Supplementary Information (SI) for New Journal of Chemistry.

Supporting Information

Ferrocene-Modified Nickel MOF: Design, Characterization, and Catalytic Application for the Synthesis of 1,2-Disubstituted Benzimidazole Scaffold

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1. General experiment information:

Characterization techniques: The ^{1}H, and ^{13}C {^{1}H} NMR spectra were acquired in $CDCl_3$ solvent at room temperature using a JEOL ECS-400 spectrometer (operating at 400 MHz for ^{1}H and 101 MHz for ^{13}C). Proton resonances are described as chemical shifts (δ) about tetramethylsilane (δ 0.0), with either the residual solvent signal or tetramethylsilane itself as an internal standard: chloroform-d (*δ* 7.19, singlet). The multiplicity is represented as s (singlet), t (triplet), and m (multiplet), with coupling constants (J) specified in hertz (Hz). The ^{13}C NMR chemical shifts are given in ppm, referenced to the central line of the triplet at 76.02 ppm for $CDCl_3$. HRMS spectra were collected using a Q-TOF spectrometer in methanol at ambient temperature. FT-IR spectra were recorded using a Perkin Elmer 10.4.00 spectrometer with attenuated total reflection (ATR) in the range of 400–4000 cm^{-1} utilising KBr pellets under an inert argon atmosphere. Oxford Instruments' ESCA+ Omicron Nanotechnology system was used to obtain the X-ray photoelectron spectroscopy (XPS) spectra. The tests were conducted using an XPS spectrometer and an XM 1000 X-ray monochromator. The XPS spectra were acquired using Al Kα (1,486.6 eV) as the radiation source and an instrumental resolution of 0.8 eV. The generated information profiles were manually assessed and deconvoluted with the Casa XPS software (Casa Software Ltd., U.K.). Powder XRD investigation was performed on a Rigaku Miniflex 600 diffractometer with CuKα radiation (λ = 1.5409 Å). The complete details of all instruments utilized in this research work, including instrument name, brand name, model name, and country of origin, have been systematically listed in **Table S1**.

Table S1 List of the instrument's name, brand and model, country of origin for all the instruments

S. No.	Instrument Name	Brand Name	Model Name	Country of Origin
1.	FE-SEM	ZEISS (Carl Zeiss)	Sigma 300	Germany
2.	TGA	Shimadzu	DTG-60H	Japan
3.	FTIR	Bruker	Tensor II	Germany
4.	BET	Quantachrome Instruments	Nova Touch LX2	USA (Quantachrome is a US-based company, acquired by Anton Paar)
5.	P-XRD	Anton Paar	High-Temperature P-XRD (like featuring Anton Paar's HTK 1200n oven attachment)	Austria

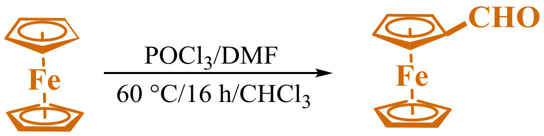
6.	XPS	Physical Electronics (Ulvac-Phi, Inc.)	PHI 5000 Versa Probe III	USA (PHI), with Japanese affiliation (ulvac-Phi)
7.	NMR	JEOL	ECS 400 MHz (JEOL NMR ECS 400)	Japan
8.	HRMS	Waters	Xevo G2-S Q-tof	USA

Chemicals and materials: Nickel nitrate hexahydrate ($Ni(NO_3)_2.6H_2O$, 98%), phosphorus(V) oxide chloride ($POCl_3$, 98%), *o*-phenylenediamine ($C_6H_8N_2$, 98%), and potassium tert-butoxide (t-BuOK, 98%) were purchased from Avra. 5-Amino isophthalic acid ($H_2NC_6H_3$-1,3-(CO_2H), 99%) (AIPA) and ferrocene ($(C_5H_5)_2Fe$, 98%) were purchased from SRL and BLD, respectively. Chloroform-d with 99.8% purity, employed as the solvent for NMR analysis, was obtained from Sigma-Aldrich. All solvents used were of analytical grade. The reactants, reagents, chemicals, and solvents were sourced from local commercial sources and utilised without additional processing.

2. General procedure for catalytic reaction

Synthesis of the starting material

Ferrocene-2-carboxaldehyde: The synthesis of ferrocene-2-carboxaldehyde was performed using the previously described methodology.[1] Initially, 10 mL of DMF at 0 °C was added to a 250 mL two-neck round-bottom flask, and N_2 gas was supplied to create an inert atmosphere throughout the assembly. 11 mL of $POCl_3$ was gradually added dropwise to the round-bottom flask after a period of 10 to 15 minutes. While pouring $POCl_3$, the round-bottom flask was submerged in an ice bath because $POCl_3$ insertion is an exothermic reaction. After 20 minutes, once the electrophile was fully formed, a solution of ferrocene (10 g, 53.7 mmol) in 80-100 mL of chloroform was added dropwise to the electrophile. The ice bath was then discarded, and the reaction was allowed to continue overnight with stirring at 60-70 °C. The reaction was performed in chloroform, and the product was isolated by column chromatography as a dark yellow solid (**Scheme S1**). Melting point: 125 °C. Yield: 90%. **^{1}H-NMR (400 MHz, $CDCl_3$)** δ 9.89 (s, 1H), 4.73 (t, *J* = 2 Hz, 2H), 4.54 (t, *J* = 2 Hz, 2H), 4.21 (s, 5H) ppm. **^{13}C-NMR (101 MHz, $CDCl_3$)** δ 192.5, 72.2, 68.6 ppm (**Fig. S1**).



Scheme S1: Synthesis of ferrocene-2-carboxaldehyde

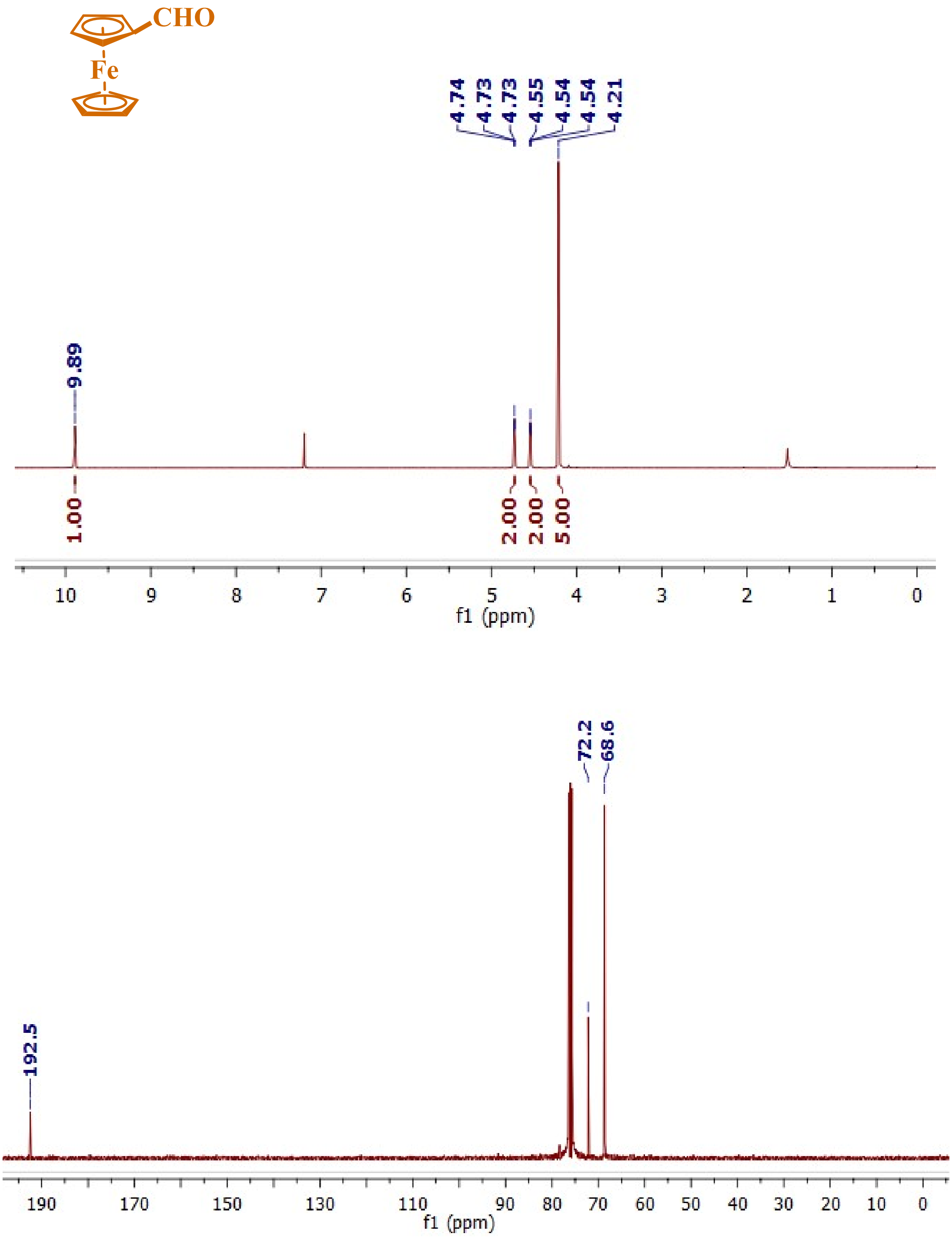


Figure S1: ^{1}H and ^{13}C-NMR spectrum of Ferrocene-2-carboxaldehyde

Catalyst development

Preparation of Fc-modified bimetallic Ni-Fc-AIPA MOF catalyst: The Ni-AIPA MOF was first prepared using a sonochemical method, and ferrocene-2-carboxaldehyde was subsequently incorporated into the synthesized Ni-AIPA MOF by following the same approach.[2] For this, the ferrocene-2-carboxaldehyde was also synthesized by the reported method (**Scheme S1**). The Fc-modified bimetallic Ni-Fc-AIPA MOF was developed as depicted in **Fig. S2** through the Schiff base reaction of Fc-CHO with NH_2 groups of amine-functionalized ligand 5-amino isophthalic acid (AIPA). For this purpose, $Ni(NO_3)_2{\cdot}6H_2O$ (1.50 g, 5.2 mmol), and AIPA (1.00 g, 5.2 mmol) was dissolved in DMF (48 mL), ethanol (3 mL), and water (3 mL) respectively using 250 mL round bottom flask and after this Fc-CHO (1.20 g, 5.2 mmol), was added to the solution followed by 30 minutes ultra-sonication of the mixture at room temperature. Subsequently, around 10 mL of triethylamine was added to the reaction mixture, which was then subjected to an additional 4 hours of ultrasonication at room temperature. The substance was then separated from the reaction mixture by centrifuging the resultant solution. After collecting a dark brown precipitate, it was repeatedly washed with ethanol and deionised water to remove any unreacted material. The developed material was then dried overnight at 150 °C for further characterization.

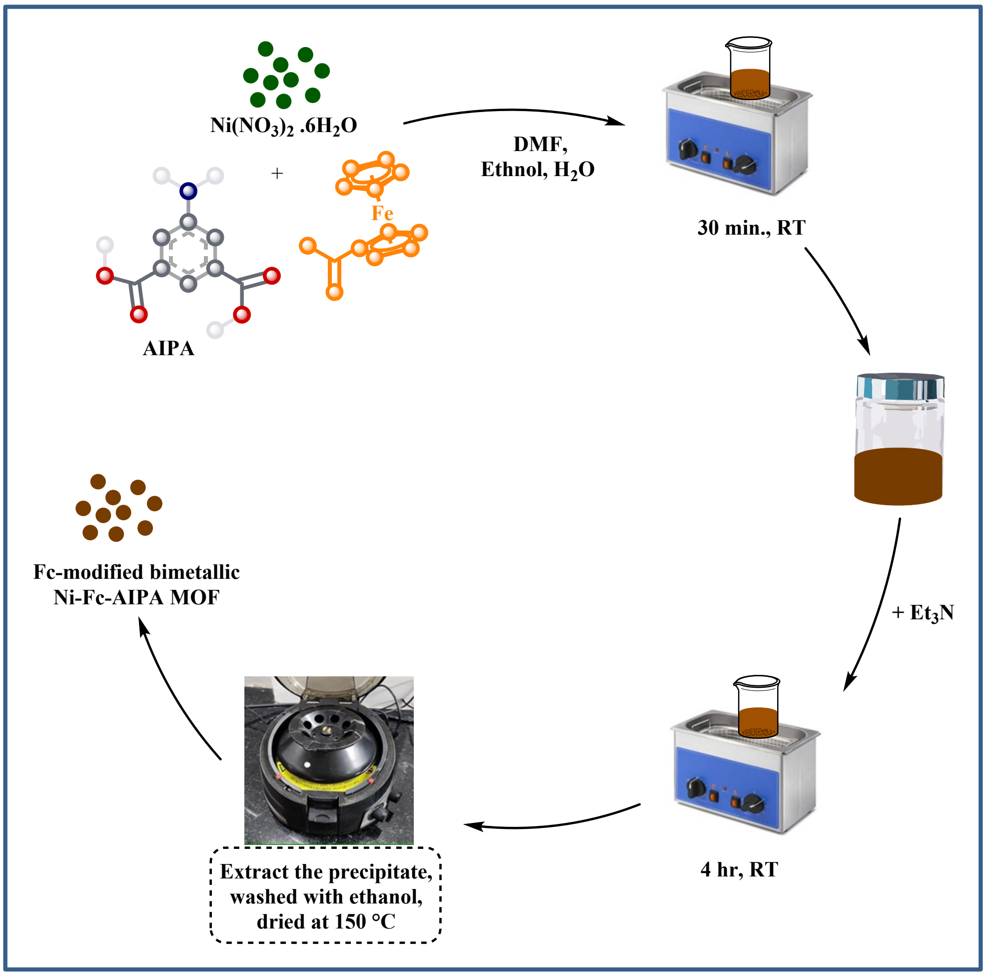
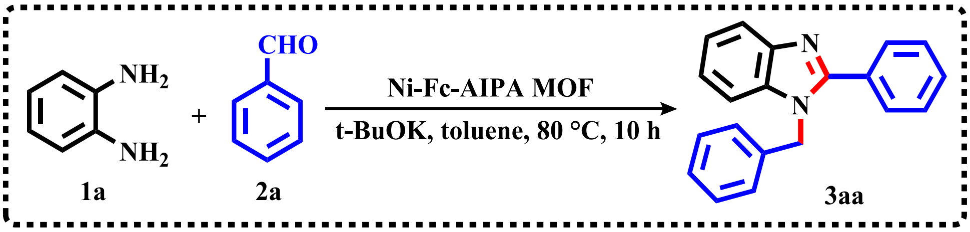


Figure. S2. Schematic representation for the synthesis of Fc-modified bimetallic Ni-Fc-AIPA MOF via the Schiff base reaction.

3. Catalytic screening of bimetallic Ni-Fc-AIPA MOF catalyst for oxidative cyclization reaction

General synthesis information: The reactions were conducted in sealed 25 mL reaction tubes and stirred using teflon®-coated magnetic stir bars. The reaction progress was monitored through thin-layer chromatography (TLC) on silica gel plates, with visualization under ultraviolet light. The product was extracted using silica gel column chromatography (230-400 mesh). Following purification, the product was vacuum-dried for several hours prior to analysis and weighing.

General experimental procedure for synthesis of 1,2-diaryl benzimidazole (3aa): In a dry, sealed 25 mL reaction tube, added *o*-phenylenediamine (**1a**) (0.50 mmol) and benzaldehyde (**2a**) (1 mmol). Add 3.5 mol% (20 mg) of the Fc-modified bimetallic Ni-Fc-AIPA MOF catalyst, along with t-BuOK (0.5 equiv.) as the base. Heated the reaction mixture at 80 °C for 10 hours under continuous stirring, using toluene as the solvent (**Scheme S2**). The reaction development was consistently studied using thin-layer chromatography. The reaction mixture was diluted with water before retrieval with ethyl acetate. The mixed organic material layers were rinsed with water and brine, followed by drying with an anhydrous solution of Na_2SO_4. After the vaporization of solvent, the residue adhered to silica gel, and column chromatography was used to purify the crude product. The reaction yield was determined using the mass of the separated compound. Product structure was verified through ^1H NMR and ^{13}C NMR spectroscopy. The spectral data of the synthesized 1,2-diaryl benzimidazole aligned with previously reported literature values.[3]



Scheme S2. Synthesis of 1,2-diaryl benzimidazole (**3aa**) utilizing the catalysts introduced in this study

4. Elemental mapping and EDAX spectra of synthesized Ni-AIPA MOF and Fc-modified bimetallic Ni-Fc-AIPA MOF

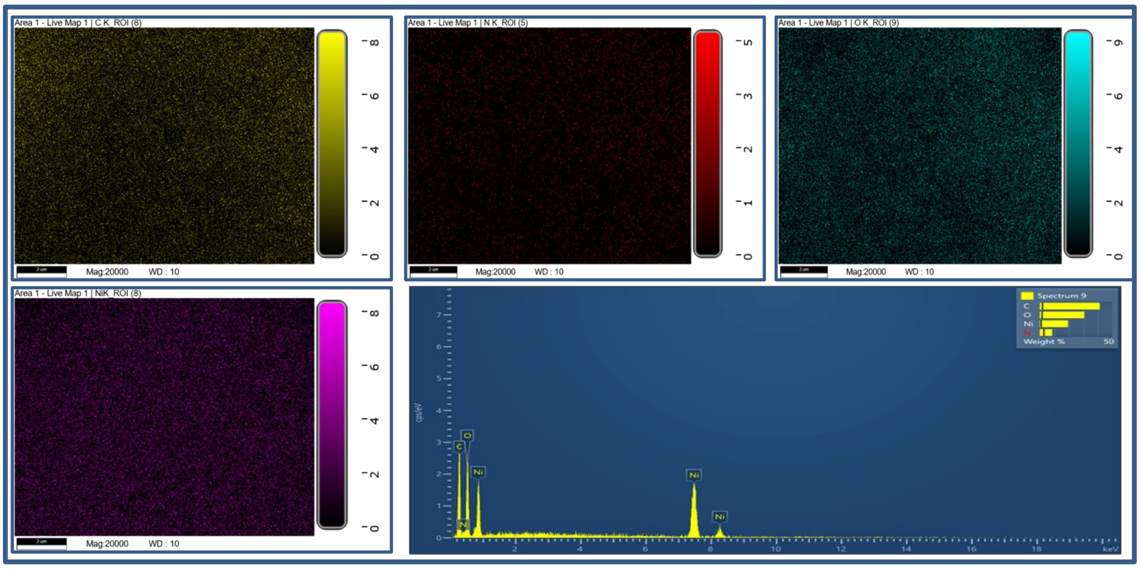


Figure S3. Elemental mapping of synthesized Ni-AIPA MOF

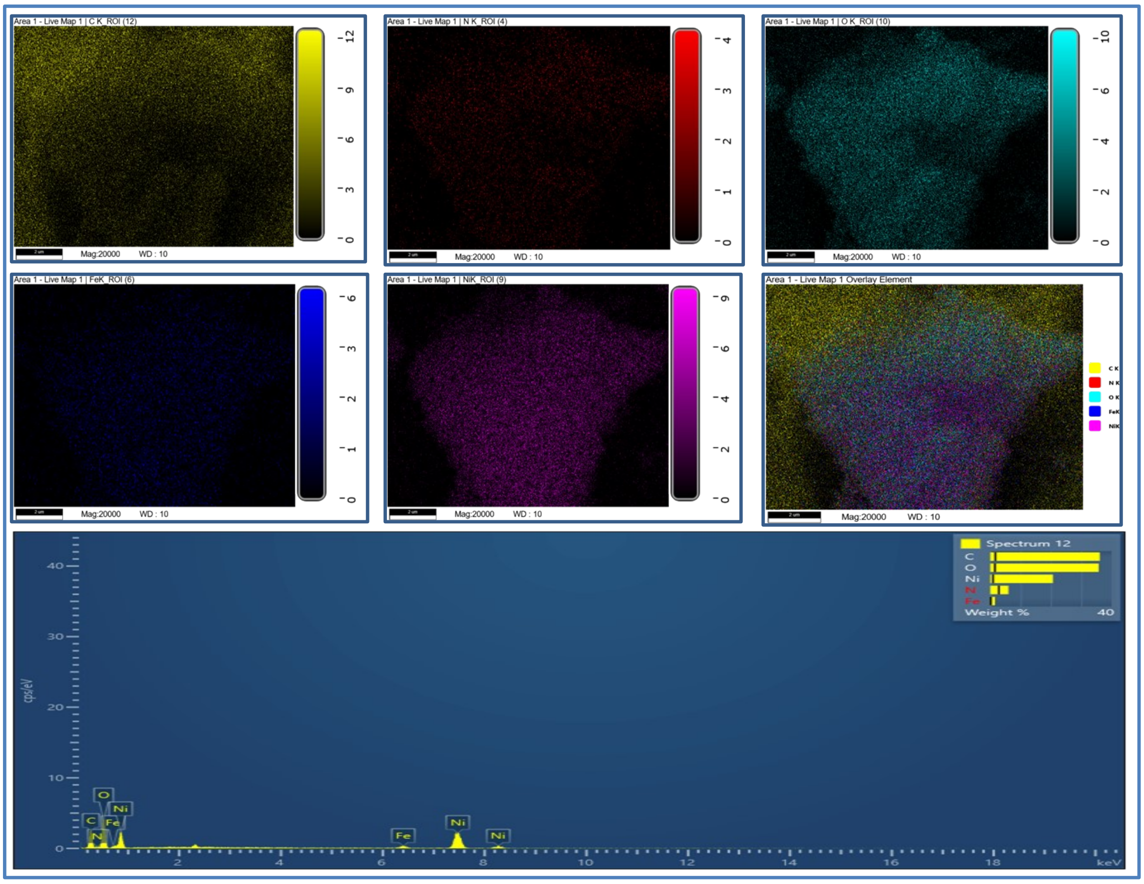


Figure S4. Elemental mapping of synthesized Fc-Modified bimetallic Ni-Fc-AIPA MOF

5. Recyclability of catalyst

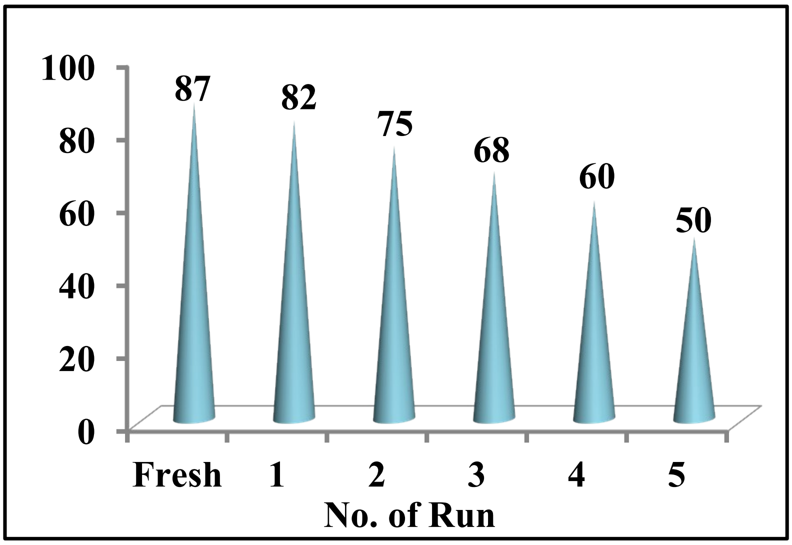


Figure S5. Recyclability of Fc-modified bimetallic Ni-Fc-AIPA MOF

6. XPS spectra of fresh and recycled catalyst

To investigate the possible change in the oxidation state of Ni during the catalytic process, the reaction mixture was collected between the reactions, and the catalyst was recovered by centrifugation. Subsequently, XPS analysis of the recovered catalyst was performed and compared with that of the freshly synthesized catalyst. The XPS spectra showed that the main Ni 2p peaks remained at binding energies characteristic of Ni(II), indicating that the oxidation state of Ni was largely preserved during the reaction. However, a noticeable decrease/disappearance of the satellite peak was observed after catalysis. The disappearance or reduction of the Ni 2p satellite peak is commonly associated with changes in the local electronic environment, charge-transfer behaviour, and coordination surroundings of the Ni species rather than a definitive alteration in oxidation state.[4] Therefore, the XPS results suggest that Ni predominantly retains its +2-oxidation state during the catalytic cycle, while undergoing modifications in its electronic coordination environment during catalysis.

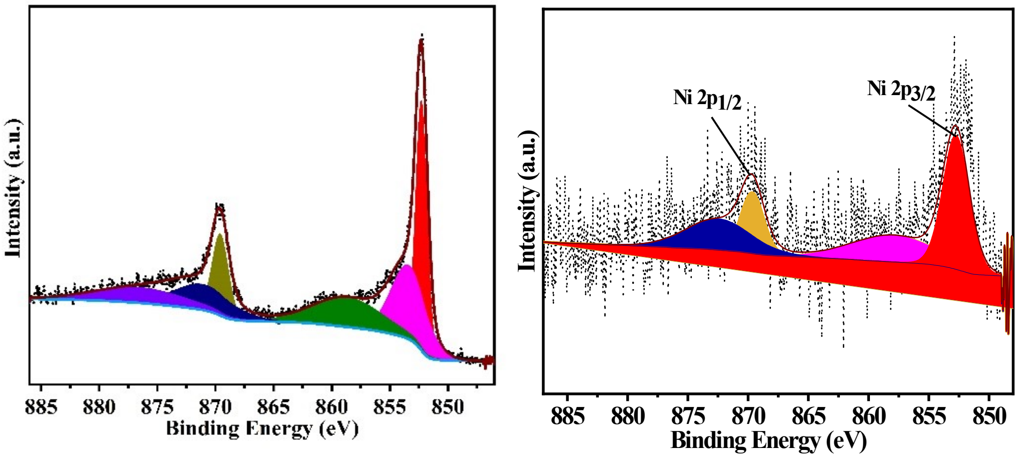
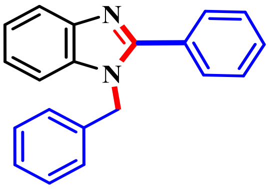
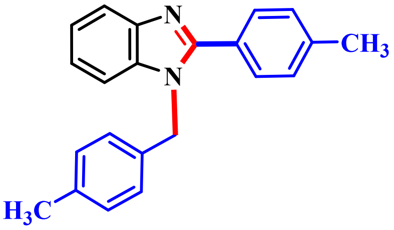
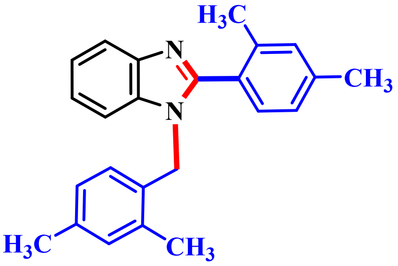
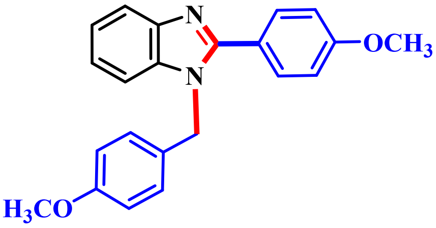
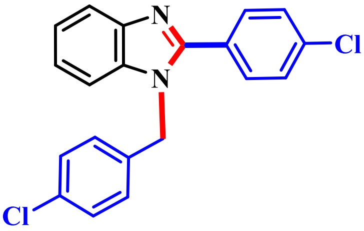
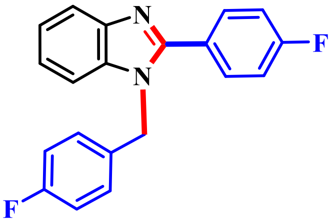


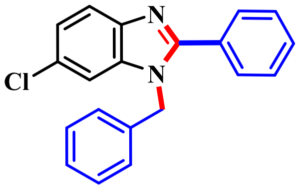
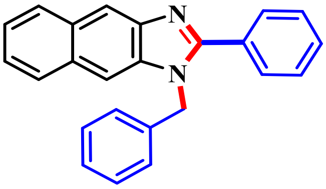
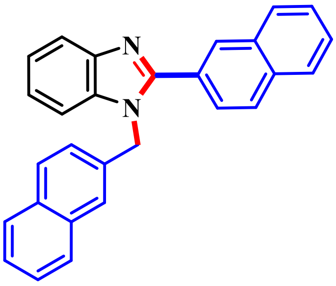
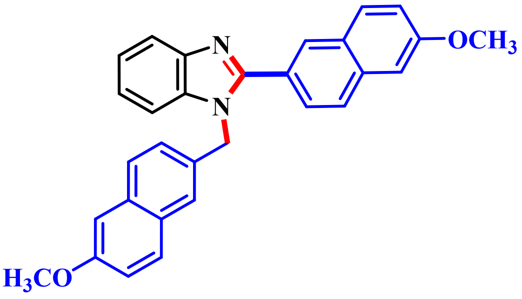
Figure S6. XPS spectra of Fesh and recycled Fc-modified bimetallic Ni-Fc-AIPA MOF

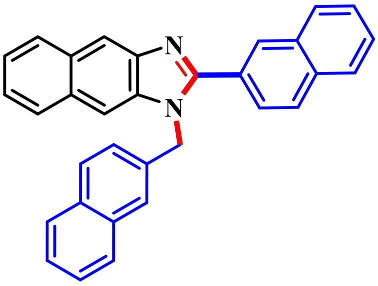
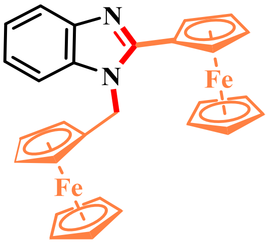
7. Spectroscopic Characterization Data

Table S2 ^{1}H NMR, ^{13}C{^{1}H} NMR and HRMS analysis of synthesized compounds

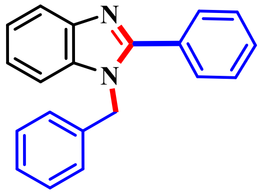
S. No.	Structure of compound	Characterization data
1.		**1-benzyl-2-phenyl-1*H*-benzo[*d*]imidazole (3aa)**[3] Brown, solid; M.P. 135 °C; Yield 77% **^{1}H-NMR (400 MHz, CDCl$_3$)** δ 7.82 (d, *J* = 8.0 Hz, 1H), 7.63-7.61 (m, 2H), 7.41-7.35 (m, 3H), 7.28-7.22 (m, 3H), 7.18-7.13 (m, 3H), 7.04-7.02 (m, 2H), 5.39 (s, 2H) ppm. **^{13}C{^{1}H}-NMR (101 MHz, CDCl$_3$)** δ 136.4, 136.1, 130.1, 129.4, 129.1, 128.9, 127.9, 126.1, 123.2, 122.9, 120.0, 110.6, 48.5 ppm.
2.		**1-(4-methylbenzyl)-2-(p-tolyl)-1*H*-benzo[*d*]imidazole (3ab)**[3] Brown, solid; M.P. 130 °C; Yield 80% **^{1}H-NMR (400 MHz, CDCl$_3$)** δ 7.82-7.79 (m, 1H), 7.49 (d, *J* = 8.0 Hz, 2H), 7.20-7.16 (m, 2H), 7.13-7.07 (m, 3H), 7.00 (d, *J* = 8.4 Hz, 2H), 6.86 (d, *J* = 8.0 Hz, 2H), 5.26 (s, 2H), 2.26 (s, 3H), 2.20 (s, 3H) ppm. **^{13}C {^{1}H}-NMR (101 MHz, CDCl$_3$)** δ 154.3, 142.9, 140.3, 137.6, 136.0, 133.5, 130.1, 129.8, 129.6, 129.3, 129.0, 127.0, 126.0, 123.1, 122.8, 119.8, 110.7, 48.3, 21.5, 21.2 ppm.
3.		**1-(2,4-dimethylbenzyl)-2-(2,4-dimethylphenyl)-1*H*-benzo[d]imidazole (3ac)**[5] Brown, semi-solid; Yield 78% **^{1}H-NMR (400 MHz, CDCl$_3$)** δ 7.84 (d, *J* = 9.2 Hz, 1H), 7.30-7.25 (m, 2H), 7.21-7.10 (m, 3H), 6.99-6.94 (m, 2H), 6.82 (d, *J* = 8.0 Hz, 1H), 6.51 (d, *J* = 7.6 Hz, 1H), 5.21 (s, 2H), 2.34 (s, 3H), 2.25 (s, 3H), 2.21 (s, 3H), 2.12 (s, 3H) ppm. **^{13}C{^{1}H}-NMR (101 MHz, CDCl$_3$)** δ 154.2, 138.2, 137.2, 131.4, 131.3, 131.1, 129.9, 127.0, 126.4, 126.1, 122.7, 122.3, 120.0, 110.7, 45.8, 21.4, 21.0, 19.9, 19.1 ppm.

4.		**1-(4-methoxybenzyl)-2-(4-methoxyphenyl)-1*H*-benzo[d]imidazole (3ad)**[5] Yellow, solid; M.P. 140 °C; Yield 79% **^{1}H-NMR (400 MHz, CDCl$_3$)** δ 7.77-7.75 (m, 1H), 7.57-7.54 (m, 2H), 7.23-7.19 (m, 1H), 7.14-7.12 (m, 2H), 6.95 (d, *J* = 8.8 Hz, 2H), 6.88 (d, *J* = 8.8 Hz, 2H), 6.77 (d, *J* = 8.8 Hz, 2H), 5.30 (s, 2H), 3.76 (s, 3H), 3.70 (s, 3H) ppm. **^{13}C{^{1}H}-NMR (101 MHz, CDCl$_3$)** δ 161.0, 159.2, 154.2, 143.2, 136.2, 130.8, 128.6, 127.3, 122.8, 122.6, 122.5, 119.8, 114.5, 114.3, 110.5, 55.4, 55.4, 48.0 ppm.
5.		**1-(4-chlorobenzyl)-2-(4-chlorophenyl)-1*H*-benzo[*d*]imidazole (3ae)**[3] Brown, solid; M.P. 155 °C; Yield 73% **^{1}H-NMR (400 MHz, CDCl$_3$)** δ 7.78 (d, *J* = 8.0 Hz, 1H), 7.52-7.48 (m, 2H), 7.37-7.33 (m, 2H), 7.27-7.23 (m, 2H), 7.22-7.17 (m, 2H), 7.12-7.10 (m, 1H), 6.93 (d, *J* = 8.4 Hz, 2H), 5.31 (s, 2H) ppm. **^{13}C{^{1}H}-NMR (101 MHz, CDCl$_3$)** δ 153.0, 143.1, 139.8, 136.5, 136.0, 134.7, 133.9, 130.5, 129.5, 129.2, 128.6, 128.4, 128.3, 127.3, 123.6, 123.2, 120.2, 110.4, 47.9 ppm.
6.		**1-(4-fluorobenzyl)-2-(4-fluorophenyl)-1*H*-benzo[d]imidazole (3af)**[5] Brown, semi-solid; Yield 70% **^{1}H-NMR (400 MHz, CDCl$_3$)** δ 7.80-7.78 (m, 1H), 7.69-7.55 (m, 2H), 7.28-7.20 (m, 2H), 7.18-7.06 (m, 4H), 6.99-6.93 (m, 3H), 5.33 (s, 2H) ppm. **^{13}C{^{1}H}-NMR (101 MHz, CDCl$_3$)** δ 165.1 ($J_{\text{C-F}}$ = 152.3 Hz), 163.6, 162.6 ($J_{\text{C-F}}$ = 148.2 Hz), 161.1, 153.2, 143.1, 135.9, 132.0, 132.0, 131.3, 131.3, 127.7, 127.7, 126.2, 123.4, 123.0, 120.1, 116.3, 116.2, 116.1, 116.0, 110.4, 47.8 ppm.
7.		**1-benzyl-6-chloro-2-phenyl-1*H*-benzo[*d*]imidazole (3ag)**[6]

		Brown, solid; M.P. < 200 °C; Yield 75% **^{1}H-NMR (400 MHz, CDCl$_3$)** δ 7.76 (d, J = 2.4 Hz, 1H), 7.60-7.57 (m, 2H), 7.41-7.37(m, 3H), 7.27-7.21 (m, 3H), 7.11-7.08 (m, 1H), 7.02-6.97 (m, 3H), 5.34 (s, 2H) ppm. **^{13}C{^{1}H}-NMR (101 MHz, CDCl$_3$)** δ 155.4, 144.0, 136.0, 130.3, 129.7, 129.3, 129.2, 129.0, 128.4, 128.1, 126.0, 123.6, 119.8, 111.4. 48.6 ppm.
8.		**1-benzyl-2-phenyl-1*H*-naphtho[2,3-*d*]imidazole (3ah)** Dark brown, solid; M.P. < 200 °C; Yield 70% **^{1}H-NMR (400 MHz, CDCl$_3$)** δ 8.27 (s, 1H), 8.05-793 (m, 2H), 7.76-7.67 (m, 2H), 7.51 (s, 1H), 7.43-7.37 (m, 4H), 7.32-7.30 (m, 2H), 7.28-7.22 (m, 3H), 7.08 (d, J = 6.8 Hz, 1H), 5.44 (s, 2H) ppm. **^{13}C{^{1}H}-NMR (101 MHz, CDCl$_3$)** δ 158.1, 143.1, 136.8, 136.4, 130.7, 130.5, 129.8, 129.5, 129.2, 128.9, 128.6, 127.9, 127.6, 126.1, 124.5, 123.7, 117.0, 106.4, 48.7 ppm; **HRMS (ESI$^+$)** calculated for $C_{24}H_{18}N_2$ $[M+H]^+$: 335.1543; found: 335.1543
9.		**2-(naphthalene-2-yl)-1-(naphthalene-2-ylmethyl)-1*H*-benzo[*d*]imidazole (3ai)**[7] White, solid; M.P. < 200 °C; Yield 80% **^{1}H-NMR (400 MHz, CDCl$_3$)** δ 8.49 (s, 1H), 8.15-8.12 (m, 4H), 7.69-7.63 (m, 4H), 7.59-7.57 (m, 2H), 7.51 (d, J = 8.0 Hz, 1H), 7.36-7.26 (m 4H), 7.16-7.14 (m, 2H), 5.20 (s, 2H) ppm. **^{13}C{^{1}H}-NMR (101 MHz, CDCl$_3$)** δ 152.4, 139.3, 134.0, 133.1, 129.0, 128.5, 127.8, 127.2, 127.0, 126.8, 124.0, 123.9, 123.2, 115.3, 53.5 ppm.
10.		**2-(6-methoxynaphthalen-2-yl)-1-((6-methoxynaphthalen-2-yl)methyl)-1*H*-benzo[d]imidazole (3aj)** Yellow, solid; M.P. < 200 °C;; Yield 82% **^{1}H-NMR (400 MHz, CDCl$_3$)** δ 8.0 (s, 1H), 7.84 (d, J = 7.6 Hz, 1H), 7.70-7.62 (m, 3H), 7.51-7.47 (m, 3H), 7.40(s, 1H), 7.26-7.15 (m, 4H), 7.06-7.00 (m, 3H), 5.51 (s, 2H), 3.81 (s, 3H), 3.80 (s, 3H) ppm. **^{13}C{^{1}H}-NMR (101 MHz, CDCl$_3$)** δ 158.8, 158.1, 154.7, 152.4, 143.2, 136.4, 135.2, 134.1,

		131.7, 130.2, 129.5, 129.2, 129.0, 128.4, 128.0, 127.5, 126.7, 126.4, 124.9, 124.8, 124.6, 123.2, 122.9, 119.7, 119.5, 110.7, 105.7, 55.4, 55.4, 48.8 ppm; **HRMS (ESI^{+})** calculated for $C_{30}H_{24}N_2O_2$ $[M+H]^{+}$: 445.1911; found: 445.6000
11.		**2-(naphthalene-2-yl)-1-(naphthalene-2-ylmethyl)-1*H*-naphtho[2,3-*d*]imidazole (3ak)** Brown, solid; M.P. 135 °C; Yield 65% **^{1}H-NMR (400 MHz, CDCl$_3$)** δ 8.64 (s, 1H), 8.31 (d, *J* = 5.6 Hz, 2H), 8.08-7.98 (m, 3H), 7.91-7.84 (m, 3H), 7.82-7.75 (m, 3H), 7.70-7.61 (m, 3H), 7.56-7.50 (m, 3H), 7.44-7.32 (m, 2H), 5.68 (s, 2H) ppm. **^{13}C{^{1}H}-NMR (101 MHz, CDCl$_3$)** δ 158.2, 143.1, 137.1, 134.1, 133.9, 133.6, 133.0, 130.9, 129.8, 129.6, 129.3, 128.8, 128.7, 128.3, 128.0, 127.9, 127.6, 126.9, 126.8, 126.7, 126.4, 126.1, 125.7, 124.8, 124.6, 124.0, 123.8, 117.1, 106.5, 49.2 ppm; **HRMS (ESI^{+})** calculated for $C_{32}H_{22}N_2$ $[M+Na]^{+}$: 457.1681; found: 457.1680
12.		**1-ferrocenylmethyl-2-ferrocenyl benzimidazole (3al)**[8] Orange, solid; M.P. 180 °C; Yield 85% **^{1}H-NMR (400 MHz, CDCl$_3$)** δ 7.69-7.67 (m, 1H), 7.34-7.31 (m, 1H), 7.18-7.16 (m, 2H), 5.33 (s, 2H), 4.93 (t, 2H), 4.40 (t, 2H), 4.17 (t, 2H), 4.12 (s, 10H), 4.05 (t, 2H) ppm. **^{13}C{^{1}H}-NMR (101 MHz, CDCl$_3$)** δ 152.7, 142.9, 135.8, 122.0, 121.8, 118.9, 109.5, 83.8, 77.2, 76.9, 76.6, 74.0, 69.8, 69.6, 69.3, 68.8, 68.4, 68.0, 43.9 ppm.

8. ^{1}H and ^{13}C-NMR (400 MHz and 101 MHz in $CDCl_3$) Spectra of Compound



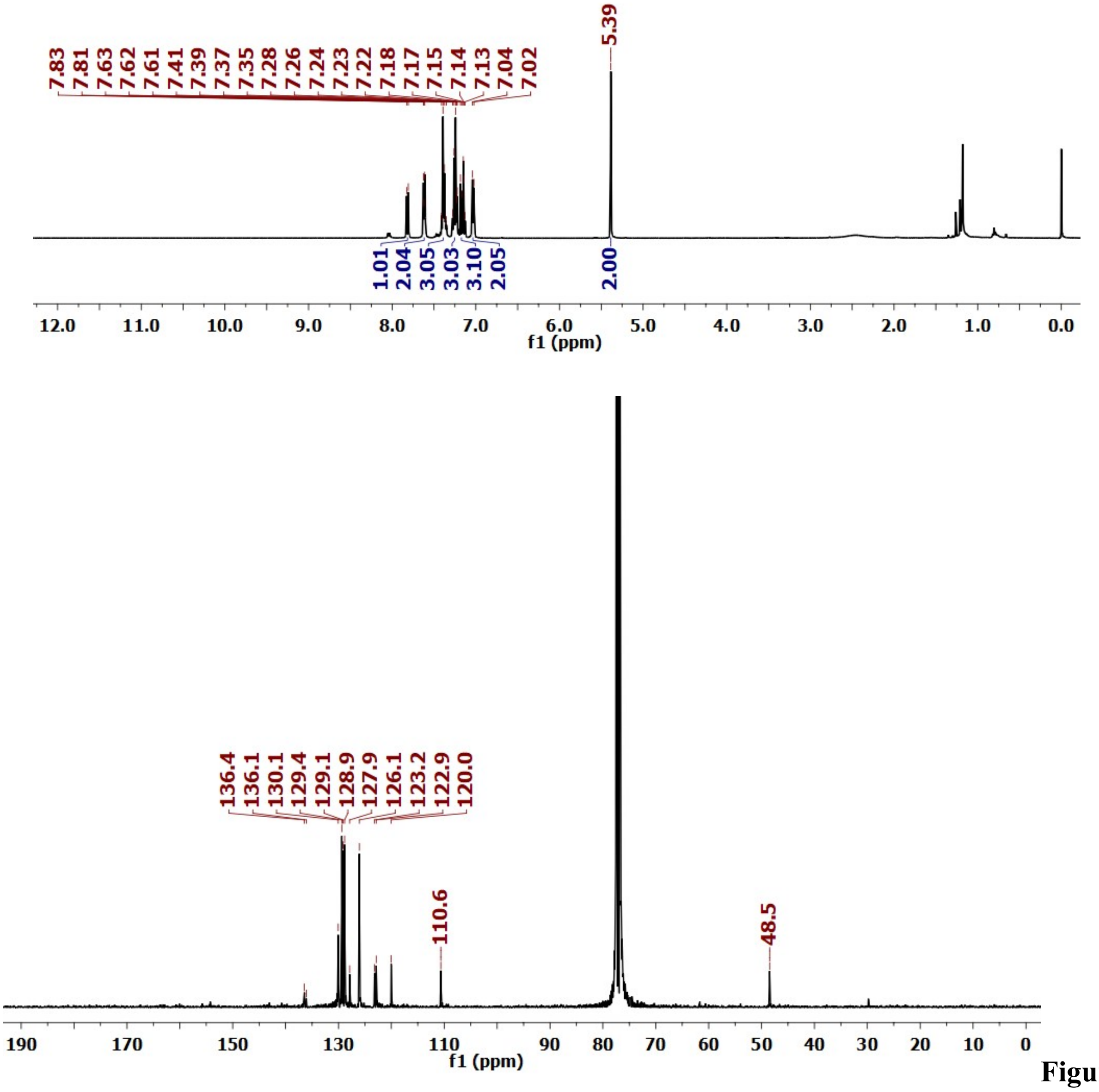


Figure S7: ^{1}H and ^{13}C-NMR spectrum of compound 3aa

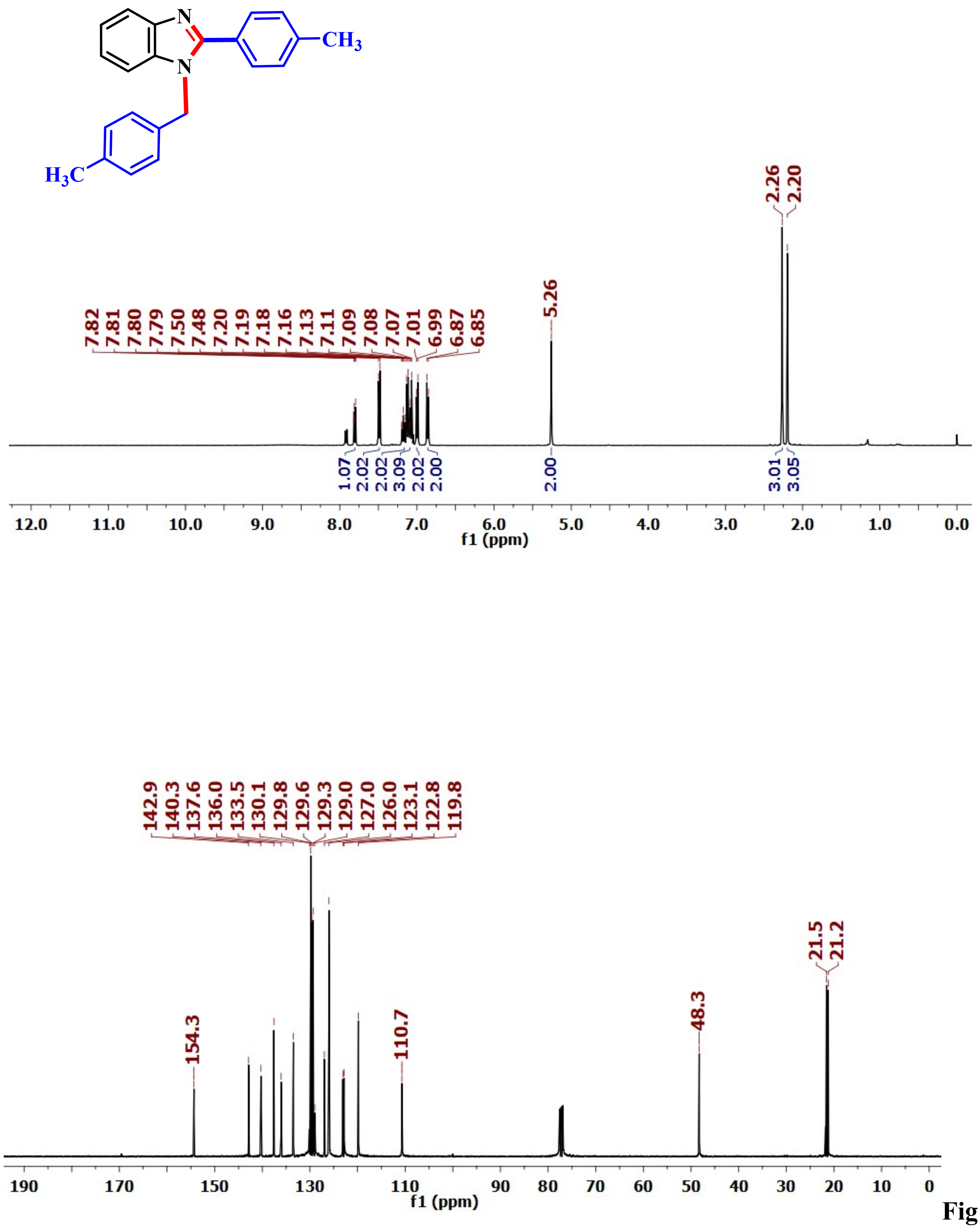


Figure S8: ^{1}H and ^{13}C-NMR spectrum of compound 3ab

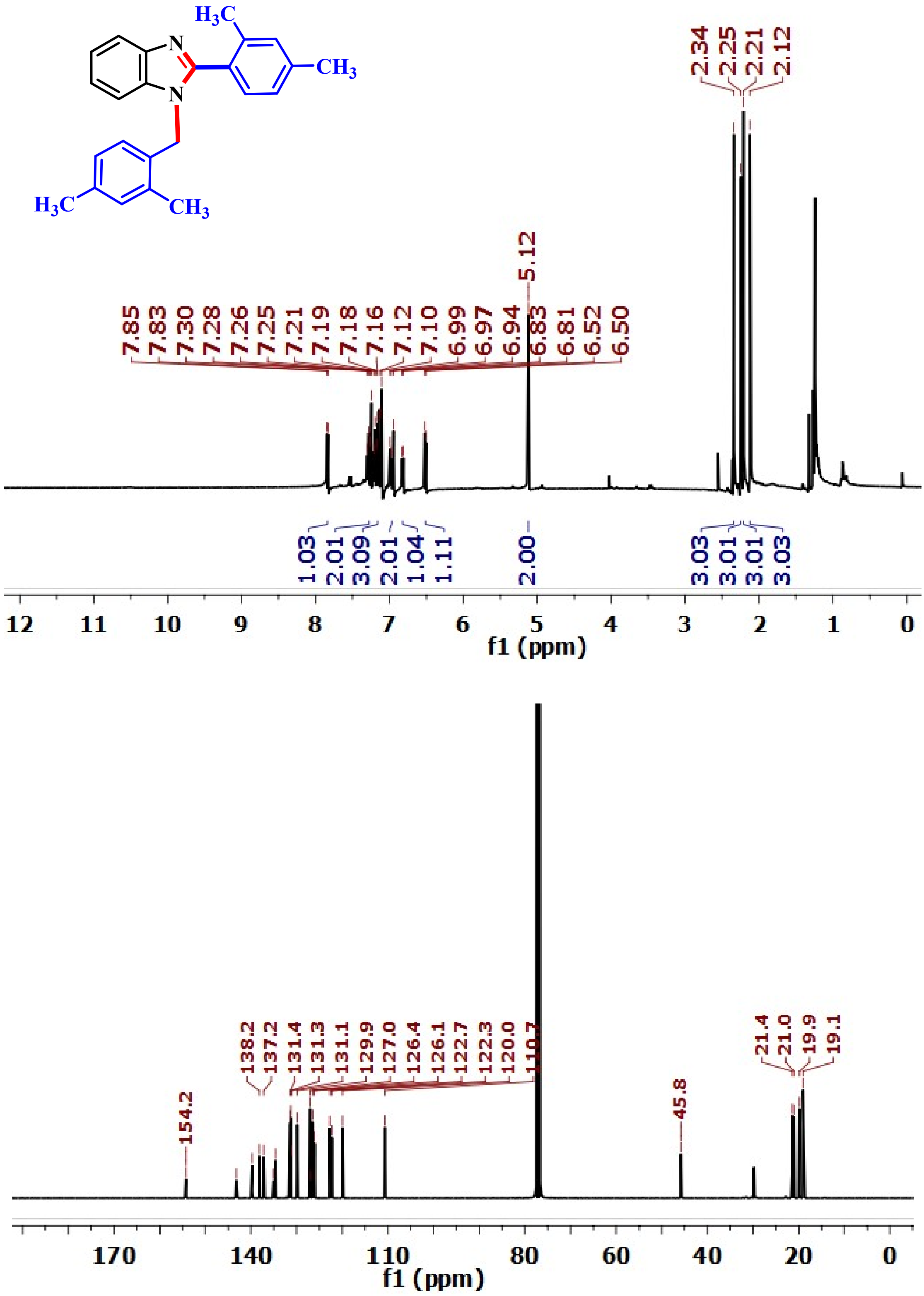


Figure S9: ^{1}H and ^{13}C-NMR spectrum of compound 3ac

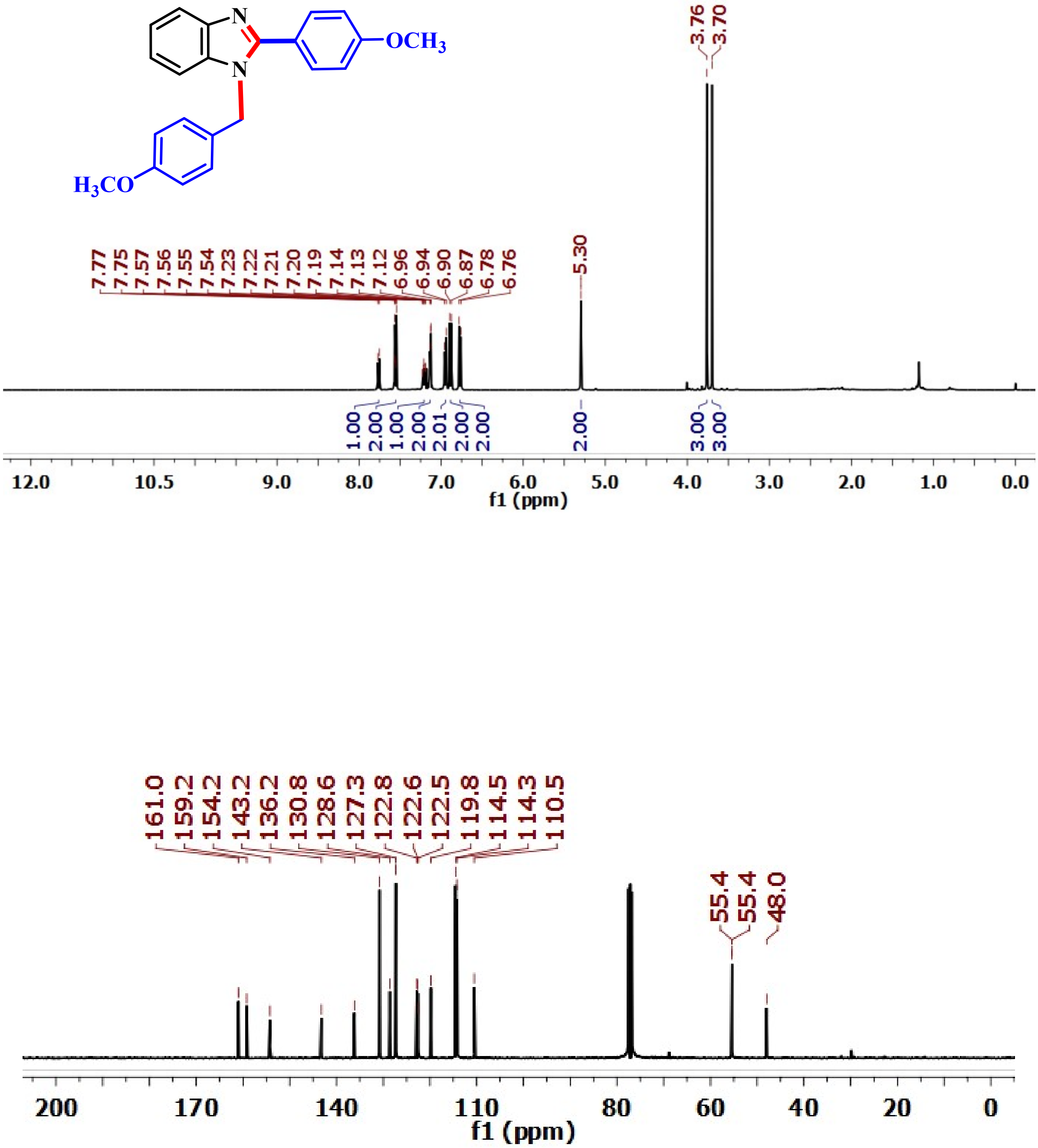
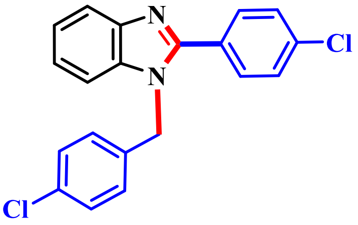


Figure S10: ^{1}H and ^{13}C-NMR spectrum of compound 3ad



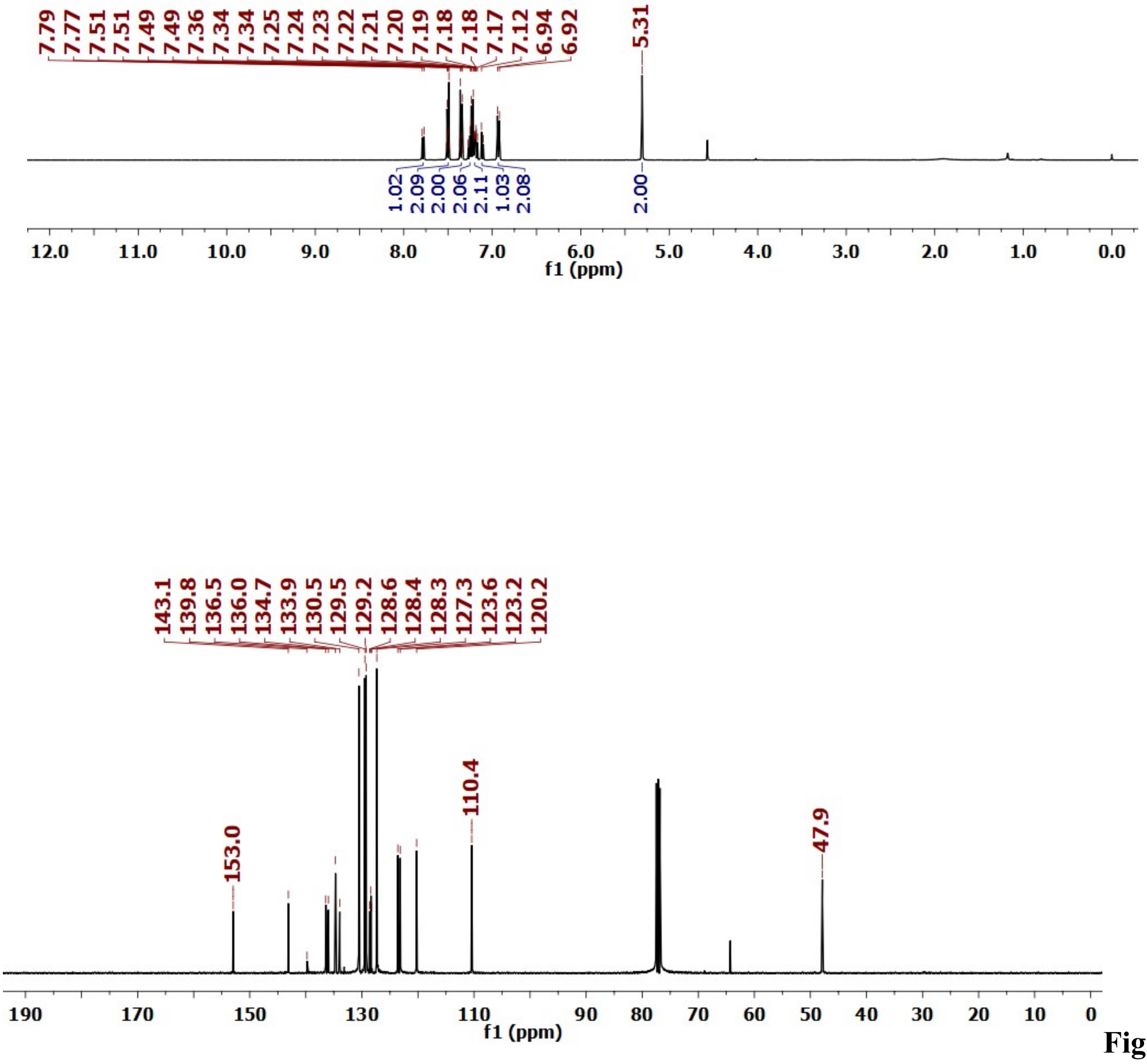


Figure S11: ^{1}H and ^{13}C-NMR spectrum of compound 3ae

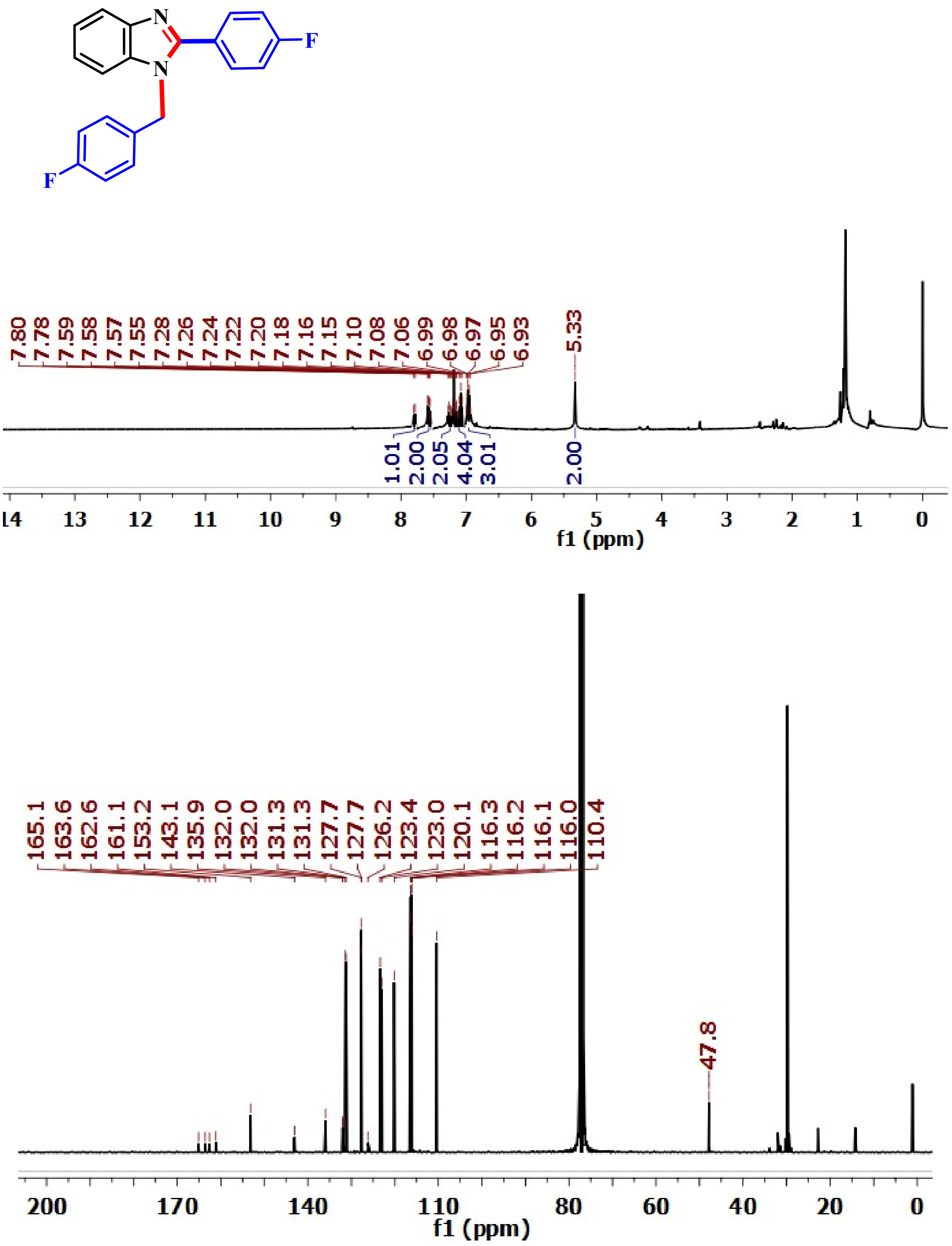


Figure S12: ^{1}H and ^{13}C-NMR spectrum of compound 3af

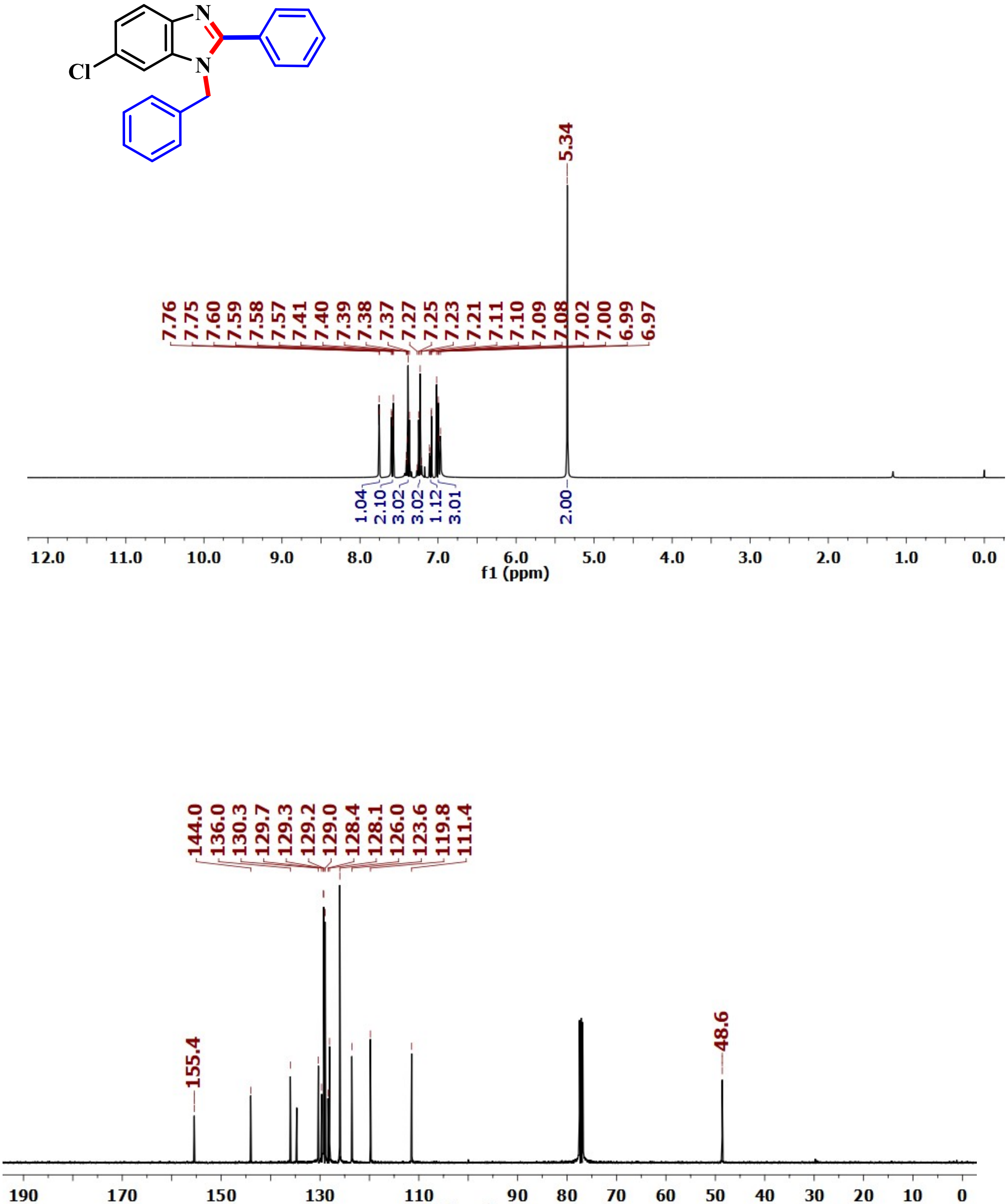


Figure S13: ^{1}H and ^{13}C-NMR spectrum of compound 3ag

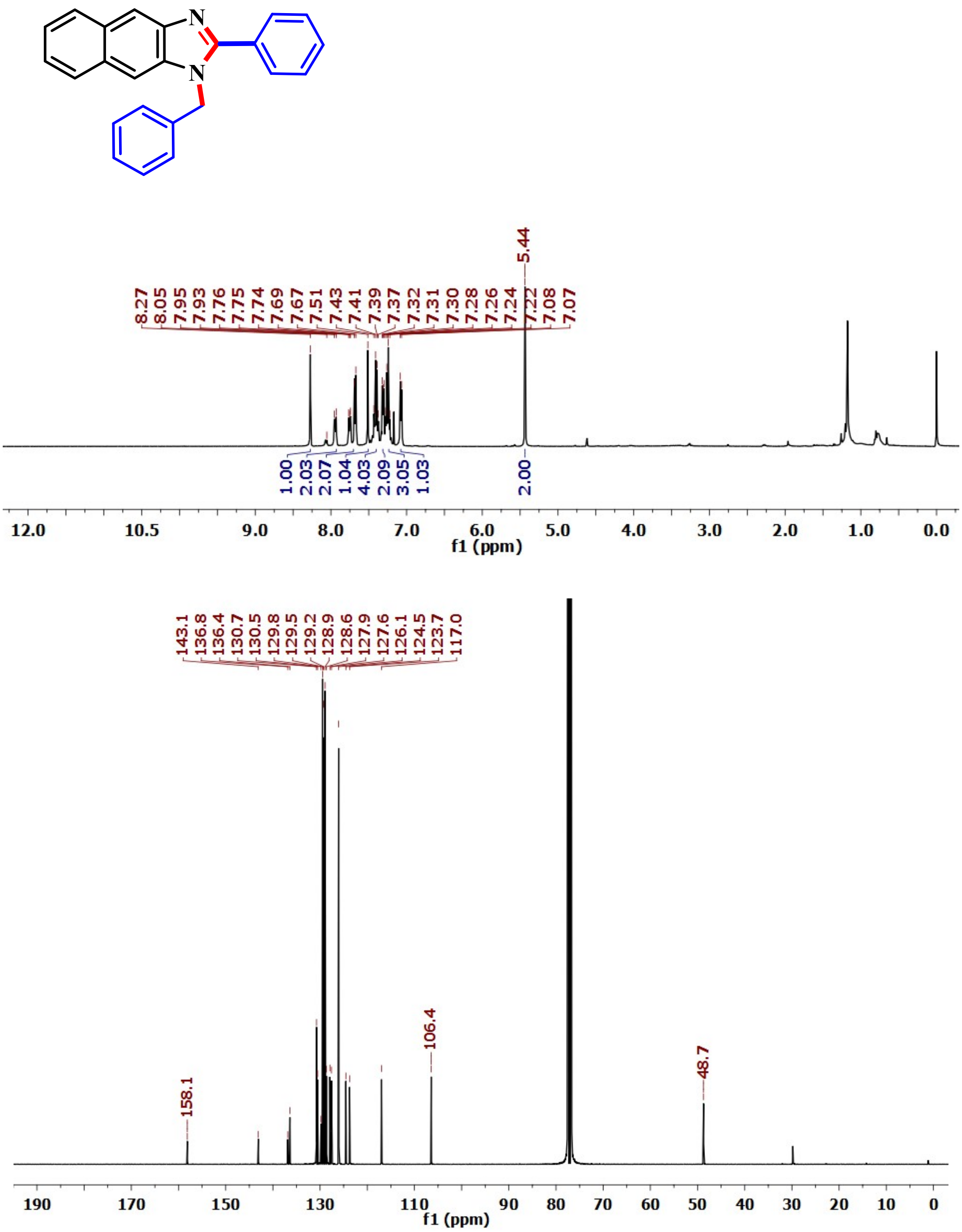


Figure S14: ^{1}H and ^{13}C-NMR spectrum of compound 3ah

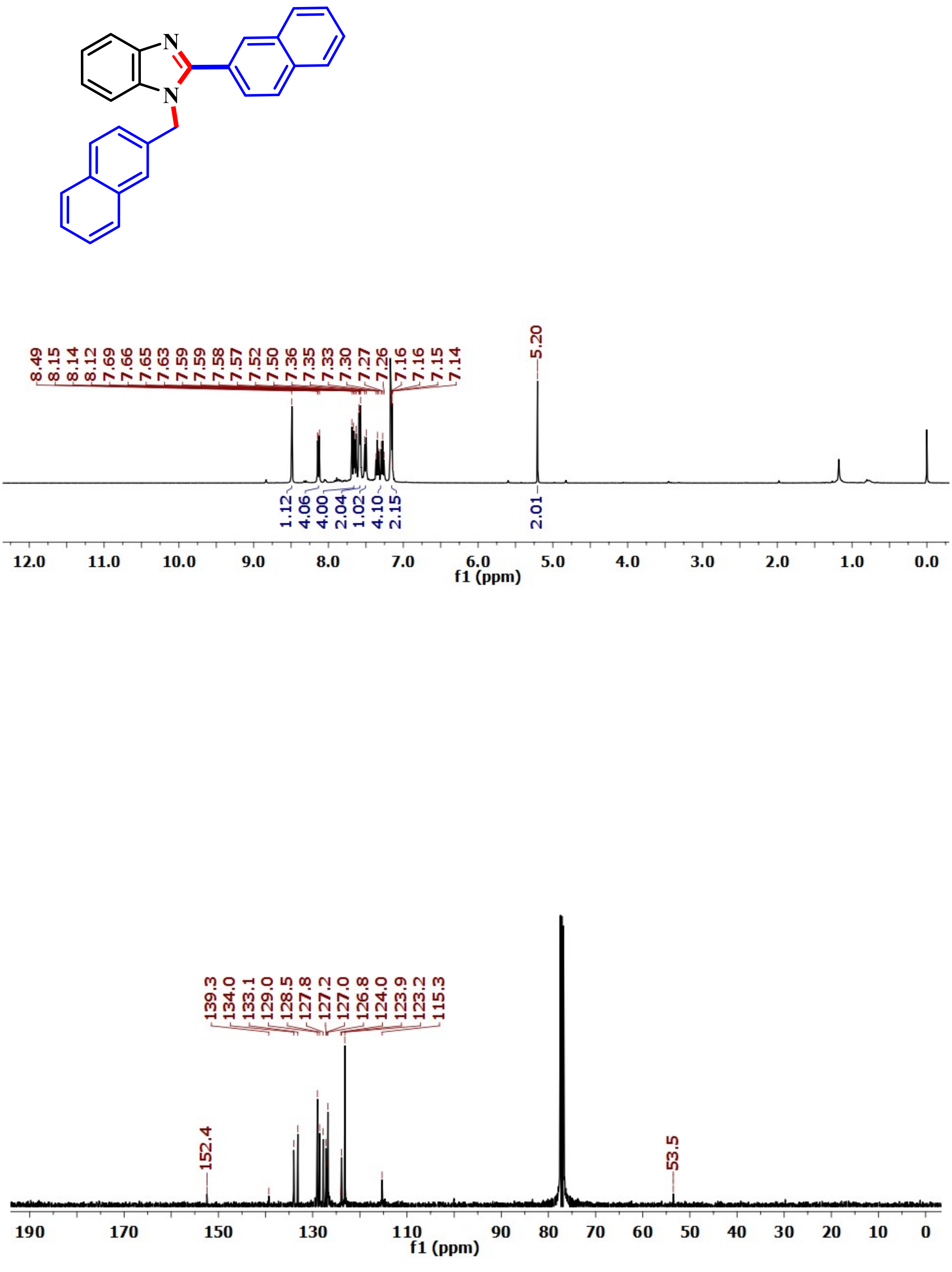


Figure S15: ^{1}H and ^{13}C-NMR spectrum of compound 3ai

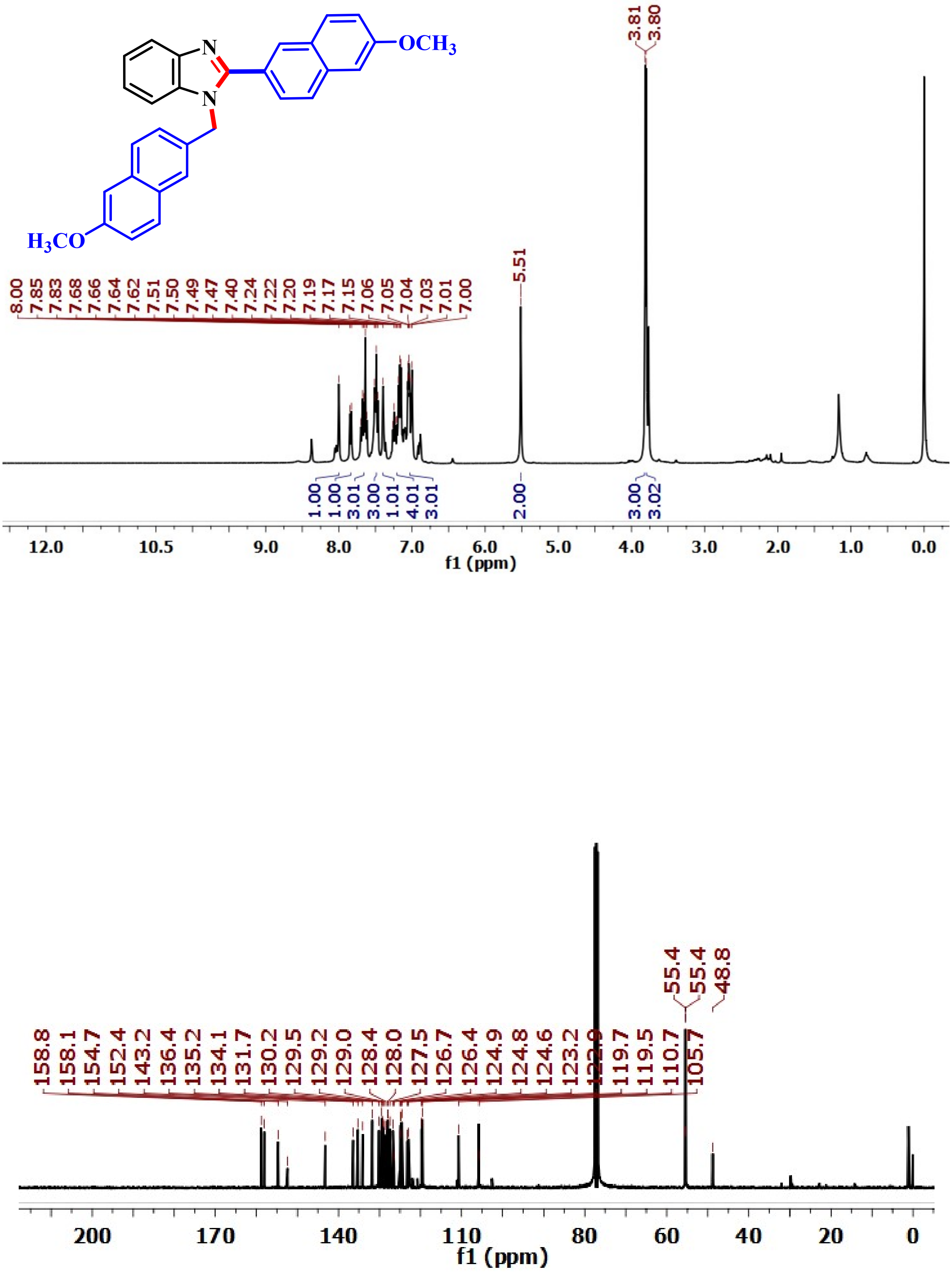


Figure S16: ^{1}H and ^{13}C-NMR spectrum of compound 3aj

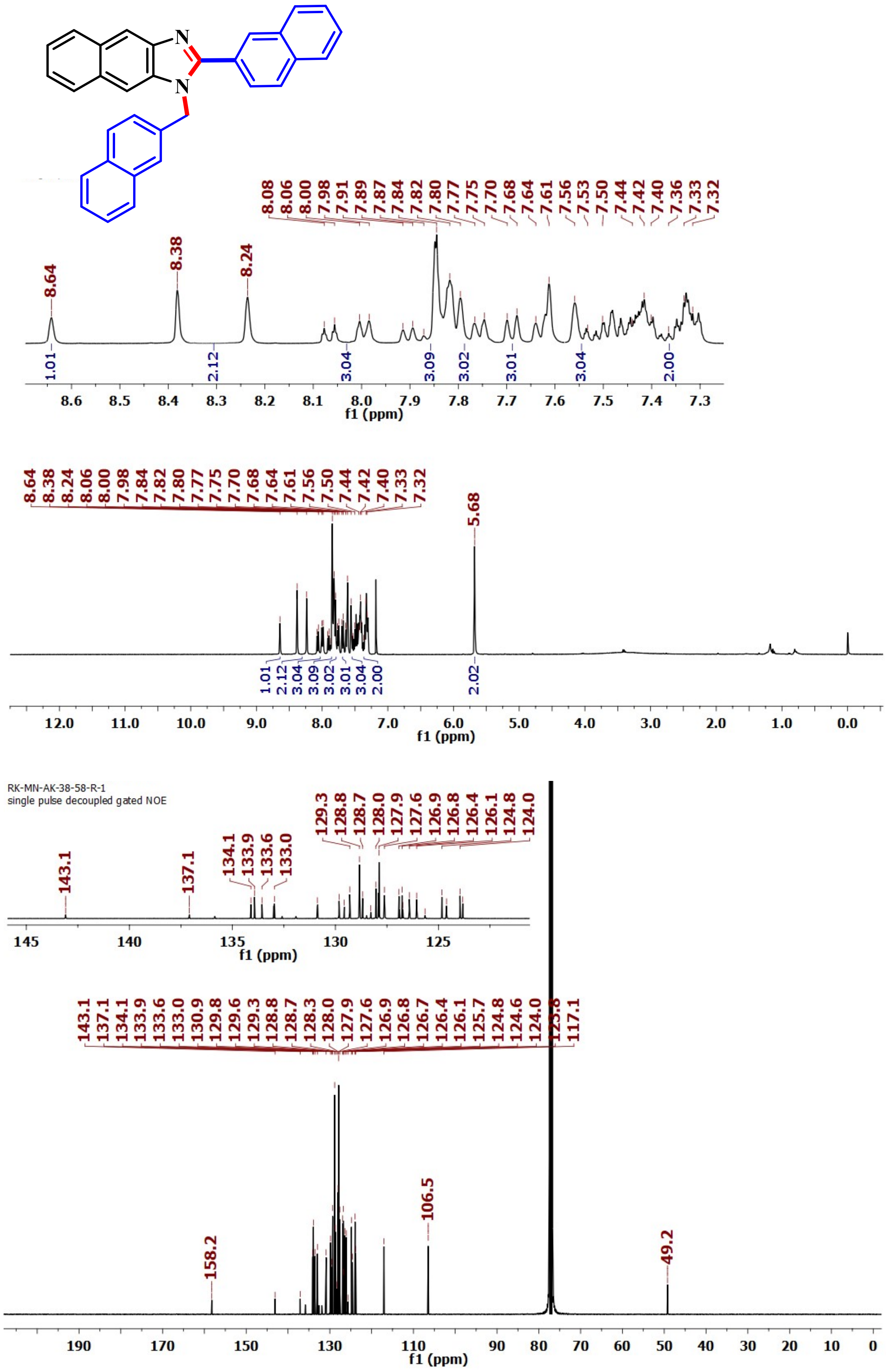


Figure S17: ^{1}H and ^{13}C-NMR spectrum of compound 3ak

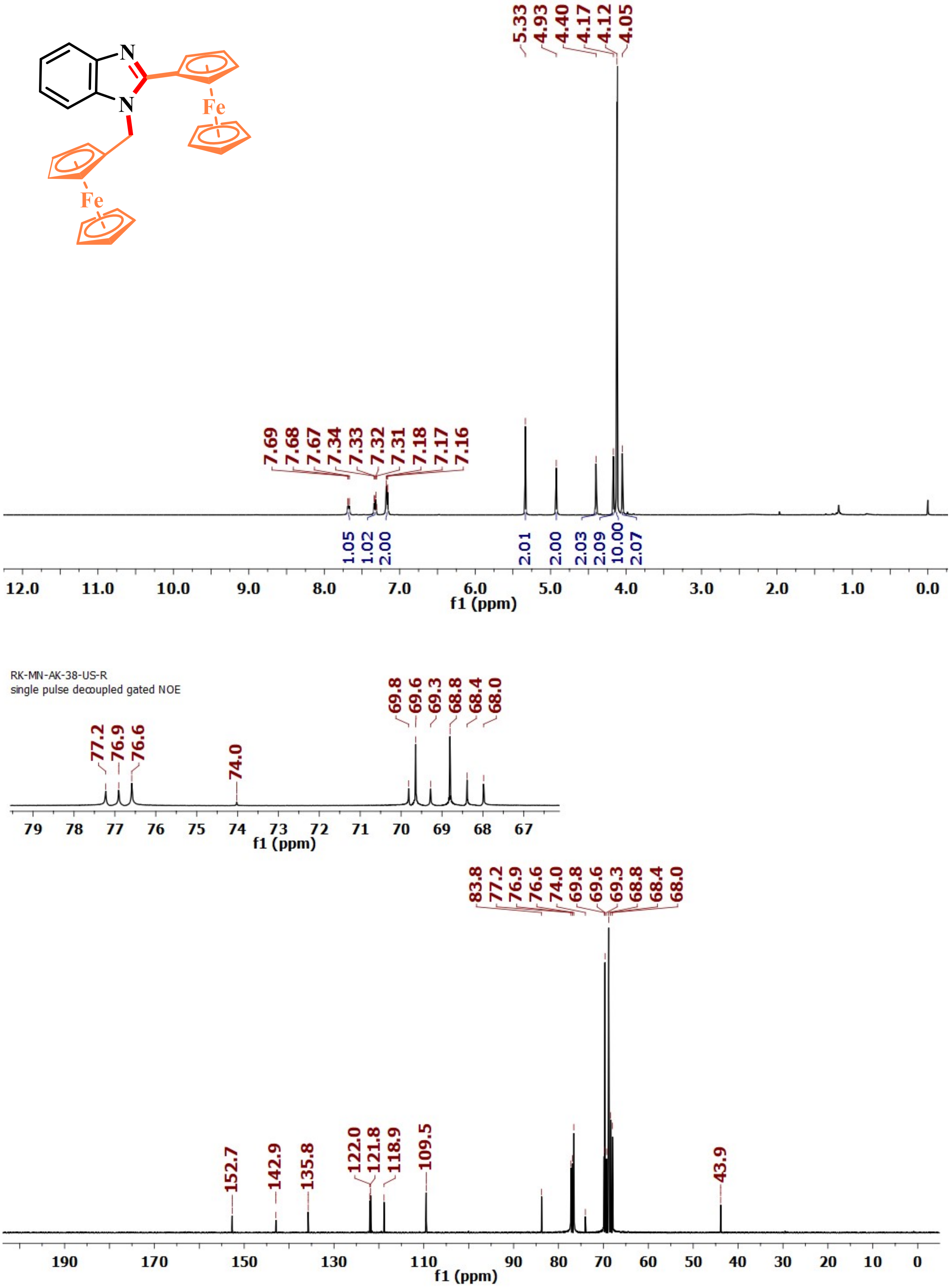


Figure S18: ^{1}H and ^{13}C-NMR spectrum of compound 3al

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