Supporting Information

For

E-Selective Partial Transfer Hydrogenation of Internal Acetylenes Enabled by Water-Promoted $Fe(CO)_5$ Catalysis

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1. Gerneral Information

1.1 Experimental Details

The ^{1}H, $^{13}C\{^{1}H\}$ NMR spectra are reported by using a JEOL ECS-400 spectrometer (operating at 400 MHz for ^{1}H and 100 MHz for $^{13}C\{^{1}H\}$). All chemical shifts for ^{1}H-NMR and $^{13}C\{^{1}H\}$-NMR spectra are given in parts per million (ppm) relative to the signals for $CDCl_3$ solvent, i.e., 7.25 ppm for ^{1}H-NMR and 77.2 ppm for $^{13}C\{^{1}H\}$-NMR spectra. $^{13}C\{^{1}H\}$-NMR spectra are single-pulse decoupled gated NOE. The frequency of the coupling constants (*J*) is stated in hertz (Hz). HRMS spectra are recorded by using a G6546A Q-Tof spectrometer (Agilent) in methanol at room temperature.

1.2 Chemicals and reagents

All the reactants (internal alkynes) specified in the manuscript were synthesized using the approaches described later. The rest of the reagents, chemicals, and solvents are bought from the best commercial suppliers in the country. Finar silica gel was used for the column chromatography (100-200 mesh). All the reactions were monitored using Merck TLC Silica gel 60 F254 precoated aluminium sheets for thin-layer chromatography (TLC). The materials obtained from commercial suppliers were used directly without further purification. All of the reactions have been performed in reaction tubes with a screw-cap, and before each usage, the magnetic stirring bar was cleaned in an acid bath. The reaction tubes were filled in the open air.

1.3 Computational Details

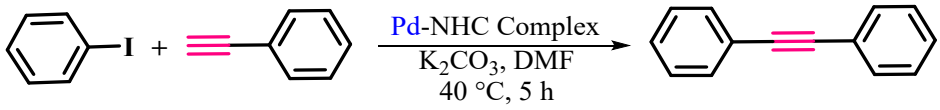
All the calculations in the current study were performed using the Gaussian 09 program.[1] Stationary points such as reactants, products, intermediates, and probable transition states were optimized in the condensed phase employing Becke's three-parameter hybrid correlation functional by Lee-Yang-Parr (B3LYP). Two basis sets have been utilized, viz., LANL2DZ for transition metal (Fe) and 6-311G** for the rest of the atoms.[2] Integral Equation Formulism Polarizable Continuum Model (IEFPCM), which is reformulated dielectric PCM (DPCM), has been used to represent statistically averaged solvent, leading to meaningful results.[3] Further, frequency calculations were carried out to characterize the nature of those

stationary points and to evaluate the thermodynamic terms and molecular partition functions. The transition states were pointed out by their distinguished imaginary frequency, characteristic of first-order saddle-points on the potential energy surface. The 3D-structures were visualized using GaussView5.0 software[4] and Chemcraft[5].

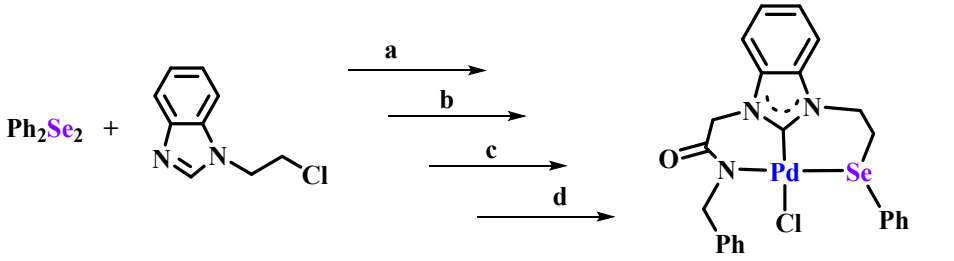
2. General procedure for the synthesis of internal alkynes

2.1 Sonogashira Coupling[6]

To a mixture of aryl bromide/iodide (1.0 mmol), K_2CO_3 (2.0 mmol), acetylene (1.2 mmol), and *N, N*-dimethylacetamide (DMA, 1.5 mL), the NHC-Pd (II) full pincer catalyst (12 mg, 0.02 mmol) was added. The reaction mixture was heated at 40 °C for 5 h with constant stirring. The resulting reaction mixture was allowed to cool down at room temperature, and the organic layer was separated by solvent extraction in ethyl acetate and water. After drying the organic layer on sodium sulphate and concentrating over a rotary evaporator, the desired product was separated by column chromatography using hexane/ethyl acetate as eluent.



Synthesis of full pincer selanated NHC-Pd (II) Complex[6]: Full pincer ligand and its Pd(II) complex was synthesized through the earlier disclosed method.

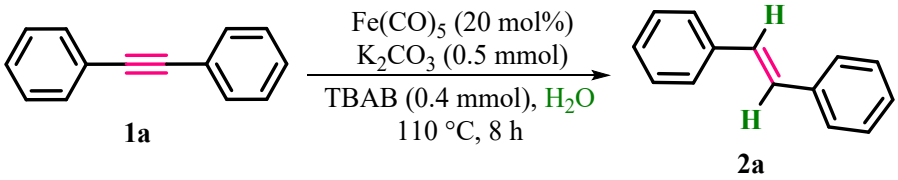


NHC-Full Pincer Complex

Scheme S1: Synthesis of tridentate selanated NHC ligand and Pd (II) complex, (a) Diphenyl diselenide, $NaBH_4$, reflux, EtOH, 15 min, N_2 atm; (b) Add 1-(2-chloroethyl)-1H benzimidazole, reflux; (c) Add N-benzyl-2-chloroacetamide, Toluene, N_2 atm, reflux, 8 h (d) $(CH_3CN)_2PdCl_2$, DMF, N_2 atm, 90 min.

3. General Procedure for Catalytic Semi-Hydrogenation of Acetylenes

In a reaction tube equipped with a magnetic stirring bar, a mixture of 1.0 mmol of internal acetylene, 0.5 mmol of potassium carbonate base, 0.4 mmol of TBAB, and 20.0 mol% of $Fe(CO)_5$ was stirred at 110 °C for 8 h in aqueous medium (using DI water). Upon completion, the mixture was cooled to room temperature and transferred to a separatory funnel for solvent extraction with ethyl acetate and water. Then, it was dried over anhydrous sodium sulfate, filtered, and concentrated under reduced pressure. The crude product was purified by column chromatography using hexane/ethyl acetate to give the pure product as a white solid. The purified product was characterized using NMR spectroscopy.

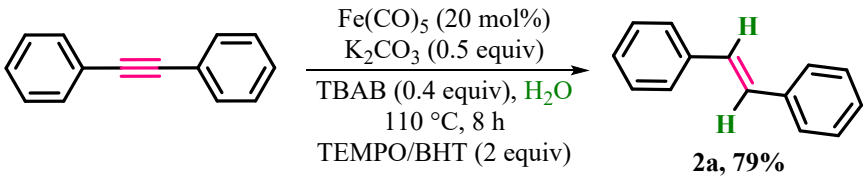


1a **2a**

4. Control Experiments

4.1 Radical Scavenger Experiment

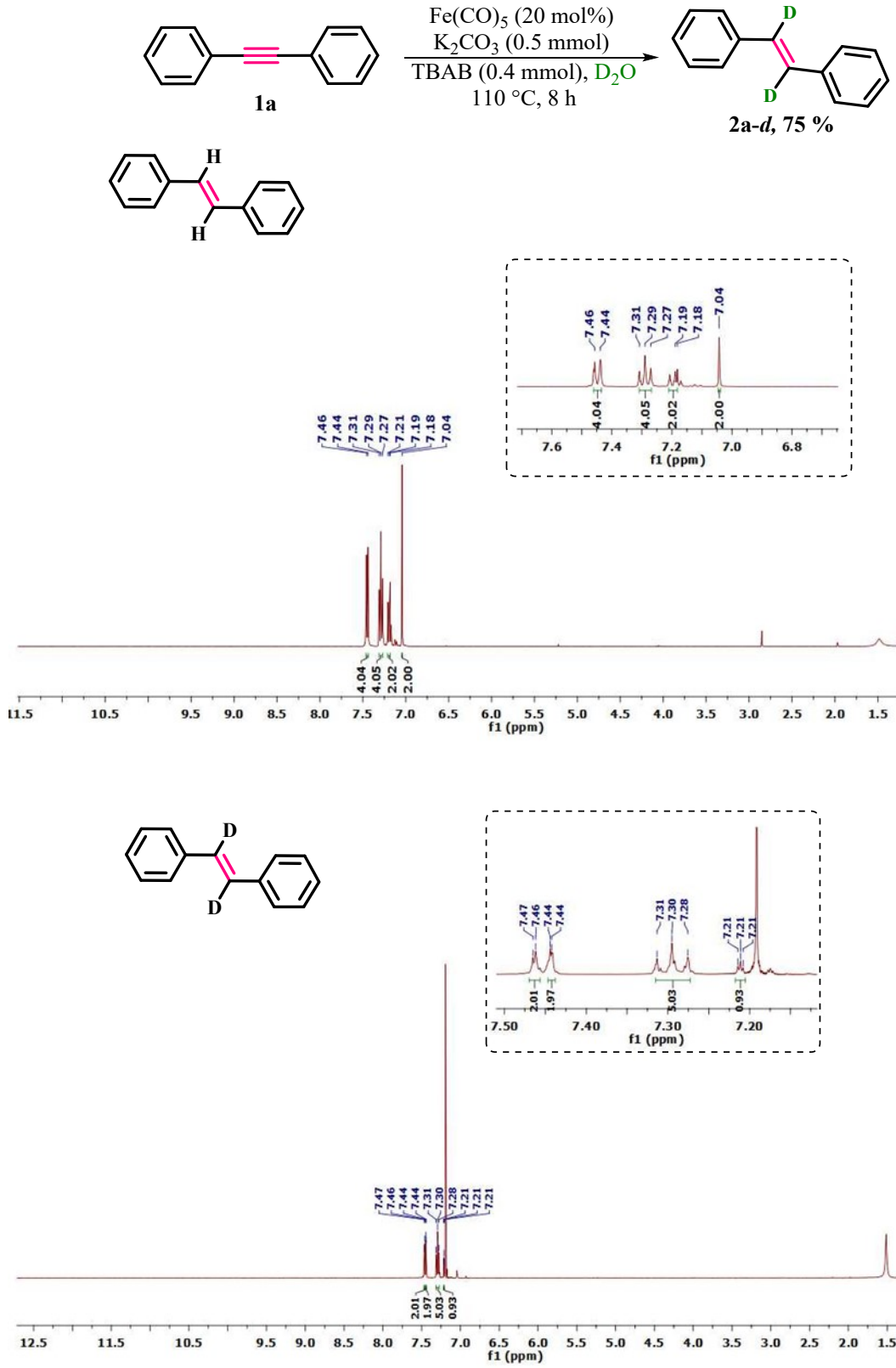
The addition of radical scavengers (TEMPO or BHT) did not significantly affect the yield of the product, and no intermediate adducts were observed, indicating that the reaction does not proceed via a free radical pathway.



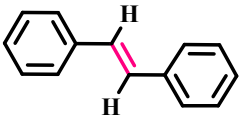
2a, 79%

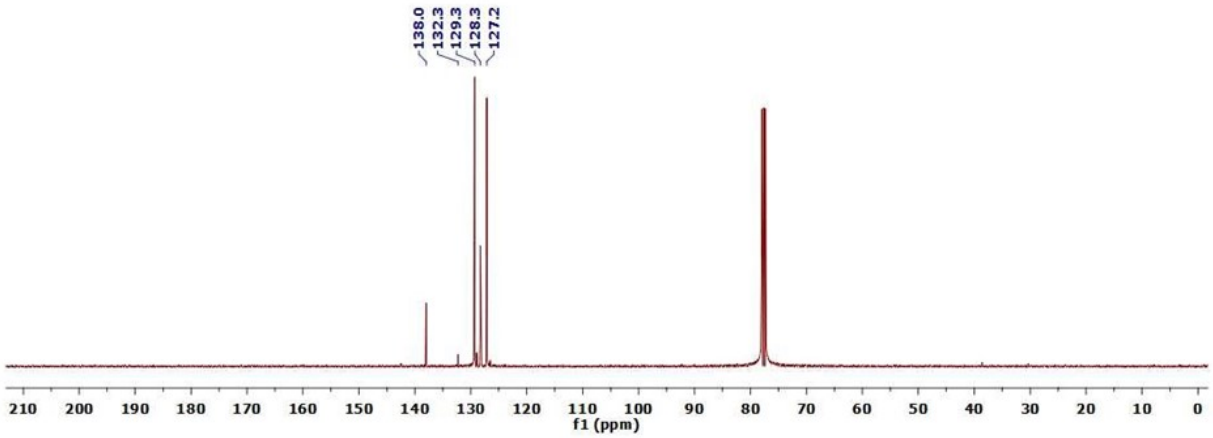
4.2 Isotopic Labeling Experiment

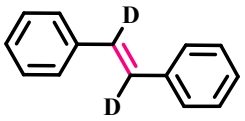
A deuterium labelling experiment was carried out using D_2O as the deuterium source under standard reaction conditions, replacing H_2O. Successful incorporation of deuterium was confirmed by ^1H and ^{13}C NMR characterization of the desired product, indicating the involvement of hydrogen transfer from H_2O in the reaction mechanism.

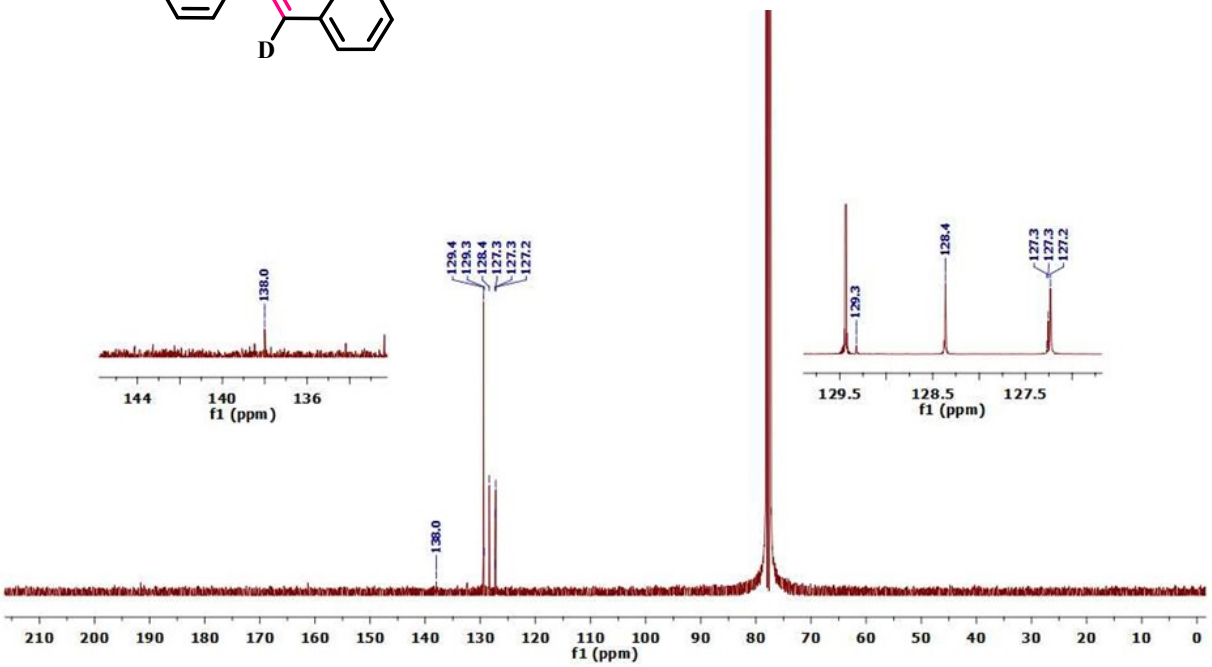


Scheme S2: ^{1}H NMR Spectrum (400 MHz, $CDCl_3$) of Compound 2a-*d*.



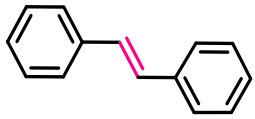
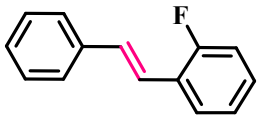
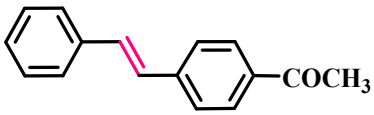


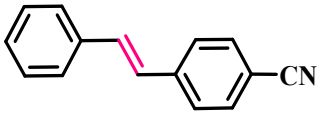
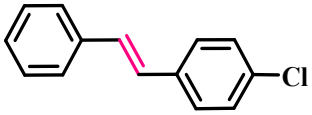
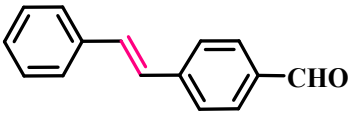
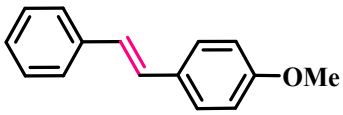


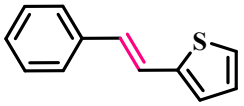
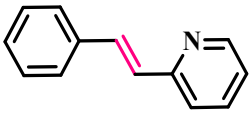
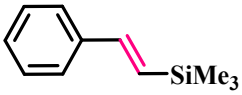
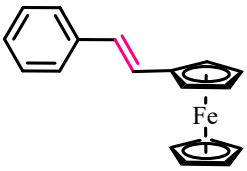
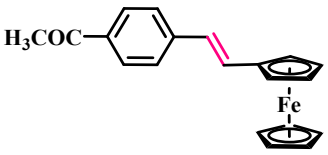


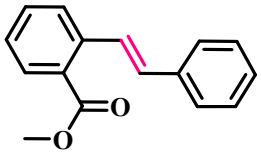
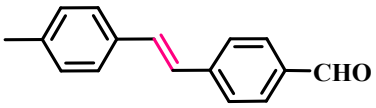
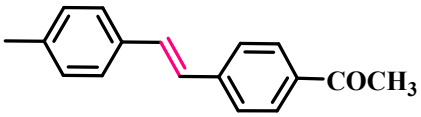
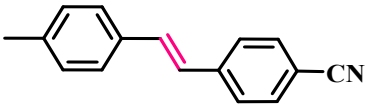
Scheme S3: $^{13}C\{^{1}H\}$ NMR Spectrum (101 MHz, $CDCl_3$) of Compound 2a-*d*.

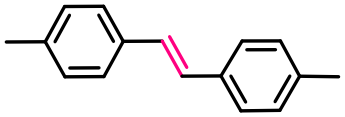
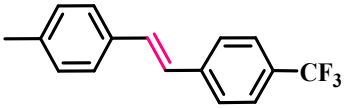
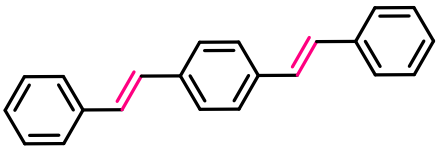
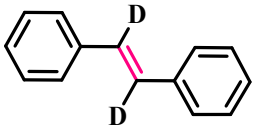
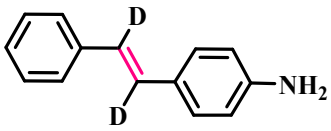
5. Characterization data Table S1:

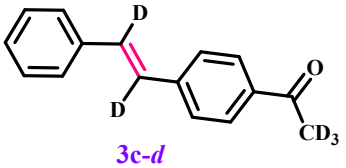
Sr. No.	Compound	Characterization
1.	 **2a** **(*E*)-1,2-diphenylethene**[7]	White Solid Yield = 81% **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.45 (d, *J* = 7.2 Hz, 4H), 7.29 (t, *J* = 7.6 Hz, 4H), 7.21 - 7.18 (m, 2H), 7.04 (s, 2H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 138.0, 132.3, 129.3, 128.3, 127.2.
2.	 **2b** **(*E*)-1-fluoro-2-styrylbenzene**[9]	White Solid Yield = 81% **^{1}H NMR (400 MHz, $CDCl_3$)** δ 6.74 (t, *J* = 7.8 Hz, 1H), 6.66 (d, *J* = 8.4 Hz, 2H), 6.49 (t, *J* = 8.0 Hz, 2H), 6.43 - 6.38 (m, 2H), 6.33 (d, *J* = 7.6 Hz, 2H), 6.28 - 6.17 (m, 2H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 160.2, 157.7, 135.7, 132.3 (d, *J* = 4.8 Hz), 127.2, 126.4, 125.4 (d, *J* = 3.8 Hz), 125.1, 123.6 (d, *J* = 12.1 Hz), 122.6 (d, *J* = 3.7 Hz), 119.3 (d, *J* = 3.9 Hz), 114.2 (d, *J* = 21.3 Hz)
3.	 **2c** **(*E*)-1-(4-styrylphenyl)ethan-1-one**[7]	White Solid Yield = 83% **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.95 (d, *J* = 8.4 Hz, 2H), 7.58 (d, *J* = 8.4 Hz, 2H), 7.53 (d, *J* = 8.0 Hz, 2H), 7.38 (t, *J* = 7.4 Hz, 2H), 7.29 (t, *J* = 7.4 Hz, 1H), 7.22 (d, *J* = 5.6 Hz, 1H), 7.12 (d, *J* = 16.0 Hz, 1H), 2.60 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 196.7, 141.2, 135.9, 135.1, 130.6, 128.0, 128.0, 127.5, 126.6, 126.0, 125.7, 25.8.
4.		White solid Yield = 81% **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.60 (q, *J* = 8.4 Hz, 4H), 7.53 (d, *J* = 7.6 Hz, 2H), 7.38 (t, *J* = 8.0 Hz, 2H), 7.31 (d, *J* = 7.2 Hz, 1H), 7.21 (d, *J* = 16.4 Hz, 1H), 7.08 (d, *J* = 16.4 Hz, 1H).

	 **2d** **(*E*)-4-styrylbenzonitrile**[8]	**^{13}C NMR (100 MHz, $CDCl_3$)** δ 140.8, 135.3, 131.5, 131.4, 127.9, 127.7, 125.9, 125.9, 125.7, 118.1, 109.6.
5.	 **2e** **(*E*)-1-chloro-4-styrylbenzene**[7]	White Solid Yield = 84% **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.43 (d, *J* = 7.6 Hz, 2H), 7.36 (d, *J* = 8.4 Hz, 2H), 7.31 - 7.26 (m, 4H), 7.20 (t, *J* = 7.6 Hz, 1H), 7.01 (d, *J* = 16.4 Hz, 1H), 6.96 (d, *J* = 16.4 Hz, 1H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 136.6, 135.4, 132.8, 128.9, 128.4, 128.3, 127.5, 127.3, 126.9, 126.1.
6.	 **2f** **(*E*)-4-styrylbenzaldehyde**[10]	White solid Yield = 83% **^{1}H NMR (400 MHz, $CDCl_3$)** δ 9.86 (s, 1H), 7.73 (d, *J* = 8.4 Hz, 2H), 7.51 (d, *J* = 8.8 Hz, 2H), 7.41 (d, *J* = 8.0 Hz, 2H), 7.28 (d, *J* = 7.2 Hz, 2H), 7.19 (t, *J* = 7.4 Hz, 1H), 7.12 (d, *J* = 14.0 Hz, 1H), 7.00 (d, *J* = 16.8 Hz, 1H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 191.1, 142.8, 135.9, 134.7, 131.6, 129.6, 128.3, 127.9, 126.7, 126.3, 126.3.
7.	 **2g** **(*E*)-1-methoxy-4-styrylbenzene**[7]	White solid Yield = 85% **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.44 (d, *J* = 7.2 Hz, 2H), 7.41 (d, *J* = 8.8 Hz, 2H), 7.29 (t, *J* = 7.6 Hz, 2H), 7.18 (t, *J* = 7.2 Hz, 1H), 7.02 (d, *J* = 16.4 Hz, 1H), 6.92 (d, *J* = 16.4 Hz, 1H), 6.85 (d, *J* = 8.8 Hz, 2H), 3.78 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 158.9, 137.3, 129.8, 128.3, 127.8, 127.3, 126.8, 126.2, 125.9, 113.8, 55.0.
8.		Yellowish solid Yield = 82% **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.44 (d, *J* = 7.6 Hz, 2H), 7.32 (t, *J* = 7.4 Hz, 2H), 7.24 - 7.15 (m, 2H),

	 **2h** **(*E*)-2-styrylthiophene[7]**	7.16 (d, *J* = 4.8 Hz, 1H), 7.04 (d, *J* = 3.6 Hz, 1H), 6.97 (m, 1H), 6.91 (d, *J* = 16.0 Hz, 1H). **^{13}C NMR (100 MHz, CDCl$_3$)** δ 142.7, 136.8, 128.5, 128.2, 127.4, 126.1, 126.0, 124.2, 121.6.
9.	 **2i** **(*E*)-2-styrylpyridine[8]**	Yellow solid Yield = 80% **^{1}H NMR (400 MHz, CDCl$_3$)** δ 8.60 (d, *J* = 4.4 Hz, 1H), 7.70 - 7.66 (m, 2H), 7.62 - 7.57 (m, 2H), 7.42 - 7.35 (m, 3H), 7.29 (t, *J* = 7.4 Hz, 1H), 7.21 - 7.14 (m, 2H). **^{13}C NMR (100 MHz, CDCl$_3$)** δ 149.2, 147.5, 136.9, 136.9, 136.4, 133.5, 133.1, 128.7, 128.4, 127.1, 122.1.
10.	 **2j** **(*E*)-trimethyl(styryl)silane[11]**	White solid Yield = 80% **^{1}H NMR (400 MHz, CDCl$_3$)** δ 7.42 (d, *J* = 7.2 Hz, 2H), 7.31 (t, *J* = 7.4 Hz, 2H), 7.20 (t, *J* = 6.6 Hz, 1H), 6.85 (d, *J* = 19.2 Hz, 1H), 6.47 (d, *J* = 19.2 Hz, 1H), 0.14 (s, 9H). **^{13}C NMR (100 MHz, CDCl$_3$)** δ 145.3, 140.1, 131.3, 130.1, 129.7, 128.1, 0.5.
11.	 **2k** **(*E*)-styrylferrocene[12]**	Orange solid Yield = 82% **^{1}H NMR (400 MHz, CDCl$_3$)** δ 7.43 (d, *J* = 7.6 Hz, 2H), 7.33 (t, *J* = 7.4 Hz, 2H), 7.23 (d, *J* = 8.8 Hz, 1H), 6.87 (d, *J* = 16.4 Hz, 1H), 6.70 (d, *J* = 16.0 Hz, 1H), 4.46 (s, 2H), 4.28 (s, 2H), 4.14 (s, 5H). **^{13}C NMR (100 MHz, CDCl$_3$)** δ 138.1, 128.8, 127.1, 126.9, 126.2, 125.9, 83.5, 69.4, 69.2, 67.0.
12.	 **2l** **(E)-1-(4-(2-(Ferrocenyl)vinyl)phenyl)ethan-1-one[12]**	Orange solid Yield = 81% **^{1}H NMR (400 MHz, CDCl$_3$)** δ 7.91 (d, *J* = 8.4 Hz, 2H), 7.48 (d, *J* = 8.4 Hz, 2H), 7.02 (d, *J* = 16.0 Hz, 1H), 6.70 (d, *J* = 16.0 Hz, 1H), 4.48 (t, *J* = 1.8 Hz, 2H), 4.33 ((t, *J* = 1.8 Hz, 2H), 4.14 (s, 5H), 2.58 (s, 3H). **^{13}C NMR (100 MHz, CDCl$_3$)** δ 197.1, 142.1, 134.7, 130.1, 128.5, 125.2, 124.2, 81.9, 69.1, 68.9, 66.8,

		26.1.
13.	 **2m** **methyl (*E*)-2-styrylbenzoate[13]**	White solid Yield = 80% **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.92 (d, *J* = 16.0 Hz, 1H), 7.86 (d, *J* = 9.7 Hz, 1H), 7.65 (d, *J* = 8.0 Hz, 1H), 7.50 - 7.41 (m, 3H), 7.31 - 7.21 (m, 3H), 7.19 (d, *J* = 6.8 Hz, 1H), 6.94 (d, *J* = 16.4 Hz, 1H), 3.85 (s, 3H).
14.	 **2p** **(*E*)-4-(4-methylstyryl)benzaldehyde[14]**	White solid Yield = 83% **^{1}H NMR (400 MHz, $CDCl_3$)** δ 9.89 (s, 1H), 7.77 (d, *J* = 8.4 Hz, 2H), 7.54 (d, *J* = 8.4 Hz, 2H), 7.36 (d, *J* = 8.4 Hz, 2H), 7.17 - 7.10 (m, 3 Hz, 3H), 7.00 (d, *J* = 16.4 Hz, 1H), 2.29 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 191.7, 143.7, 138.6, 135.1, 133.8, 132.2, 130.3, 129.6, 126.9, 126.8, 126.3, 21.4.
15.	 **2q** **(*E*)-1-(4-(4-methylstyryl)phenyl) ethan-1-one[10]**	White solid Yield = 84% **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.84 (d, *J* = 8.4 Hz, 2H), 7.47 (d, *J* = 8.4 Hz, 2H), 7.34 (d, *J* = 8.0 Hz, 2H), 7.14 (d, *J* = 13.6 Hz, 1H), 7.09 (d, *J* = 6.8 Hz, 2H), 6.98 (d, *J* = 16.0 Hz, 1H), 2.50 (s, 3H), 2.28 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 196.6, 141.3, 137.5, 134.7, 133.0, 130.5, 128.6, 128.0, 125.9, 125.5, 125.5, 25.7, 20.4.
16.	 **2r** **(*E*)-4-(4-methylstyryl)benzonitrile[14]**	White solid Yield = 82% **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.56 (d, *J* = 8.4 Hz, 2H), 7.50 (d, *J* = 8.4 Hz, 2H), 7.36 (d, *J* = 8.0 Hz, 2H), 7.12 (t, *J* = 8.0 Hz, 3H), 6.97 (d, *J* = 16.4 Hz, 1H), 2.31 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 140.9, 137.6, 132.3, 131.3, 131.2, 128.4, 125.7, 125.5, 124.5, 117.9, 109.1, 20.1.
17.		White solid Yield = 85% **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.40 (d, *J* = 8.0 Hz,

	 **2s** **(*E*)-1,2-di-*p*-tolylethene[8]**	4H), 7.16 (d, *J* = 8.0 Hz, 4H), 7.04 (s, 2H), 2.35 (s, 6H). **^{13}C NMR (100 MHz, CDCl$_3$)** δ 137.2, 134.7, 129.3, 127.6, 126.3, 21.2.
18.	 **2t** **(*E*)-1-methyl-4-(4-(trifluoromethyl) styryl)benzene[15]**	White solid Yield = 86% **^{1}H NMR (400 MHz, CDCl$_3$)** δ 7.54 (s, 4H), 7.39 (d, *J* = 8.0 Hz, 2H), 7.18 (d, *J* = 20.0 Hz, 1H), 7.14 - 7.10 (m, 2H), 7.02 (d, *J* = 16.4 Hz, 1H), 2.33 (s, 3H). **^{13}C NMR (100 MHz, CDCl$_3$)** δ 140.8, 138.1, 133.6, 130.9, 129.3, 129.0, 128.6, 126.5, 126.2, 125.4 (q, *J* = 4.0 Hz), 122.7, 21.1.
19.	 **2u** **1,4-di((*E*)-styryl)benzene[12]**	White solid Yield = 79% **^{1}H NMR (400 MHz, CDCl$_3$)** δ 7.55 (d, *J* = 1.2 Hz, 1H), 7.53 (s, 4H), 7.38 (t, *J* = 7.4 Hz, 5H), 7.29 (t, *J* = 1.2 Hz, 1H), 7.27 (s, 3H), 7.14 (s, 2H), 7.13 (s, 2H). **^{13}C NMR (100 MHz, CDCl$_3$)** δ 137.3, 136.7, 128.7, 128.5, 128.2, 127.6, 126.8, 126.5.
20.	 **3a-*d*** **(*E*)-1,2-diphenylethene-1,2-d_2**	White solid, Yield = 75% **^{1}H NMR (400 MHz, CDCl$_3$)** δ 7.46 (d, *J* = 1.2 Hz, 2H), 7.44 (d, *J* = 0.8 Hz, 2H), 7.29 (t, *J* = 7.4 Hz, 5H), 7.21 (t, *J* = 1.2 Hz, 1H). **^{13}C NMR (100 MHz, CDCl$_3$)** δ 138.0, 129.4, 129.3, 128.4, 127.3 (t, *J* = 2.4 Hz).
21.	 **3b-*d*** **(E)-4-(2-phenylvinyl-1,2-d_2)aniline**	White Solid Yield = 79% **^{1}H NMR (400 MHz, CDCl$_3$)** δ 7.43 - 7.40 (m, 2H), 7.27 - 7.24 (m, 3H), 7.23 - 7.19 (m, 2H), 6.54 (d, *J* = 8.8 Hz, 2H), 3.72 (s, 2H).

22.	 **3c-*d*** **[(*E*)-1-(4-(2-phenylvinyl-1,2-d_2)phenyl) ethan-1-one-2,2,2-d_3] [16]**	White Solid Yield = 77% **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.91 (d, *J* = 8.8 Hz, 2 H), 7.52 (dd, *J* = 19.6, 8.4 Hz, 4 H), 7.34 (t, *J* = 8.0 Hz, 2 H), 7.26 (t, *J* = 8.0 Hz, 1H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 197.7, 142.0, 136.7, 136.0, 129.0, 128.9, 128.4, 126.9, 126.6 - 25.7 (m).

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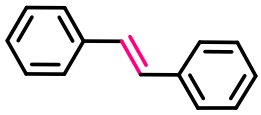
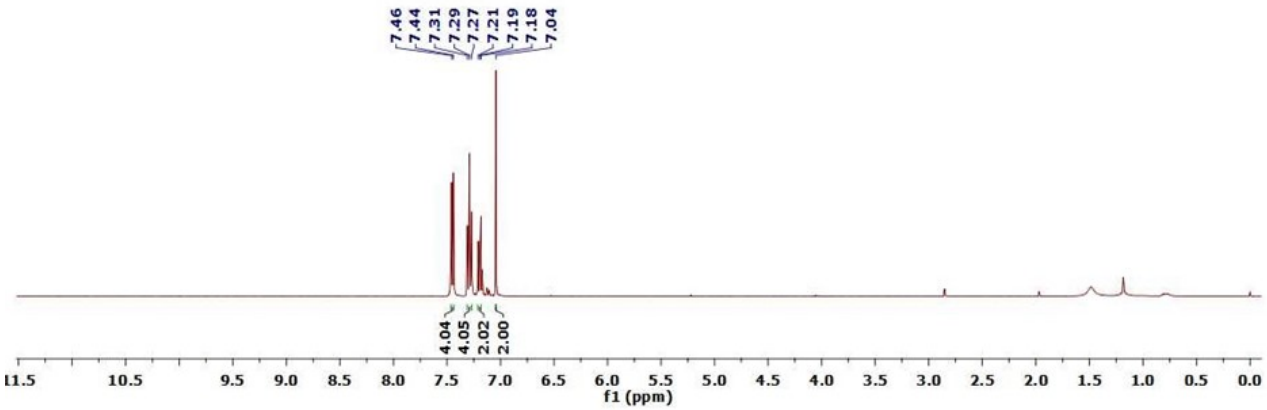
7. Copies of NMR Spectra





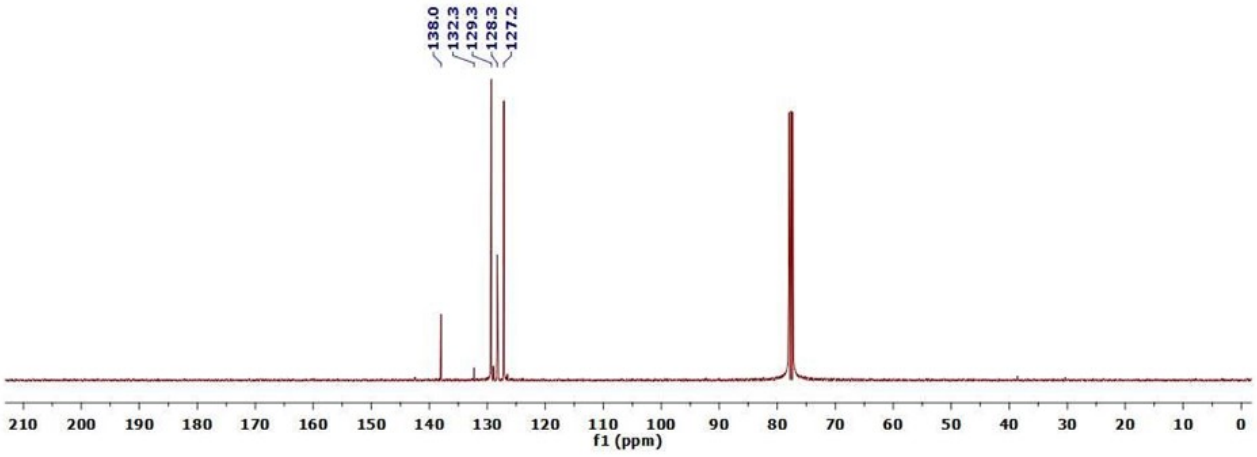
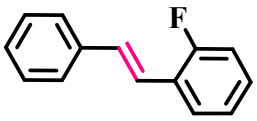
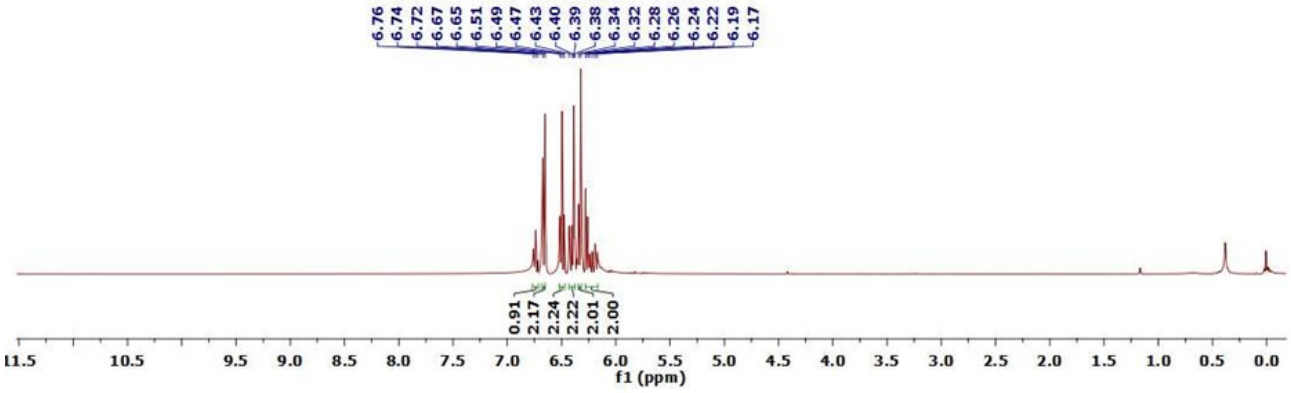


Figure S1: ^{1}H & $^{13}C\{^{1}H\}$-NMR Spectrum (400 MHz & 101 MHz, $CDCl_3$) of Compound 2a.





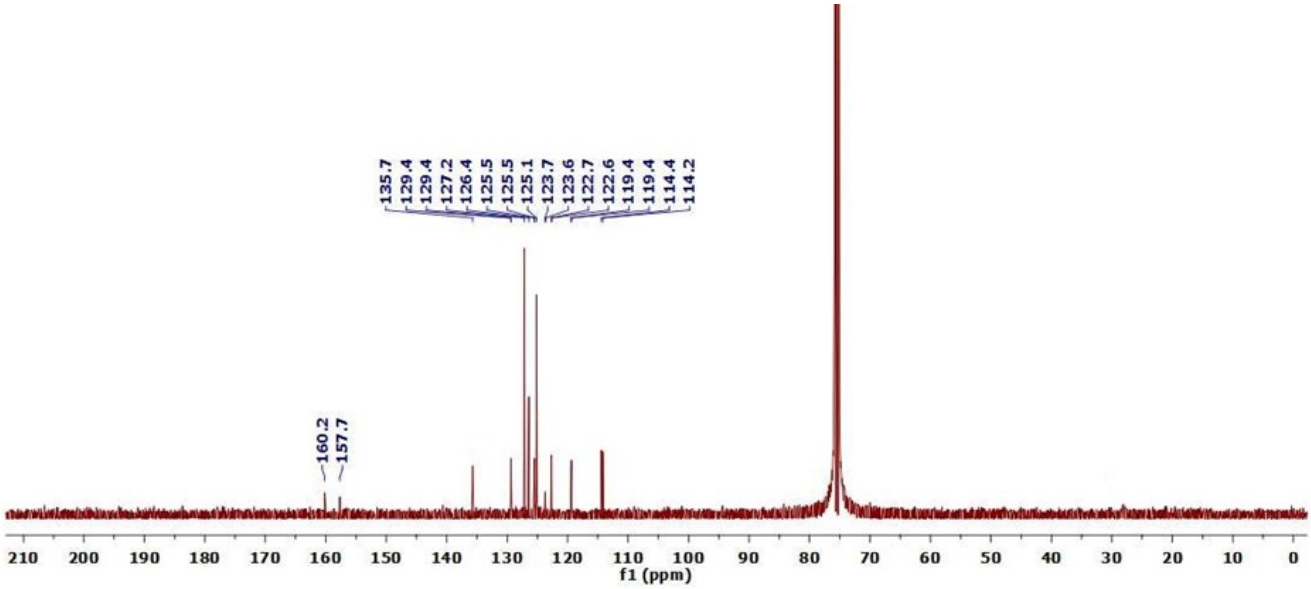


Figure S2: ^{1}H & $^{13}C\{^{1}H\}$–NMR Spectrum (400 MHz & 101 MHz, $CDCl_3$) of Compound 2b.

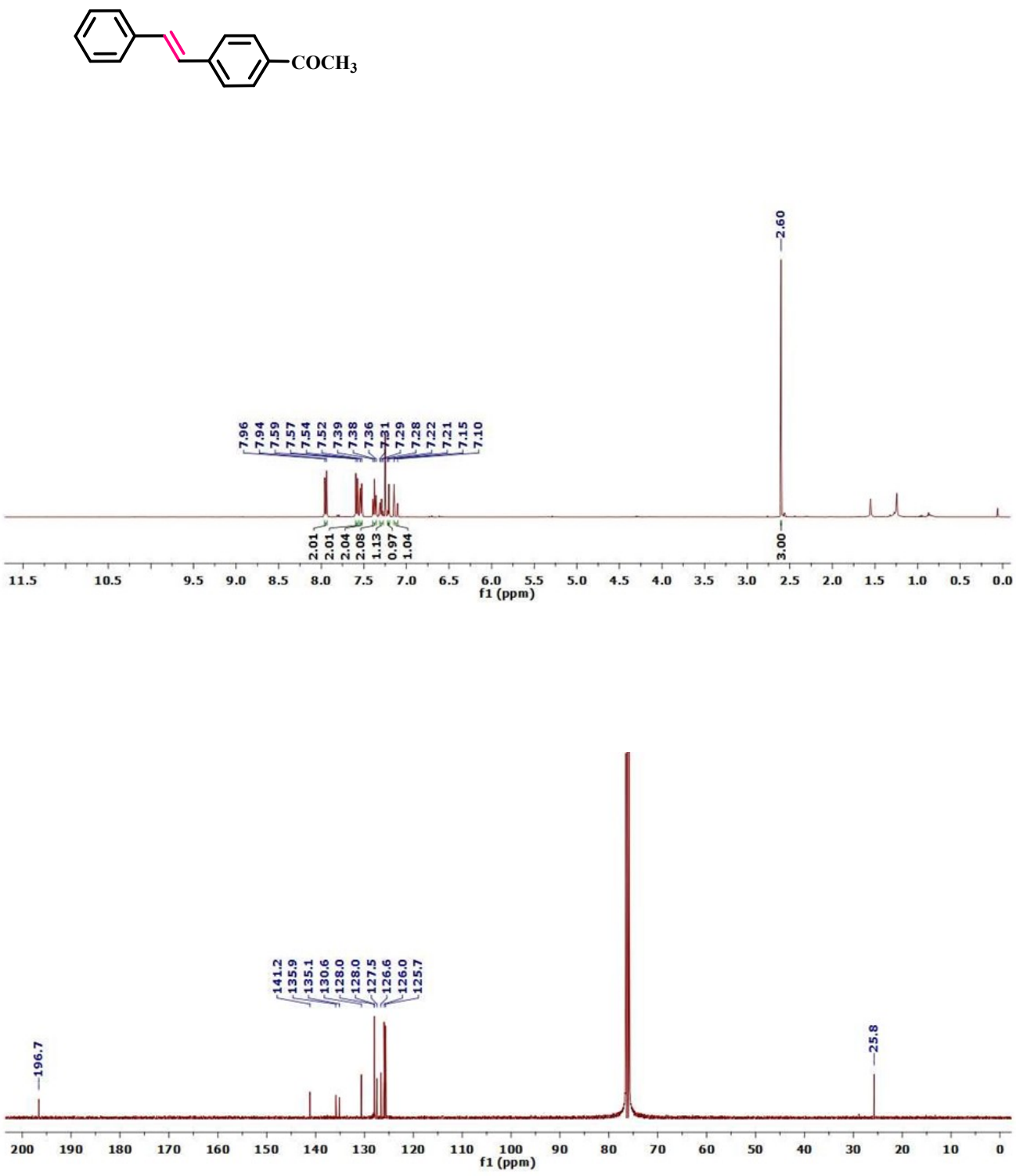
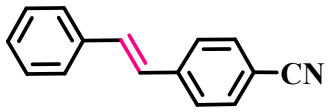
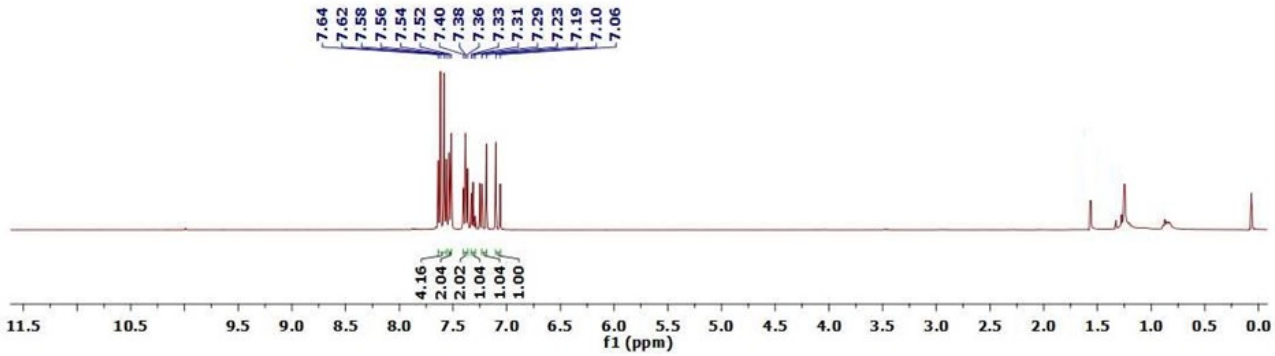


Figure S3: ^{1}H & $^{13}C\{^{1}H\}$–NMR Spectrum (400 MHz & 101 MHz, $CDCl_3$) of Compound 2c





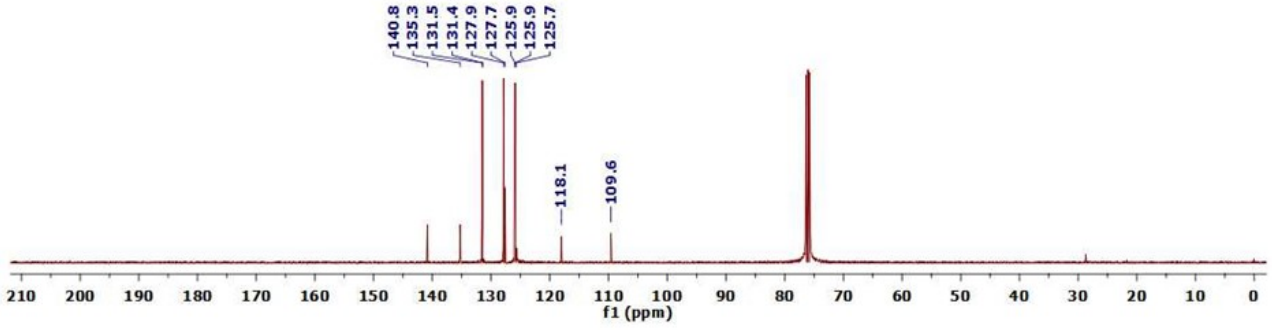
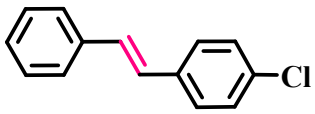
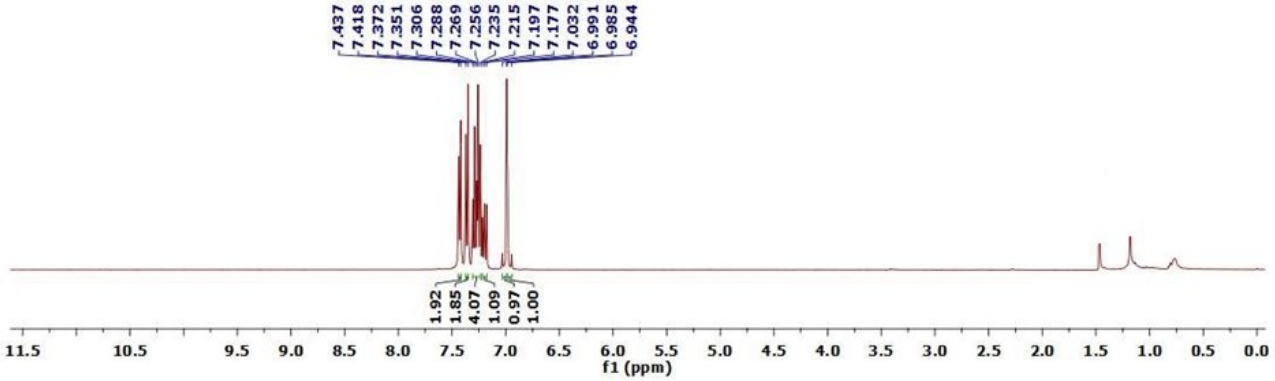


Figure S4: ^{1}H & $^{13}C\{^{1}H\}$–NMR Spectrum (400 MHz & 101 MHz, $CDCl_3$) of Compound 2d





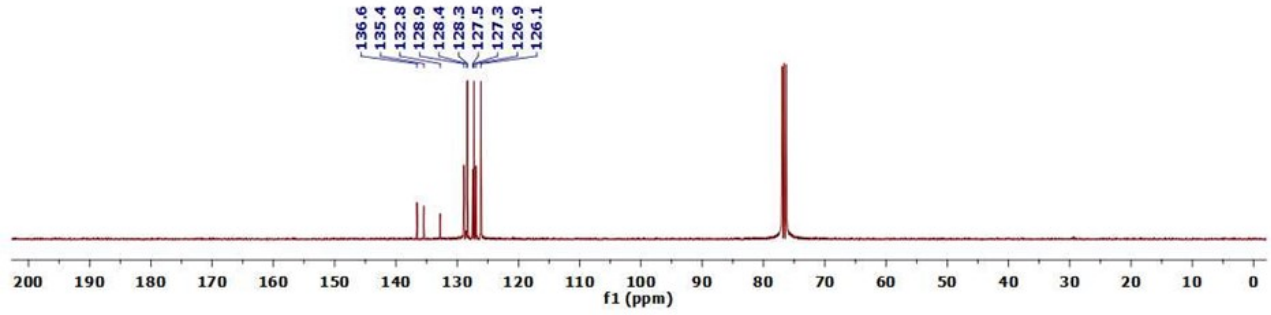
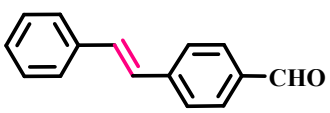
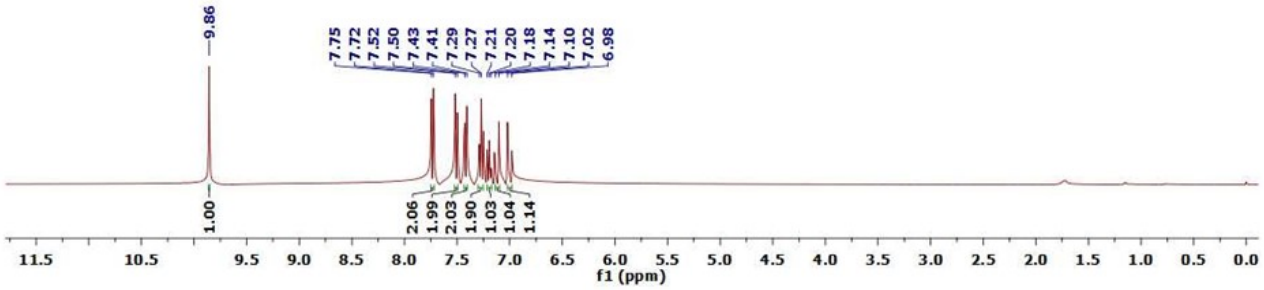


Figure S5: ^{1}H & $^{13}C\{^{1}H\}$–NMR Spectrum (400 MHz & 101 MHz, $CDCl_3$) of Compound 2e





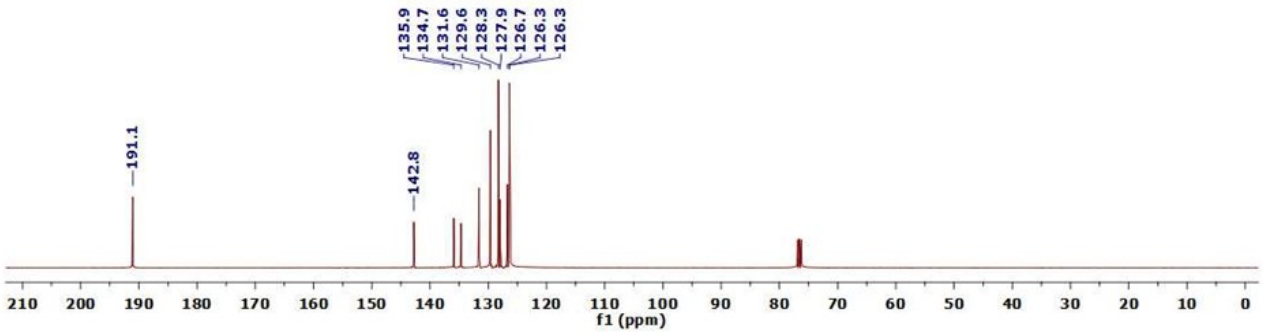
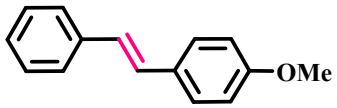
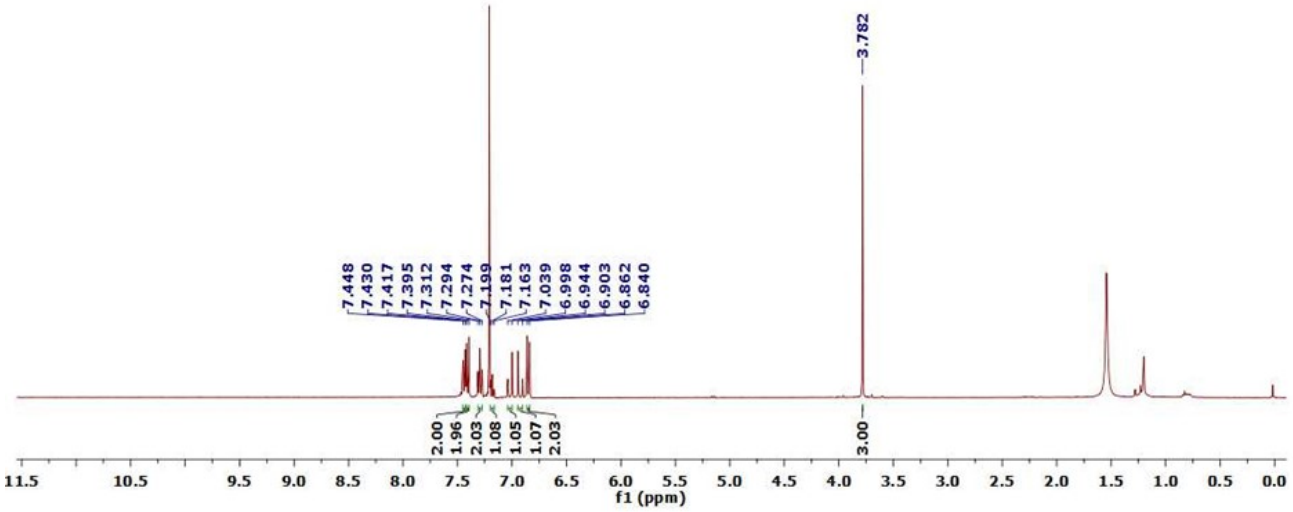


Figure S6: ^{1}H & $^{13}C\{^{1}H\}$–NMR Spectrum (400 MHz & 101 MHz, $CDCl_3$) of Compound 2f





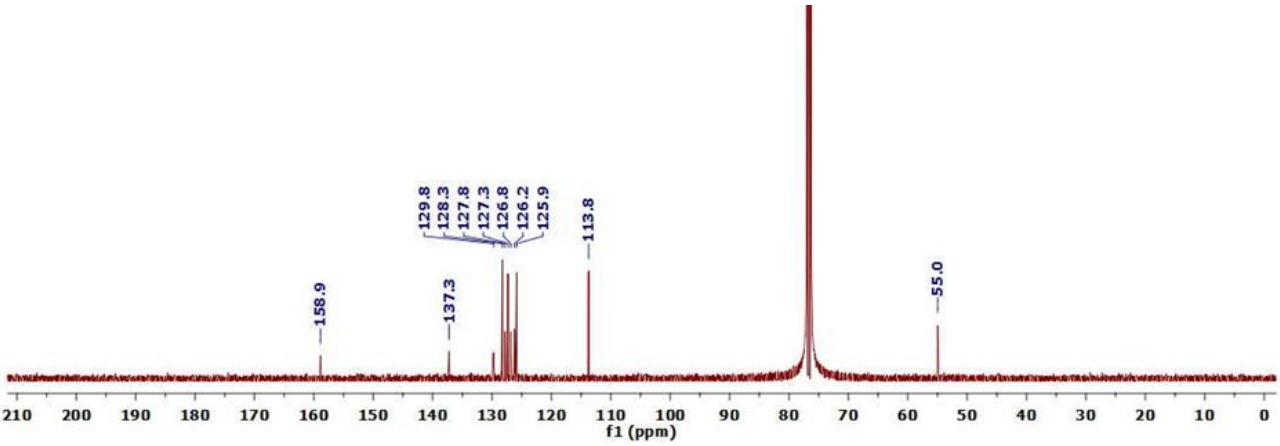
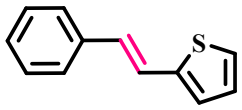
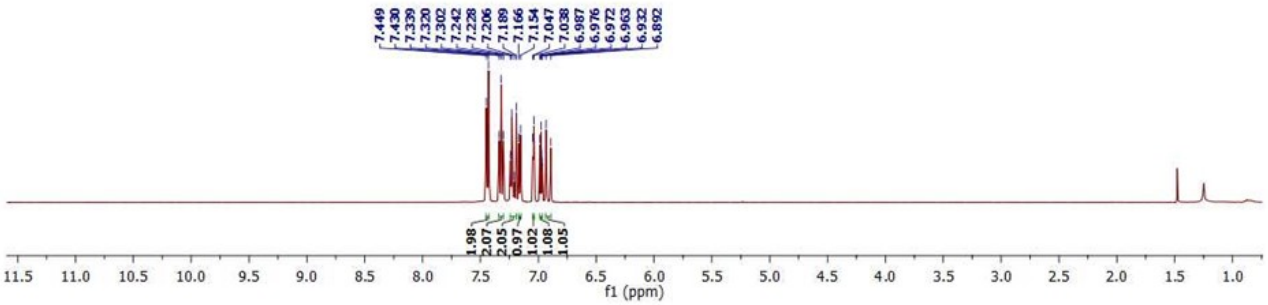


Figure S7: ^{1}H & $^{13}C\{^{1}H\}$–NMR Spectrum (400 MHz & 101 MHz, $CDCl_3$) of Compound 2g





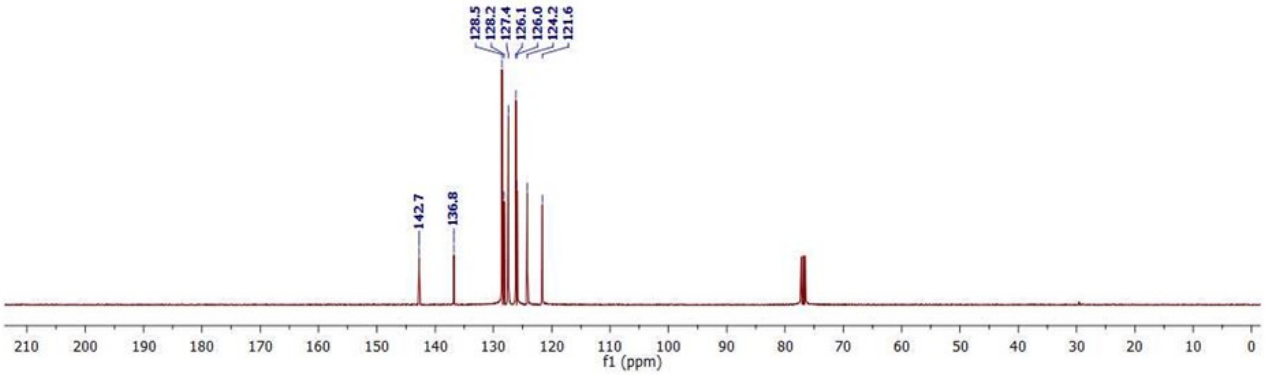
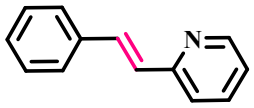
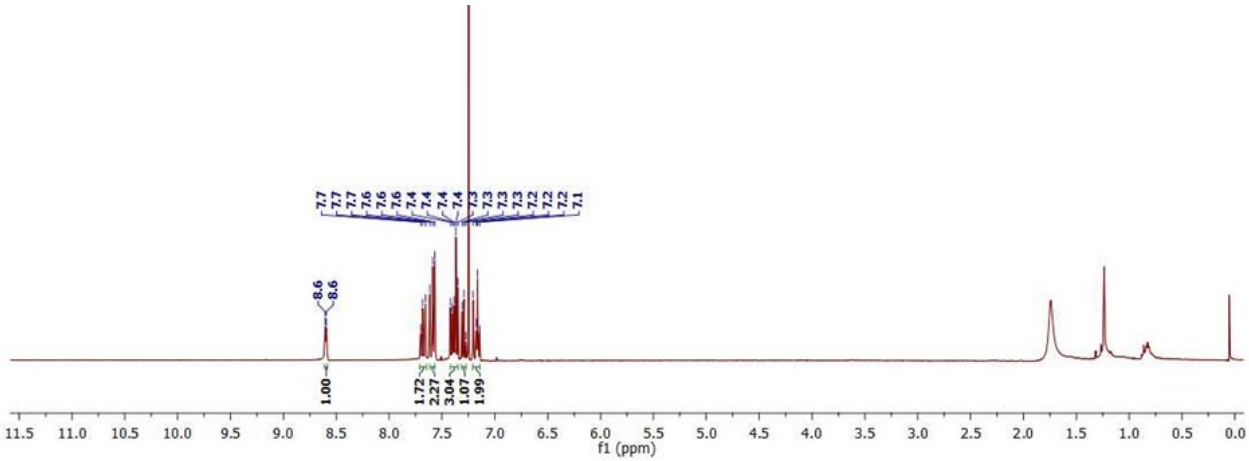


Figure S8: ^{1}H & $^{13}C\{^{1}H\}$–NMR Spectrum (400 MHz & 101 MHz, $CDCl_3$) of Compound 2h





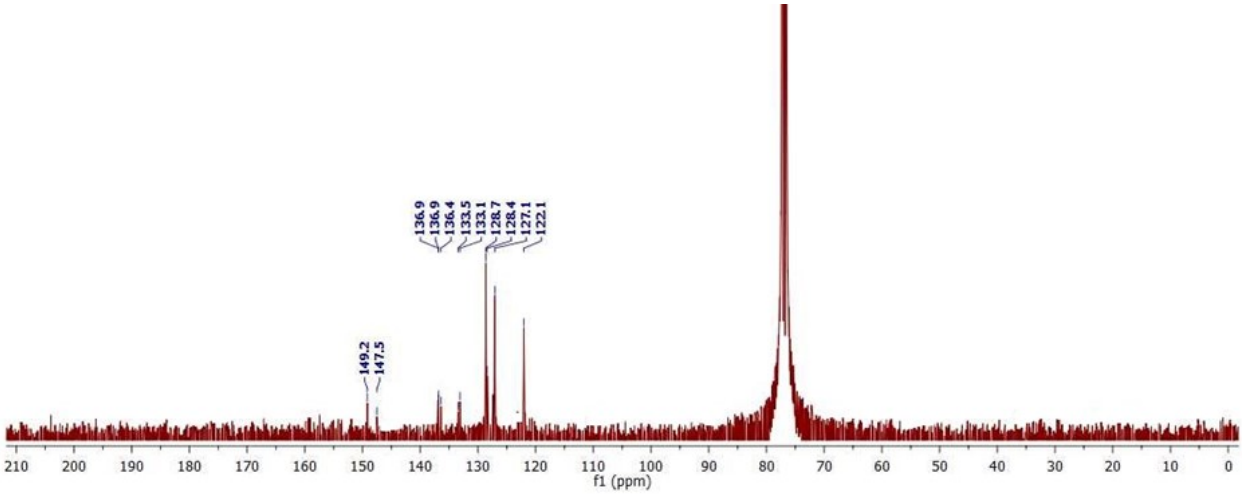
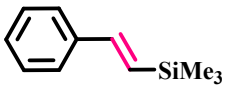
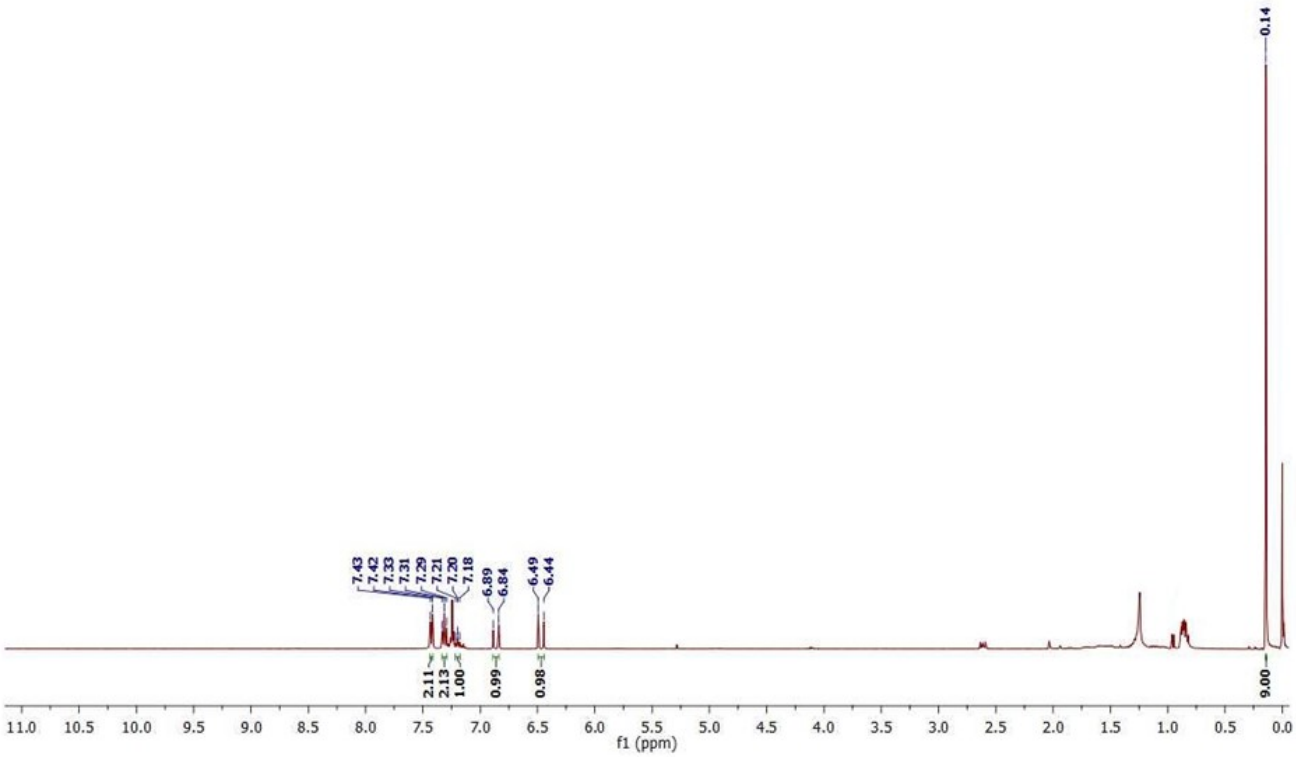


Figure S9: ^{1}H & $^{13}C\{^{1}H\}$–NMR Spectrum (400 MHz & 101 MHz, $CDCl_3$) of Compound 2i





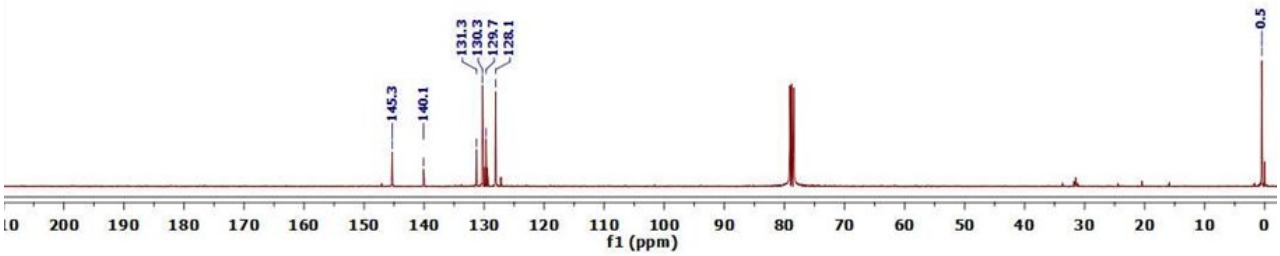
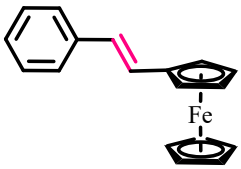
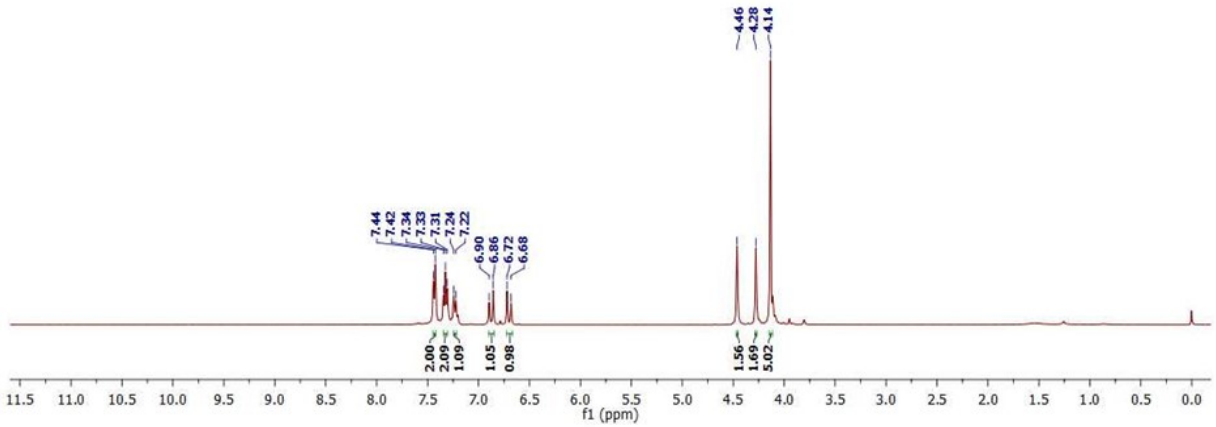


Figure S10: ^{1}H & $^{13}C\{^{1}H\}$–NMR Spectrum (400 MHz & 101 MHz, $CDCl_3$) of Compound 2j





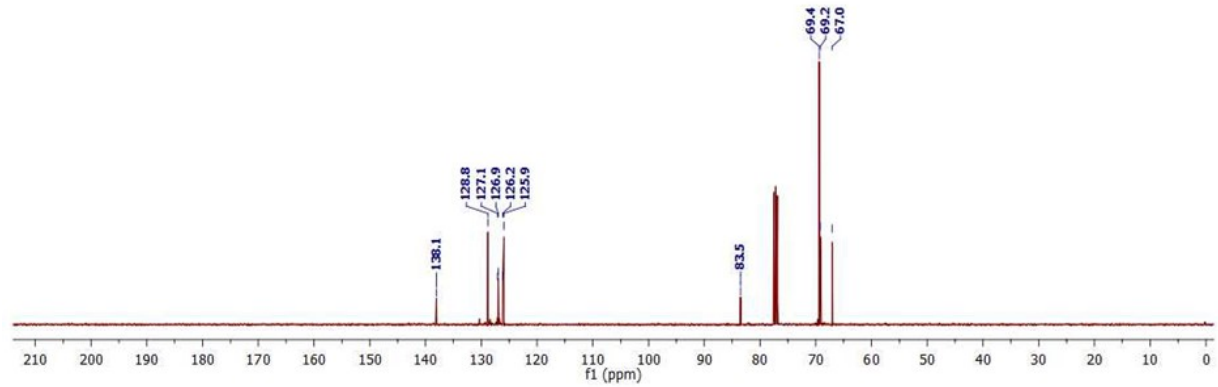
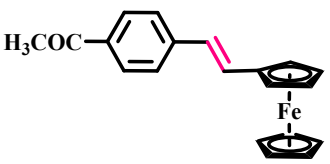
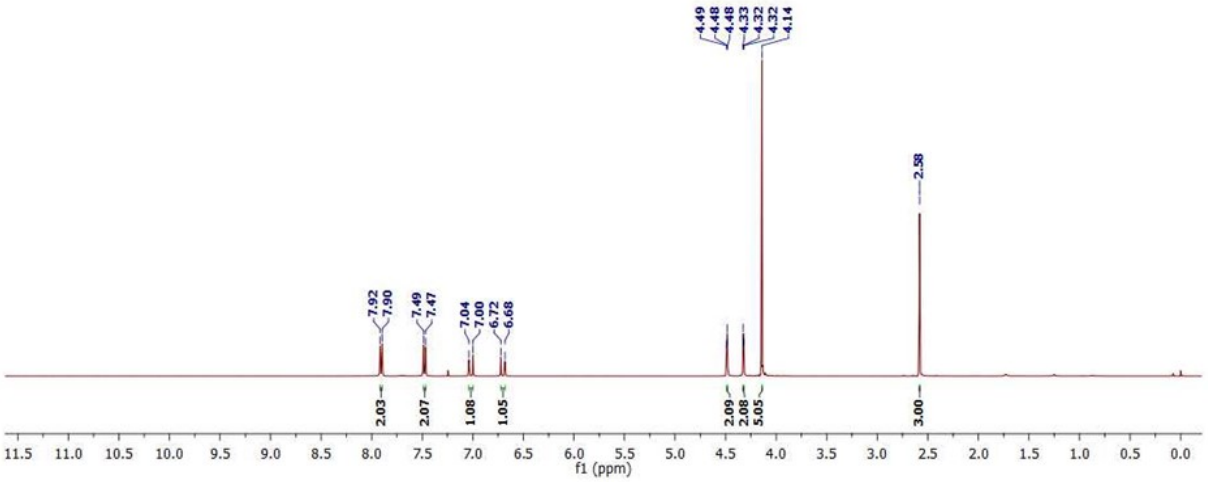


Figure S11: ^{1}H & $^{13}C\{^{1}H\}$–NMR Spectrum (400 MHz & 101 MHz, $CDCl_3$) of Compound 2k





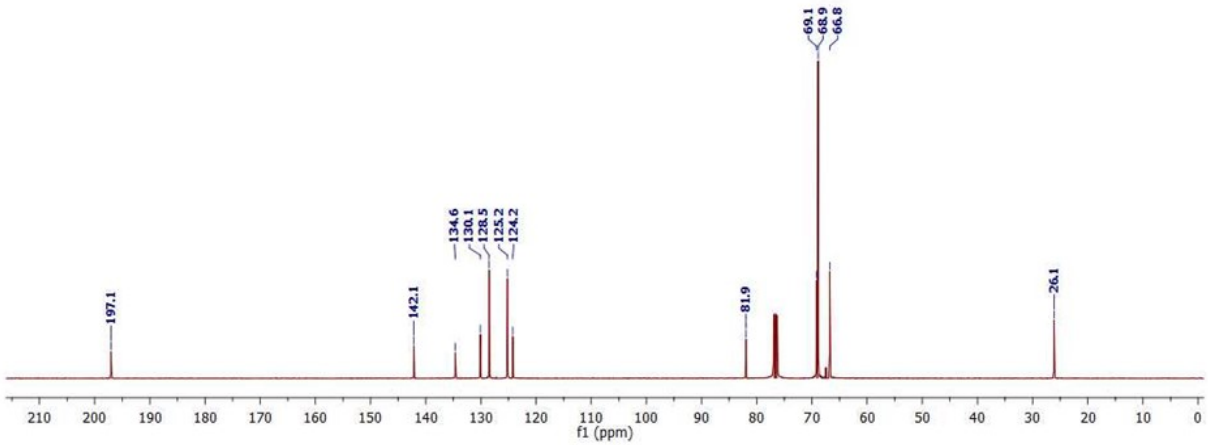


Figure S12: ^{1}H & $^{13}C\{^{1}H\}$–NMR Spectrum (400 MHz & 101 MHz, $CDCl_3$) of Compound 2l.

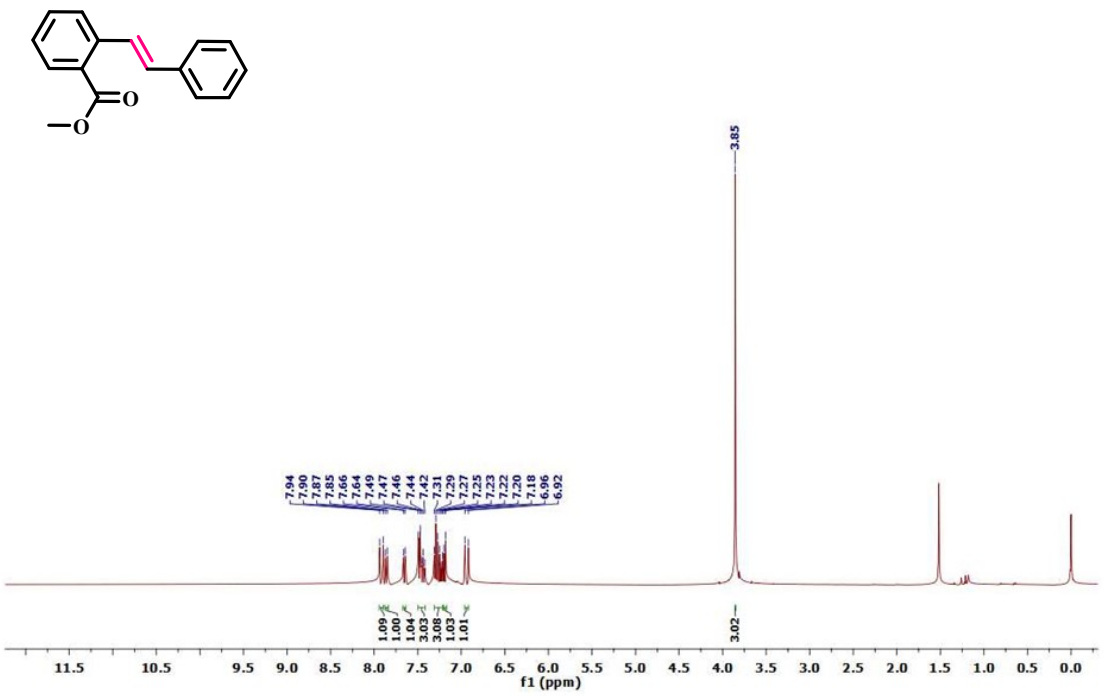
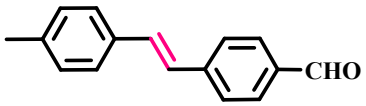
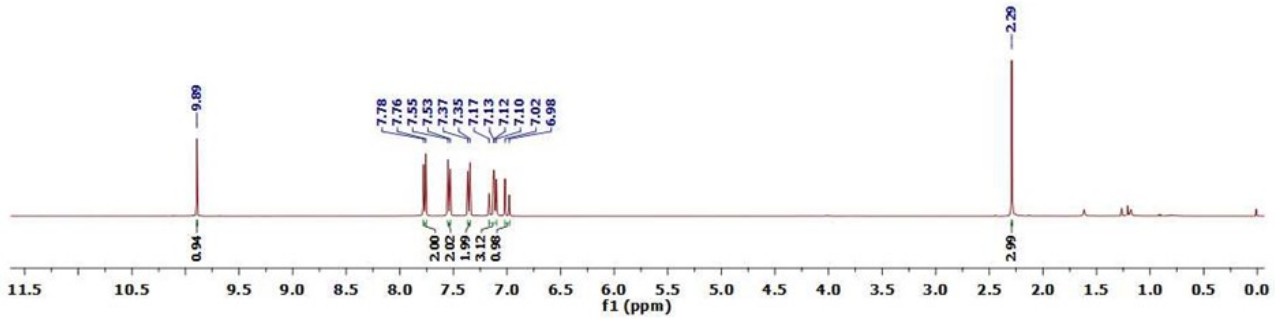


Figure S13: ^{1}H & $^{13}C\{^{1}H\}$–NMR Spectrum (400 MHz & 101 MHz, $CDCl_3$) of Compound 2m.





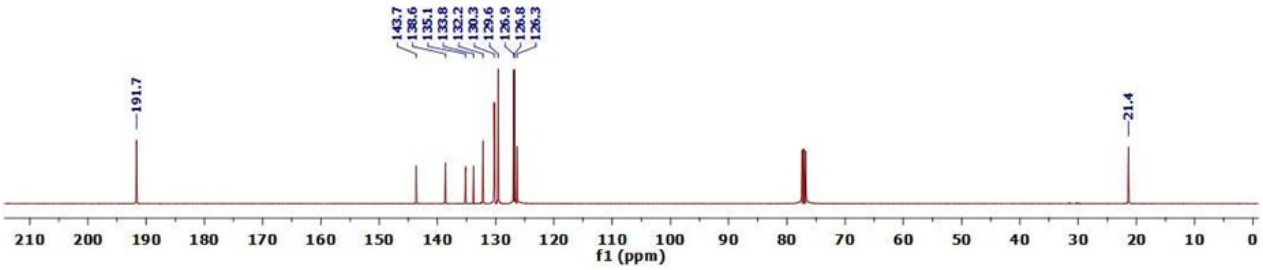
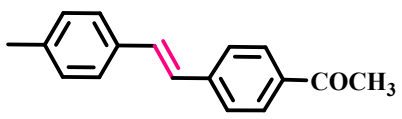
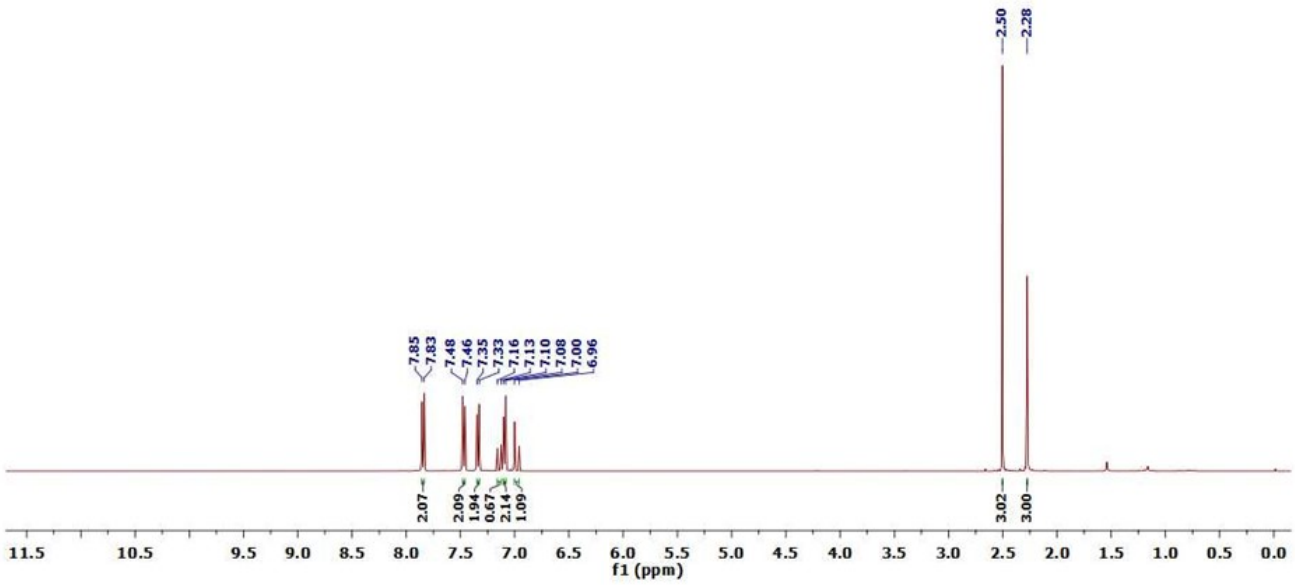


Figure S14: ^{1}H & $^{13}C\{^{1}H\}$–NMR Spectrum (400 MHz & 101 MHz, $CDCl_3$) of Compound 2p





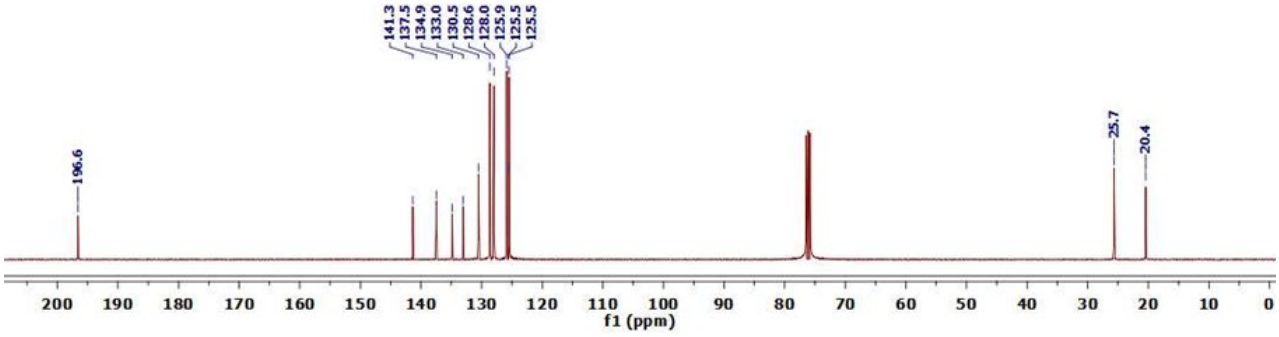
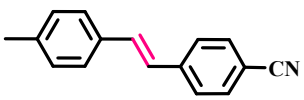
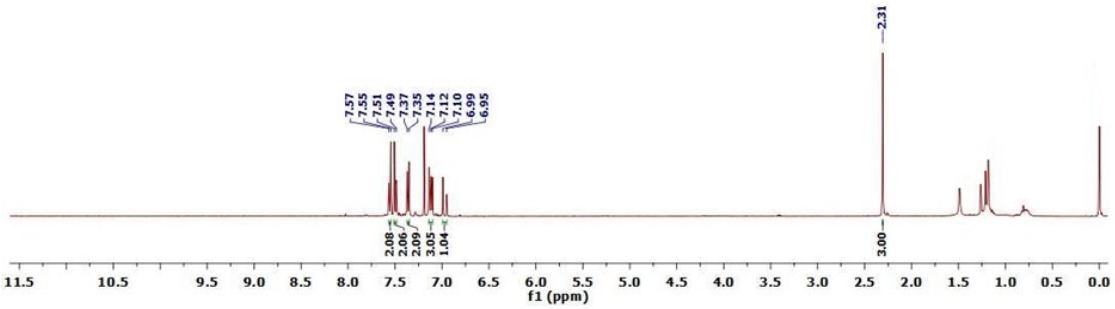


Figure S15: ^{1}H & $^{13}C\{^{1}H\}$–NMR Spectrum (400 MHz & 101 MHz, $CDCl_3$) of Compound 2q





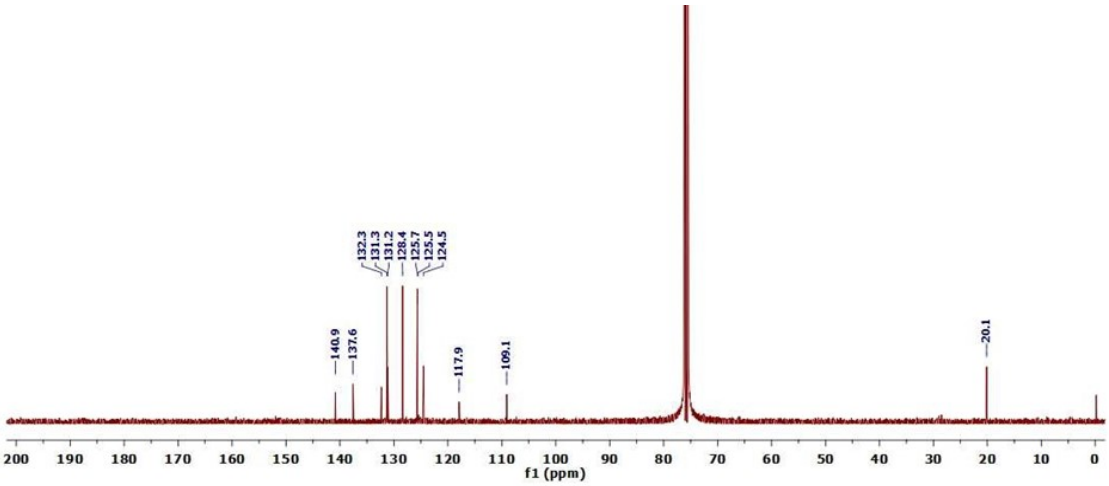
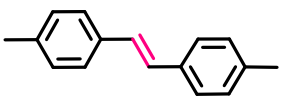
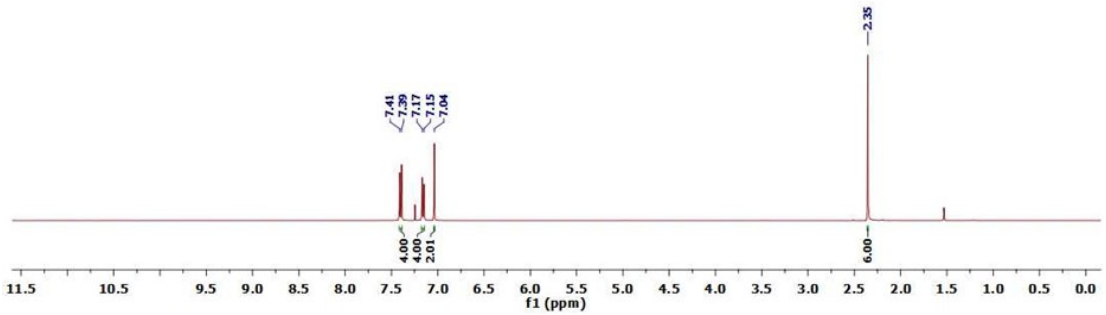


Figure S16: ^{1}H & $^{13}C\{^{1}H\}$–NMR Spectrum (400 MHz & 101 MHz, $CDCl_3$) of Compound 2r





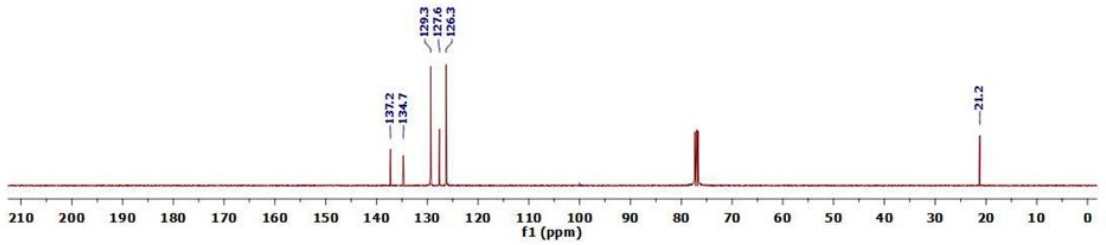


Figure S17: ^{1}H & $^{13}C\{^{1}H\}$–NMR Spectrum (400 MHz & 101 MHz, $CDCl_3$) of Compound 2s

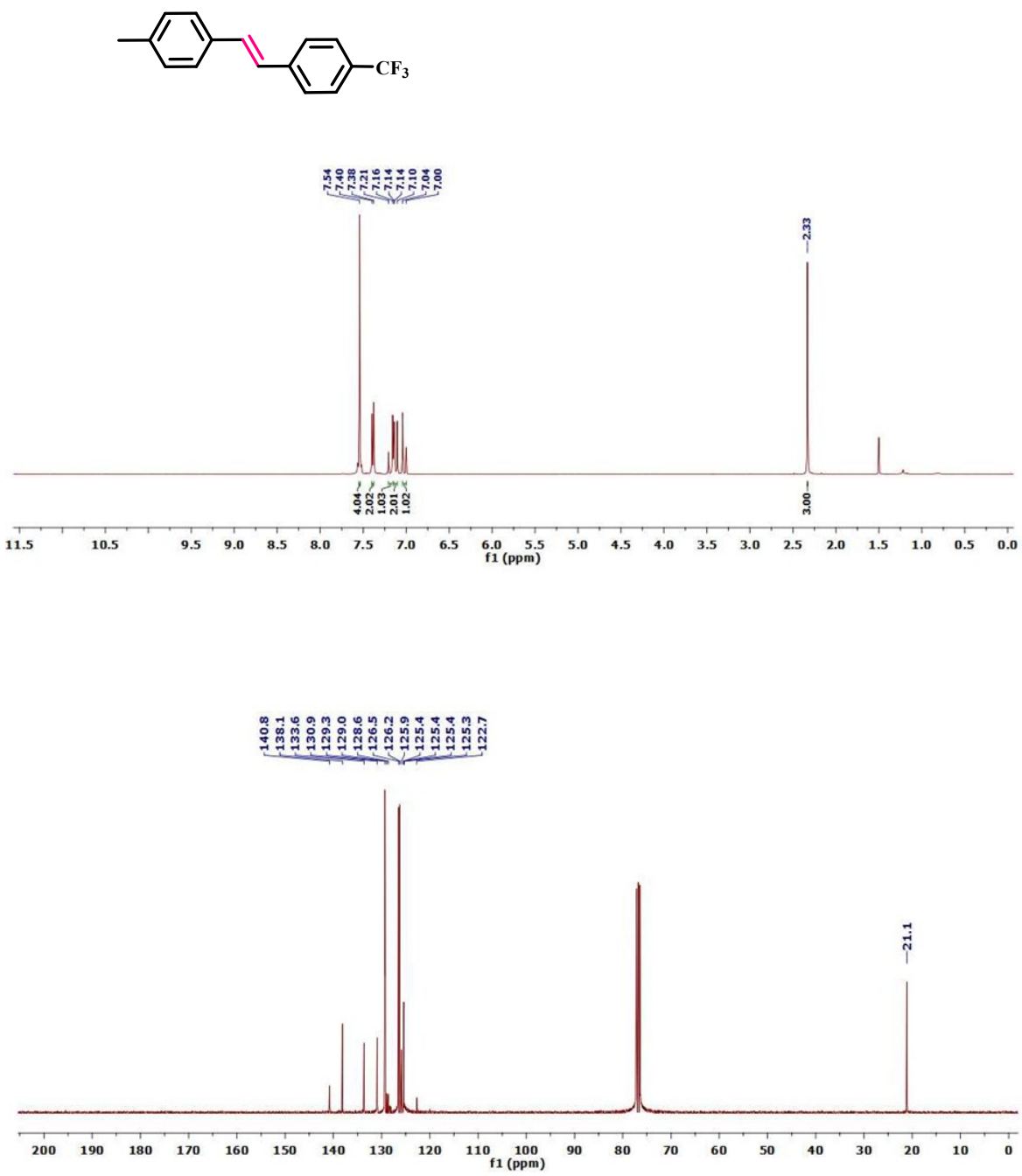
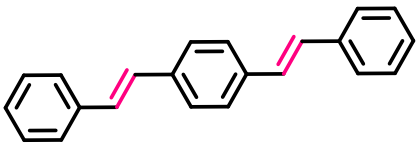
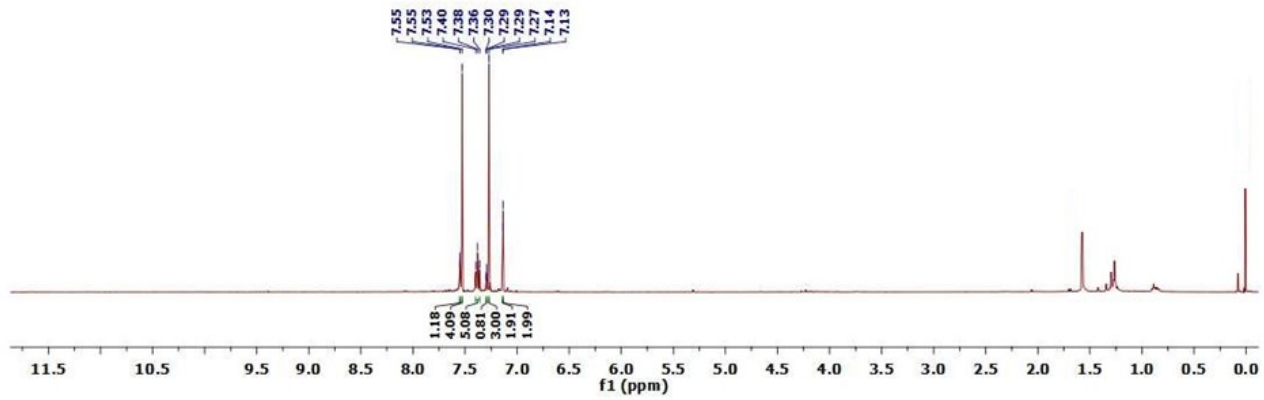


Figure S18: ^{1}H & $^{13}C\{^{1}H\}$–NMR Spectrum (400 MHz & 101 MHz, $CDCl_3$) of Compound 2t





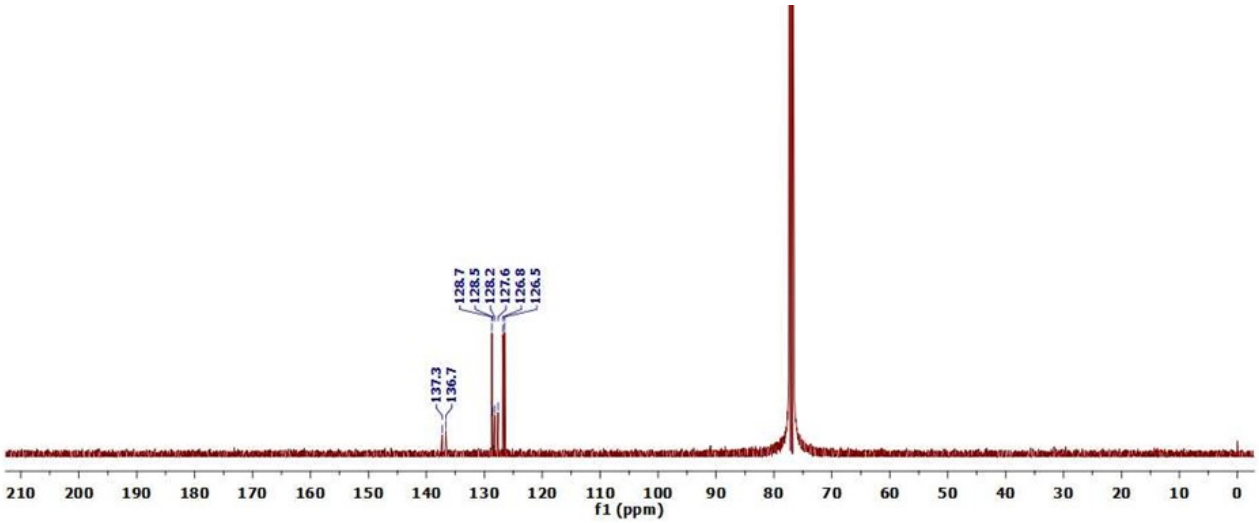


Figure S19: ^{1}H & $^{13}C\{^{1}H\}$–NMR Spectrum (400 MHz & 101 MHz, $CDCl_3$) of Compound 2u

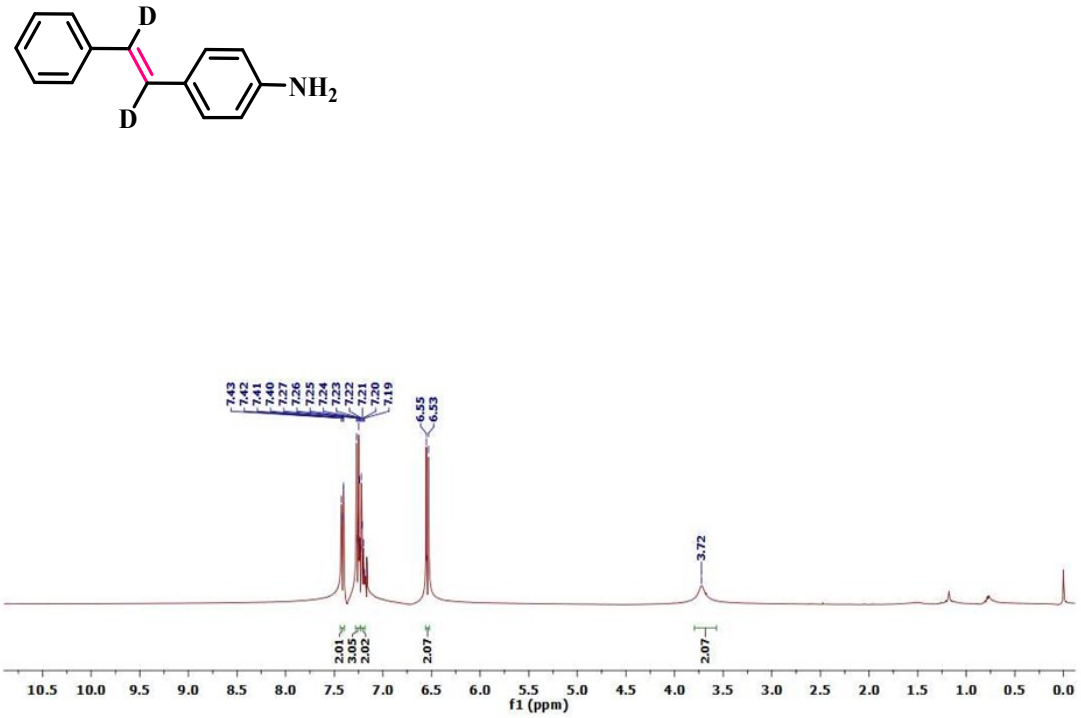
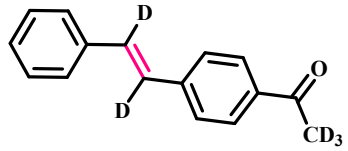


Figure S20: ^{1}H & $^{13}C\{^{1}H\}$–NMR Spectrum (400 MHz & 101 MHz, $CDCl_3$) of Compound 3b-*d*



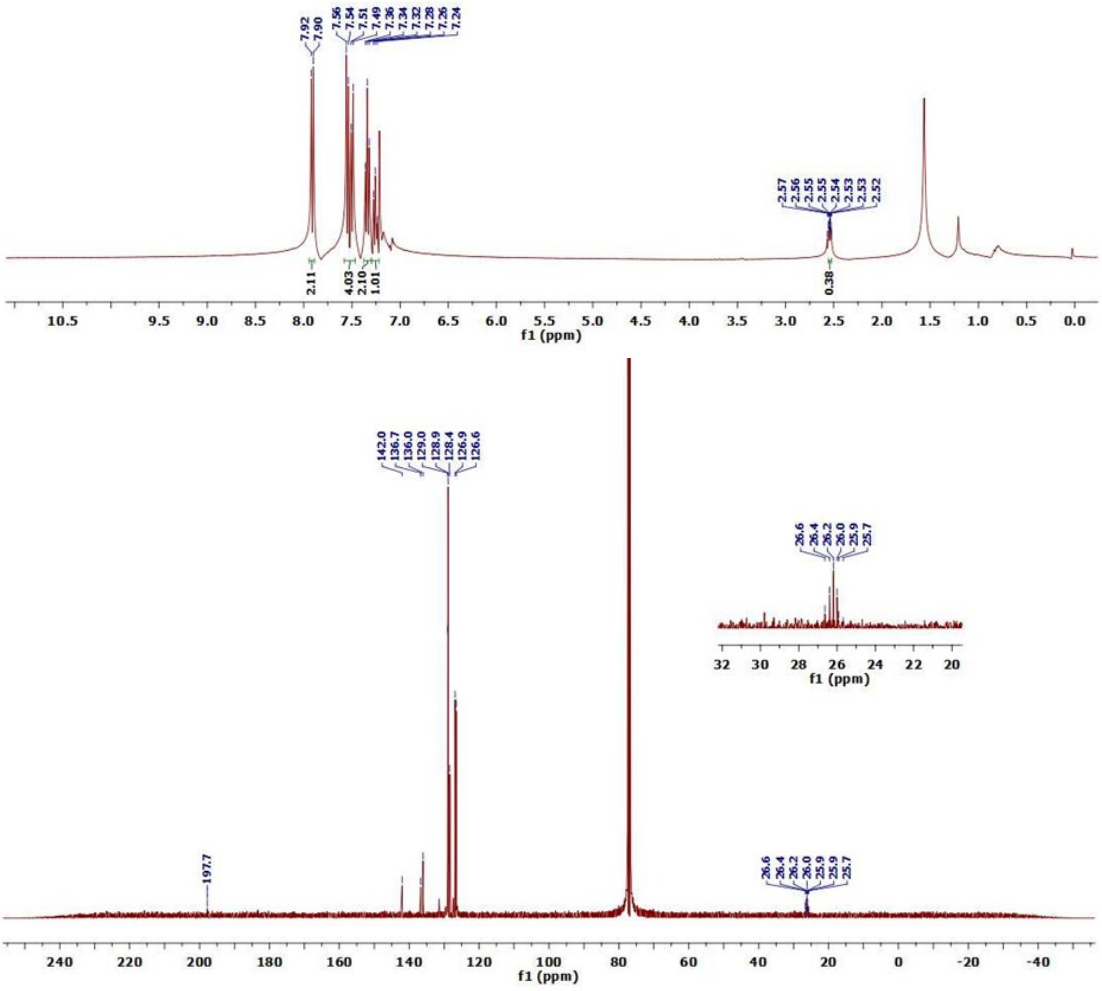
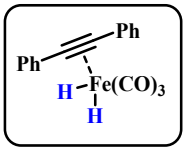


Figure S21: ^{1}H & $^{13}C\{^{1}H\}$–NMR Spectrum (400 MHz & 101 MHz, $CDCl_3$) of Compound 3c-*d*

8. Copies of HRMS spectra to support mechanism



Calc. $(M+H)^+$ = 321.0214
Obs. $(M+H)^+$ = 321.0216

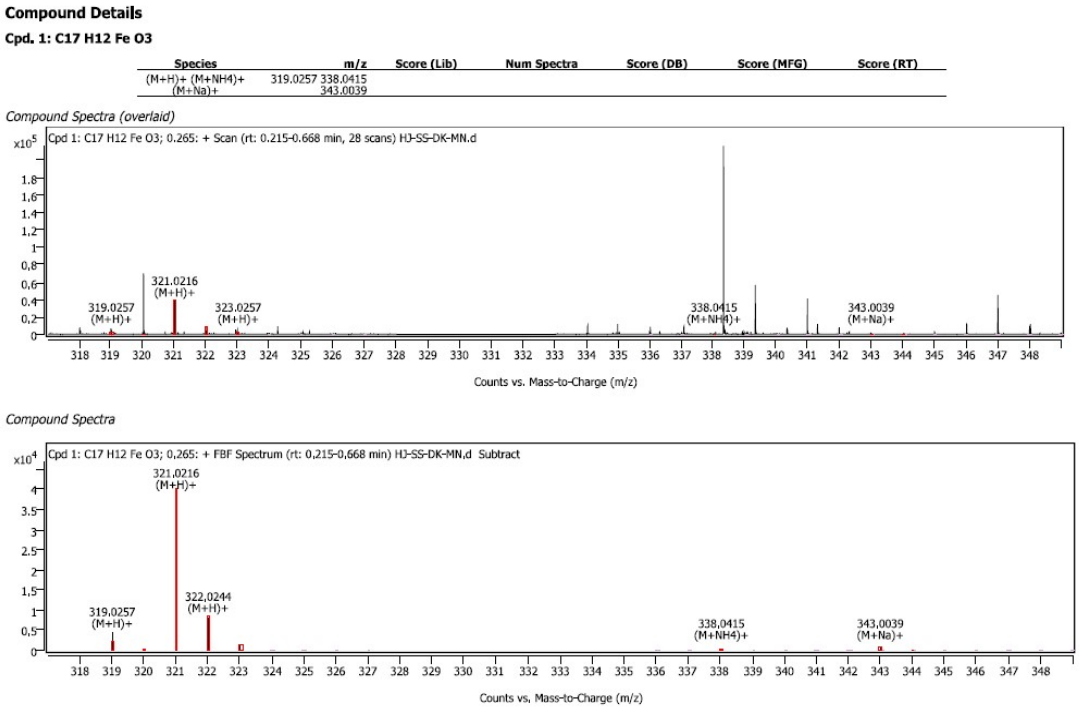
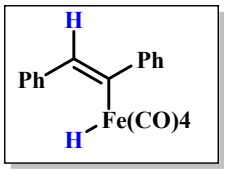


Figure S22: HRMS of intermediate D



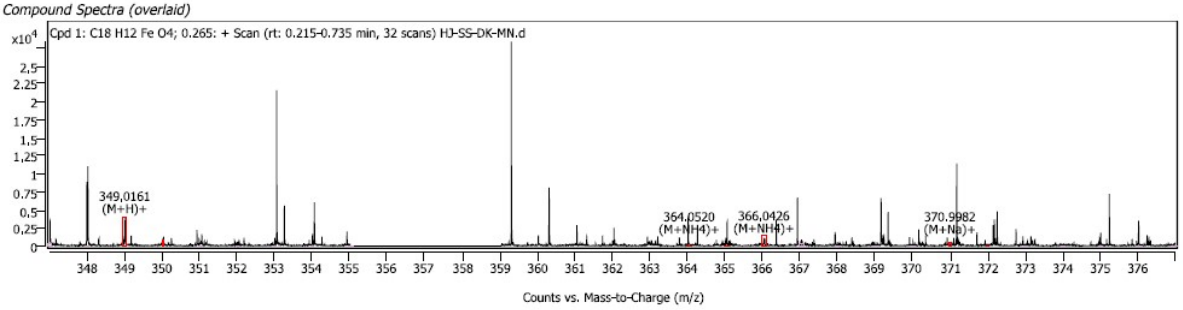
Calc. $(M+H)^+$ = 349.0163
Obs. $(M+H)^+$ = 349.0161

Compound Details

Cpd. 1: C18 H12 Fe O4

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Score (MFG)	Score (RT)
(M+H)+ (M+NH4)+ (M+Na)+	349.0161 364.0520 370.9982					

Compound Spectra (overlaid)



Compound Spectra

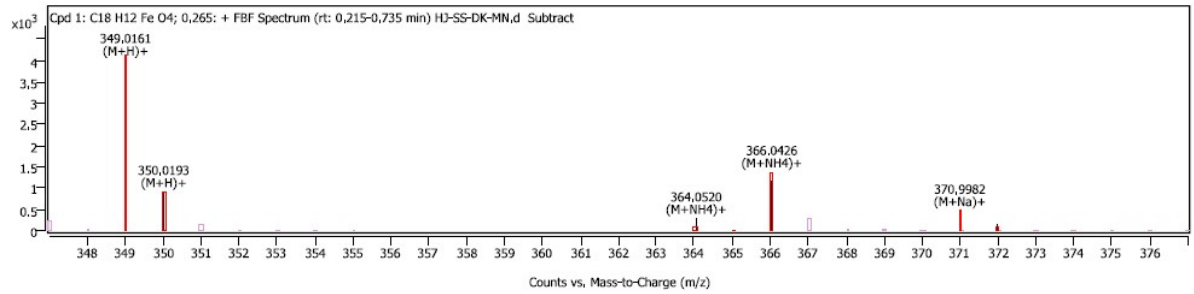
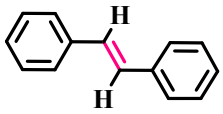


Figure S23: HRMS of intermediate E



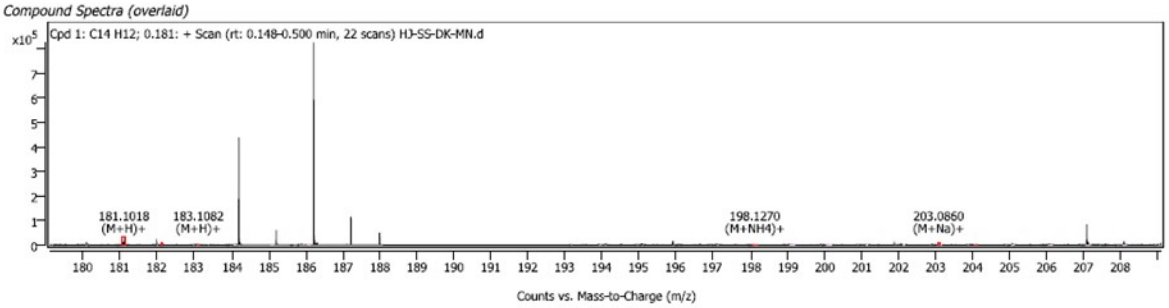
Calc. $(M+H)^+$ = 181.1017
Obs. $(M+H)^+$ = 181.1018

Compound Details

Cpd. 1: C14 H12

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Score (MFG)	Score (RT)
(M+H)+ (M+NH4)+ (M+Na)+	181.1018 198.1270 203.0860					

Compound Spectra (overlaid)



Compound Spectra

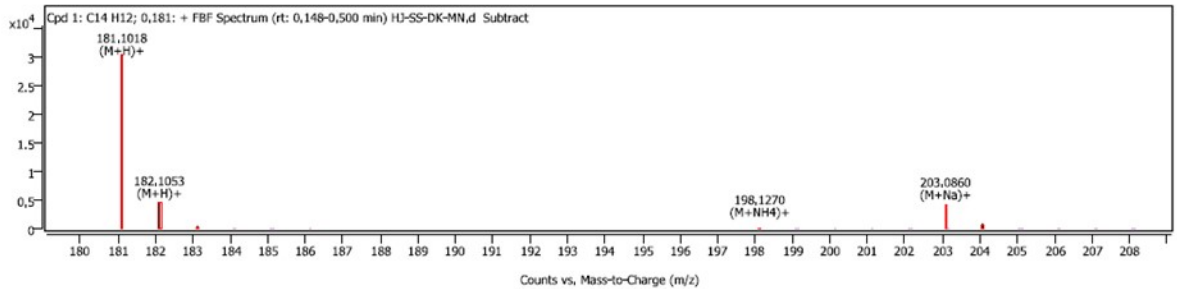


Figure S24: HRMS of intermediate product (*E*-stilbene)