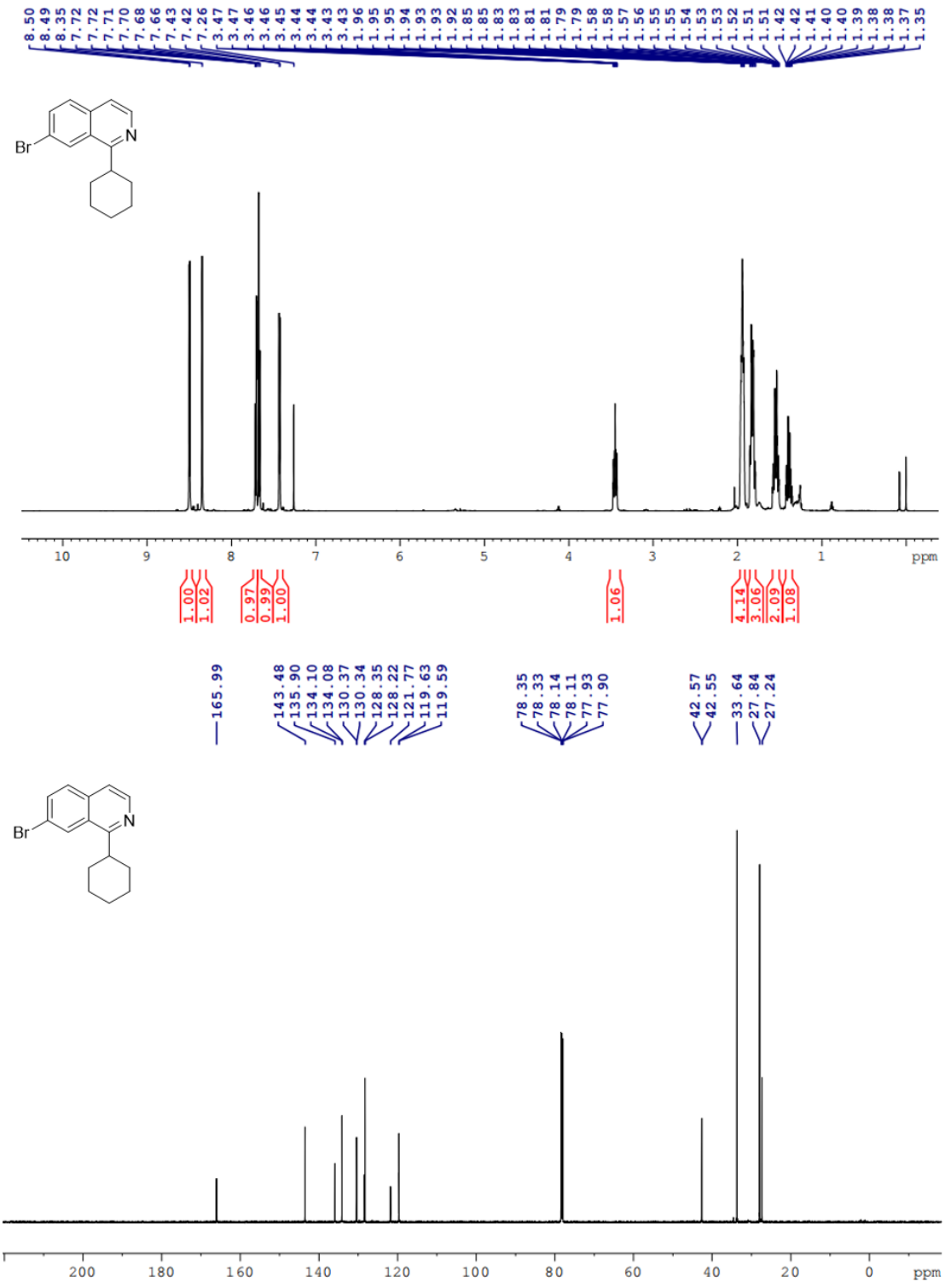


Figure S44. ^{1}H NMR and ^{13}C NMR spectra of **18**.

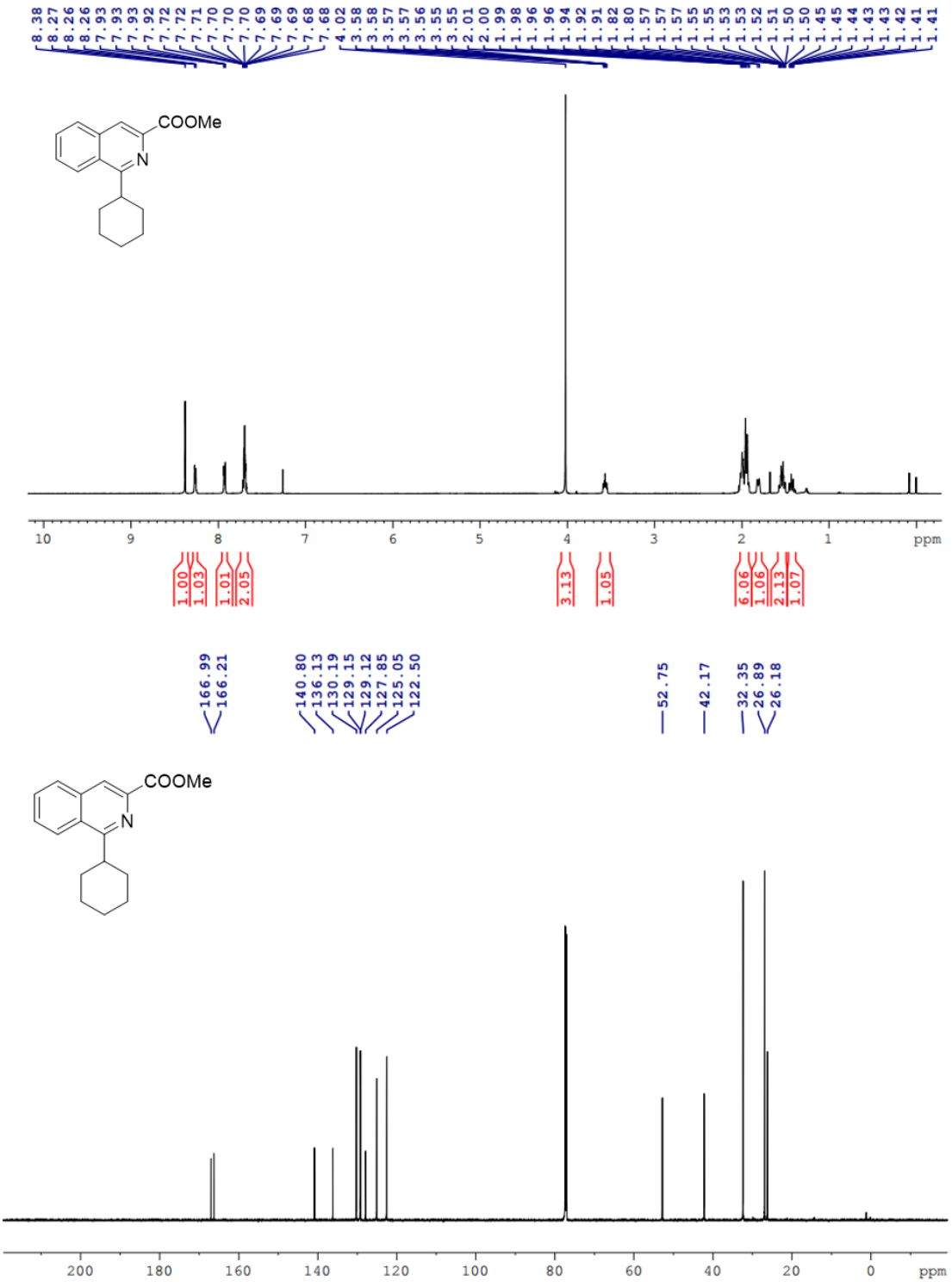


Figure S45. ^{1}H NMR and ^{13}C NMR spectra of **19**.

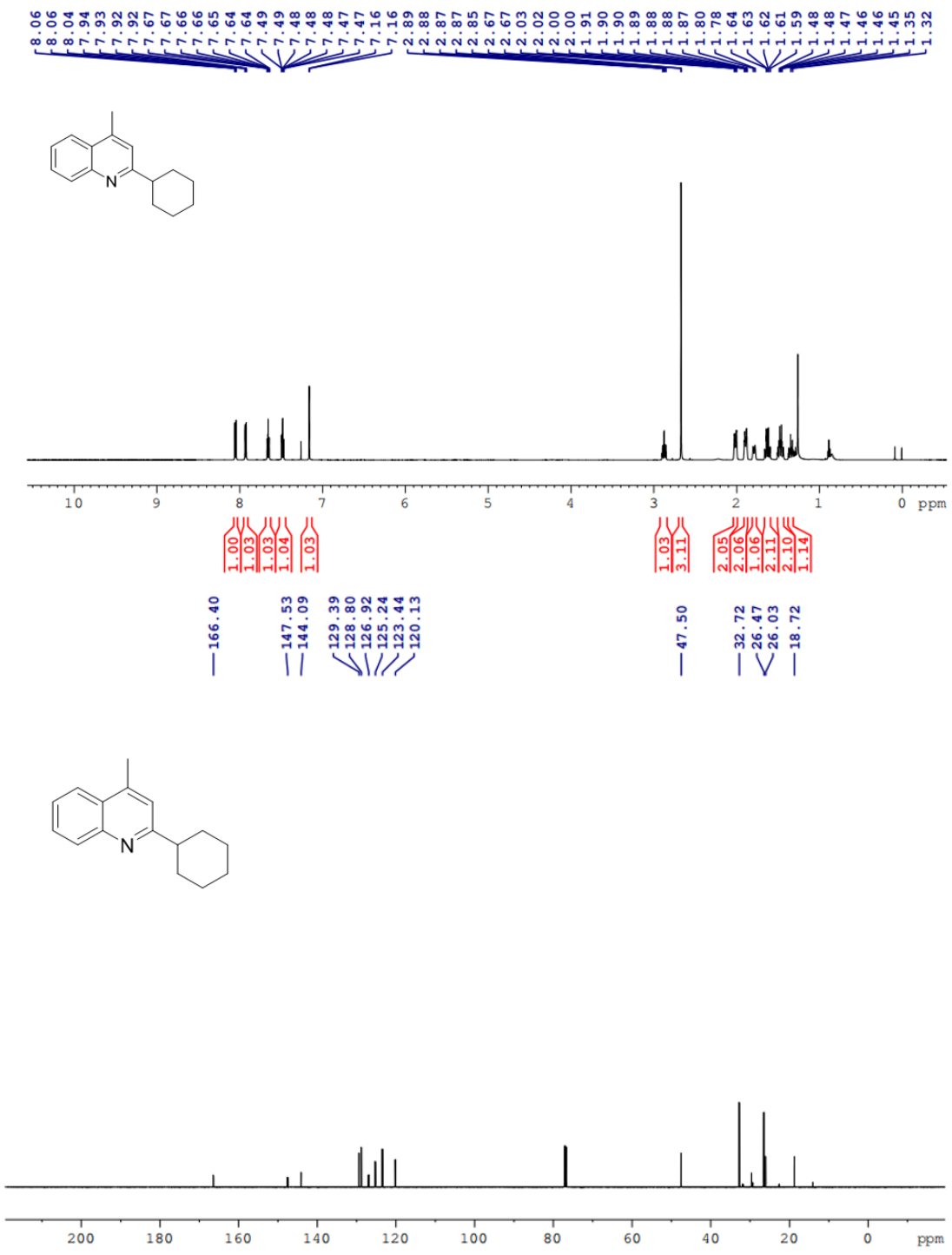


Figure S46. [1]H NMR and [13] C NMR spectra of **20**.

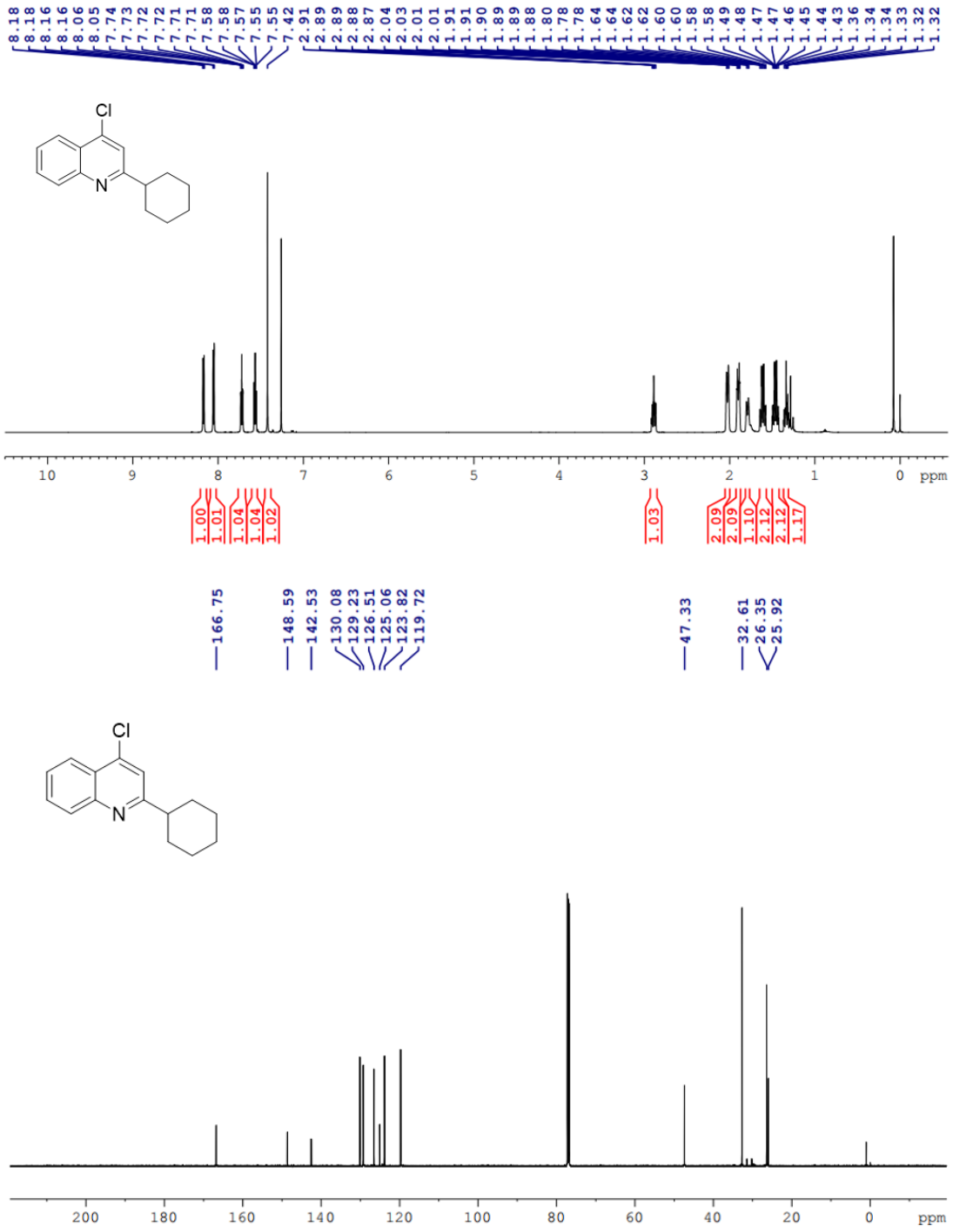


Figure S47. ^{1}H NMR and ^{13}C NMR spectra of **21**.

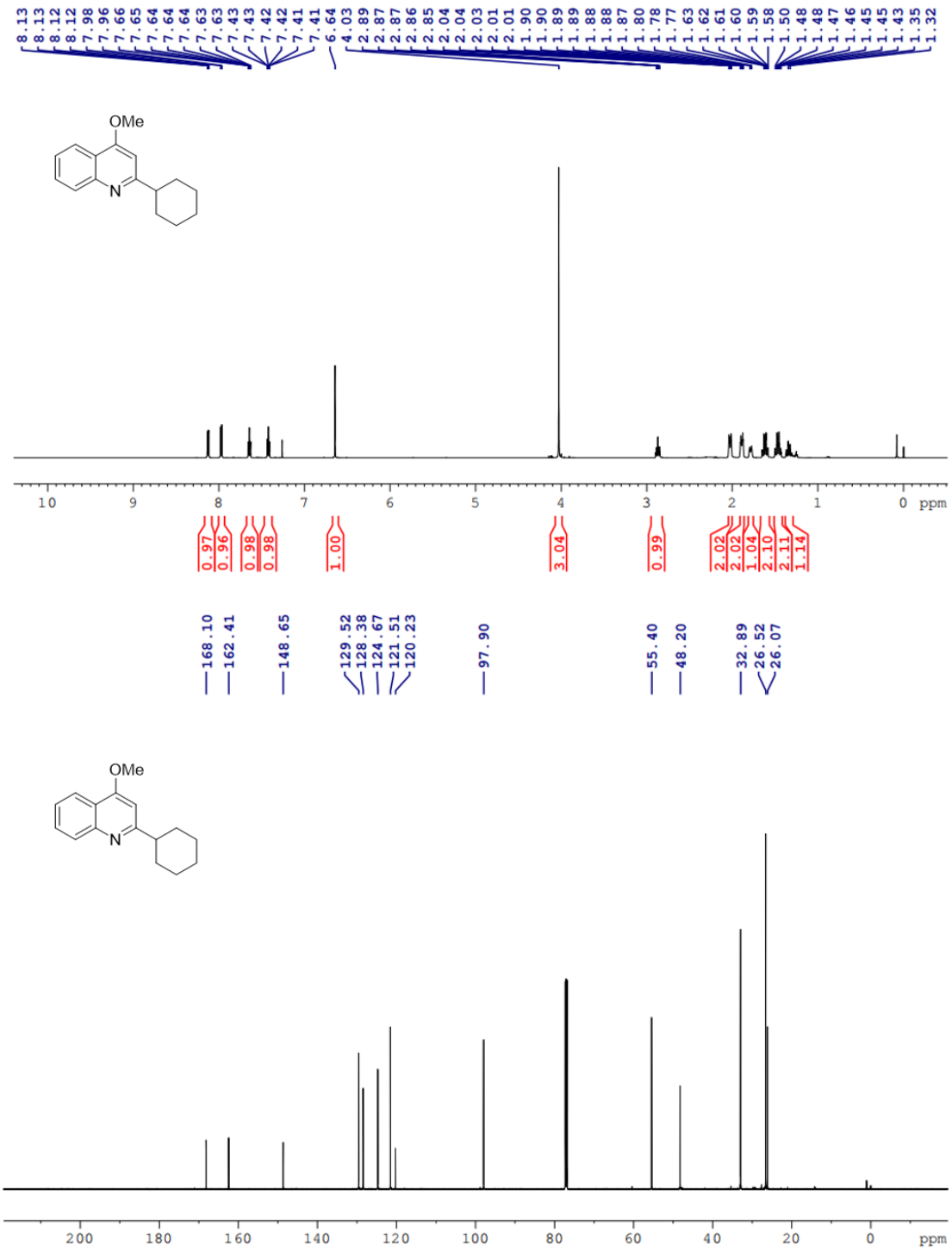


Figure S48. ^{1}H NMR and ^{13}C NMR spectra of **22**.

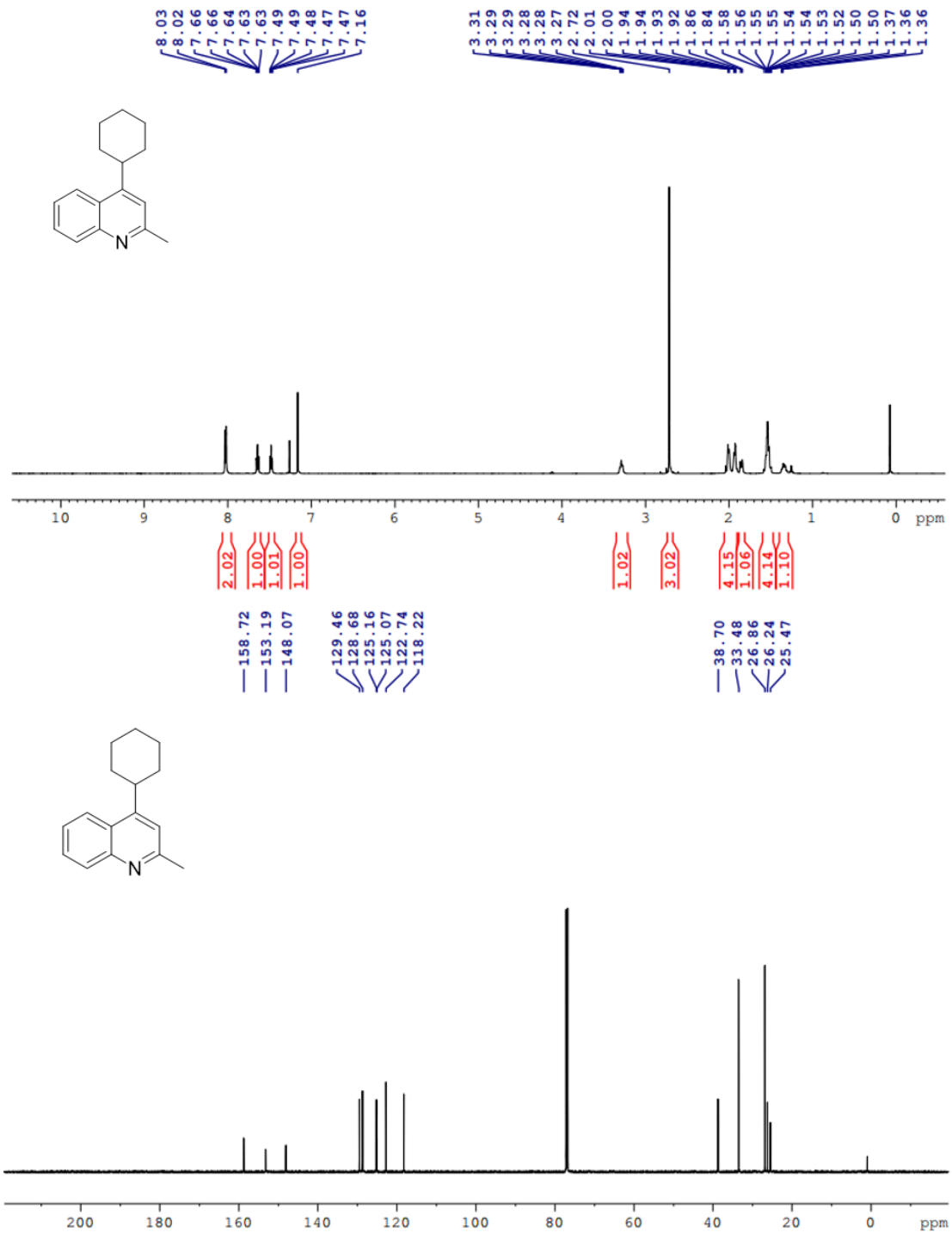


Figure S49. [1]H NMR and [13] C NMR spectra of **23**.

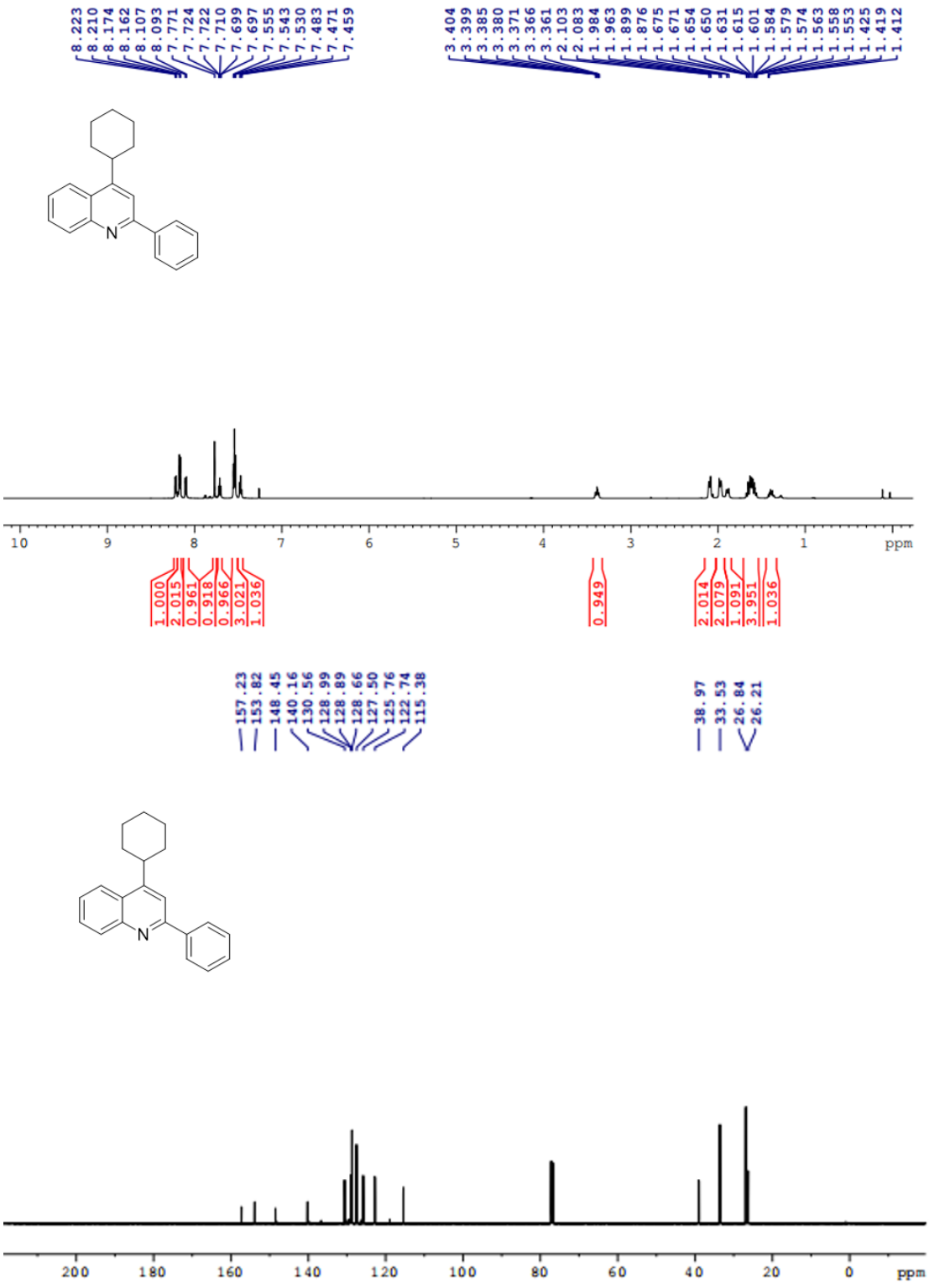


Figure S50. [1]H NMR and [13] C NMR spectra of **24**.

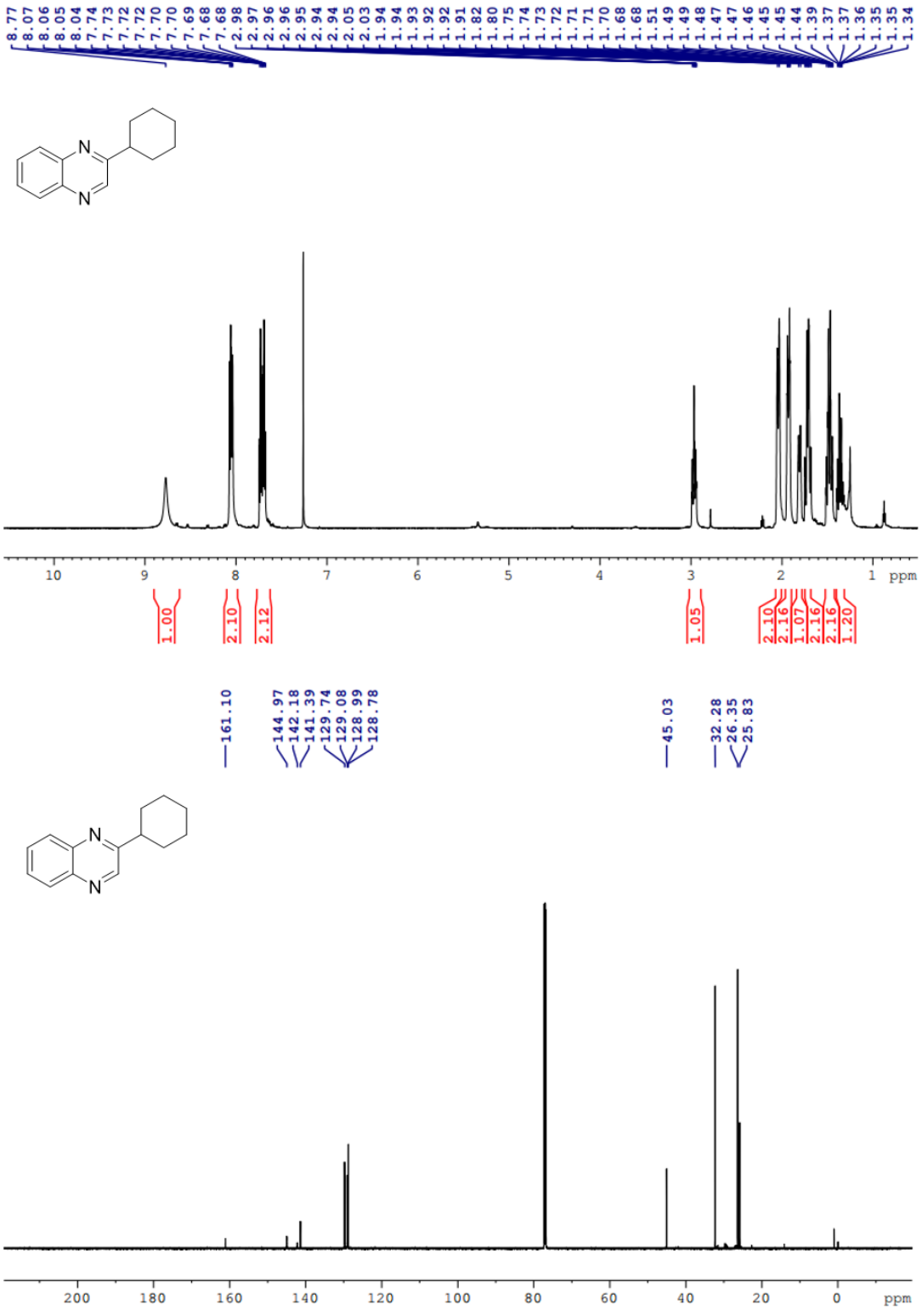


Figure S51. ^{1}H NMR and ^{13}C NMR spectra of **25**.

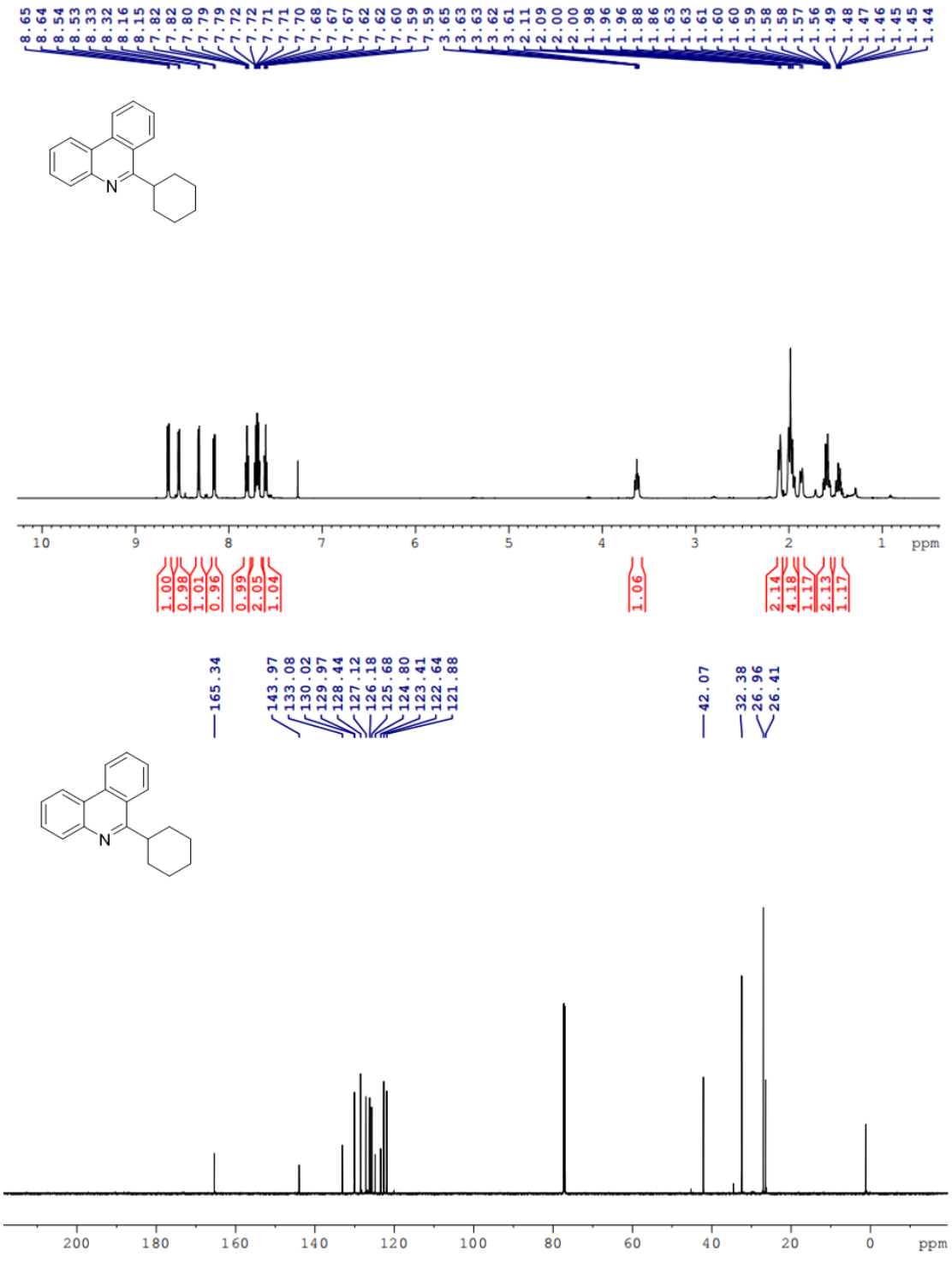


Figure S52. [1]H NMR and [13] C NMR spectra of **26**.

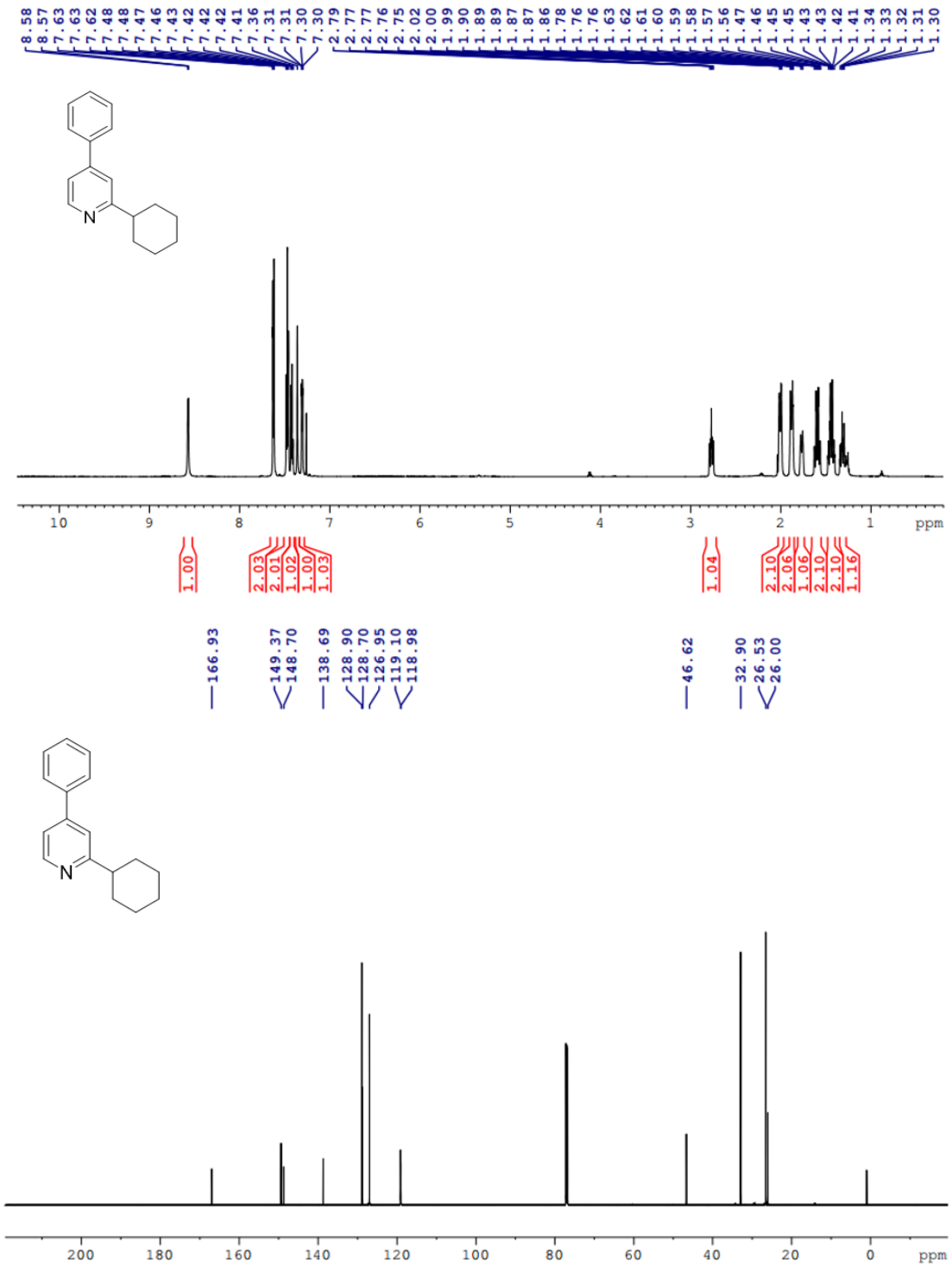


Figure S53. ^{1}H NMR and ^{13}C NMR spectra of **27-mono**.

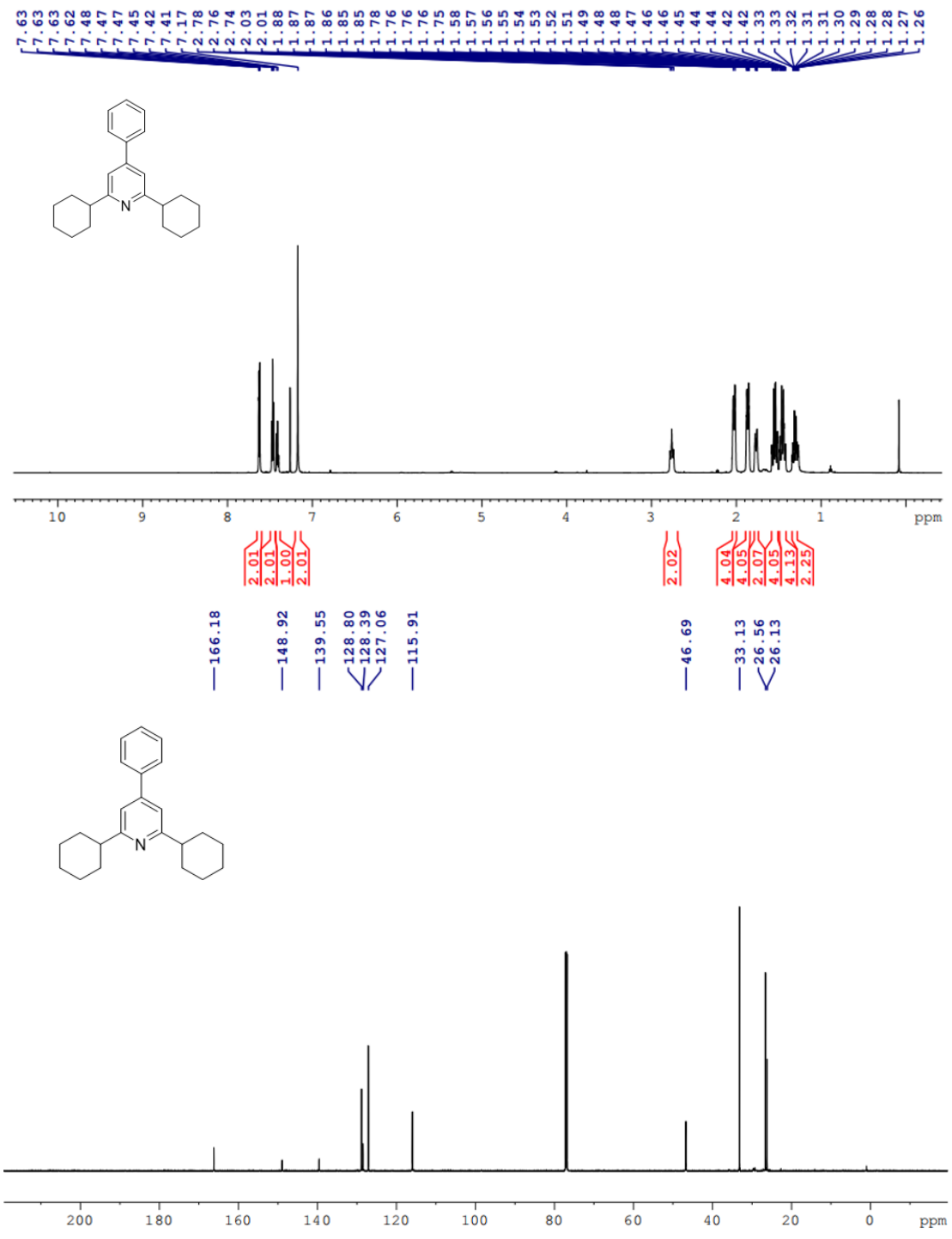


Figure S54. [1]H NMR and [13] C NMR spectra of **27-di**.

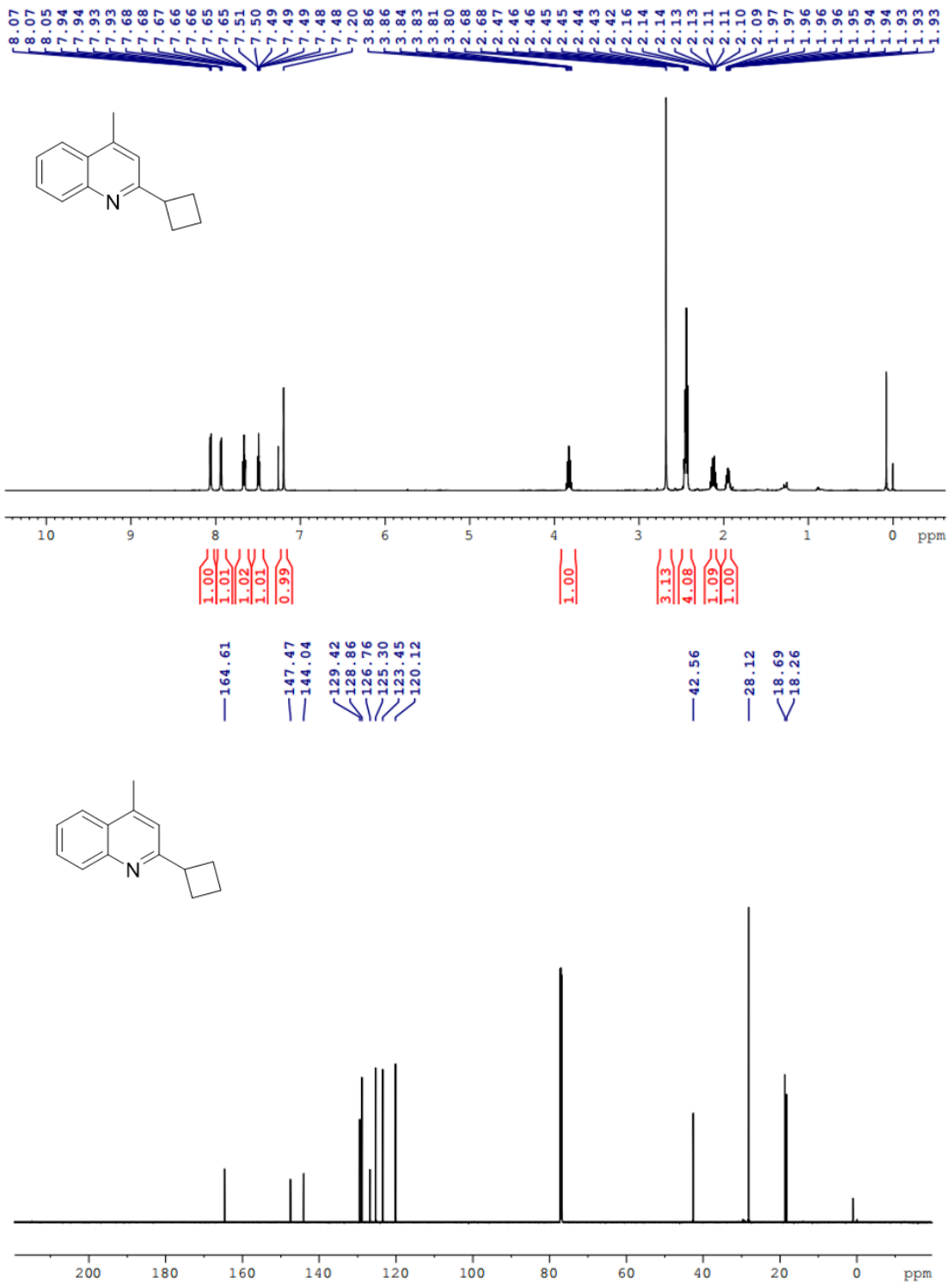


Figure S55. [1]H NMR and [13] C NMR spectra of **28**.

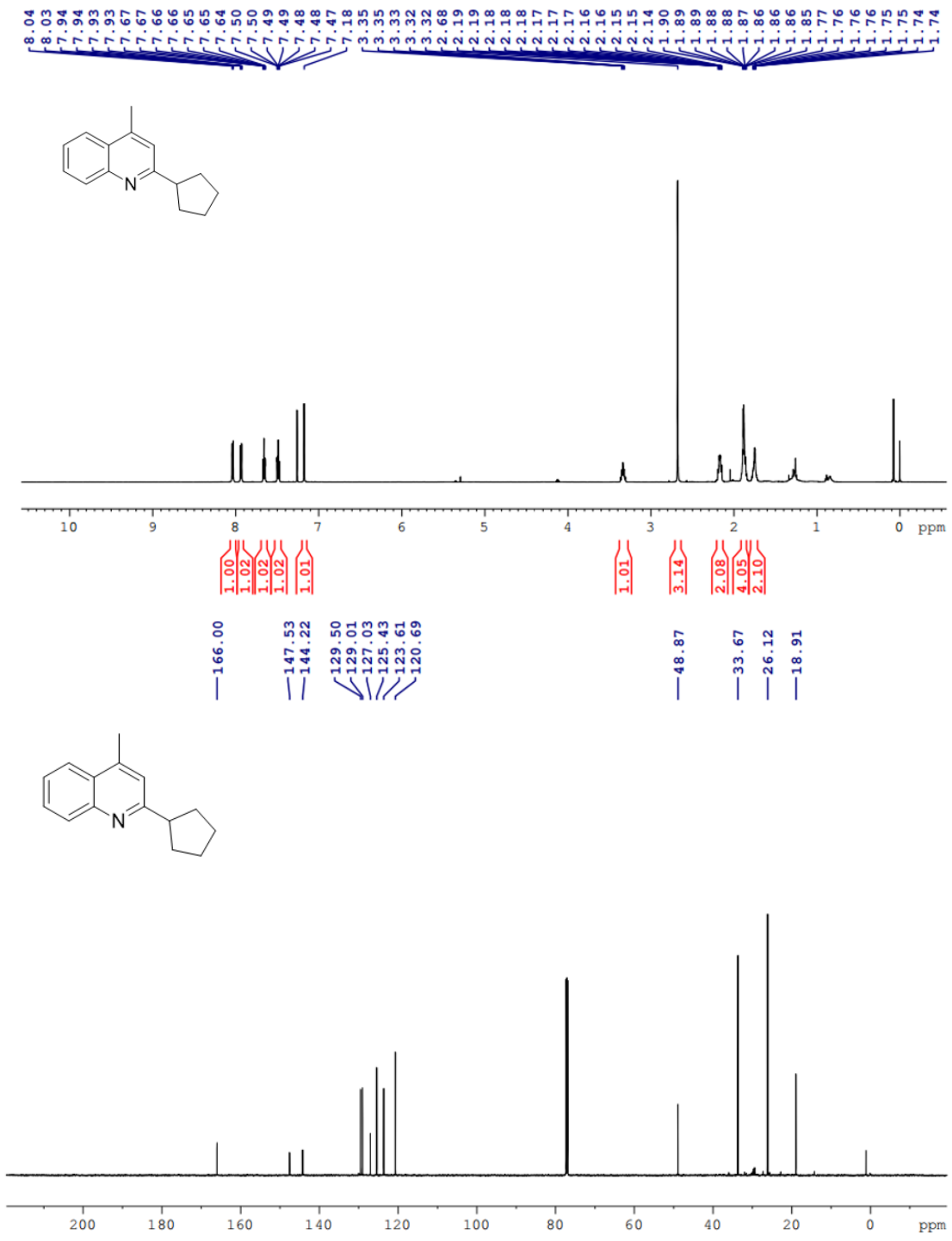


Figure S56. [1]H NMR and [13] C NMR spectra of **29**.

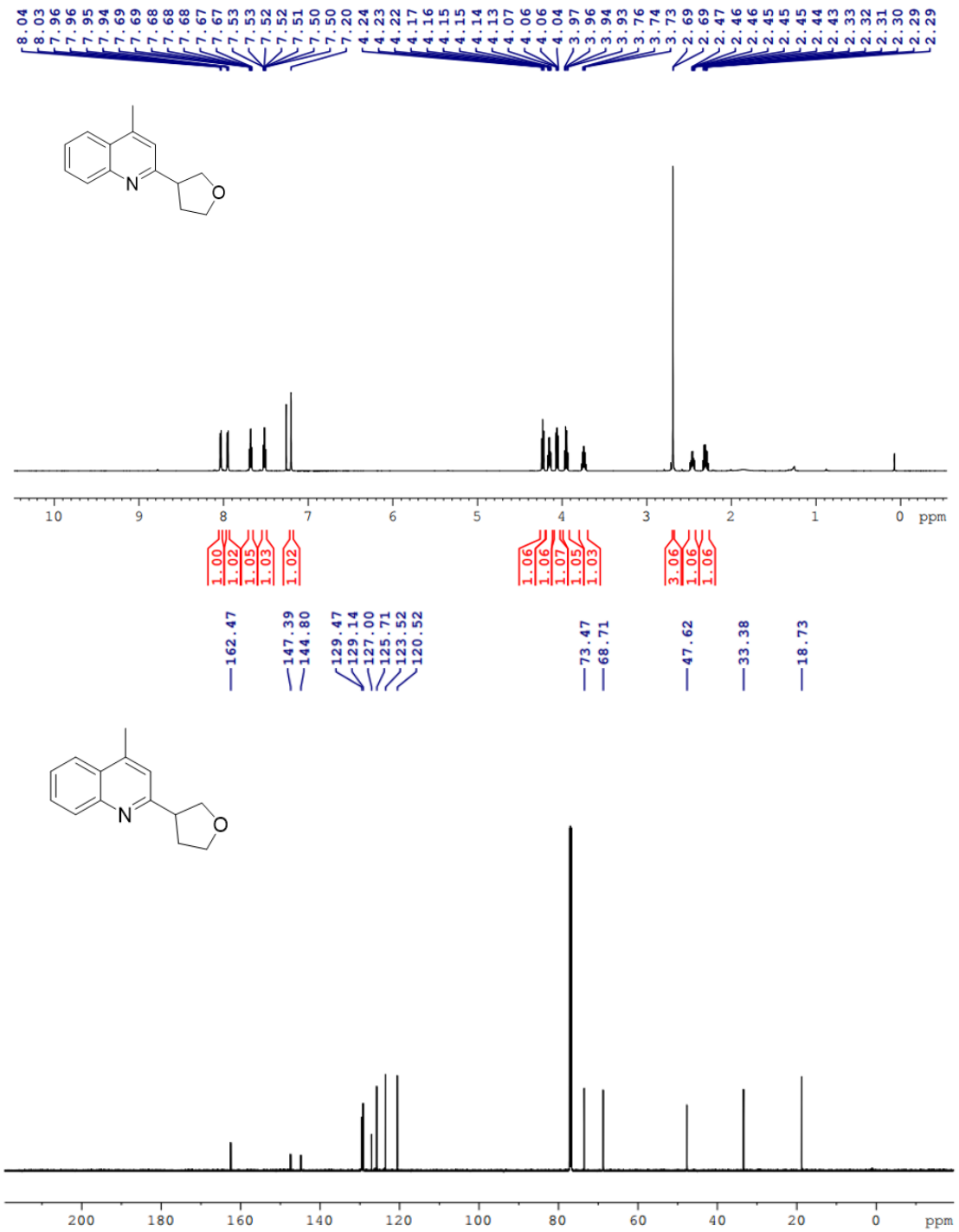


Figure S57. ^{1}H NMR and ^{13}C NMR spectra of **30**.

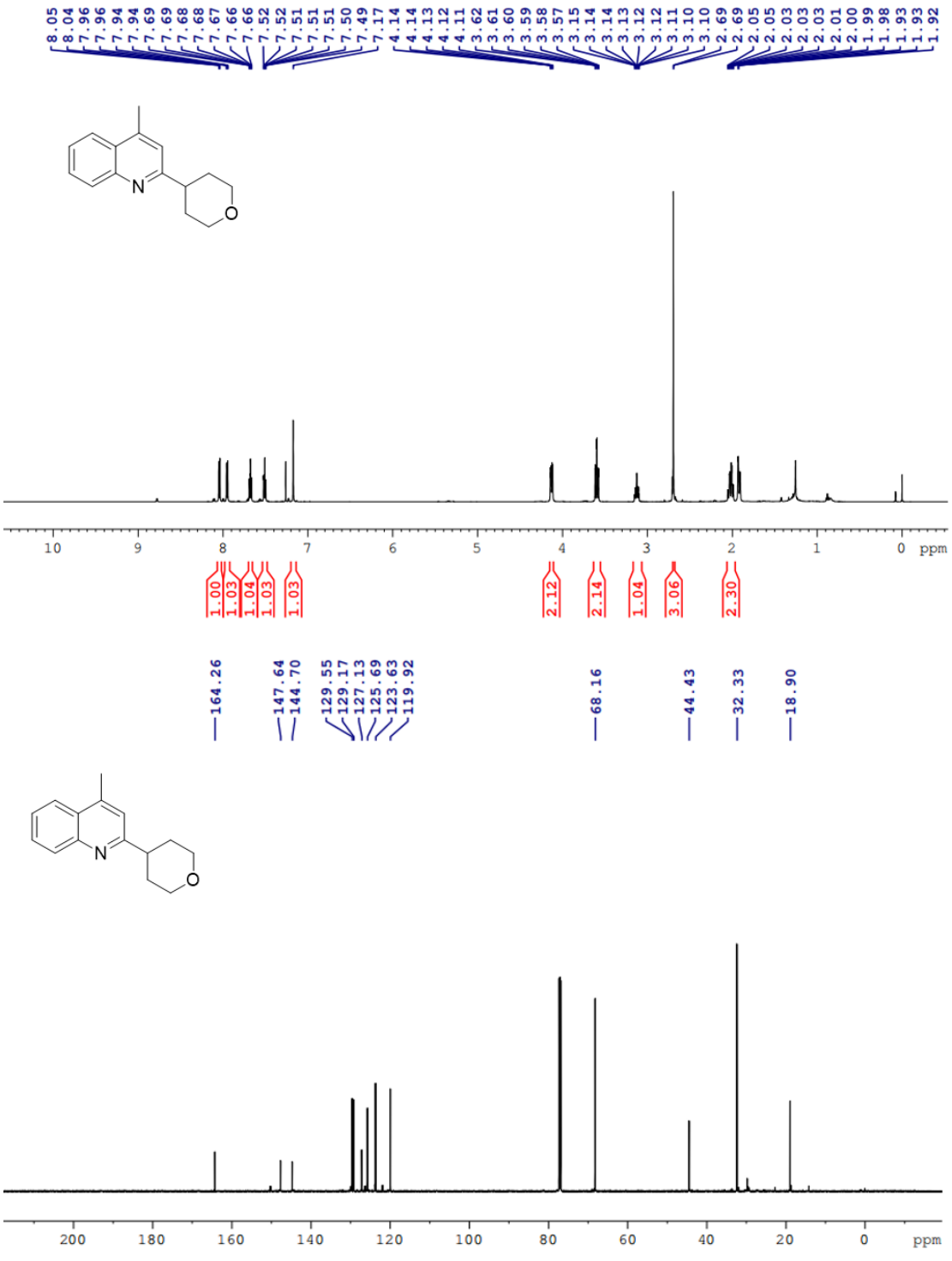


Figure S58 . [1]H NMR and [13] C NMR spectra of **31**.

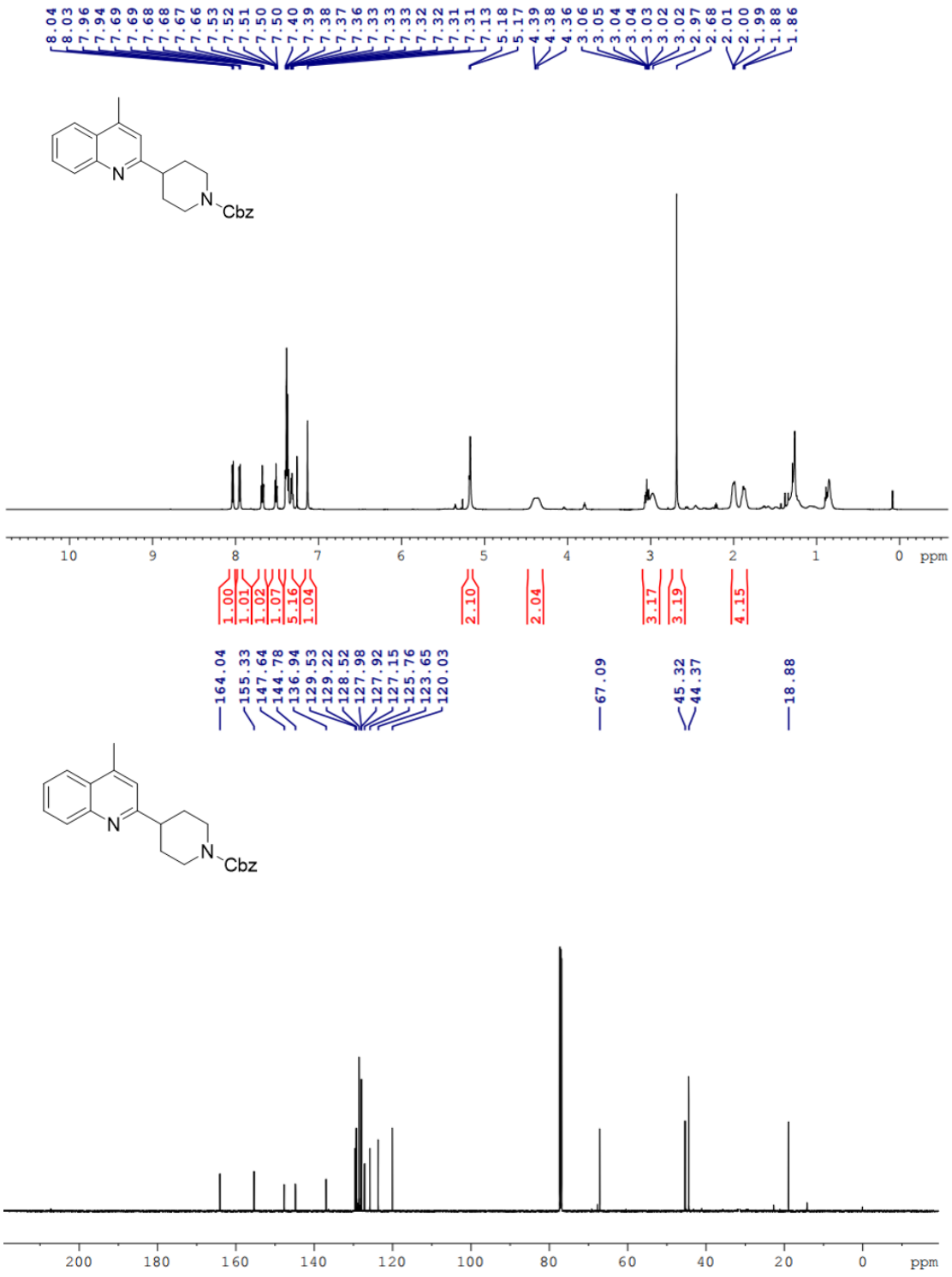


Figure S59. ^{1}H NMR and ^{13}C NMR spectra of **32.**

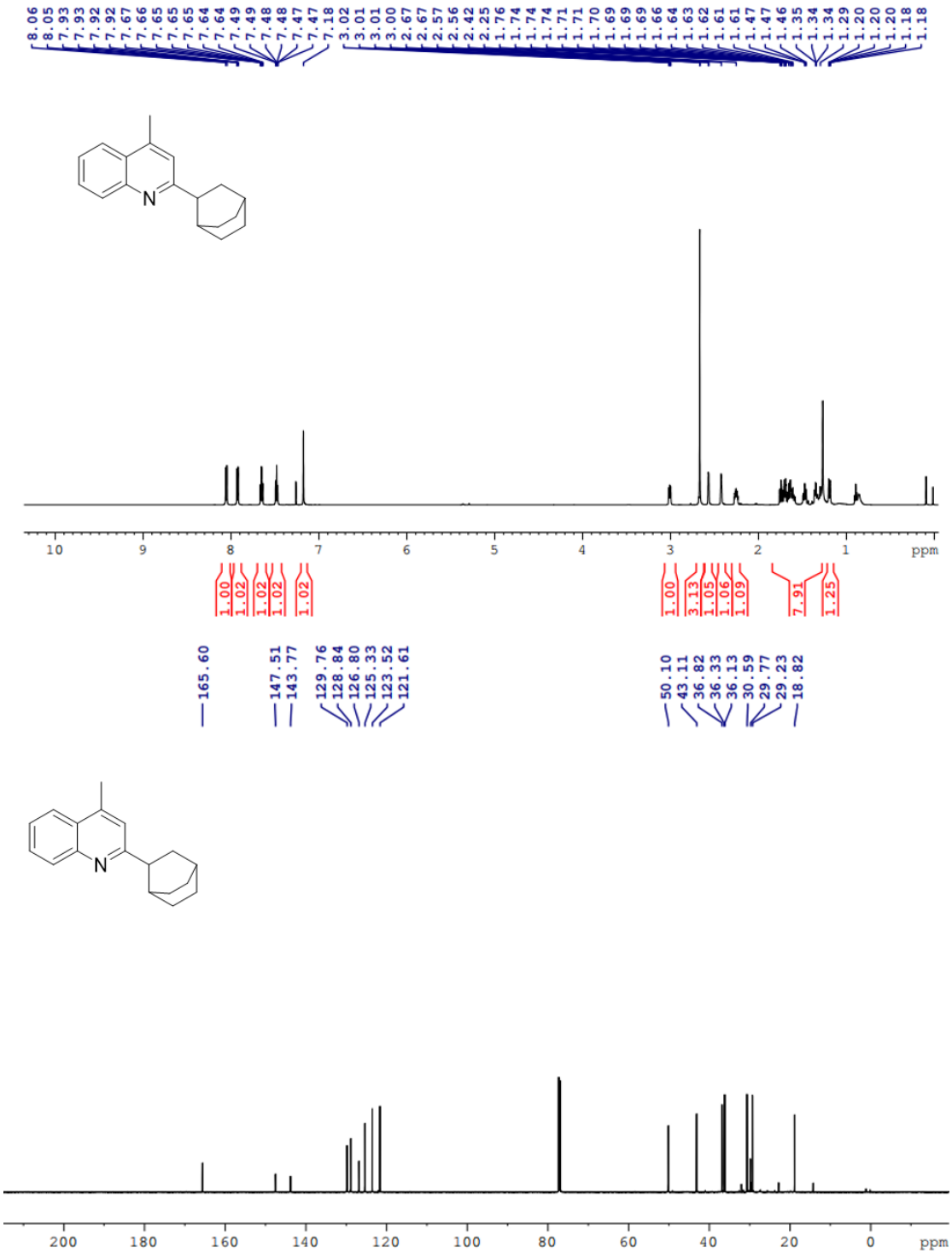
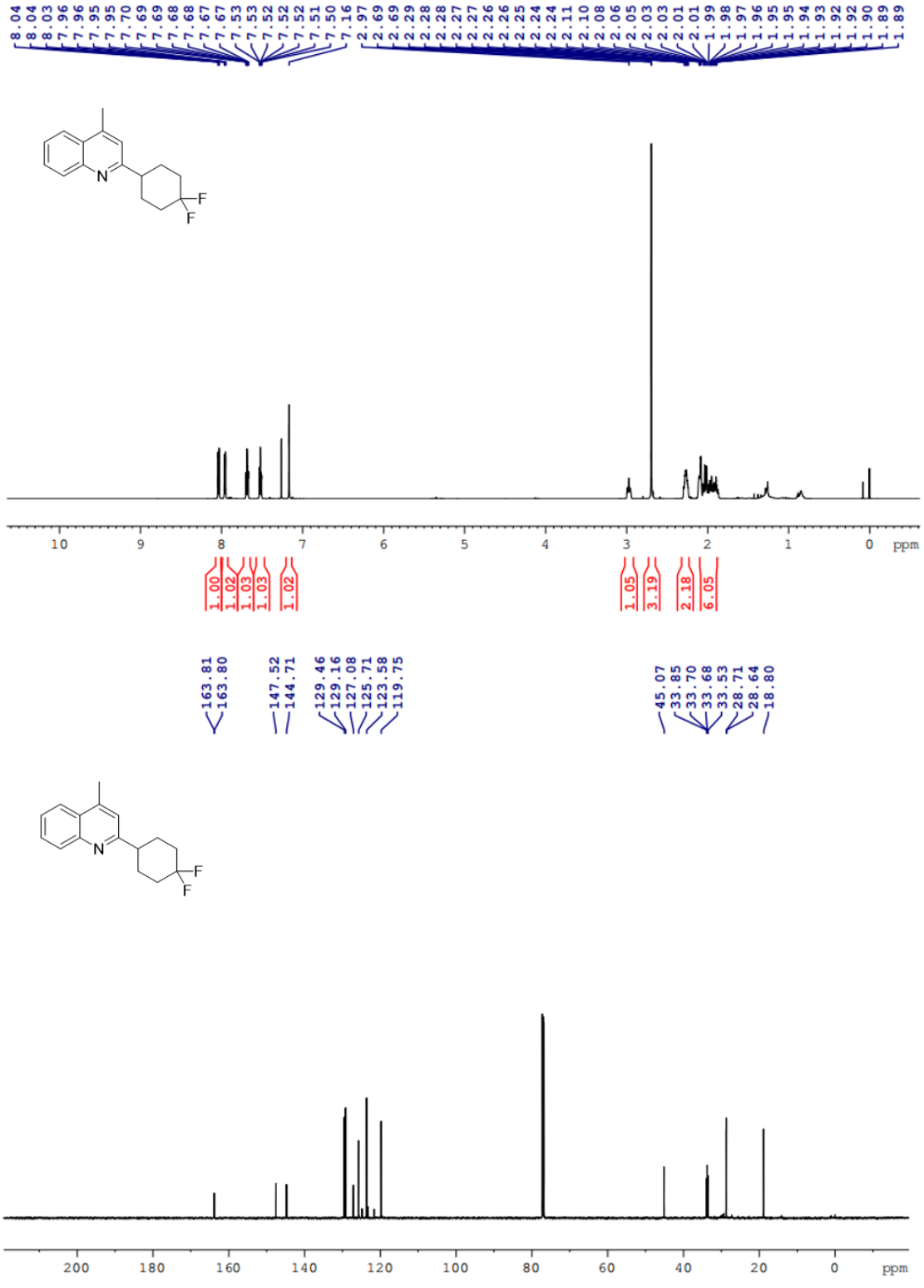


Figure S60. ^{1}H NMR and ^{13}C NMR spectra of **33.**


8.04 8.04 8.03 7.96 7.96 7.95 7.95 7.70 7.69 7.69 7.68 7.68 7.67 7.67 7.53 7.53 7.52 7.52 7.52 7.51 7.50 7.16
2.97 2.69 2.69 2.29 2.28 2.28 2.27 2.27 2.26 2.26 2.25 2.24 2.24 2.11 2.10 2.08 2.06 2.05 2.03 2.03 2.01 2.01 1.99 1.98 1.97 1.96 1.95 1.95 1.94 1.93 1.92 1.92 1.90 1.89 1.89
N
F
F
10 9 8 7 6 5 4 3 2 1 0 ppm
1.00 1.02 1.03 1.03 1.02
1.05 3.19 2.18 6.05
163.81 163.80 147.52 144.71 129.46 129.16 127.08 125.71 123.58 119.75
45.07 33.85 33.70 33.68 33.53 28.71 28.64 18.80
N
F
F
200 180 160 140 120 100 80 60 40 20 0 ppm

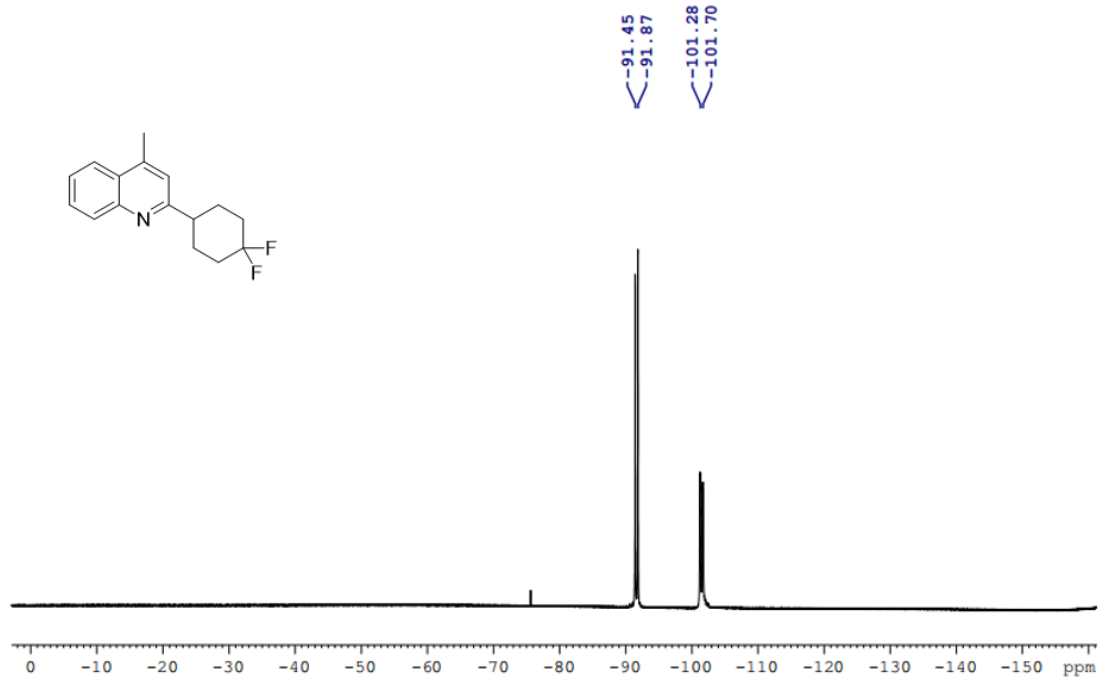


Figure S61. ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra of **34.**

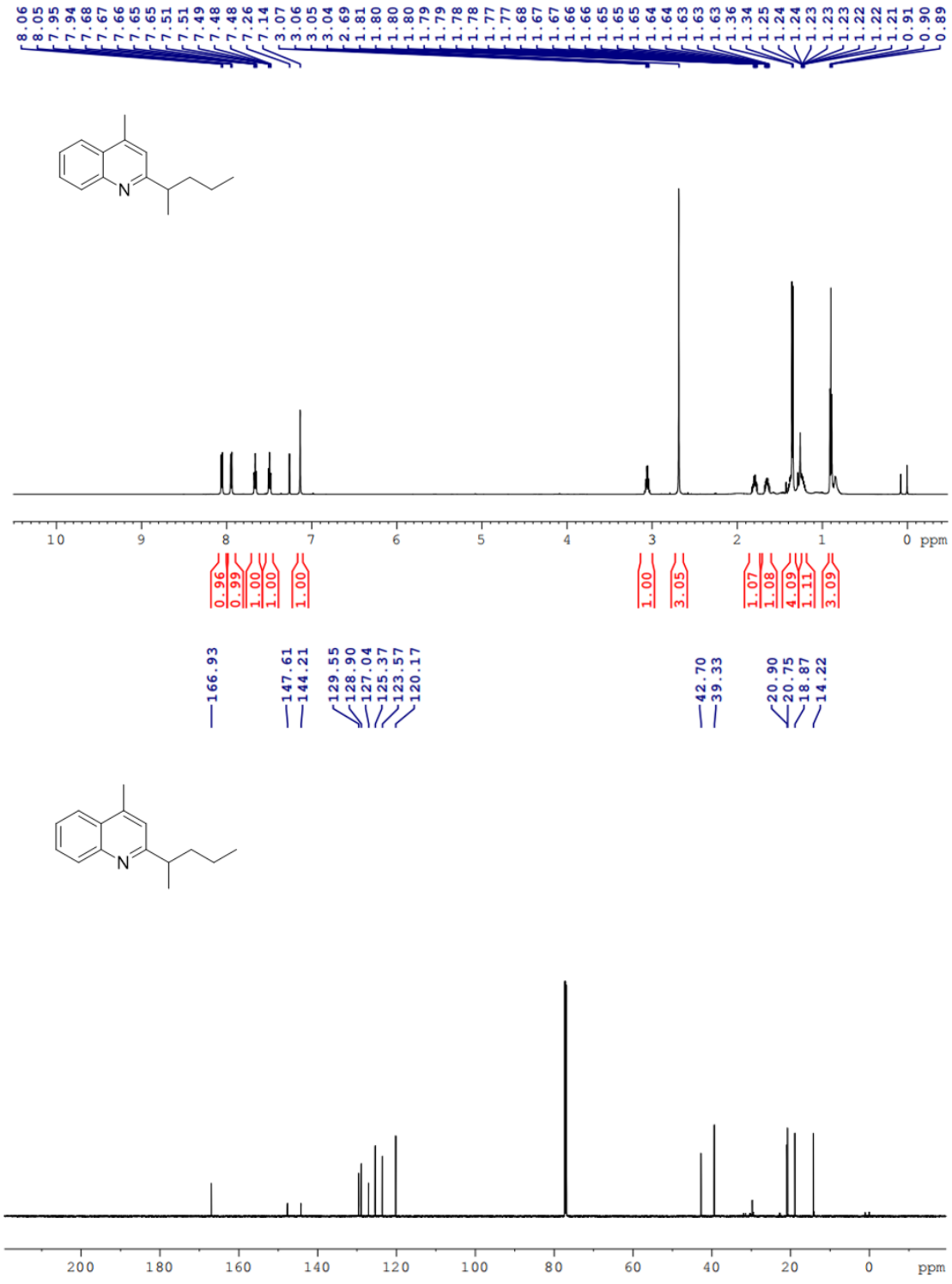


Figure S62. ^{1}H NMR and ^{13}C NMR spectra of **35.**

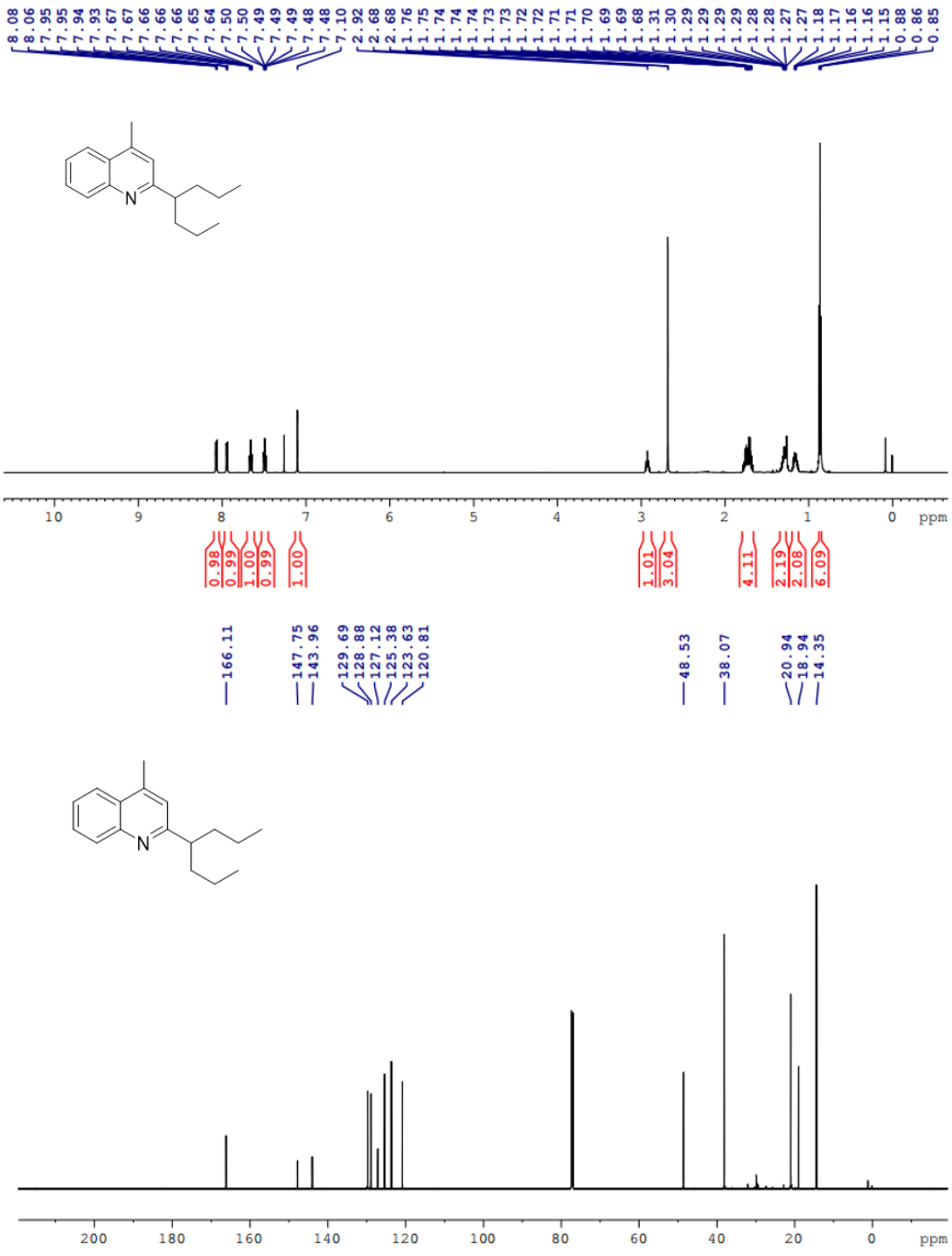


Figure S63. ^{1}H NMR and ^{13}C NMR spectra of **36.**

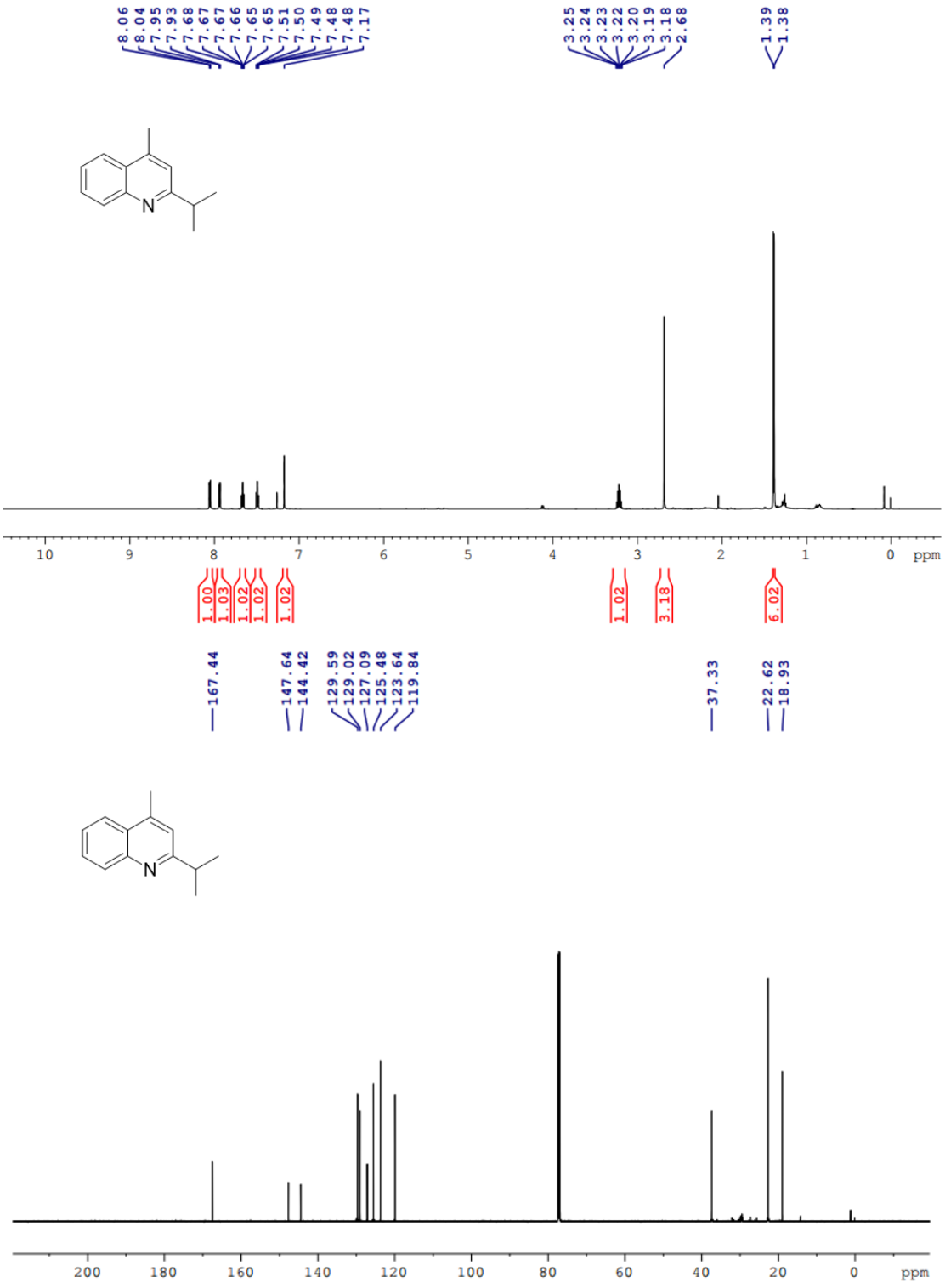


Figure S64. ^{1}H NMR and ^{13}C NMR spectra of **37.**

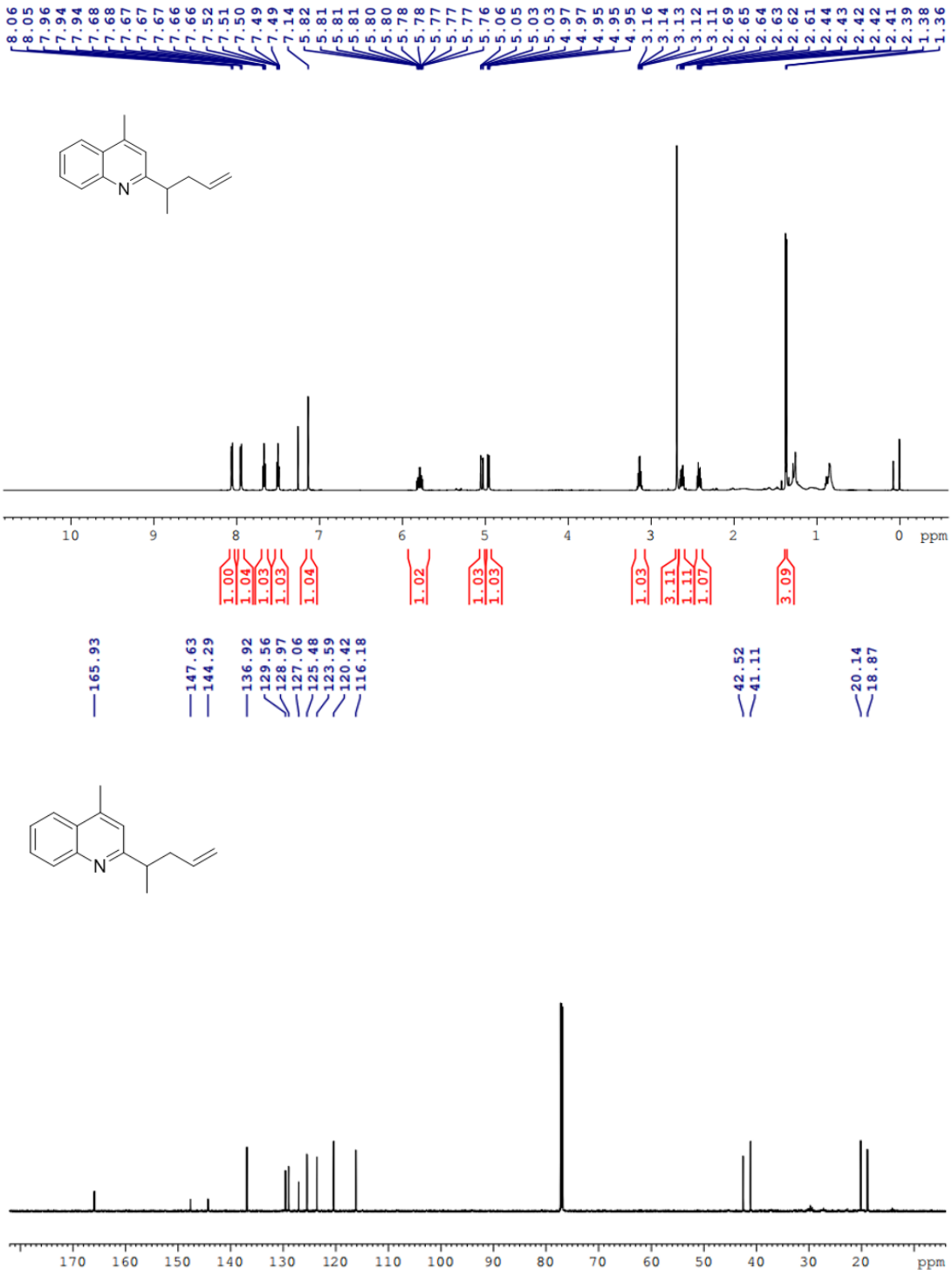


Figure S65. ^{1}H NMR and ^{13}C NMR spectra of **38.**

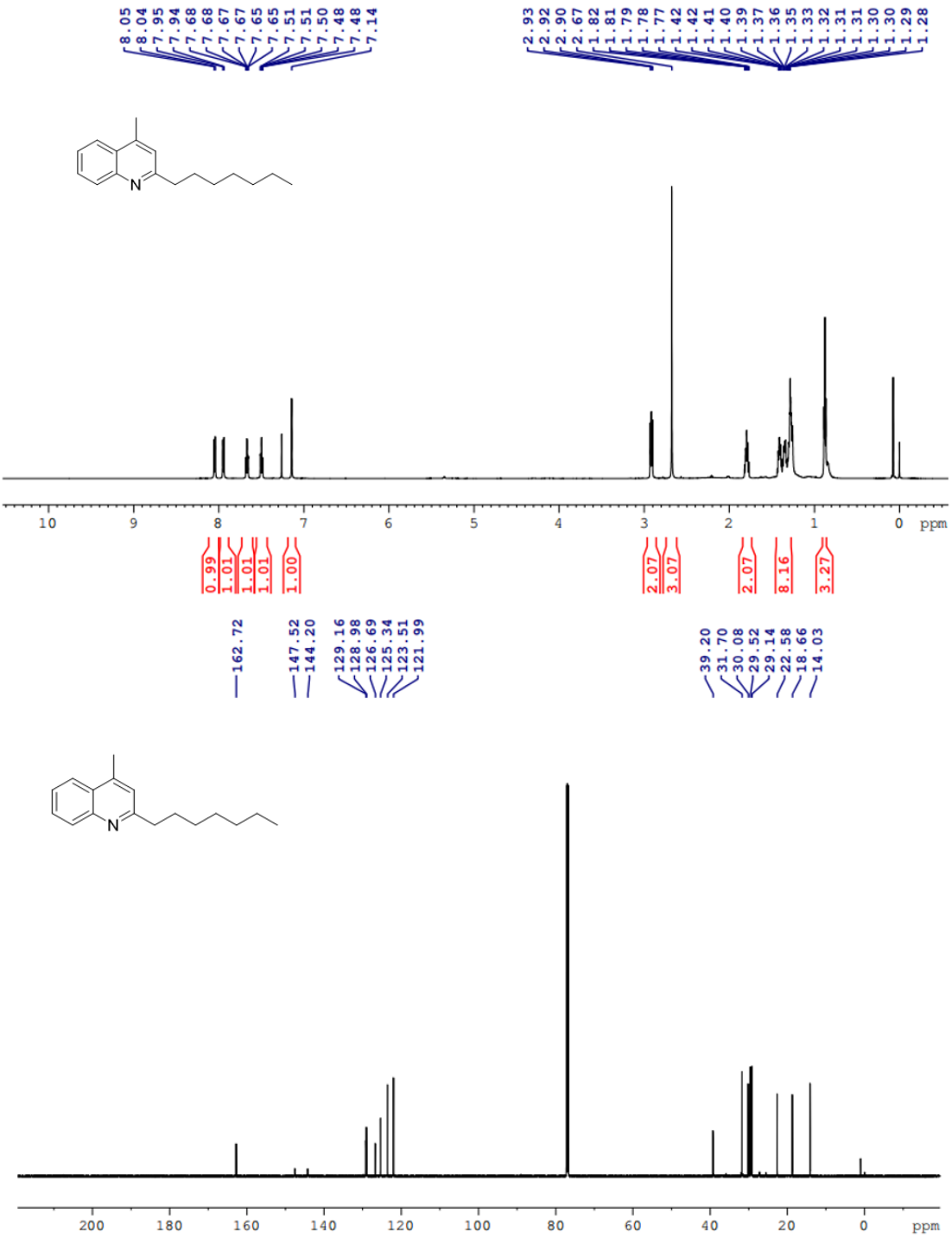


Figure S66. ^{1}H NMR and ^{13}C NMR spectra of **39.**

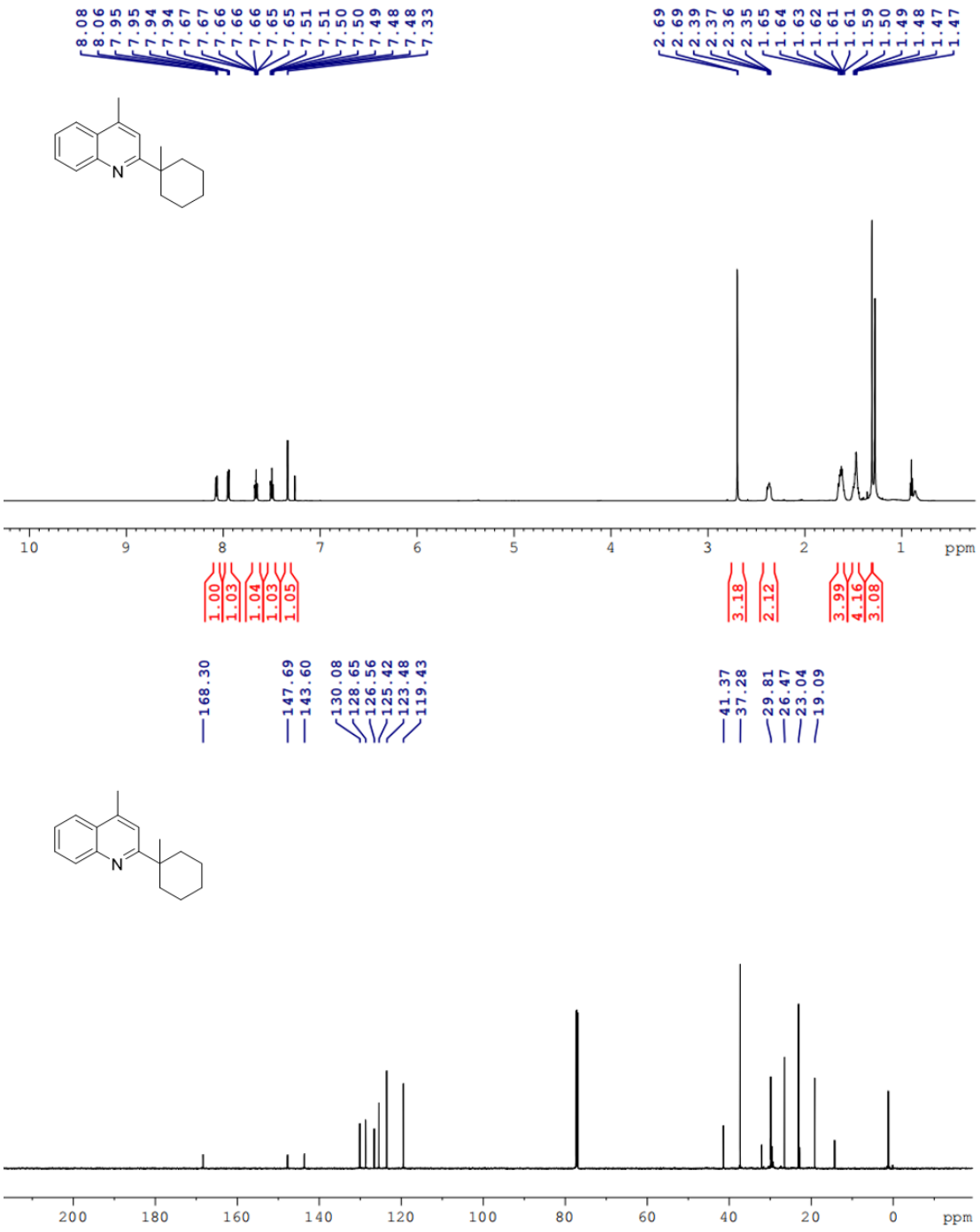


Figure S67. ^{1}H NMR and ^{13}C NMR spectra of **40.**

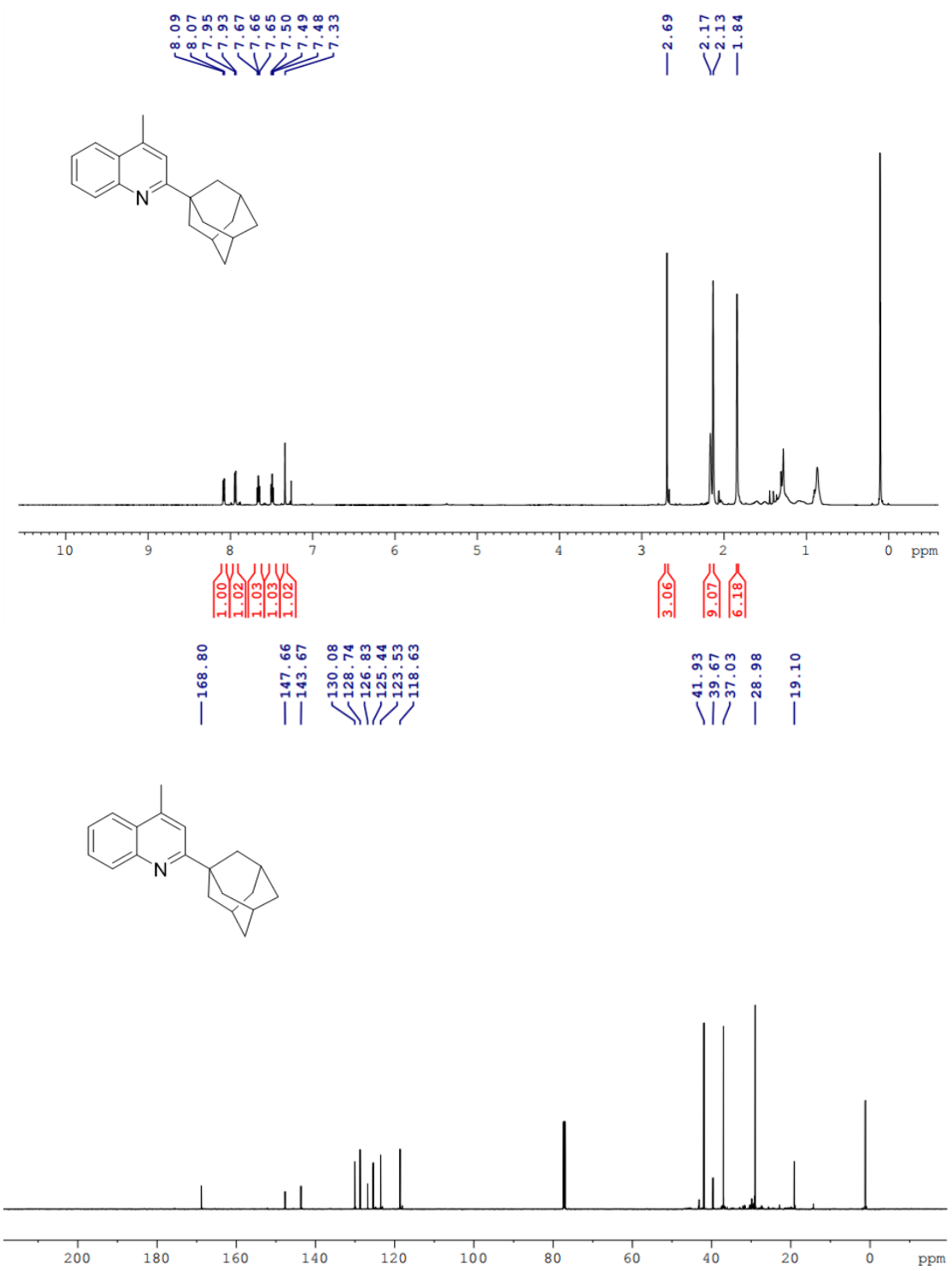


Figure S68. ^{1}H NMR and ^{13}C NMR spectra of **41.**

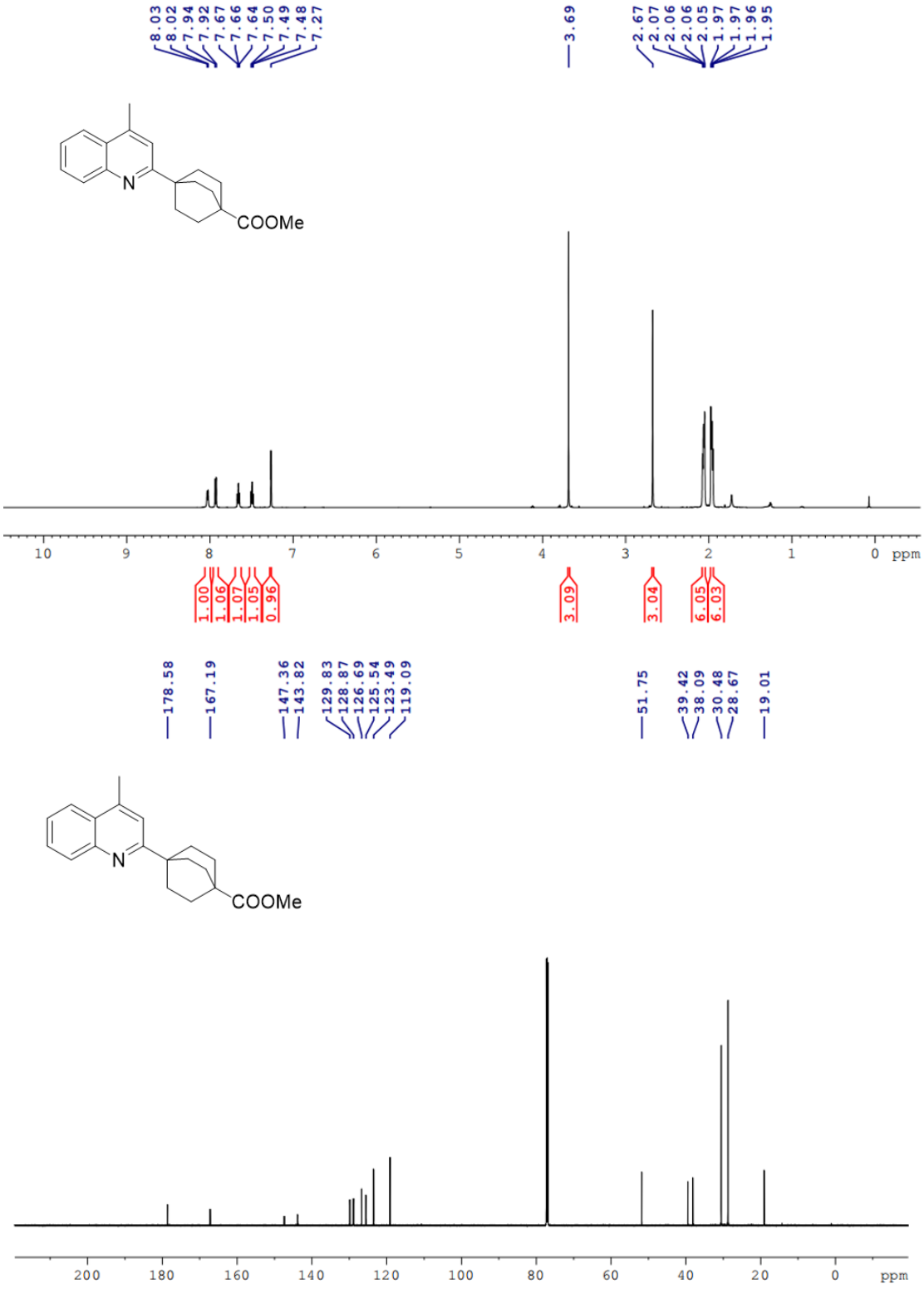


Figure S69. ^{1}H NMR and ^{13}C NMR spectra of **42.**

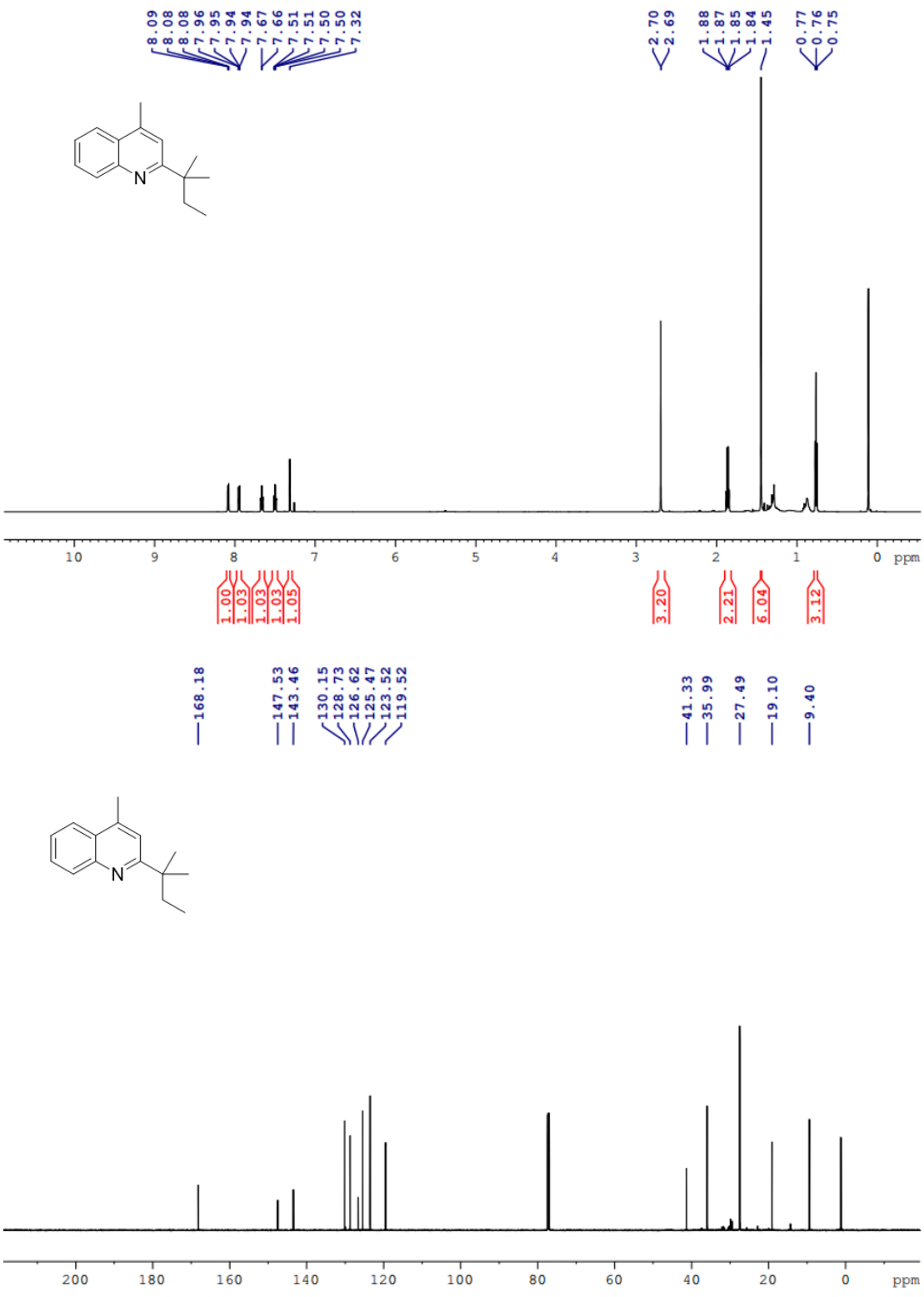


Figure S70. ^{1}H NMR and ^{13}C NMR spectra of **43.**

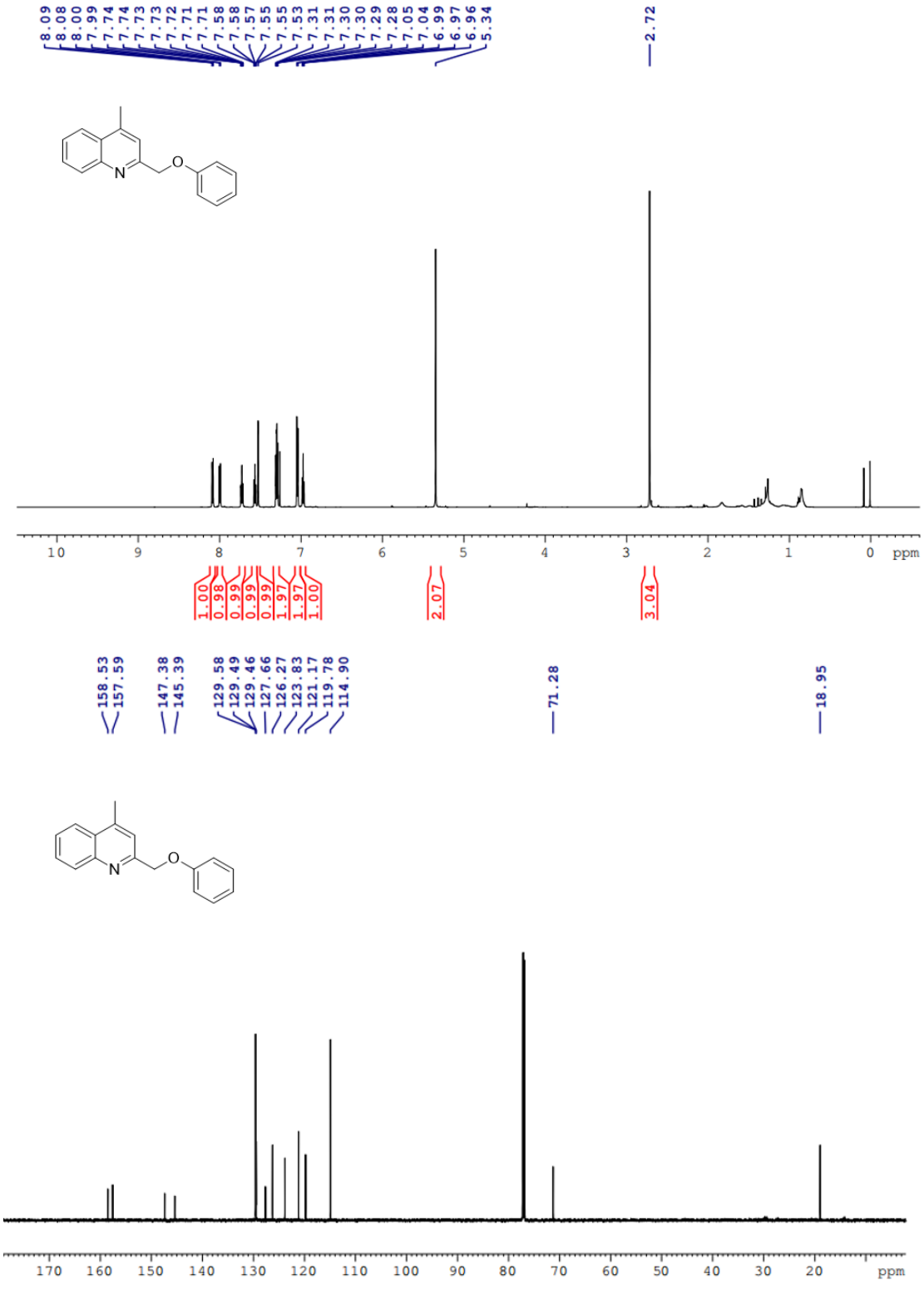


Figure S71. ^{1}H NMR and ^{13}C NMR spectra of **44.**

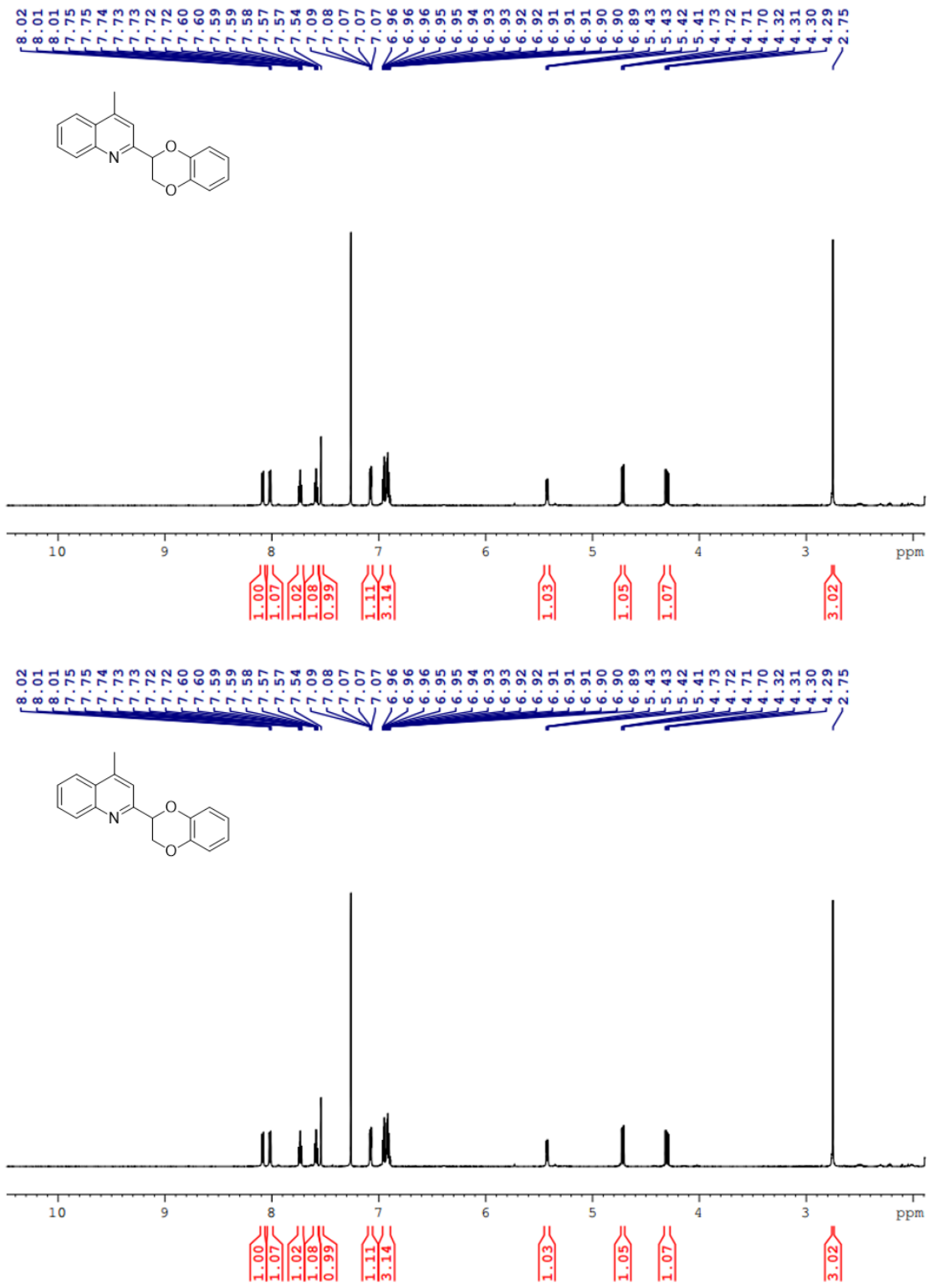


Figure S72. [1]H NMR and [13] C NMR spectra of **45.**

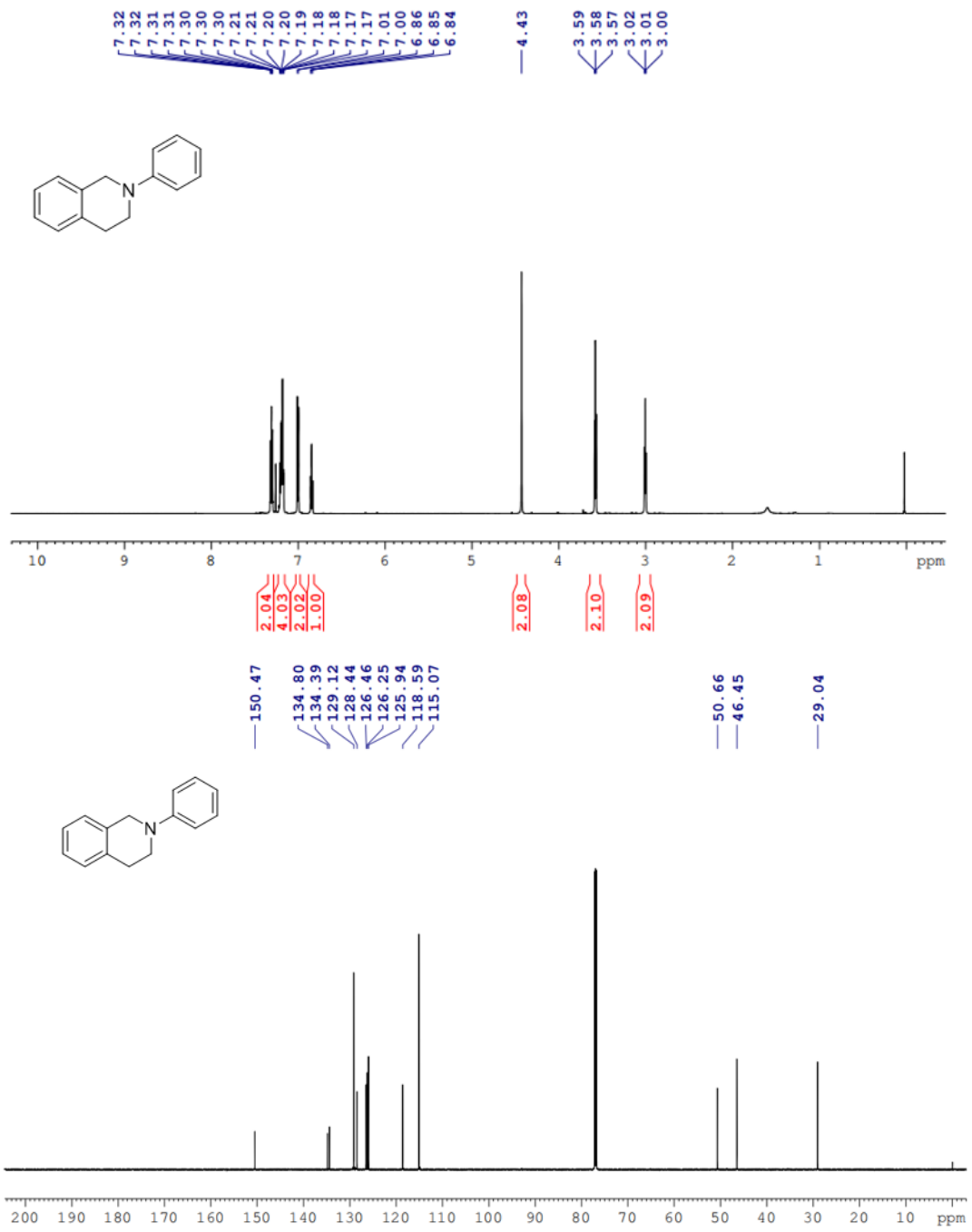


Figure S73. [1]H NMR and [13] C NMR spectra of **2-phenyl-1,2,3,4-tetrahydroisoquinoline**.

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