Supporting Information

Ligand-modulated phosphine-free Ni(II) complexes for *Z*-selective semi-transfer hydrogenation of alkynes and dual transfer hydrogenation of α,β-unsaturated ketones using ammonia-borane

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1. General Consideration

1.1 Reagent Information: All the experiments were carried out under air. The Glass apparatus were oven-dried immediately before use. Solvents were dried according to the literature. HPLC-grade Methanol was used. All commercially available reagents were purchased from Sigma-Aldrich, Alfa-Aesar, TCI, SD-fine, Avra, and Spectrochem. Silica gel was used for column chromatography unless otherwise stated. A gradient elution using hexane/ethyl acetate was performed, based on a silica TLC plate.

1.2 Analytical Information: ^{1}H and ^{13}C spectra were recorded on JEOL 400 MHz, and 500 MHz Spectrometer using $CDCl_3$, DMSO-d_6, and CD_3OD. All ^{1}H NMR experiments were reported in parts per million (ppm) units and were measured relative to the signals for residual chloroform (7.26 ppm), residual DMSO (2.5 ppm), and CD_3OD (3.31) in the deuterated solvent, unless otherwise stated and coupling constant (J) was reported in hertz (Hz). All ^{1}H decoupled ^{13}C NMR spectra were reported in ppm relative to deuterated chloroform (77.16 ppm), and DMSO-d_6 (39.5). All the GC analyses were performed using Perkin Elmer Clarus 600 Gas Chromatograph and GC-MS were taken using Agilent 7890A Gas Chromatograph equipped with Agilent 5890 triple-quadrupole mass system.

2. Synthesis of Alkynes Derivatives:[1]

The corresponding aryl iodide (1 equiv), $Pd(PPh_3)_4$ (5 mol%), CuI (1-2 mol%), and phenylacetylene (1-1.1 equiv) were added to a 50 mL Schlenk flask with a stir bar under an atmosphere of nitrogen. Then tetrahydrofuran (10 mL) and triethylamine (10 mL) were added sequentially. The reaction mixture was then stirred at room temperature overnight. Afterward, 15 mL of water was added and the reaction mixture was extracted with EtOAc (3 × 15 mL). The combined organic fractions were washed with brine and dried over Na_2SO_4. After filtration, the solvent was removed under reduced pressure. The residue was purified by silica gel column chromatography using petroleum ether and ethyl acetate as the eluent. All the substrates were characterized by GC-MS analysis and ^{1}H NMR spectroscopy.

3. Synthesis of α,β-Unsaturated Ketone Derivatives:[2]

An oven-dried 25 mL round bottom flask (RB) was charged with a magnetic stir-bar, aryl ketone derivative (1.0 mmol), and aldehyde derivative (1.0 mmol), followed by the addition of ethanol (5.0 mL). Then 10% aqueous solution of NaOH (1.5 equiv.) was added dropwise in the stirring solution under ice-cold conditions. The stirring was continued for 5 h. After completion of the reaction, the reaction mixture was cooled in the refrigerator overnight and a yellowish-white precipitate was obtained. Then the precipitate was collected through filtration and washed with an ice-cold water-ethanol mixture until the pH of the filtrate becomes 7. Finally, the desired α, β-unsaturated ketone was purified through column chromatography (silica gel) using hexane-ethyl acetate as eluent. All the substrates were characterized by GC-MS analysis and ^{1}H NMR spectroscopy.

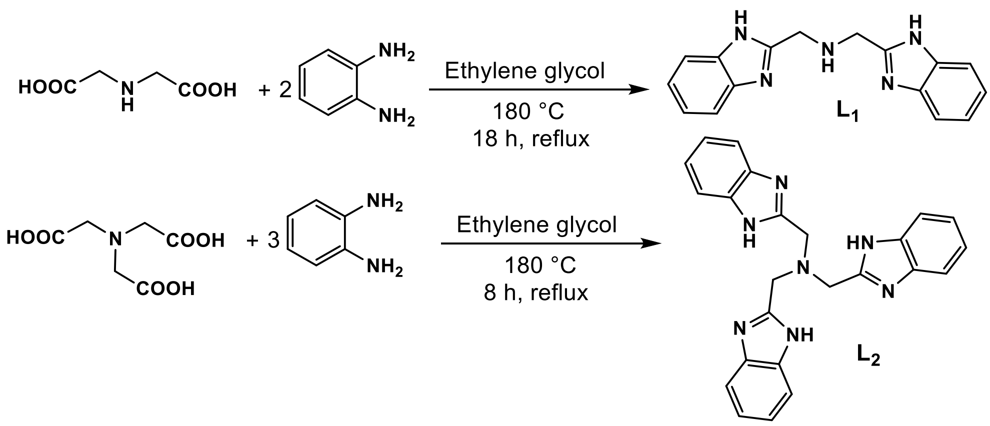
4. Optimization for Transfer Hydrogenation of Alkynes:

An oven-dried 4 mL screw cap vial was taken and charged with a magnetic stir-bar, alkyne **1a** (35.64 mg, 0.20 mmol), Cat. **4** (5 mol%), and AB (9.2 mg, 0.3 mmol), followed by the addition of methanol (1 mL). Then, the vial was sealed and placed in a preheated oil bath at 55 °C (oil bath temperature) for 12 h. After completion of the reaction, the tube was allowed to cool at room temperature. Then, the 25 μL reaction mixture was syringed out and filtered through a small plug of silica and subjected to GC analysis using mesitylene as an internal standard to determine the conversion and yield of the product.

5. Optimization for Dual Transfer Hydrogenation of Chalcones:

An oven-dried 4 mL screw cap vial was taken and charged with a magnetic stir-bar, chalcone **22a** (41.6 mg, 0.20 mmol), Cat. **1** (3 mol%), and AB (2 equiv), followed by the addition of methanol (1 mL). Then, the tube was sealed and placed in a preheated oil bath at 40 °C (oil bath temperature) for 3 h. After completion of the reaction, the tube was allowed to cool at room temperature. Then, the reaction mixture was subjected to ^{1}H NMR analysis using 1,3,5-trimethoxybenzene as an internal standard to determine the conversion and yield of the product.

6. Experimental Section



Scheme S1 Synthesis of ligands

Synthesis of ligand bis((1H-benzoimidazol-2-yl)methyl)amine (L_1)

The ligand (L_1 = bis(2-benzimidazolylmethyl)amine) was synthesized after slightly modifying the literature methods.[3] Aminodiacetic acid (0.665 g, 5 mmol) and *o*-phenylenediamine (1.081 g, 10 mmol) were refluxed in 30 mL ethylene glycol at 180 °C for 18 h. After cooling down to room temperature, a reddish crude product was obtained by adding water. Yield 0.915 g (66%). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.26 (s, 2H), 7.51 (s, 4H), 7.14 (dd, J = 6.0, 3.1 Hz, 4H), 4.00 (s, 4H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 154.5, 139.2, 122.0, 115.3, 47.0. ESI-MS (positive ion mode, CH_3OH) calcd *m/z*: 278.1406; found at *m/z*, 278.1402, which are assigned as $[L_1H]^+$.

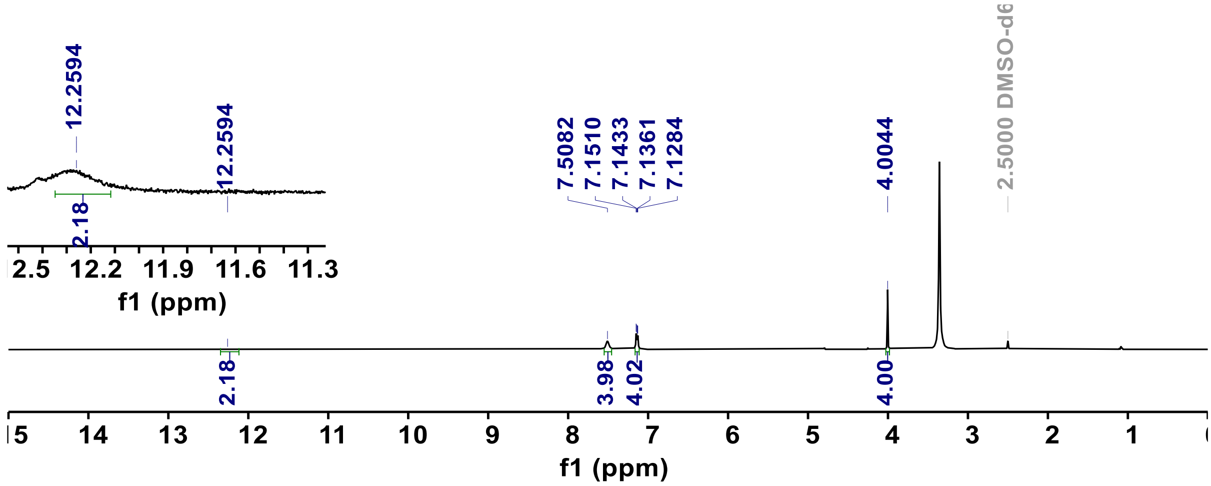


Fig. S1 ^{1}H NMR spectrum (400 MHz, DMSO-d^6) of ligand $\mathbf{L_1}$.

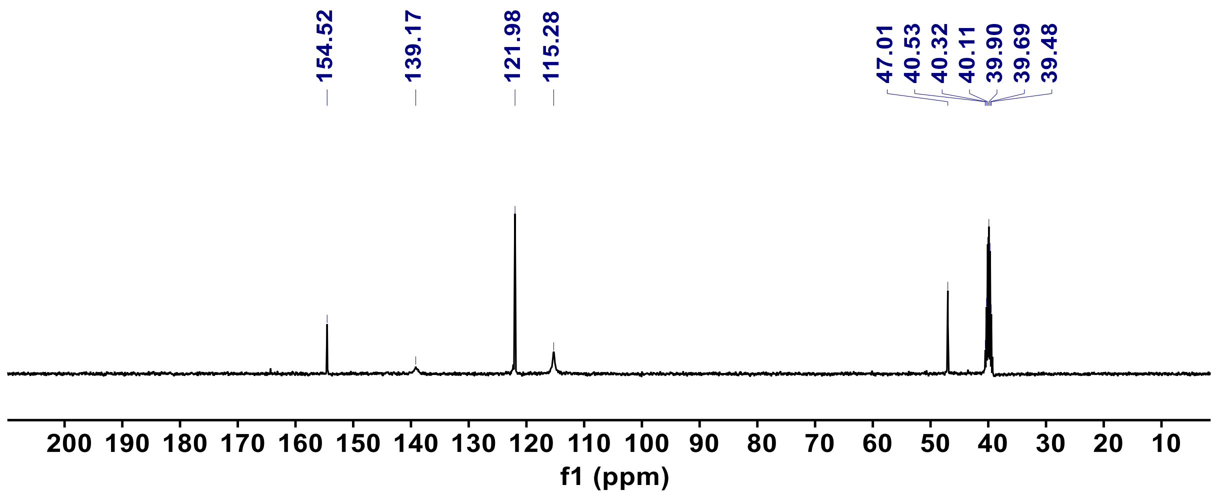


Fig. S2 ^{13}C NMR spectrum (100 MHz, DMSO-d_6) of ligand $\mathbf{L_1}$.

Synthesis of ligand tris((1H-benzoimidazol-2-yl)methyl)amine (L_2)

The ligand (L_2 = tris(2-benzimidazolylmethyl)amine) was synthesized following the methods reported earlier.[4] Aminotriacetic acid (0.9557 g, 5 mmol) and *o*-phenylenediamine (1.622 g, 15 mmol) were refluxed in 30 mL ethylene glycol at 180 °C for 8 h. After cooling down to room temperature, a reddish crude product was obtained by adding water. Colorless crystals of the ligand were obtained upon recrystallization from ethanol. Yield 1.46 g (72%). ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.46 (s, 3H), 7.56 (s, 6H), 7.20–7.14 (m, 6H), 4.14 (s, 6H).^{13}C NMR (100 MHz, DMSO-d_6) δ 152.3, 121.7, 51.5, 40.1, 39.9, 39.7, 39.5, 39.3, 39.1, 38.9. ESI-MS (positive ion mode, CH_3OH) calcd *m*/*z*: 408.1937; found at *m*/*z*, 408.1934, which are assigned as $[L_2H]^+$.

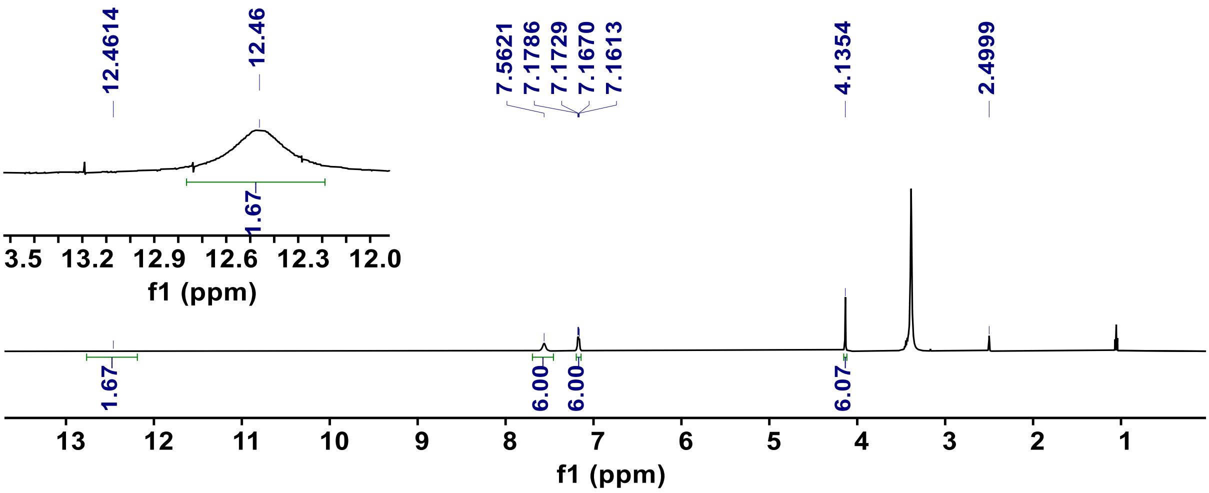


Fig. S3 ^{1}H NMR spectrum (500 MHz, DMSO-d_6) of ligand $\mathbf{L_2}$.

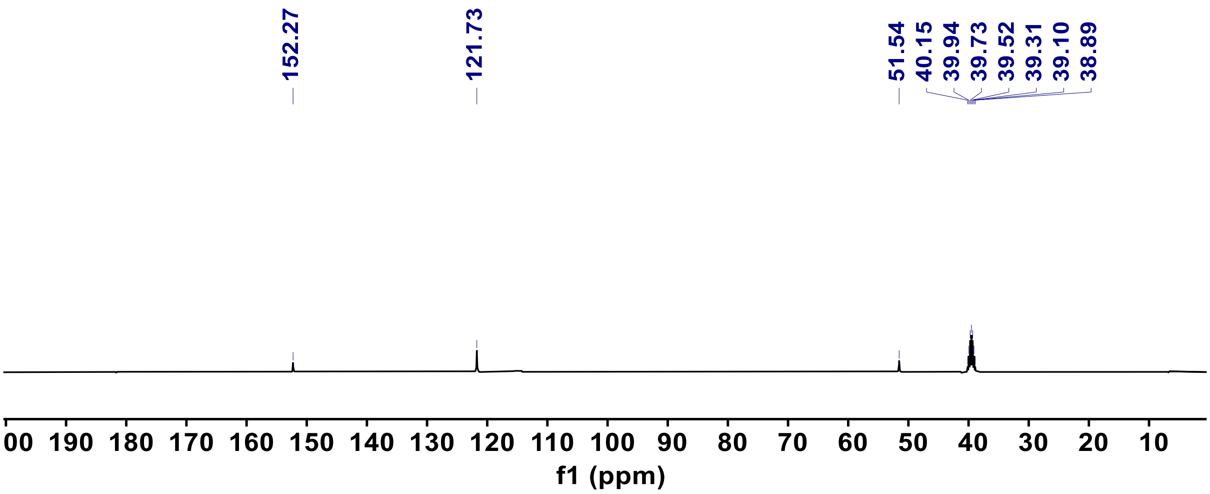


Fig. S4 ^{13}C NMR spectrum (100 MHz, DMSO-d_6) of ligand $\mathbf{L_2}$.

Synthesis of complex [NiL$_1$Br]Br (Cat. **1)**

An acetonitrile solution of ligand L$_1$ (0.277 g, 1 mmol) was added to the solution (10 mL) of NiBr$_2$ (0.218 g, 1 mmol) with constant stirring. A red-colored compound was obtained after removing the solvent under reduced pressure.

Cat. **1** Yield 0.382 g (77%) $C_{16}H_{15}Br_2N_5Ni_1$ (495.83). Calculated C, 38.76; H, 3.05; N, 14.12; Found C, 38.63; H, 2.94; N, 14.21. ESI-MS (positive ion mode, CH_3OH) calcd *m*/*z*: 415.98; found at *m*/*z*, 415.98, which are assigned as $[NiL_1Br]^+$.

Light green colored single crystals for X-ray diffraction were obtained by slow diffusion of diethyl ether into the DMF solution.

Synthesis of complexes and [NiBrL$_2$CH$_3$CN][NiL$_2$(CH$_3$CN)$_2$]Br$_3$ (Cat. **2)**

Complex Cat. **2** was synthesized following the same procedure as Cat. **1**, using ligand **L$_2$** (0.408 g, 1 mmol) instead of **L$_1$**. Blue crystals were obtained after slowly evaporating the solvent.

Cat. **2**. Yield 0.508 g (74%) $C_{54}H_{51}Br_4N_{17}Ni_2$ (1375.12). Calculated C, 47.17; H, 3.74; N, 17.32; Found C, 47.08; H, 3.67; N, 17.41; IR (cm^{-1}): $\nu_{(C\equiv N)}$ = 2306, 2282. ESI-MS (positive ion mode, CH_3OH) calcd *m*/*z*: 546.03; found at *m*/*z*, 546.03, which are assigned as $[NiL_2Br]^+$.

Synthesis of complexes [NiL$_2$(CH$_3$CN)$_2$]$_2$PF$_6$ (Cat. **3**) and **[NiL$_2$(CH$_3$CN)$_2$]$_2$BF$_4$** (Cat. **4**)

Both complexes Cat. **3** and Cat. **4** were prepared similarly by dissolving Cat. **2** (0.668 g, 1 mmol) in acetonitrile solution (20 mL) and then, aqueous solution of NH_4PF_6 (0.407 g, 2.5 mmol) for **3** and NH_4BF_4 (0.262 g, 2.5 mmol) for **4** was added to it. The resulting solution was filtered, and the filtrate was evaporated to obtain a light blue solid. Single crystals were obtained by diffusing Et_2O into a concentrated solution of Cat. **3** and Cat. **4** in CH_3CN. ESI-MS (positive ion mode, CH_3OH) calcd *m*/*z*: 232.56; found at *m*/*z*, 232.56, which are assigned as $[NiL_2]^{2+}$.

Cat. **3**. Yield 0.746 g (85%) $C_{30}H_{30}F_{12}N_{10}NiP_2$ (879.29). Calculated C, 40.98; H, 3.44; N, 15.93; Found C, 40.90; H, 3.31; N, 16.01; IR (cm^{-1}): $\nu_{(C\equiv N)}$ = 2309, 2280, $\nu_{(PF6)}$ = 832. ESI-MS (positive ion mode, CH_3OH) calcd *m*/*z*: 232.56; found at *m*/*z*, 232.56, which are assigned as $[NiL_2]^{2+}$.

Cat. **4**. Yield 0.679 g (87%) $C_{62}H_{63}B_4F_{16}N_{21}Ni_2$ (1566.93). Calculated C, 47.52; H, 4.05; N, 18.77; Found C, 47.63; H, 3.91; N, 18.63; IR (cm^{-1}): $\nu_{(C\equiv N)}$ = 2305, 2285, $\nu_{(BF4)}$ = 1046. ESI-

MS (positive ion mode, CH_3OH) calcd *m*/*z*: 232.56; found at *m*/*z*, 232.56, which are assigned as $[NiL_2]^{2+}$.

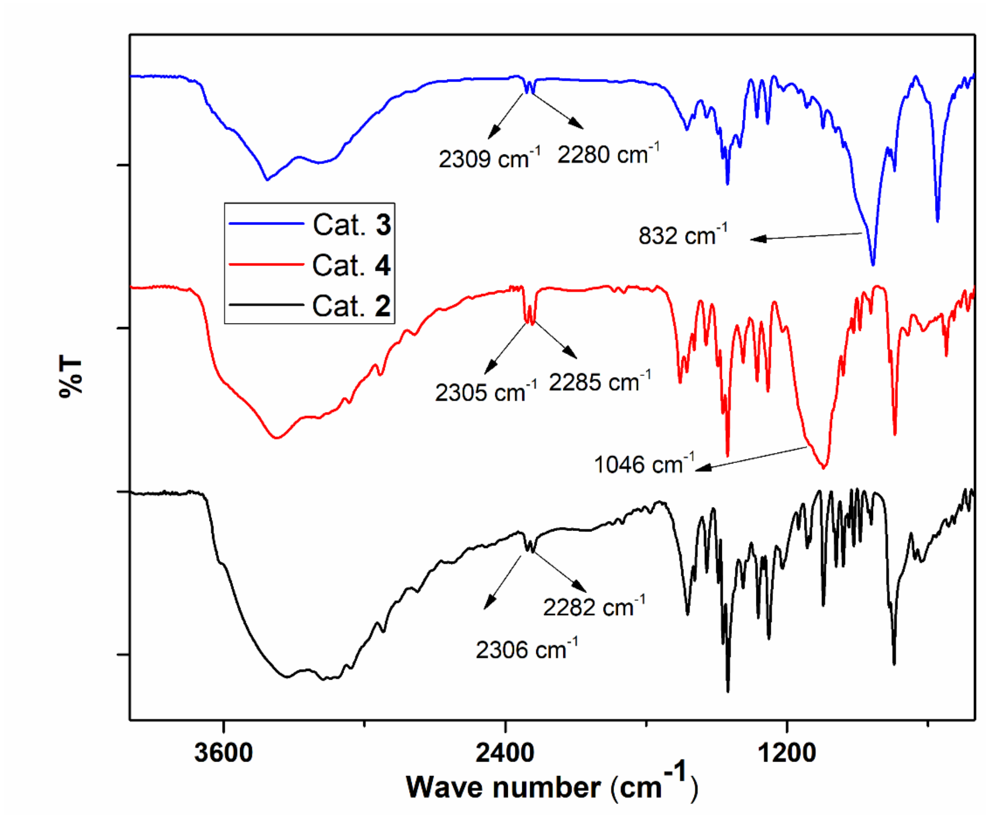


Fig. S5 IR spectra of complexes Cat. **2**–Cat. **4**.

Synthesis of complex $[CoBrL_2]_2Br_2$ (Cat. **5)** and **$[MnBrL_2]Br$** (Cat. **6**)[5]

Both complexes Cat. **5** and Cat. **6** were synthesized by following the same procedure as for Cat. **2**, using $CoBr_2$ (0.218 g, 1 mmol) and $MnBr_2$ (0.214 g, 1 mmol) instead of $NiBr_2$. The dark blue and white-colored compound was obtained after evaporating solvent for Cat. **5** and Cat. **6** respectively. Single crystals were obtained by diffusing Et_2O into a concentrated solution of Cat. **5** CH_3CN.

Cat. **5**. Yield 0.451 g (72%) $C_{24}H_{21}BrCoN_7$ (626.22). Calculated C, 46.03; H, 3.38; N, 15.66; Found C, 45.90; H, 3.21; N, 15.75; ESI-MS (positive ion mode, CH_3OH) calcd *m*/*z*: 547.03; found at *m*/*z*, 547.03, which are assigned as $[CoL_2Br]^{+}$.

Cat. **6**. Yield 0.746 g (75%) $C_{24}H_{21}BrMnN_7$ (622.23). Calculated C, 46.33; H, 3.40; N, 15.76; Found C, 46.22; H, 3.30; N, 15.70; ESI-MS (positive ion mode, CH_3OH) calcd *m*/*z*: 541.04; found at *m*/*z*, 541.04, which are assigned as $[MnL_2Br]^{+}$.

7. X-ray Crystallographic data collection and refinement

Suitable single crystals of complex Cat. **1**$(DMF)_2$–Cat. **5** was mounted on a Bruker-AXS SMART APEX II diffractometer equipped with a graphite monochromator and Mo-Kα (λ = 0.71073Å) radiation. The structure was solved by direct methods and refined by full-matrix least-squares on F^2 using the SHELXL2018/3 package and OLEX2 program.[6-8] Absorption corrections were carried out using the SADABS program.[9] All other hydrogen atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms. Successful convergence was indicated by the maximum shift/error of 0.001 for the last cycle of the least squares refinement. Data collection, structure refinement parameters, and crystallographic data for complexes Cat. **1**$(DMF)_2$–Cat. **5** is given in Table S1. The CCDC numbers of Cat. **1**$(DMF)_2$–Cat. **5** are 2400610-2400614.

Table S1 Crystallographic data and structure refinement of complexes Cat. **1**$(DMF)_2$–Cat. **5**

Complex	Cat. **1**$(DMF)_2$	Cat. **2**	Cat. **3**	Cat. **4**	Cat. **5**
Chemical formula	$C_{22}H_{31}Br_2N_7NiO_3$	$C_{54}H_{51}Br_4N_{17}Ni_2$	$C_{30}H_{30}F_{12}N_{10}P_2Ni_2$	$C_{124}H_{126}B_8F_{32}N_{41}Ni_4$	$C_{24}H_{21}Br_2CoN_7$
Formula weight	660.03	1375.10	879.29	3119.97	626.21
Crystal system	Monoclinic	Triclinic	Triclinic	Orthorhombic	Monoclinic
Space group	*P*21/*c*	$P\bar{1}$	$P\bar{1}$	*Fdd*2	*P*21/*c*
a(Å)	15.3924(4)	9.7261(4)	11.8948(6)	73.099(3)	14.0083(5)
b (Å)	9.4602(2)	15.9789(6)	13.3449(7)	19.0547(6)	24.0679(8)
c (Å)	18.6459(5)	19.4875(7)	13.5674(6)	19.8088(6)	17.5113(6)
α(°)	90	88.756(1)	85.767(2)	90	90
β (°)	91.876(1)	86.997(1)	66.498(2)	90	90.476(1)
γ(°)	90	81.808(1)	81.303(2)	90	90
V (Å)³	2713.67(12)	2993.3(2)	1952.04(17)	27591.3(17)	5903.7(4)
Z	4	2	2	8	8
ρ_{calc}(g cm^{-3})	1.615	1.526	1.496	1.502	1.409

T (K)	296	296	296	296	296
μ (Mo Kα) (mm^{-1})	3.696	3.349	0.673	0.646	3.311
F(000)	1336	1380	892	12776	2488
R(int)	0.042	0.043	0.051	0.062	0.062
Total reflections	45101	50926	52816	116287	98104
Unique reflections	6775	14541	9731	16061	14749
Reflections with I > 2σ(I)	5946	11371	8380	14088	11603
[I>2σ(I)]R_1^a, wR_2^b	0.0264, 0.0601	0.1022, 0.3211	0.0330, 0.0855	0.0688, 0.1798	0.0507, 0.1317
R(all data)	0.0330	0.1208	0.0403	0.0794	0.0658
GOF^{c}on F^2	1.05	1.09	1.03	1.06	1.01
Residual electron Density, e/Å^{-3}	-1.14, 0.76	-5.80, 5.43	-0.44, 0.41	-0.77, 1.95	-2.81, 1.29

$^aR_1 = \sum||F_o|-|F_c||/\sum|F_o|$, $^bwR_2\ (F_o^2) = \sum[w(F_o^2 - F_c^2)^2/\sum w\ F_o^4]^{½}$ and ^{c}GOF $= \sum[w(F_o^2 - F_c^2)^2/(N_{obs} - N_{params})]^{½}$

8. Description of the Structures

In Cat. **1**(DMF)$_2$, the metal atom is hexacoordinated with an octahedral environment. It is bonded to two benzimidazole nitrogen atoms (N2 and N4), one amine nitrogen atom N1, two oxygen atoms (O1 and O2) of solvent DMF molecules, and one non-coordinated bromine and one solvent water molecule. The structure of Cat. **1**(DMF)$_2$ is shown in Scheme 2 together with the selective atomic numbering scheme. The asymmetric unit of Cat. **2** contains two independent mononuclear Ni(II) units (A and B) and three bromine anions. The structure of Cat. **2** is shown in Scheme 2 (unit A) together with the selective atomic numbering scheme. The Ni(II) centers are six-coordinated with distorted octahedral geometry. The Ni1 atom is coordinated by three benzimidazole nitrogen atoms (N2A, N4A, and N6A), one amine nitrogen atom (N1A) from ligand **L$_2$**, one acetonitrile molecule, and one bromide ion in unit A. In contrast, unit B has a similar coordination environment, but an acetonitrile molecule is coordinated instead of a bromide ion. The structures of Cat. **3** and Cat. **4** shares the same basic framework as Cat. **2**, but with PF_6^- (in Cat. **3**) and BF_4^- (in Cat. **4**) anions replacing the Br^- anion (Scheme 2). In both complexes, the Ni(II) centers are six-coordinated, exhibiting a distorted octahedral geometry. The solid-state structure of Cat. **5** reveals that the asymmetric unit contains two independent cationic complexes (A and B) and two bromide ions that balance the charge. A perspective view of Cat. **5** together with the selective atomic numbering scheme is shown in Scheme 2 (unit A). Both units have an equivalent structure with slight bond length and angle differences. Co(II) center possesses a penta-coordinated distorted trigonal bipyramidal geometry ($\tau^5 \approx 0.94$) being coordinated by three benzimidazole nitrogen atoms (N2A, N4A, and N6A), one amine nitrogen atom (N1A) of the ligand (**L_2**) and one bromide ion (for unit A). Selected bond lengths and angles of Cat. **1**$(DMF)_2$–Cat. **5** are given in Table S2-S6.

Table S2 Selected bond lengths (Å) and angles (°) complex Cat. **1**$(DMF)_2$

Bond lengths (Å)	
Ni(1)–Br(1)	2.4990(4)
Ni(1)–O(1)	2.1201(13)
Ni(1)–O(2)	2.1100(13)
Ni(1)–N(1)	2.1145(16)
Ni(1)–N(2)	2.0561(15)
Ni(1)–N(4)	2.0733(15)
Bond angles (°)	
Br(1)–Ni(1)–O(1)	96.32(4)
Br(1)–Ni(1)–O(2)	97.58(4)
Br(1)–Ni(1)–N(1)	178.51(4)
Br(1)–Ni(1)–N(2)	100.03(5)
Br(1)–Ni(1)–N(4)	99.92(5)
O(1)–Ni(1)–O(2)	166.06(6)

O(1)−Ni(1)−N(1)	82.21(6)
O(1)−Ni(1)−N(2)	87.84(6)
O(1)−Ni(1)−N(4)	85.91(6)
O(2)−Ni(1)−N(1)	83.90(6)
O(2)−Ni(1)−N(2)	88.60(6)
O(2)−Ni(1)−N(4)	92.84(6)
N(1)−Ni(1)−N(2)	80.18(6)
N(1)−Ni(1)−N(4)	79.77(6)
N(2)−Ni(1)−N(4)	159.62(6)

Table S3 Selected bond lengths (Å) and angles (°) complex Cat. **2**

Bond lengths (Å)			
Ni(1)−Br(1A)	2.569(16)	Ni(2)−N(1B)	2.172(6)
Ni(1)−N(1A)	2.224(6)	Ni(2)−N(2B)	2.037(7)
Ni(1)−N(2A)	2.062(6)	Ni(2)−N(4B)	2.068(6)
Ni(1)−N(4A)	2.082(6)	Ni(2)−N(6B)	2.060(6)
Ni(1)−N(6A)	2.065(6)	Ni(2)−N(8B)	2.050(6)
Ni(1)−N(8A)	2.137(6)	Ni(2)−N(9B)	2.148(8)
Bond angles (°)			
N(1A)−Ni(1)−N(2A)	78.3(2)	N(1B)−Ni(2)−N(2B)	83.1(3)
N(1A)−Ni(1)−N(4A)	79.0(2)	N(1B)−Ni(2)−N(4B)	79.4(3)
N(1A)−Ni(1)−N(6A)	81.6(2)	N(1B)−Ni(2)−N(6B)	79.9(3)
N(1A)−Ni(1)−N(8A)	87.8(2)	N(1B)−Ni(2)−N(8B)	178.8(3)

N(2A)–Ni(1)–N(4A)	157.2(2)	N(1B)–Ni(2)–N(9B)	90.8(3)
N(2A)–Ni(1)–N(6A)	91.2(2)	N(2B)–Ni(2)–N(4B)	90.5(3)
N(2A)–Ni(1)–N(8A)	87.1(2)	N(2B)–Ni(2)–N(6B)	89.7(3)
N(4A)–Ni(1)–N(6A)	86.5(2)	N(2B)–Ni(2)–N(8B)	98.1(2)
N(4A)–Ni(1)–N(8A)	91.1(2)	N(2B)–Ni(2)–N(9B)	173.5(2)
N(6A)–Ni(1)–N(8A)	169.3(2)	N(4B)–Ni(2)–N(6B)	159.1(3)
Br(1A)–Ni(1)–N(1A)	175.9(3)	N(4B)–Ni(2)–N(8B)	100.8(2)
Br(1A)–Ni(1)–N(2A)	97.6(3)	N(4B)–Ni(2)–N(9B)	90.8(3)
Br(1A)–Ni(1)–N(4A)	105.2(3)	N(6B)–Ni(2)–N(8B)	99.9(2)
Br(1A)–Ni(1)–N(6A)	100.8(2)	N(6B)–Ni(2)–N(9B)	86.9(3)
Br(1A)–Ni(1)–N(8A)	92.2(4)	N(8B)–Ni(2)–N(9B)	88.0(2)

Table S4 Selected bond lengths (Å) and angles (°) complex Cat. **3**

Bond lengths (Å)	
Ni(1)–N(1)	2.1928(15)
Ni(1)–N(2)	2.0588(13)
Ni(1)–N(4)	2.0797(13)
Ni(1)–N(6)	2.0514(13)
Ni(1)–N(8)	2.0424(16)
Ni(1)–N(9)	2.1163(15)
Bond angles (°)	
N(1)–Ni(1)–N(2)	80.92(5)
N(1)–Ni(1)–N(4)	78.77(5)

N(1)−Ni(1)−N(6)	81.65(5)
N(1)−Ni(1)−N(8)	177.18(5)
N(1)−Ni(1)−N(9)	92.82(6)
N(2)−Ni(1)−N(4)	158.86(6)
N(2)−Ni(1)−N(6)	87.43(5)
N(2)−Ni(1)−N(8)	101.90(6)
N(2)−Ni(1)−N(9)	88.20(5)
N(4)−Ni(1)−N(6)	95.36(5)
N(4)−Ni(1)−N(8)	98.42(6)
N(4)−Ni(1)−N(9)	86.99(5)
N(6)−Ni(1)−N(8)	98.46(6)
N(6)−Ni(1)−N(9)	173.43(6)
N(8)−Ni(1)−N(9)	87.24(6)

Table S5 Selected bond lengths (Å) and angles (°) complex Cat. **4**

Bond lengths (Å)			
Ni(1)−N(1A)	2.180(5)	Ni(2)−N(1B)	2.192(5)
Ni(1)−N(2A)	2.064(6)	Ni(2)−N(2B)	2.080(6)
Ni(1)−N(4A)	2.059(6)	Ni(2)−N(4B)	2.037(6)
Ni(1)−N(6A)	2.050(6)	Ni(2)−N(6B)	2.070(6)
Ni(1)−N(8A)	2.047(6)	Ni(2)−N(8B)	2.063(6)
Ni(1)−N(9A)	2.130(6)	Ni(2)−N(9B)	2.133(6)
Bond angles (°)			

N(1A)−Ni(1)−N(2A)	80.7(2)	N(1B)−Ni(2)−N(2B)	78.2(2)
N(1A)−Ni(1)−N(4A)	78.6(2)	N(1B)−Ni(2)−N(4B)	81.6(2)
N(1A)−Ni(1)−N(6A)	82.5(2)	N(1B)−Ni(2)−N(6B)	81.2(2)
N(1A)−Ni(1)−N(8A)	178.5(2)	N(1B)−Ni(2)−N(8B)	177.7(2)
N(1A)−Ni(1)−N(9A)	92.1(2)	N(1B)−Ni(2)−N(9B)	93.7(2)
N(2A)−Ni(1)−N(4A)	158.8(2)	N(2B)−Ni(2)−N(4B)	92.7(2)
N(2A)−Ni(1)−N(6A)	90.4(2)	N(2B)−Ni(2)−N(6B)	158.5(2)
N(2A)−Ni(1)−N(8A)	100.8(2)	N(2B)−Ni(2)−N(8B)	100.4(2)
N(2A)−Ni(1)−N(9A)	90.1(2)	N(2B)−Ni(2)−N(9B)	86.9(2)
N(4A)−Ni(1)−N(6A)	91.0(2)	N(4B)−Ni(2)−N(6B)	90.4(2)
N(4A)−Ni(1)−N(8A)	100.0(2)	N(4B)−Ni(2)−N(8B)	96.6(2)
N(4A)−Ni(1)−N(9A)	86.4(2)	N(4B)−Ni(2)−N(9B)	175.2(2)
N(6A)−Ni(1)−N(8A)	97.7(2)	N(6B)−Ni(2)−N(8B)	100.3(2)
N(6A)−Ni(1)−N(9A)	174.4(2)	N(6B)−Ni(2)−N(9B)	88.2(2)
N(8A)−Ni(1)−N(9A)	87.7(2)	N(8B)−Ni(2)−N(9B)	88.2(2)

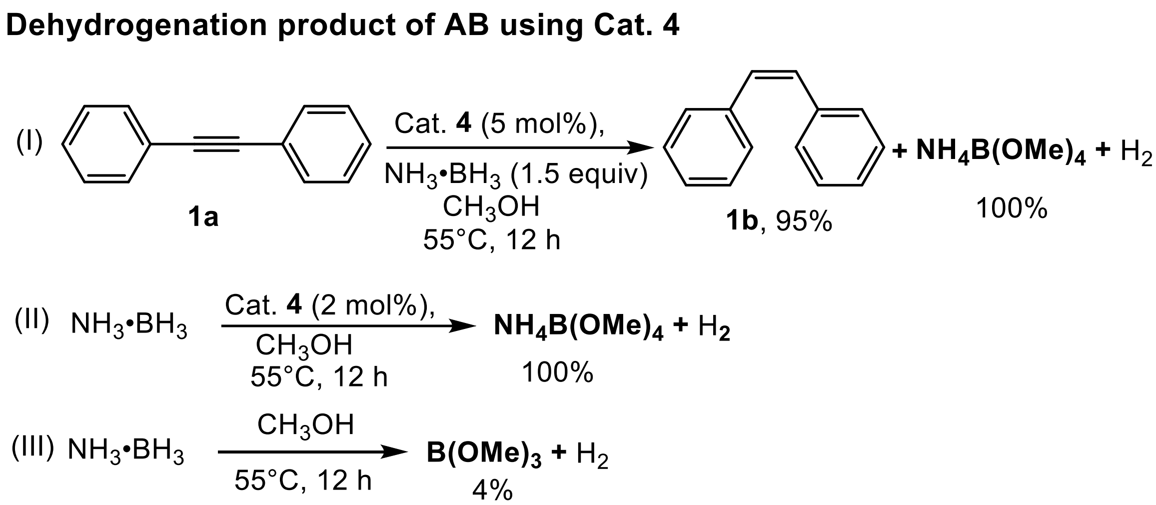
Table S6 Selected bond lengths (Å) and angles (°) complex Cat. **5**

Bond lengths (Å)			
Co(1)−N(1A)	2.339(3)	Co(2)−N(1B)	2.346(3)
Co(1)−Br(1A)	2.4451(6)	Co(2)−Br(1B)	2.4659(6)
Co(1)−N(2A)	2.054(3)	Co(2)−N(2B)	2.051(3)
Co(1)−N(4A)	2.061(3)	Co(2)−N(4B)	2.045(3)
Co(1)−N(6A)	2.047(3)	Co(2)−N(6B)	2.057(3)

Bond angles (°)			
Br(1A)−Co(1)−N(1A)	177.89(8)	Br(1B)−Co(2)−N(1B)	177.96(7)
Br(1A)−Co(1)−N(2A)	105.50(9)	Br(1B)−Co(2)−N(2B)	103.40(9)
Br(1A)−Co(1)−N(4A)	101.86(9)	Br(1B)−Co(2)−N(4B)	105.74(9)
Br(1A)−Co(1)−N(6A)	104.53(10)	Br(1B)−Co(2)−N(6B)	102.29(8)
N(1A)−Co(1)−N(2A)	75.73(11)	N(1B)−Co(2)−N(2B)	76.98(11)
N(1A)−Co(1)−N(4A)	76.04(12)	N(1B)−Co(2)−N(4B)	75.93(11)
N(1A)−Co(1)−N(6A)	76.61(12)	N(1B)−Co(2)−N(6B)	75.88(11)
N(2A)−Co(1)−N(4A)	115.03(12)	N(2B)−Co(2)−N(4B)	109.34(12)
N(2A)−Co(1)−N(6A)	106.71(13)	N(2B)−Co(2)−N(6B)	121.17(12)
N(4A)−Co(1)−N(6A)	121.43(12)	N(4B)−Co(2)−N(6B)	113.02(12)

9. Control Experiments

9.1 Determination of the dehydrogenation product of ammonia-borane



An oven-dried 4 mL screw cap vial was taken and charged with a magnetic stir-bar, alkyne **1a** (36.58 mg, 0.20 mmol), Cat. **4** (5 mol%), and AB (9.2 mg, 0.3 mmol), followed by the addition of methanol (1 mL). Then, the vial was sealed and placed in a preheated oil bath at 55 °C (oil bath temperature) for 12 h. After completion of the reaction, the tube was allowed to cool at room temperature. After this, the solvent was removed and dissolved in THF, then submitted for ^{11}B NMR which shows the complete conversion of AB into $NH_4(BOMe)_4$.

The above experiment was carried in the absence of **1a** and 100% of $NH_4(BOMe)_4$ was observed. When the experiment was carried out without Cat. **4** then only 4% of $B(OMe)_3$ was observed.

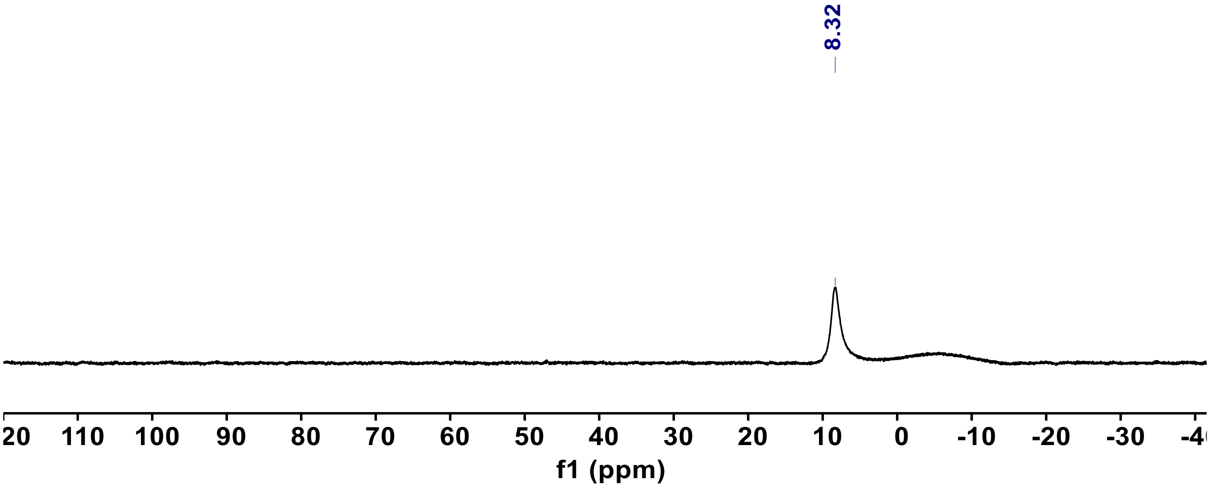


Fig. S6 ^{11}B NMR spectrum (in THF) of the reaction mixture

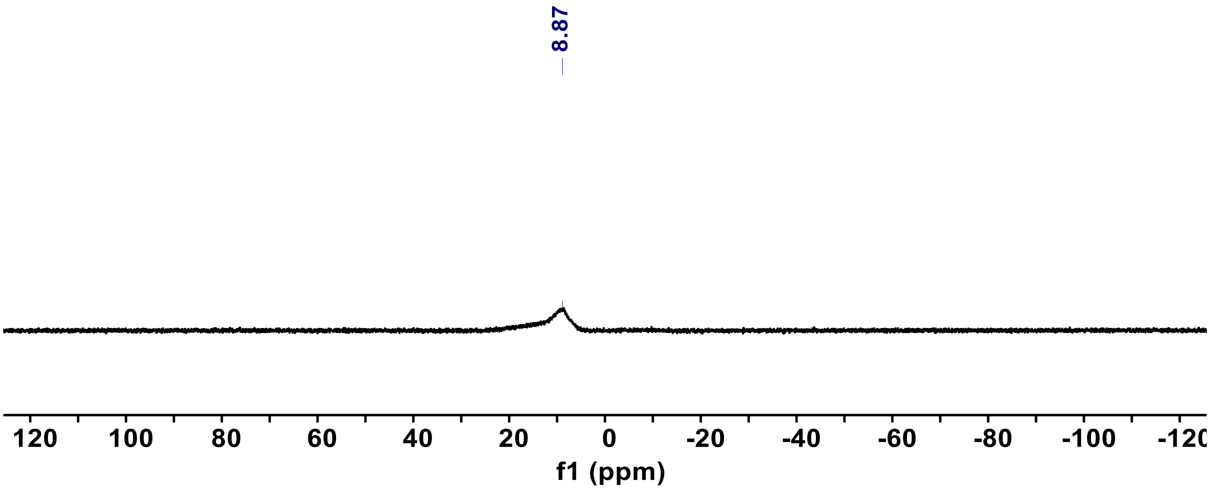


Fig. S7 ^{11}B NMR spectrum (in THF) in the absence of substrate

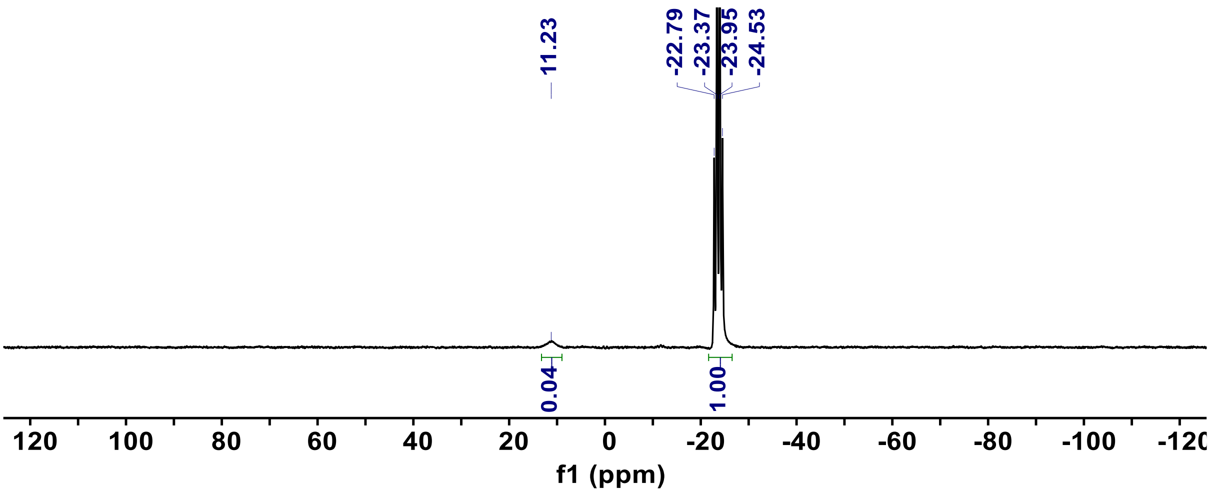
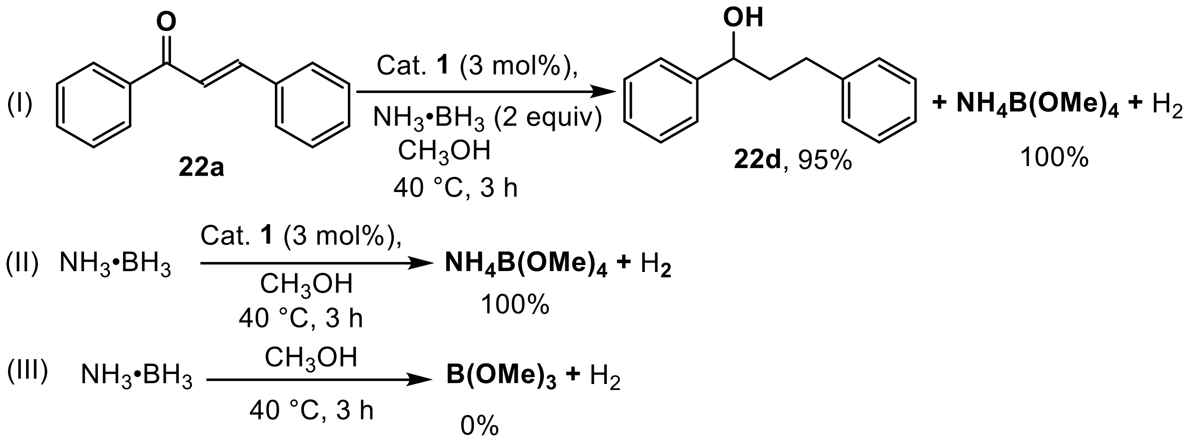


Fig. S8 ^{11}B NMR spectrum (in THF) under catalyst and substrate-free reaction condition

Dehydrogenation product of AB using Cat. 1



An oven-dried 4 mL screw cap vial was taken and charged with a magnetic stir-bar, alkyne **22a** (41.6 mg, 0.20 mmol), Cat. **1** (3 mol%), and AB (12.4 mg, 0.4 mmol), followed by the addition of methanol (1 mL). Then, the vial was sealed and placed in a preheated oil bath at 40 °C (oil bath temperature) for 3 h. After completion of the reaction, the tube was allowed to cool at room temperature. After this, the solvent was removed and dissolved in THF, then submitted for ^{11}B NMR which shows the complete conversion of AB into $NH_4(BOMe)_4$.

The above experiment was carried out under identical conditions in the absence of **22a** and 100% of $NH_4(BOMe)_4$ was observed. When the experiment was carried out without Cat. **1** then no conversion was observed.

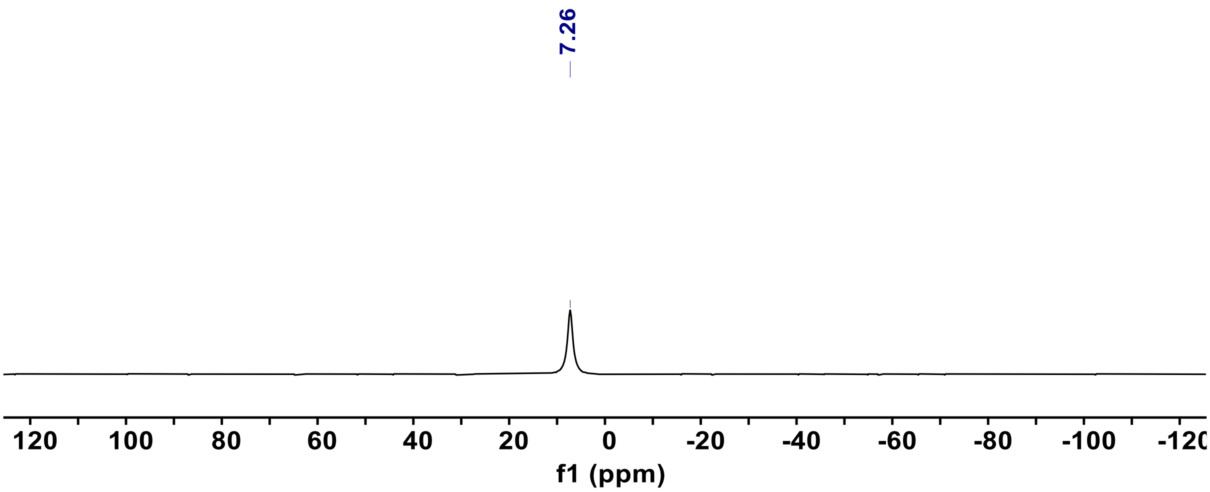


Fig. S9 ^{11}B NMR spectrum (in THF) of the reaction mixture

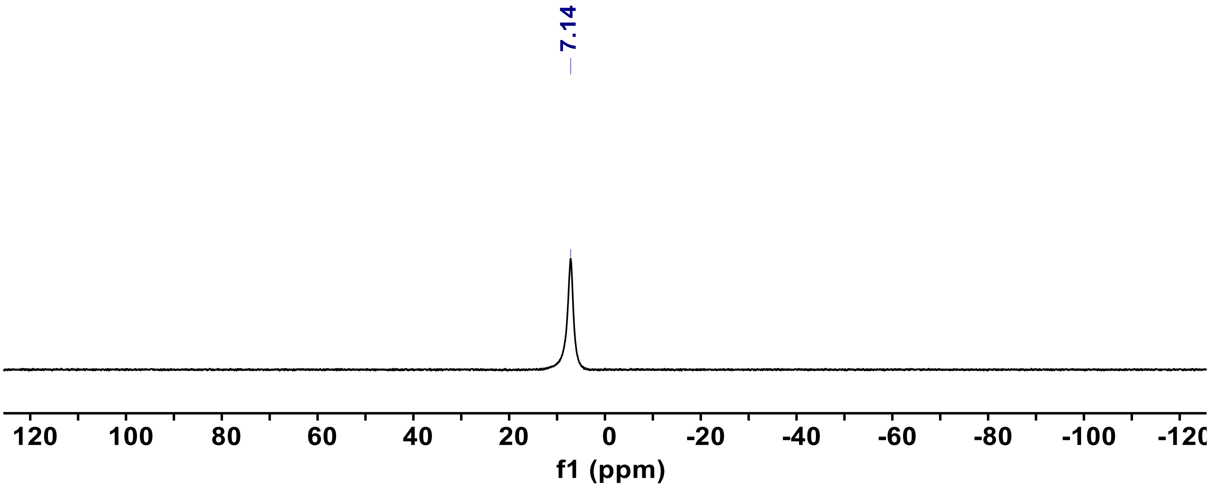


Fig. S10 ^{11}B NMR spectrum (in THF) in the absence of substrate

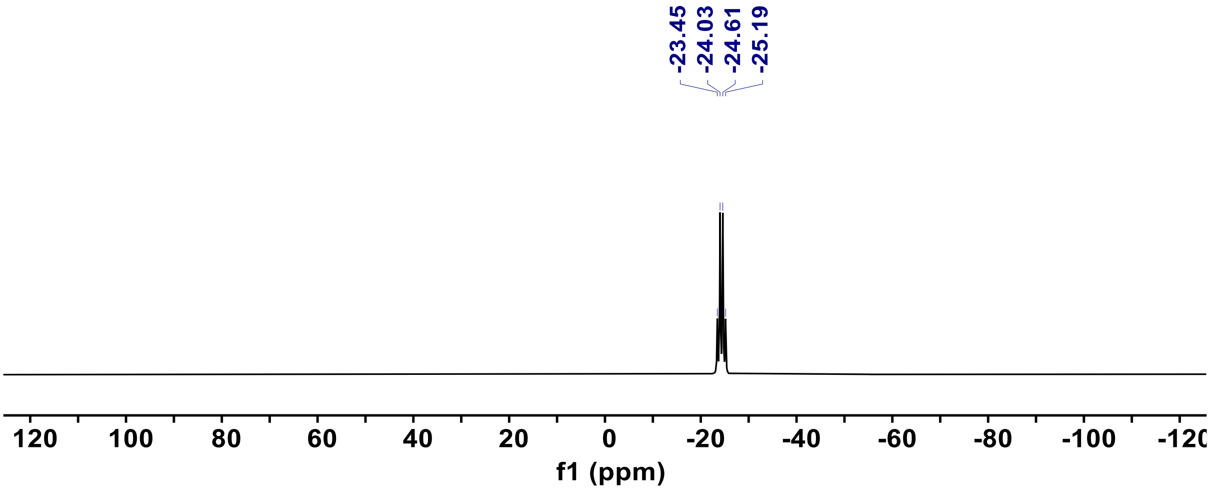


Fig. S11 ^{11}B NMR spectrum (in THF) under catalyst and substrate-free reaction condition

9.2 Procedure for Rate of Reaction (Electronic Effect).

An oven-dried 4 mL screw cap vial was taken and charged with a magnetic stir-bar, 1-methoxy-4-(phenylethynyl)benzene (**3a**, 48.4 mg, 0.2 mmol) or 1-(phenylethynyl)-4-

(trifluoromethyl)benzene (**4a**, 49.2 mg, 0.2 mmol), Cat. **4** (5 mol%), and AB (9.2 mg, 0.3 mmol), followed by the addition of methanol (1 mL). Then, the vial was sealed and placed in a preheated oil bath at 55 °C (oil bath temperature). The reaction vessel was taken at regular intervals (5, 10, 20, 30, and 40 min), and an aliquot of sample was withdrawn to the GC vial. The sample was diluted with MeOH and subjected to GC analysis. The data of the concentration of the product **3b** or **4b** versus time (min) plot was drawn (Figure S12) with Origin Pro 9.1, and the rate was determined by the initial rate method (up to 40 min). The initial rate obtained for the transfer hydrogenation of 1-methoxy-4(phenylethynyl)benzene (**3a**) was 9.48×10^{-4} $Mmin^{-1}$. Similarly, the rate for the transfer hydrogenation of 1-(phenylethynyl)-4-(trifluoromethyl)benzene (**4a**) was 8.06×10^{-4} $Mmin^{-1}$. Therefore, the rate (4-OMe)/ rate (4-CF_3) = $9.48\times10^{-4}/8.06\times10^{-4}$ = 1.18.

Table S7 Time-dependent formation of product **3b** or **4b** from **3a** and **4a**.

Time(min)	3b[M]	4b[M]
5	0.02538	0.01316
10	0.03054	0.01722
20	0.04084	0.02804
30	0.05004	0.0344
40	0.05842	0.04106

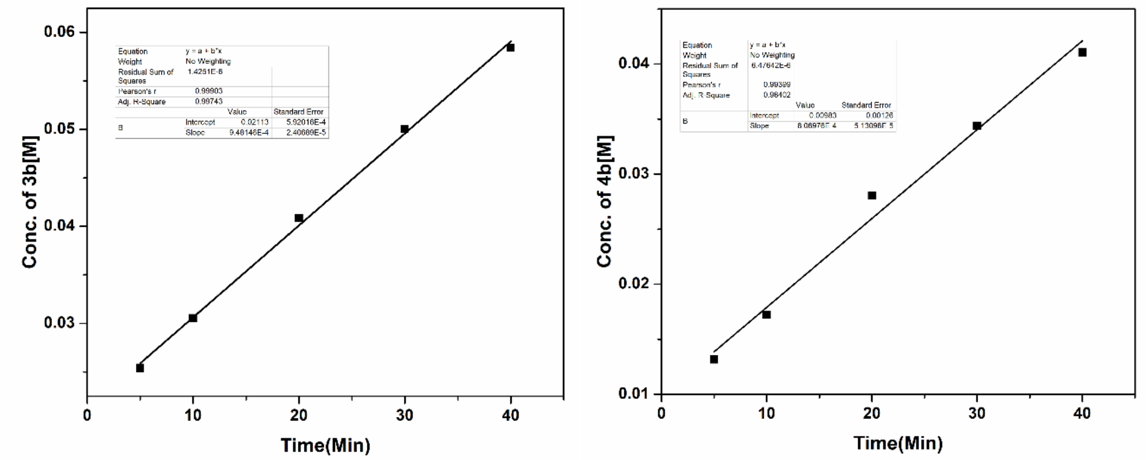
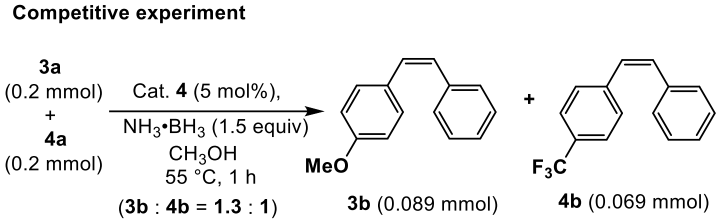


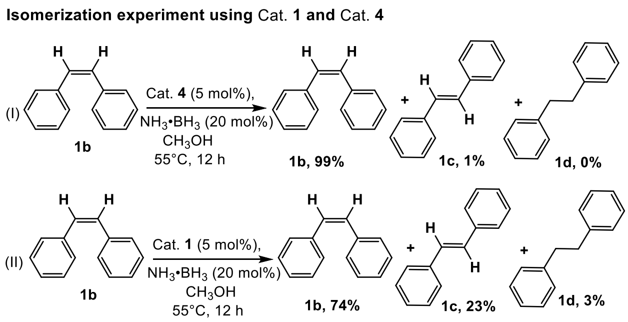
Fig. S12 Time-dependent formation of products **3b** and **4b**.

9.3 Procedure for Competition Experiment



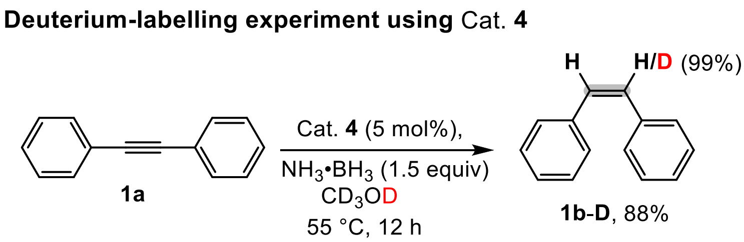
An oven-dried 4 mL screw cap vial was taken and charged with a magnetic stir-bar, 1-methoxy-4-(phenylethynyl)benzene (**3a**, 48.4 mg, 0.2 mmol) and 1-(phenylethynyl)-4-(trifluoromethyl)benzene (**4a**, 49.2 mg, 0.2 mmol), Cat. **4** (5 mol%), and AB (9.2 mg, 0.3 mmol), followed by the addition of methanol (1 mL). Then, the vial was sealed and placed in a preheated oil bath at 55 °C (oil bath temperature) for 1 h. The yields of alkenes (**3b** (0.0899 mmol) and **4b** (0.0689 mmol)) were determined by GC.

9.4 Isomerisation experiment



An oven-dried 4 mL screw cap vial was taken and charged with a magnetic stir-bar, 1-methoxy-(*Z*)-1,2-diphenylethene (**1a**, 36 mg, 0.2 mmol), Cat. **4** (5 mol%) or Cat. **1** (5 mol%), and AB (20 mol%), followed by the addition of methanol (1 mL). Then, the vial was sealed and placed in a preheated oil bath at 55 °C (oil bath temperature) for 12 h. Product yields were determined by GC.

9.5 Procedure for Deuterium Labelling Experiment.



An oven-dried 4 mL screw cap vial was taken and charged with a magnetic stir-bar, alkyne (**1a**, 89.0 mg, 0.5 mmol), Cat. **4** (5 mol%), and AB (23.1 mg, 0.75 mmol), followed by the addition of CD_3OD (2 mL). Then, the vial was sealed and placed in a preheated oil bath at 55 °C (oil bath temperature) for 12h. The crude reaction mixture was then purified by flash chromatography using petroleum ether as eluent to obtain deuterated Z-stilbene **1b-D** (79.2 mg, 86%). ^1H NMR (400 MHz, $CDCl_3$) δ 7.28–7.16 (m, 10H), 6.60 (s, 1H).

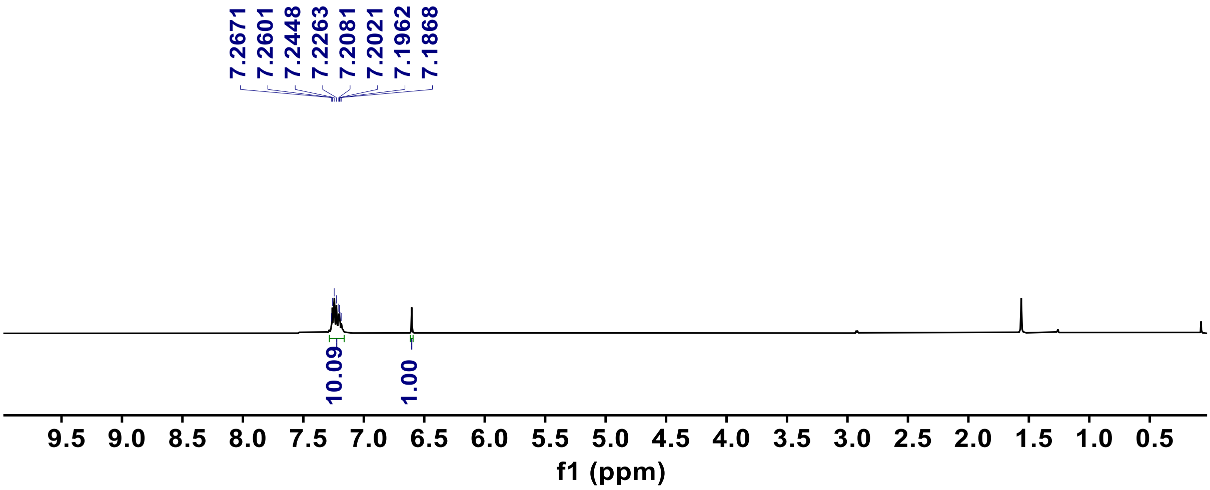
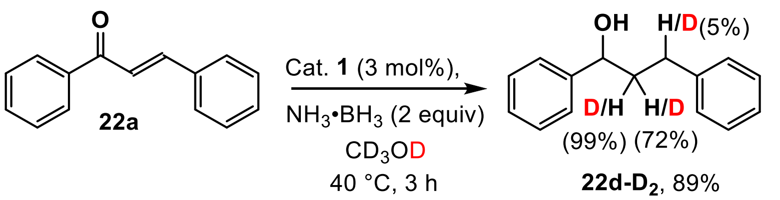


Fig. S13 ^1H NMR spectrum (in $CDCl_3$) for the reaction of alkyne and AB (1.5 equiv) in under standard reaction conditions.

Deuterium-labelling experiment using Cat. **1**



An oven-dried 4 mL screw cap vial was taken and charged with a magnetic stir-bar, chalcone **22a** (41.6 mg, 0.20 mmol), Cat. **1** (3 mol%), and AB (2 equiv), followed by the addition of CD_3OD (1 mL). Then, the tube was sealed and placed in a preheated oil bath at 40 °C (oil bath temperature) for 3 h. After completion of the reaction, the tube was allowed to cool at room temperature. Then, the reaction mixture was subjected to ^1H and ^2H NMR analysis.

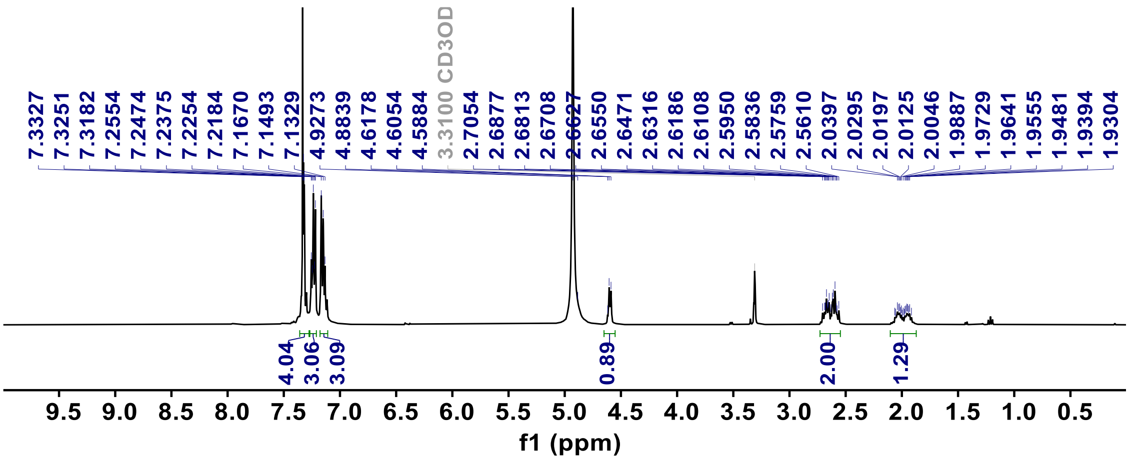


Fig. S14 ^{1}H NMR spectrum (in CD_3OD) for the reaction of chalcone and AB (2 equiv) in CD_3OD under standard reaction conditions.

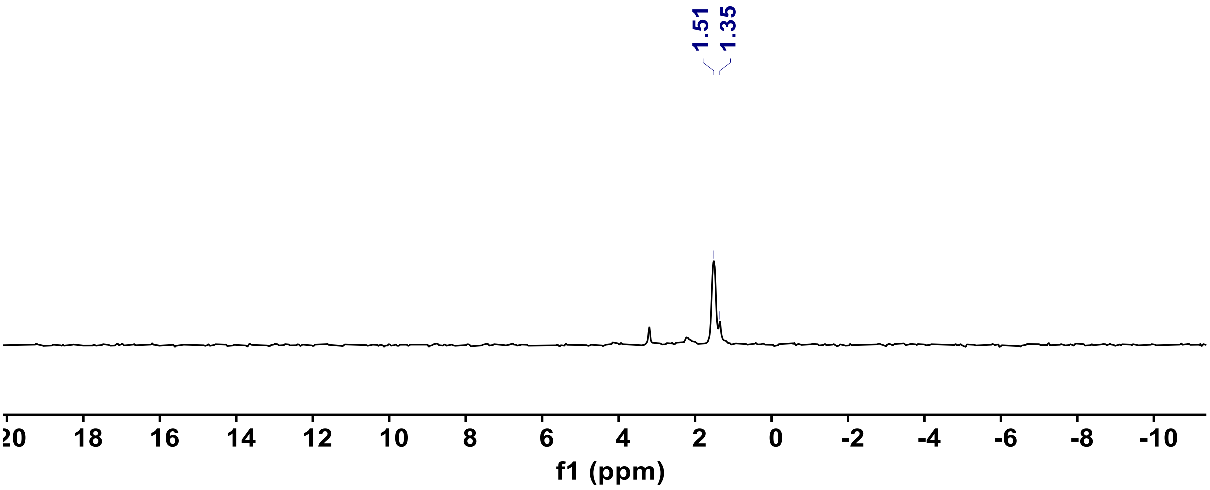
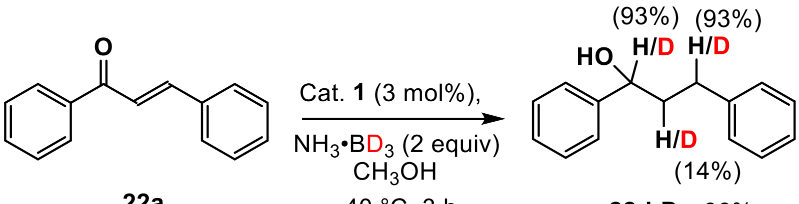


Fig. S15 ^{2}H NMR spectrum (in THF) for the reaction of chalcone and AB (2 equiv) under standard reaction conditions.



22a

22d-D2, 86%

An oven-dried 4 mL screw cap vial was taken and charged with a magnetic stir-bar, chalcone **22a** (41.6 mg, 0.20 mmol), Cat. **1** (3 mol%), and $NH_3•BD_3$ (2 equiv), followed by the addition of CH_3OH (1 mL). Then, the tube was sealed and placed in a preheated oil bath at 40 °C (oil bath temperature) for 3 h. After completion of the reaction, the tube was allowed to cool at room temperature. Then, the reaction mixture was subjected to ^{1}H and ^{2}H NMR analysis.

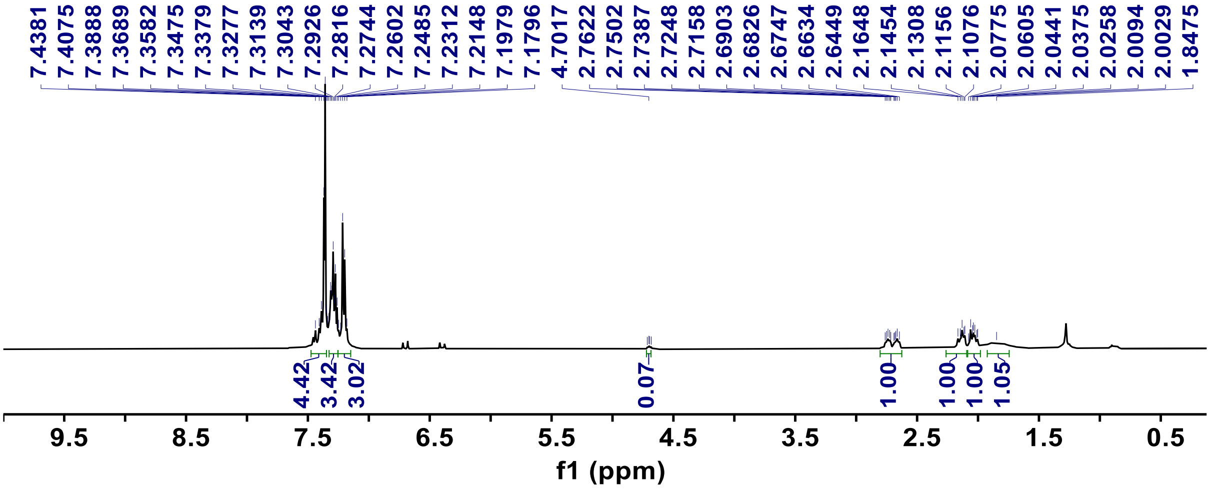


Fig. S16 ^{1}H NMR spectrum (in $CDCl_3$) for the reaction of chalcone and NH_3•BD_3 (2 equiv) in CH_3OH under standard reaction conditions.

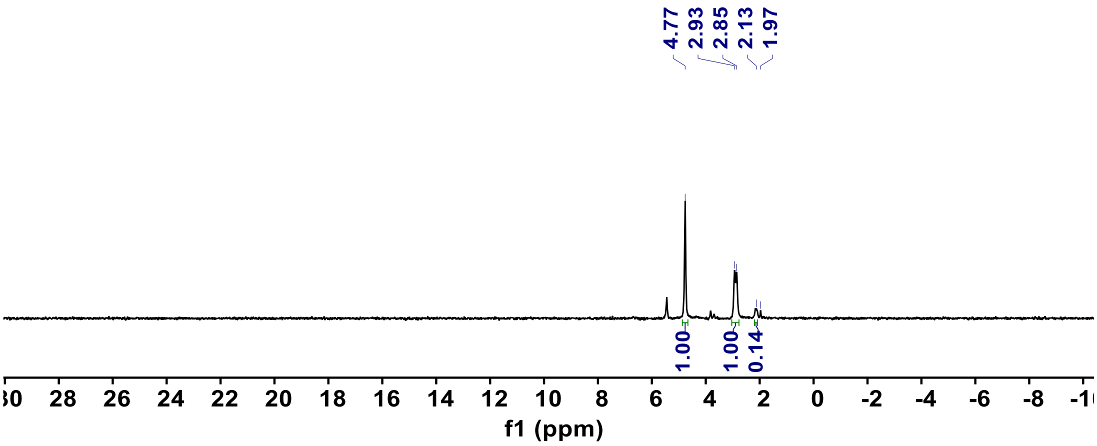
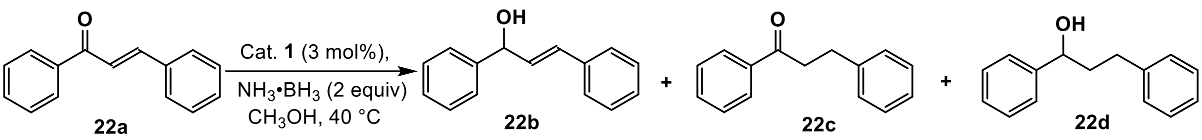
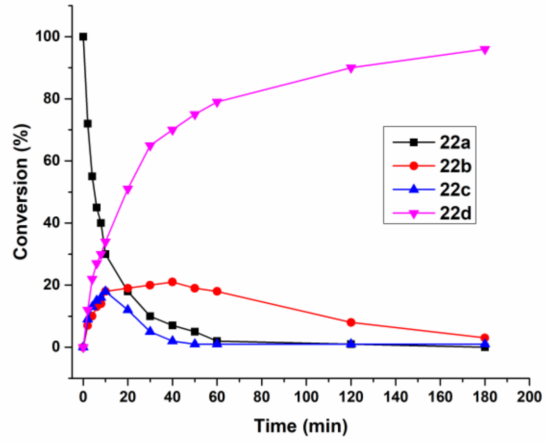


Fig. S17 ^{2}H NMR spectrum (in THF) for the reaction of chalcone and NH_3•BD_3 (2 equiv) in CH_3OH under standard reaction conditions.

9.6 Procedure for time-dependent product distribution study

Time-dependent product distribution study





An oven-dried 4 mL screw cap vial was taken and charged with a magnetic stir-bar, chalcone **22a** (41.6 mg, 0.20 mmol), Cat. **1** (3 mol%), and AB (2 equiv), followed by the addition of CH_3OH (1 mL). Then, the tube was sealed and placed in a preheated oil bath at 40 °C (oil bath temperature) for 2-180 Min. After completion of the reaction, the tube was allowed to cool at room temperature. Then, the reaction mixture was subjected to ^{1}H NMR analysis.

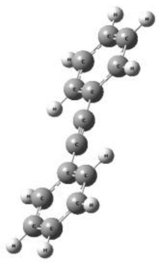
9.7 Procedure for the validation of possible intermediates

The intermediates **22b** and **22c** were synthesized according to procedures reported in the literature.[2] Each of them was independently subjected under standard reaction conditions. An oven-dried 4 mL screw cap vial was taken and charged with a magnetic stir-bar, each intermediate (0.20 mmol), Cat. **1** (3 mol%), and AB (2 equiv), followed by the addition of CH_3OH (1 mL). Then, the tube was sealed and placed in a preheated oil bath at 40 °C (oil bath temperature) for 3 h. After completion of the reaction, the tube was allowed to cool at room temperature. Then, the reaction mixture was subjected to ^{1}H NMR analysis.

10. Computational Studies:

All the calculations were performed using the Gaussian 09 package.[10] Full geometry optimization followed by energy calculations on the stationary points were carried out to ascertain the nature of the stationary points as minima or first order saddle point. Hybrid functional, M062X was used with the LANL2DZ basis set[11] for Ni and 6-31G** basis set[12] for non-metal elements. The transition states (TS) were further confirmed by performing intrinsic reaction coordinate (IRC) calculations using the same method. The effect of solvent (methanol) during the calculation was incorporated in the manuscript. The solvent effect was incorporated using the conductor-like polarizable continuum model (CPCM) with methanol[13] at 328.15 K.

Diphenylacetylene:



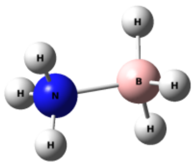
Diphenylacetylene	
SCF Done: E (RM062X)	**-539.074689**
SCF done for solvent	**-539.235122**
Thermal correction to Gibbs Free Energy	**0.154441**
Temperature	**328.15 K**

Coordinates

C	0.19838	4.4279	-0.7951
C	0.21946	3.05049	-1.00029
C	1.4375	2.35896	-0.96973
C	2.63296	3.07048	-0.7724
C	2.60103	4.44472	-0.56745
C	1.3824	5.12481	-0.56698
H	-0.74665	4.9604	-0.82931
H	-0.69328	2.49724	-1.20554
H	3.57546	2.5291	-0.78561
H	3.52784	4.99038	-0.42208
H	1.36112	6.19797	-0.40964
C	1.49485	0.92639	-1.15095
C	1.5622	-0.30702	-1.31482
C	1.64046	-1.74047	-1.50527
C	0.61381	-2.61842	-1.14377
C	2.8382	-2.24747	-2.02978

C	0.7785	-3.98693	-1.32134
H	-0.30079	-2.22401	-0.711
C	2.99274	-3.61599	-2.20529
H	3.63768	-1.56252	-2.29446
C	1.96357	-4.48792	-1.85411
H	-0.02099	-4.66455	-1.04098
H	3.92008	-4.00289	-2.61434
H	2.08736	-5.55693	-1.99247

Ammonia-borane:

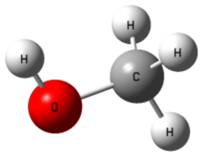


Ammonia-borane	
SCF Done: E (RM062X)	**-83.116827**
SCF done for solvent	**-83.181686**
Thermal correction to Gibbs Free Energy	**0.047453**
Temperature	**328.15 K**

Coordinates

B	-2.96182	1.4507	2.35068
H	-2.26455	0.41715	2.31118
H	-2.77905	1.9752	3.40767
H	-2.88203	2.18717	1.40043
N	-4.49157	0.87494	2.32621
H	-5.13062	1.65231	2.49035
H	-4.65776	0.18731	3.05907
H	-4.73813	0.46438	1.42366

Methanol:

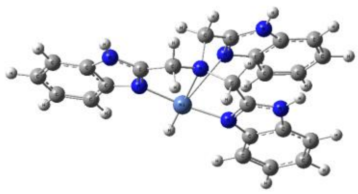


Methanol	
SCF Done: E (RM062X)	**-115.632634**
SCF done for solvent	**-115.667286**
Thermal correction to Gibbs Free Energy	**0.029621**
Temperature	**328.15 K**

Coordinates

```
C                    -1.35352   0.97033   0.0
H                    -0.99685   1.47473   0.87365
H                    -0.99685   1.47473  -0.87365
H                    -2.42352   0.97035   0.0
O                    -0.87687  -0.37789   0.0
H                    -1.19522  -0.83033   0.78457
```

L_2Ni-H:



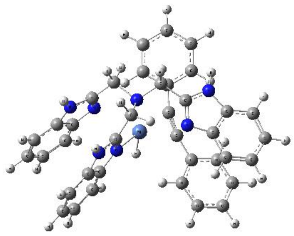
L_2Ni-H:	
SCF Done: E (RM062X)	**-1479.371007**
SCF done for solvent	**-1479.833624**
Thermal correction to Gibbs Free Energy	**0.373486**
Temperature	**328.15 K**

Coordinates

Ni	23.16	11.9351	10.1659
N	21.054	12.376	10.5858
N	22.2119	11.0765	8.5257
N	20.3427	10.1314	7.7967
H	19.5288	9.8539	7.7828
N	23.0795	13.8032	9.3577
N	21.88	15.642	8.9754
H	21.1986	16.1664	8.9388
N	23.3771	12.7457	12.0576
N	22.3537	13.6374	13.8087
H	21.7154	13.9165	14.3135
C	20.3084	11.2023	10.0965
H	19.3761	11.427	9.9535
H	20.3574	10.4766	10.7393
C	20.9568	10.8002	8.801
C	21.2652	9.9885	6.8162
C	21.198	9.3444	5.5643
H	20.4416	8.8821	5.2819
C	22.3347	9.4492	4.7838
H	22.3113	9.1049	3.9202
C	23.4991	10.0361	5.2216
H	24.2472	10.0305	4.6694
C	23.581	10.6287	6.4616
H	24.3605	11.0462	6.7502
C	22.445	10.5773	7.2579
C	20.6658	13.6012	9.8212
H	20.1609	13.3454	9.0325
H	20.1007	14.1635	10.3721
C	21.8836	14.3615	9.4092
C	23.168	15.9507	8.603
C	23.7235	17.0997	8.0285
H	23.2181	17.8617	7.8555
C	25.0576	17.0311	7.7353
H	25.4752	17.7839	7.3847
C	25.8171	15.884	7.9394
H	26.7152	15.884	7.6976
C	25.2674	14.7502	8.4881
H	25.7778	13.9847	8.6275
C	23.9231	14.7884	8.8288
C	20.9027	12.5856	12.0497
H	20.6172	11.7611	12.4743
H	20.2287	13.2631	12.2185
C	22.2133	13.022	12.6182
C	23.6841	13.7422	14.0662
C	24.3902	14.2739	15.128
H	23.9475	14.6762	15.8406
C	25.755	14.1977	15.1062
H	26.2445	14.5207	15.829
C	26.4246	13.6413	14.0108
H	27.3534	13.5998	14.0185
C	25.7308	13.1516	12.9173

H	26.1821	12.7953	12.1864
C	24.3507	13.203	12.9431
H	24.54691	11.67043	9.83585

IntA:



IntA:	
SCF Done: E (RM062X)	-2018.433248
SCF done for solvent	-2019.062940
Thermal correction to Gibbs Free Energy	0.560326
Temperature	328.15 K

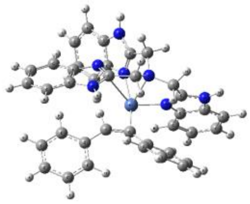
Coordinates

Ni	-0.18164	0.1234	-0.30627
N	-0.19732	1.37446	1.57141
N	1.92371	-0.53363	1.93632
N	3.45722	1.04993	1.5831
H	3.82926	1.97451	1.4256
N	-1.65244	-0.75031	0.64033
N	-2.79114	-1.10163	2.50162
H	-3.02641	-1.07849	3.48241
N	-2.09483	1.91629	-0.81109
N	-3.48449	1.84045	0.93255
H	-3.83872	2.01183	1.8611
C	1.12989	1.83436	2.02732
H	1.082	2.19046	3.0685
H	1.4261	2.68185	1.40087
C	2.15714	0.75012	1.8725
C	4.11956	-0.15245	1.41176
C	5.43351	-0.46652	1.06061
H	6.18147	0.29939	0.88559
C	5.73529	-1.81442	0.95165
H	6.7427	-2.1101	0.67877

C	4.76822	-2.81153	1.19092
H	5.05134	-3.85359	1.08836
C	3.46934	-2.49064	1.54402
H	2.71846	-3.25354	1.71691
C	3.14143	-1.13496	1.65008
C	-0.79004	0.46593	2.58536
H	0.01763	-0.12581	3.0234
H	-1.288	1.03815	3.38295
C	-1.74661	-0.46777	1.91732
C	-3.42702	-1.85258	1.51782
C	-4.55536	-2.66991	1.54364
H	-5.11057	-2.8556	2.45626
C	-4.93211	-3.23436	0.33499
H	-5.80529	-3.87659	0.30297
C	-4.21488	-2.99229	-0.85214
H	-4.55682	-3.44798	-1.77488
C	-3.09097	-2.183	-0.87015
H	-2.54035	-1.97164	-1.78048
C	-2.69778	-1.61425	0.34246
C	-1.08554	2.54821	1.33463
H	-0.50204	3.30173	0.8014
H	-1.41933	2.97871	2.28994
C	-2.24046	2.16547	0.46315
C	-4.19867	1.32796	-0.1375
C	-5.4861	0.79971	-0.24992
H	-6.16567	0.75256	0.59395
C	-5.84774	0.32519	-1.49964
H	-6.83534	-0.10205	-1.63618
C	-4.96722	0.38075	-2.59981
H	-5.3019	-0.00085	-3.5583
C	-3.6936	0.90809	-2.48087
H	-3.00722	0.95121	-3.31967
C	-3.3058	1.38471	-1.22332
H	-0.46651	-0.70116	-1.42951
C	1.15374	4.70175	-1.3928
C	0.83815	3.34501	-1.41791
C	1.85536	2.39553	-1.25951
C	3.1882	2.81796	-1.11638
C	3.49045	4.17376	-1.09656
C	2.47172	5.11873	-1.22342
H	0.36547	5.43637	-1.52129
H	-0.18489	3.00784	-1.56234
H	3.97199	2.06938	-1.03838
H	4.52176	4.49602	-0.9961
H	2.70978	6.17703	-1.20908
C	1.59774	0.97734	-1.2496
C	1.72348	-0.24672	-1.30492
C	2.18356	-1.59974	-1.49107
C	1.40488	-2.7264	-1.20196
C	3.4994	-1.7587	-1.95167
C	1.9361	-3.99645	-1.39264
H	0.39554	-2.59915	-0.82559
C	4.01853	-3.03241	-2.13863
H	4.10406	-0.88088	-2.15613

C	3.23798	-4.15299	-1.86316
H	1.32992	-4.86841	-1.17089
H	5.03523	-3.14931	-2.4983
H	3.64567	-5.14744	-2.01163

IntA1:



IntA1:	
SCF Done: E (RM062X)	-2018.474930
SCF done for solvent	-2019.104633
Thermal correction to Gibbs Free Energy	0.561215
Temperature	328.15 K

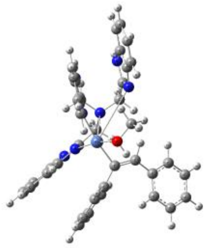
Coordinates

Ni	-0.6418	0.30805	0.38345
N	-0.75998	0.2794	-2.184
N	2.00947	0.80882	-1.62346
N	2.57596	-1.30064	-2.07731
H	2.48172	-2.25527	-2.38756
N	-0.16944	2.18945	-0.04303
N	0.55317	3.68659	-1.49684
H	0.7928	4.08838	-2.39038
N	-2.55569	0.47258	-0.05786
N	-4.34499	0.29427	-1.33837
H	-4.902	0.12617	-2.16281
C	0.2787	-0.56329	-2.77218
H	0.34821	-0.42947	-3.86601
H	0.00071	-1.60615	-2.58443
C	1.62137	-0.32173	-2.14517
C	3.67447	-0.7505	-1.44048
C	4.91553	-1.26844	-1.07314
H	5.19995	-2.29162	-1.29273
C	5.76106	-0.41284	-0.38375

H	6.73643	-0.77195	-0.07288
C	5.38525	0.90815	-0.06793
H	6.07979	1.53564	0.47996
C	4.15407	1.41895	-0.44727
H	3.85391	2.43481	-0.20881
C	3.29156	0.57212	-1.15134
C	-0.64417	1.71228	-2.4688
H	0.00365	1.88462	-3.33903
H	-1.63559	2.11062	-2.72142
C	-0.09643	2.51327	-1.31425
C	0.9889	4.13098	-0.25735
C	1.73493	5.23782	0.14515
H	2.09565	5.97601	-0.56235
C	1.99936	5.34331	1.50263
H	2.57982	6.18547	1.86287
C	1.53328	4.38718	2.42502
H	1.76411	4.51474	3.47677
C	0.78786	3.29271	2.0176
H	0.42281	2.55384	2.72443
C	0.51919	3.17204	0.65275
C	-2.10155	-0.25266	-2.38077
H	-2.05073	-1.34786	-2.3346
H	-2.54706	0.02063	-3.35173
C	-2.99464	0.19391	-1.26094
C	-4.81562	0.6531	-0.08297
C	-6.09657	0.88169	0.41876
H	-6.98128	0.79847	-0.20238
C	-6.18061	1.21859	1.76032
H	-7.15574	1.40219	2.19768
C	-5.03514	1.32597	2.57383
H	-5.15593	1.58808	3.61892
C	-3.76549	1.10386	2.06859
H	-2.87618	1.18027	2.68597
C	-3.66728	0.76572	0.71667
H	1.01246	-0.22829	1.00665
C	-3.53883	-3.71338	-0.04189
C	-2.74335	-2.68976	0.46208
C	-1.36821	-2.65671	0.18713
C	-0.81655	-3.66893	-0.61727
C	-1.61821	-4.68221	-1.13137
C	-2.98255	-4.70672	-0.84589
H	-4.59798	-3.73588	0.19397
H	-3.17771	-1.91157	1.08366
H	0.25197	-3.65087	-0.8206
H	-1.17806	-5.45837	-1.74925
H	-3.6072	-5.50025	-1.24206
C	-0.54356	-1.53319	0.60776
C	0.70224	-1.33325	1.01273
C	1.80716	-2.16524	1.51464
C	3.08101	-1.61559	1.69211
C	1.58998	-3.51223	1.84001
C	4.12522	-2.40203	2.16805
H	3.26275	-0.57133	1.44428
C	2.63517	-4.29189	2.3166

H	0.59669	-3.93692	1.73214
C	3.90685	-3.74046	2.47924
H	5.10962	-1.96247	2.29198
H	2.45649	-5.33139	2.57136
H	4.72014	-4.35267	2.85466

IntB:



IntB:	
SCF Done: E (RM062X)	-2134.125681
SCF done for solvent	-2134.812523
Thermal correction to Gibbs Free Energy	0.616195
Temperature	328.15 K

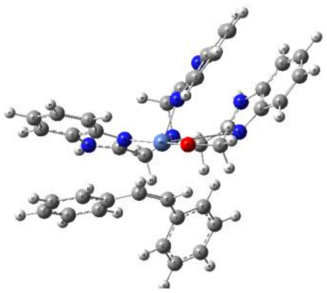
Coordinates

Ni	-0.29757	-0.54709	-0.55286
N	0.45334	0.93086	1.80968
N	2.67339	1.75384	-0.12875
N	3.67648	1.96697	1.85835
H	3.79467	2.2744	2.81227
N	1.45413	-1.33322	0.15808
N	3.29007	-1.22187	1.39113
H	3.90688	-0.92768	2.13361
N	-1.37063	-1.02147	1.04553
N	-2.64856	-0.70412	2.8185
H	-3.01125	-0.26728	3.65267
C	1.17644	2.2004	1.80303
H	1.32692	2.59326	2.82511
H	0.58149	2.92969	1.24619
C	2.50694	2.02409	1.13533
C	4.68562	1.6488	0.96738

C	6.05512	1.43315	1.13008
H	6.54604	1.55057	2.0904
C	6.76291	1.07348	-0.00643
H	7.83064	0.89779	0.06869
C	6.1322	0.94642	-1.25934
H	6.7285	0.67322	-2.12287
C	4.7747	1.16959	-1.41231
H	4.30125	1.08939	-2.38425
C	4.03281	1.51349	-0.27445
C	1.23454	-0.16889	2.36813
H	1.94818	0.17262	3.13409
H	0.56626	-0.88309	2.85701
C	1.97746	-0.90582	1.2885
C	3.66059	-1.8896	0.23784
C	4.88159	-2.3977	-0.20323
H	5.78538	-2.31166	0.3896
C	4.87916	-3.00478	-1.44763
H	5.80367	-3.41496	-1.83872
C	3.70365	-3.10689	-2.21855
H	3.75132	-3.59891	-3.1839
C	2.49545	-2.59671	-1.77442
H	1.58973	-2.65547	-2.36928
C	2.48531	-1.96758	-0.52489
C	-0.89299	1.04572	2.34049
H	-1.39105	1.8752	1.81887
H	-0.92866	1.25807	3.42442
C	-1.63664	-0.22352	2.05528
C	-3.09185	-1.88745	2.2449
C	-4.12027	-2.76995	2.57239
H	-4.75293	-2.62046	3.44007
C	-4.29874	-3.84538	1.71772
H	-5.08826	-4.55932	1.9251
C	-3.48641	-4.03683	0.58245
H	-3.67613	-4.88914	-0.06049
C	-2.46226	-3.16099	0.26872
H	-1.84235	-3.28934	-0.61299
C	-2.27151	-2.07412	1.12392
H	-0.47091	2.10173	-0.73284
C	-4.51114	-1.72411	-2.40397
C	-3.32656	-1.00161	-2.29566
C	-3.12151	-0.10484	-1.23902
C	-4.14002	0.03993	-0.28593
C	-5.31367	-0.69891	-0.37872
C	-5.50429	-1.58419	-1.43836
H	-4.65258	-2.40745	-3.2352
H	-2.54255	-1.14197	-3.03708
H	-3.99373	0.73806	0.53621
H	-6.08415	-0.5836	0.37739
H	-6.4213	-2.15947	-1.50957
C	-1.80934	0.54527	-1.05762
C	-1.52201	1.85435	-0.93173
C	-2.39746	3.04611	-0.87895
C	-1.87843	4.19841	-0.27144
C	-3.71949	3.08158	-1.34443

C	-2.65925	5.33286	-0.08237
H	-0.83786	4.20471	0.04706
C	-4.49952	4.2172	-1.15957
H	-4.13644	2.21944	-1.85235
C	-3.98079	5.3409	-0.51787
H	-2.23515	6.21037	0.39497
H	-5.52168	4.22735	-1.52398
H	-4.59841	6.22129	-0.37411
C	1.56419	0.42366	-2.76059
H	2.3919	-0.0492	-2.23915
H	1.70801	0.34705	-3.84116
H	1.49052	1.46446	-2.44105
H	-0.38678	0.16184	-2.77254
O	0.37758	-0.30321	-2.39898

IntB1:



IntB1:	
SCF Done: E (RM062X)	-2134.122712
SCF done for solvent	-2134.814136
Thermal correction to Gibbs Free Energy	0.619678
Temperature	328.15 K

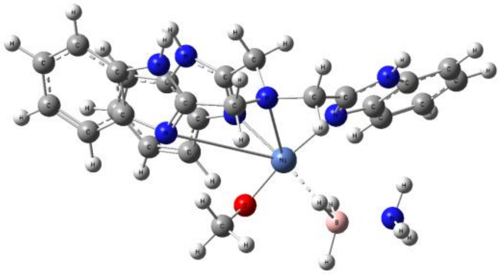
Coordinates

Ni	-0.40039	-0.45922	-0.84529
N	0.32702	1.01582	1.73737
N	2.75724	1.64612	0.07516
N	3.64727	1.59213	2.12707
H	3.74678	1.82694	3.10344
N	1.15699	-1.34454	0.03336
N	2.86569	-1.50059	1.42608
H	3.4519	-1.28895	2.21997
N	-1.59087	-0.70335	0.72931

N	-2.89097	-0.4352	2.48978
H	-3.27646	-0.01221	3.32097
C	1.20734	2.16453	1.94466
H	1.32884	2.39468	3.01889
H	0.75899	3.03412	1.45959
C	2.54833	1.86464	1.34277
C	4.65709	1.182	1.27401
C	5.96677	0.75344	1.49809
H	6.4078	0.74128	2.48934
C	6.68322	0.3516	0.3812
H	7.70589	0.01116	0.50354
C	6.12008	0.38372	-0.90955
H	6.72177	0.06525	-1.75359
C	4.8227	0.81653	-1.12333
H	4.39191	0.85183	-2.11766
C	4.07453	1.21526	-0.00826
C	0.90362	-0.21519	2.27242
H	1.5985	-0.01403	3.10173
H	0.1174	-0.85688	2.67911
C	1.62815	-1.00103	1.21623
C	3.24121	-2.21301	0.30055
C	4.41235	-2.90103	-0.01493
H	5.25465	-2.93588	0.66687
C	4.439	-3.52877	-1.24756
H	5.32469	-4.08007	-1.54376
C	3.3378	-3.47223	-2.12487
H	3.40178	-3.98459	-3.0787
C	2.18334	-2.77636	-1.81039
H	1.34765	-2.69086	-2.49353
C	2.14654	-2.12434	-0.57151
C	-1.04813	1.26407	2.13874
H	-1.39845	2.15546	1.60043
H	-1.17295	1.45454	3.22042
C	-1.86831	0.06771	1.75614
C	-3.32163	-1.6075	1.88438
C	-4.32832	-2.52464	2.18903
H	-4.99231	-2.39041	3.03552
C	-4.43395	-3.62166	1.3496
H	-5.19847	-4.3649	1.54743
C	-3.57118	-3.80626	0.2501
H	-3.68993	-4.68882	-0.36873
C	-2.58099	-2.88889	-0.05266
H	-1.9126	-3.01911	-0.89988
C	-2.47241	-1.77352	0.7824
H	-0.70223	1.22253	-2.68794
C	-5.78043	-1.04242	-1.04397
C	-4.57004	-0.80055	-1.68392
C	-3.71926	0.23019	-1.26318
C	-4.11902	1.01561	-0.17135
C	-5.3289	0.77615	0.46809
C	-6.1644	-0.25275	0.03578
H	-6.42042	-1.84855	-1.38638
H	-4.26986	-1.4257	-2.52081
H	-3.47806	1.81402	0.18471

H	-5.62509	1.39926	1.3067
H	-7.10989	-0.4351	0.53599
C	-2.436	0.37756	-1.97654
C	-1.52123	1.38692	-1.99537
C	-1.50241	2.72092	-1.35746
C	-0.26817	3.22066	-0.91877
C	-2.62626	3.5564	-1.32498
C	-0.17573	4.51584	-0.41472
H	0.62195	2.59237	-0.97295
C	-2.52808	4.85003	-0.82325
H	-3.57283	3.19562	-1.71597
C	-1.30502	5.33024	-0.35844
H	0.78849	4.89741	-0.09023
H	-3.40367	5.49047	-0.81362
H	-1.22741	6.34363	0.02132
C	1.53467	0.12111	-2.7648
H	2.29487	0.04405	-1.97628
H	1.96728	-0.27896	-3.69227
H	1.34796	1.19891	-2.92632
H	-2.22264	-0.42421	-2.68681
O	0.37215	-0.58988	-2.46197

IntC:



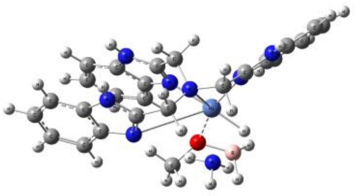
IntC:	
SCF Done: E (RM062X)	-1676.950634
SCF done for solvent	-1677.520005
Thermal correction to Gibbs Free Energy	0.481668
Temperature	328.15 K

Coordinates

Ni	-1.17568	0.77966	0.75111
N	-0.26672	-2.08997	0.50867
N	2.4119	-0.9111	1.43909
N	3.08718	-2.68831	0.26132
H	3.12664	-3.65689	-0.01883
N	0.29943	0.59106	-0.574
N	1.90124	-0.38246	-1.74742
H	2.46926	-1.12782	-2.12204
N	-2.51442	-0.51032	-0.09797
N	-3.83167	-2.27928	-0.29263
H	-4.11937	-3.24676	-0.26255
C	0.78235	-2.77126	1.27432
H	0.85044	-3.8394	0.99878
H	0.52781	-2.70761	2.33591
C	2.11077	-2.11405	1.04842
C	4.11707	-1.76656	0.17037
C	5.3417	-1.7739	-0.50047
H	5.69019	-2.63744	-1.05706
C	6.09849	-0.61524	-0.41112
H	7.06002	-0.57359	-0.91183
C	5.65331	0.50989	0.31215
H	6.27804	1.3959	0.34082
C	4.43884	0.50901	0.97506
H	4.07648	1.37493	1.51903
C	3.66288	-0.6536	0.90468
C	0.08889	-1.88155	-0.89353
H	0.7561	-2.66953	-1.27509
H	-0.81334	-1.90567	-1.51045
C	0.74417	-0.54376	-1.06855
C	2.2572	0.95331	-1.67094
C	3.36304	1.64541	-2.16227
H	4.15261	1.14263	-2.70969
C	3.40552	3.00059	-1.88746
H	4.24612	3.5884	-2.24025
C	2.38231	3.63399	-1.15377
H	2.45924	4.69868	-0.96151
C	1.29179	2.93877	-0.66053
H	0.52497	3.40545	-0.05711
C	1.2387	1.56417	-0.92423
C	-1.56747	-2.68767	0.70426
H	-1.73796	-2.79026	1.78331
H	-1.66985	-3.69854	0.26509
C	-2.62814	-1.80356	0.11669
C	-4.56066	-1.21909	-0.80651
C	-5.84502	-1.13014	-1.34537
H	-6.49422	-1.99453	-1.42789
C	-6.24511	0.12464	-1.77562
H	-7.23338	0.24607	-2.20498
C	-5.39593	1.24561	-1.68219
H	-5.74797	2.20328	-2.0491
C	-4.12091	1.15141	-1.14736
H	-3.46053	2.00917	-1.08436
C	-3.70913	-0.10809	-0.69167
C	0.43472	1.66281	2.72971

H	1.12855	0.8336	2.53509
H	1.02523	2.51553	3.09236
H	-0.24583	1.3693	3.54888
O	-0.25726	2.06578	1.58299
B	-2.88837	1.74899	2.13745
H	-2.22018	0.69392	2.17835
H	-2.64597	2.36924	3.12896
H	-2.83259	2.38104	1.11589
N	-4.43154	1.21645	2.24283
H	-5.04226	2.02714	2.34084
H	-4.58048	0.62552	3.05929
H	-4.73006	0.70973	1.40636

IntC1:



IntC1:	
SCF Done: E (RM062X)	-1676.983428
SCF done for solvent	-1677.535689
Thermal correction to Gibbs Free Energy	0.481818
Temperature	328.15 K

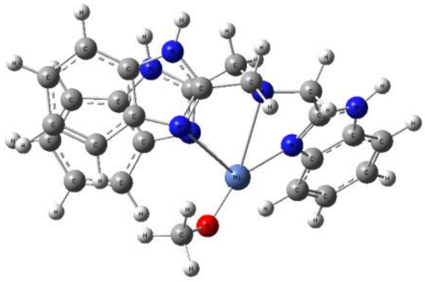
Coordinates

Ni	-1.18529	0.70824	0.64667
N	-0.2912	-2.08272	0.48528
N	2.36366	-0.84192	1.44284
N	3.0711	-2.65565	0.34172
H	3.11488	-3.63187	0.08915
N	0.28426	0.54521	-0.65756

N	1.92772	-0.42521	-1.76666
H	2.51062	-1.16807	-2.12426
N	-2.5064	-0.50717	-0.13354
N	-3.87437	-2.22941	-0.29112
H	-4.21092	-3.17732	-0.2091
C	0.74747	-2.72658	1.29571
H	0.83816	-3.80093	1.05456
H	0.46492	-2.63773	2.34827
C	2.07411	-2.05987	1.08248
C	4.10305	-1.73817	0.24702
C	5.34455	-1.77151	-0.39118
H	5.70267	-2.65405	-0.91053
C	6.10635	-0.61546	-0.31662
H	7.08138	-0.59363	-0.79158
C	5.64931	0.53072	0.36438
H	6.28041	1.41228	0.3907
C	4.41761	0.55443	0.99454
H	4.06084	1.43884	1.51191
C	3.6319	-0.60315	0.93557
C	0.09271	-1.92531	-0.9169
H	0.75935	-2.72944	-1.2642
H	-0.80202	-1.95456	-1.54498
C	0.75602	-0.59424	-1.11793
C	2.26536	0.91744	-1.70247
C	3.37678	1.6246	-2.15727
H	4.19392	1.13292	-2.67315
C	3.38969	2.983	-1.88962
H	4.23386	3.57979	-2.21704
C	2.33283	3.61002	-1.19983
H	2.38578	4.67776	-1.01784
C	1.23307	2.9009	-0.74724
H	0.42612	3.37598	-0.20144
C	1.21301	1.52499	-1.00225
C	-1.59632	-2.68737	0.6728
H	-1.77174	-2.79271	1.75003
H	-1.6879	-3.69468	0.22733
C	-2.65315	-1.79473	0.09335
C	-4.58977	-1.14077	-0.76579
C	-5.89595	-0.99965	-1.23031
H	-6.57564	-1.84121	-1.30191
C	-6.28518	0.28233	-1.58765
H	-7.29222	0.44494	-1.95555
C	-5.40683	1.37975	-1.48851
H	-5.75936	2.36289	-1.77955
C	-4.10837	1.22952	-1.02926
H	-3.43146	2.07377	-0.93828
C	-3.70847	-0.05708	-0.66455
C	0.70957	1.79157	2.46703
H	1.56105	1.66013	1.79911
H	0.87815	2.62438	3.1522
H	0.55111	0.86786	3.03068
O	-0.43685	2.1017	1.66385
B	-1.76659	2.07167	2.30639
H	-2.27422	0.91425	1.79925

H	-1.76369	1.82299	3.47748
H	-2.50361	2.91738	1.8792
N	-4.88996	0.49448	2.08382
H	-4.49764	1.43294	2.07113
H	-5.26351	0.36478	3.02061
H	-5.69451	0.52813	1.46083

Ni-OMe:



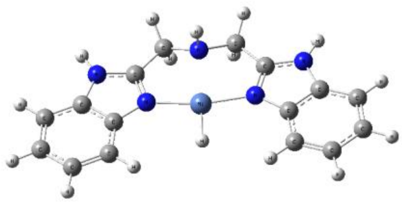
Ni-OMe:	
SCF Done: E (RM062X)	-1593.817077
SCF done for solvent	-1594.311066
Thermal correction to Gibbs Free Energy	0.413816
Temperature	328.15 K

Coordinates

Ni	-0.40039	-0.45922	-0.84529
N	0.32702	1.01582	1.73737
N	2.75724	1.64612	0.07516
N	3.64727	1.59213	2.12707
H	3.74678	1.82694	3.10344
N	1.15699	-1.34454	0.03336
N	2.86569	-1.50059	1.42608
H	3.4519	-1.28895	2.21997
N	-1.59087	-0.70335	0.72931
N	-2.89097	-0.4352	2.48978
H	-3.27646	-0.01221	3.32097
C	1.20734	2.16453	1.94466
H	1.32884	2.39468	3.01889

H	0.75899	3.03412	1.45959
C	2.54833	1.86464	1.34277
C	4.65709	1.182	1.27401
C	5.96677	0.75344	1.49809
H	6.4078	0.74128	2.48934
C	6.68322	0.3516	0.3812
H	7.70589	0.01116	0.50354
C	6.12008	0.38372	-0.90955
H	6.72177	0.06525	-1.75359
C	4.8227	0.81653	-1.12333
H	4.39191	0.85183	-2.11766
C	4.07453	1.21526	-0.00826
C	0.90362	-0.21519	2.27242
H	1.5985	-0.01403	3.10173
H	0.1174	-0.85688	2.67911
C	1.62815	-1.00103	1.21623
C	3.24121	-2.21301	0.30055
C	4.41235	-2.90103	-0.01493
H	5.25465	-2.93588	0.66687
C	4.439	-3.52877	-1.24756
H	5.32469	-4.08007	-1.54376
C	3.3378	-3.47223	-2.12487
H	3.40178	-3.98459	-3.0787
C	2.18334	-2.77636	-1.81039
H	1.34765	-2.69086	-2.49353
C	2.14654	-2.12434	-0.57151
C	-1.04813	1.26407	2.13874
H	-1.39845	2.15546	1.60043
H	-1.17295	1.45454	3.22042
C	-1.86831	0.06771	1.75614
C	-3.32163	-1.6075	1.88438
C	-4.32832	-2.52464	2.18903
H	-4.99231	-2.39041	3.03552
C	-4.43395	-3.62166	1.3496
H	-5.19847	-4.3649	1.54743
C	-3.57118	-3.80626	0.2501
H	-3.68993	-4.68882	-0.36873
C	-2.58099	-2.88889	-0.05266
H	-1.9126	-3.01911	-0.89988
C	-2.47241	-1.77352	0.7824
C	1.53467	0.12111	-2.7648
H	2.29487	0.04405	-1.97628
H	1.96728	-0.27896	-3.69227
H	1.34796	1.19891	-2.92632
O	0.37215	-0.58988	-2.46197

L_1Ni-H:



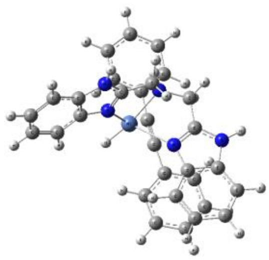
L$_1$Ni-H:	
SCF Done: E (RM062X)	-1061.659215
SCF done for solvent	-1061.999681
Thermal correction to Gibbs Free Energy	0.262426
Temperature	328.15 K

Coordinates

```
Ni   3.2724   4.6653   6.0293
 N   5.3534   4.4113   6.3051
 H   5.4875   3.5086   6.6622
 N   3.7896   3.9619   4.1677
 N   5.4327   3.3694   2.7967
 H   6.2307   3.2564   2.4966
 N   3.4821   5.4069   7.954
 N   4.8651   6.4267   9.3658
 H   5.6022   6.6975   9.7164
 C   6.0472   4.469    5.0011
 H   6.8549   3.9321   5.0251
 H   6.2901   5.3834   4.7885
 C   5.0938   3.9303   3.9756
 C   4.2588   3.0093   2.1606
 C   4.0049   2.3565   0.959
 H   4.6928   2.1036   0.3864
 C   2.6811   2.1011   0.6575
 H   2.4725   1.6654  -0.1372
 C   1.6463   2.4824   1.5192
 H   0.7674   2.2938   1.2808
 C   1.8943   3.1323   2.7167
 H   1.2031   3.3856   3.2849
 C   3.2238   3.3871   3.0296
 C   5.8653   5.3526   7.3107
 H   6.2027   6.1523   6.8778
 H   6.5899   4.9453   7.8106
 C   4.7372   5.7019   8.2309
 C   3.5926   6.6525   9.8591
 C   3.1308   7.3979  10.9443
```

H	3.7125	7.8509	11.5114
C	1.7645	7.4263	11.1295
H	1.4138	7.9235	11.833
C	0.8914	6.7281	10.2874
H	-0.0214	6.7475	10.4642
C	1.3551	6.0053	9.1923
H	0.771	5.5489	8.631
C	2.7281	5.9944	8.9719
H	1.85123	4.87627	5.8337

IntA′:



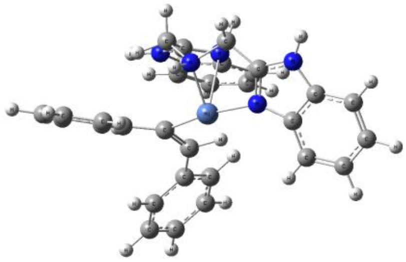
IntA′	
SCF Done: E (RM062X)	-1600.727311
SCF done for solvent	-1601.233183
Thermal correction to Gibbs Free Energy	0.438564
Temperature	328.15 K

Coordinates

Ni	0.76041	-0.57108	-0.63591
N	0.61734	-2.07743	0.94587
N	-0.64111	0.22379	1.87602
N	-2.66787	-0.70953	1.78292
H	-3.36559	-1.4345	1.71341
N	2.5869	-0.53756	-0.02022
N	4.07319	-0.90466	1.57038
H	4.46539	-1.23322	2.44027
C	-0.6817	-2.24051	1.62611
H	-0.55661	-2.73478	2.59943
H	-1.32001	-2.87917	1.01027
C	-1.3157	-0.89123	1.78758
C	-2.8899	0.65505	1.86394
C	-4.05412	1.42479	1.86821
H	-5.04118	0.97719	1.82522

C	-3.88257	2.79797	1.93216
H	-4.75707	3.43974	1.93751
C	-2.60157	3.38296	1.99443
H	-2.51923	4.46356	2.03979
C	-1.45305	2.61134	1.99644
H	-0.4646	3.0554	2.03915
C	-1.60426	1.22228	1.92727
C	1.69454	-1.74996	1.90611
H	1.28623	-1.02274	2.61533
H	2.0429	-2.63159	2.45825
C	2.80281	-1.09184	1.15241
C	4.73161	-0.15757	0.5984
C	6.03356	0.33378	0.51368
H	6.76643	0.15953	1.29315
C	6.34069	1.06534	-0.62238
H	7.33945	1.47247	-0.73371
C	5.39094	1.29484	-1.63689
H	5.68126	1.8724	-2.5073
C	4.10078	0.8002	-1.54908
H	3.36169	0.96589	-2.32527
C	3.77733	0.06623	-0.40607
H	1.15429	0.26915	-1.72158
C	-1.36762	-4.54723	-1.74955
C	-0.89086	-3.24048	-1.76819
C	-1.74825	-2.18072	-1.44207
C	-3.09136	-2.44199	-1.1277
C	-3.55914	-3.75028	-1.11678
C	-2.69646	-4.80455	-1.41619
H	-0.70552	-5.36639	-2.00923
H	0.1373	-3.02848	-2.05205
H	-3.75073	-1.60944	-0.90139
H	-4.59938	-3.95005	-0.88196
H	-3.0643	-5.82484	-1.4062
C	-1.284	-0.82194	-1.37795
C	-1.12043	0.39382	-1.31453
C	-1.23059	1.82914	-1.3142
C	-0.1332	2.68824	-1.18087
C	-2.52524	2.35903	-1.43105
C	-0.33355	4.0632	-1.18629
H	0.86355	2.27545	-1.07087
C	-2.71171	3.73434	-1.43428
H	-3.37308	1.68647	-1.51228
C	-1.61718	4.58849	-1.31677
H	0.51806	4.7282	-1.08969
H	-3.71366	4.13943	-1.52719
H	-1.7653	5.66328	-1.32293
H	0.84772	-2.95782	0.48648

IntA1′:



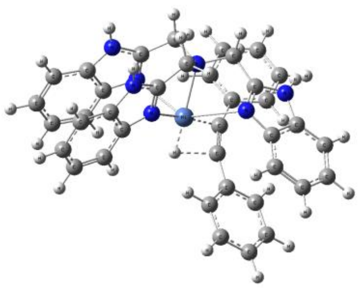
IntA1′	
SCF Done: E (RM062X)	**-1600.744372**
SCF done for solvent	**-1601.258042**
Thermal correction to Gibbs Free Energy	**0.443536**
Temperature	**328.15 K**

Coordinates

Ni	0.80808	-0.7365	-0.42439
N	0.82676	-2.29649	0.94826
N	-0.42118	0.01886	1.95274
N	-2.45069	-0.89919	1.79986
H	-3.14336	-1.61092	1.61944
N	2.67418	-0.47991	0.14479
N	4.25615	-1.01923	1.58624
H	4.70599	-1.44951	2.38063
C	-0.48417	-2.44697	1.62885
H	-0.36471	-2.98866	2.57642
H	-1.1337	-3.0407	0.97897
C	-1.1012	-1.092	1.83969
C	-2.66427	0.46735	1.83949
C	-3.82208	1.24328	1.76479
H	-4.80906	0.7986	1.69496
C	-3.64308	2.61742	1.77864
H	-4.51119	3.26484	1.7157
C	-2.36182	3.19658	1.87018
H	-2.27238	4.27736	1.86781
C	-1.22019	2.41763	1.95697
H	-0.23199	2.85961	2.02709
C	-1.37717	1.02733	1.94162
C	1.90713	-1.96911	1.92127
H	1.46451	-1.33237	2.69376
H	2.31547	-2.87111	2.39036
C	2.96402	-1.17568	1.21893
C	4.84971	-0.15281	0.67294

C	6.14524	0.34798	0.54874
H	6.93103	0.09372	1.25087
C	6.37797	1.191	-0.52636
H	7.37025	1.60553	-0.66483
C	5.36414	1.52362	-1.44622
H	5.6007	2.18346	-2.27331
C	4.08029	1.02368	-1.31782
H	3.29483	1.26694	-2.02611
C	3.83309	0.17644	-0.23571
H	0.42764	0.80441	-0.97474
C	-1.98276	-4.26038	-1.79556
C	-1.22359	-3.0993	-1.71547
C	-1.80799	-1.87089	-1.35756
C	-3.18653	-1.83563	-1.10305
C	-3.94336	-3.00305	-1.17055
C	-3.34552	-4.21699	-1.50768
H	-1.51439	-5.19624	-2.0824
H	-0.16004	-3.12486	-1.94184
H	-3.65091	-0.89304	-0.82538
H	-5.00869	-2.9651	-0.9665
H	-3.94279	-5.12112	-1.55731
C	-0.91239	-0.74106	-1.17227
C	-0.67703	0.5469	-1.28373
C	-1.26098	1.87051	-1.53452
C	-0.42547	2.99306	-1.46255
C	-2.63522	2.05101	-1.71535
C	-0.94783	4.27425	-1.56366
H	0.64267	2.85729	-1.30561
C	-3.15704	3.3366	-1.80879
H	-3.28935	1.18647	-1.76808
C	-2.31979	4.44818	-1.7292
H	-0.2893	5.13427	-1.50548
H	-4.2257	3.47258	-1.93827
H	-2.73715	5.44716	-1.79846
H	1.05153	-3.18172	0.49667

TS1:



TS1	
SCF Done: E (RM062X)	**-2018.430683**

SCF done for solvent	-2019.061749
Thermal correction to Gibbs Free Energy	0.561750
Temperature	328.15 K

Coordinates

Ni	23.16	11.9351	10.1659
N	21.19457	11.90024	10.55486
N	21.82036	10.62608	8.49475
N	19.84175	10.15127	7.59593
H	18.84544	10.01303	7.52105
N	23.8506	13.50169	9.59864
N	22.39643	15.1376	9.24544
H	21.52	15.62105	9.22403
N	23.59326	12.61803	12.00886
N	22.43446	13.81054	13.48648
H	21.63828	14.2147	13.94761
C	20.07449	11.04408	10.1434
H	19.14345	11.56815	10.13496
H	19.97226	10.2119	10.81004
C	20.5318	10.59006	8.72551
C	20.77141	9.93749	6.60499
C	20.68804	9.5132	5.25549
H	19.75338	9.25414	4.7882
C	21.87288	9.44298	4.53071
H	21.84575	9.12891	3.5037
C	23.09773	9.76138	5.1001
H	23.99994	9.72923	4.51335
C	23.1765	10.12881	6.40935
H	24.12506	10.34019	6.88599
C	21.99343	10.22383	7.12456
C	21.20587	13.02851	9.5968
H	21.01131	12.63193	8.61722
H	20.42165	13.70506	9.8638
C	22.53724	13.84527	9.50854
C	23.5488	15.67961	9.01147
C	23.76808	16.97074	8.65615
H	22.95408	17.66265	8.62548
C	25.03214	17.33737	8.34084
H	25.2098	18.34596	8.0326
C	26.11204	16.39272	8.40548
H	27.10524	16.69844	8.11502
C	25.88008	15.08902	8.84623
H	26.68712	14.36849	8.94276
C	24.53262	14.75359	9.14428
C	21.06088	12.34284	11.95011
H	20.81467	11.49636	12.54864
H	20.28634	13.0694	12.03409
C	22.38392	12.92102	12.46424
C	23.7012	14.04651	13.78497

C	24.20628	14.81376	14.76563
H	23.5659	15.36721	15.42213
C	25.5639	14.85946	14.9015
H	25.99862	15.43336	15.70569
C	26.39696	14.14537	13.98355
H	27.46458	14.18813	14.07219
C	25.83768	13.3948	12.97166
H	26.44725	12.86178	12.25765
C	24.48728	13.34859	12.91358
H	24.84216	10.93793	9.68798
C	24.12235	7.00955	14.05641
C	24.51596	7.81609	12.96251
C	23.54984	8.23625	12.01017
C	22.22286	7.79027	12.11553
C	21.83775	6.98422	13.20194
C	22.78069	6.59079	14.16774
H	24.83799	6.7111	14.7919
H	25.54278	8.11558	12.84341
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C	23.93685	9.19749	10.839
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C	25.1201	8.86746	8.32005
C	26.07974	9.67099	7.65025
C	24.8191	7.58508	7.83432
C	26.79914	9.13923	6.55461
H	26.25495	10.6796	7.98456
C	25.53282	7.06322	6.73957
H	24.05004	6.99317	8.2846
C	26.5183	7.83487	6.09922
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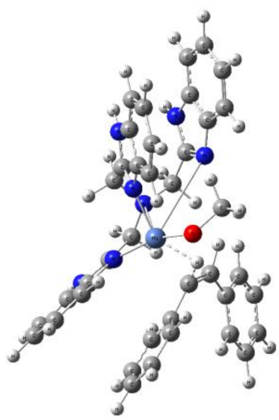
TS2:



TS2	
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SCF done for solvent	**-2134.783724**
Thermal correction to Gibbs Free Energy	**0.611051**
Temperature	**328.15 K**

Coordinates

Ni	-0.18377	-0.39382	-0.53502
N	0.40941	0.46035	1.96627
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N	3.55246	1.83555	2.04514
H	3.64772	2.09971	3.01456
N	1.55776	-1.34588	0.03574
N	3.33512	-1.56325	1.33813
H	3.91161	-1.5001	2.16342
N	-1.2954	-1.38122	0.78473
N	-2.65406	-1.45247	2.52545
H	-3.08907	-1.18126	3.3945
C	1.04927	1.76761	2.07978
H	1.21302	2.07296	3.12841
H	0.38875	2.50415	1.61229
C	2.37081	1.75053	1.36236
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C	5.9705	1.66917	1.25605
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C	1.24604	-0.65142	2.41292
H	1.9425	-0.34887	3.21108
H	0.61204	-1.44179	2.82692
C	2.02636	-1.21366	1.25482
C	3.75687	-1.92826	0.06965
C	4.99715	-2.32286	-0.43046
H	5.86866	-2.4195	0.20737
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H	6.00202	-2.87307	-2.23267
C	3.92676	-2.43285	-2.62039
H	4.0247	-2.64166	-3.68011
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C	-0.95861	0.42365	2.46014

H	-1.47942	1.30926	2.07224
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C	-2.28866	2.65899	-0.76718
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C	-4.06591	5.76881	0.41988
H	-2.25232	4.7309	0.91938
C	-5.34098	4.8326	-1.39689
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H	-1.92542	1.18346	-3.58034
H	-0.19596	1.60386	-3.69744
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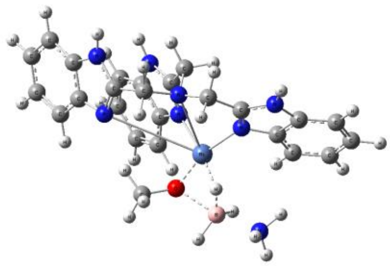
TS3:



TS3	
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SCF done for solvent	**-1677.494845**
Thermal correction to Gibbs Free Energy	**0.479020**
Temperature	**328.15 K**

Coordinates

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N                        -2.23537  -0.5813   -1.45954
N                        -2.84608  -2.67087  -0.94495
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N                        -1.57792  -1.09919   1.74074
H                        -2.12598  -1.92808   1.92069
N                         2.66942  -0.53023  -0.13229
N                         4.03814  -2.24816  -0.3316
H                         4.37699  -3.15715  -0.61098
C                        -0.58818  -2.36169  -2.00504
H                        -0.64807  -3.45891  -2.11933
H                        -0.36133  -1.92906  -2.98366
C                        -1.9109   -1.84095  -1.5248
C                        -3.87268  -1.8617   -0.49063
C                        -5.05985  -2.13278   0.19294
H                        -5.37179  -3.14475   0.42897
C                        -5.829    -1.03548   0.54959
H                        -6.76352  -1.19481   1.07686
C                        -5.43144   0.28083   0.23928
H                        -6.06497   1.10687   0.54359
C                        -4.25485   0.54017  -0.44194
H                        -3.94268   1.55318  -0.67409
C                        -3.46225  -0.55288  -0.81434
C                         0.15473  -2.24741   0.32449
H                        -0.50691  -3.11881   0.44375
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H	-3.72063	0.08034	3.29972
C	-2.98867	2.09474	3.00031
H	-3.78669	2.55318	3.57404
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H	-2.07579	3.99281	2.54685
C	-0.96944	2.39454	1.66093
H	-0.22554	3.02328	1.18294
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C	1.78973	-2.44454	-1.46672
H	1.93712	-2.20293	-2.52634
H	1.92723	-3.53596	-1.35799
C	2.82753	-1.72961	-0.64848
C	4.72711	-1.30736	0.42369
C	5.99737	-1.29914	0.99965
H	6.67647	-2.13925	0.90935
C	6.34874	-0.15154	1.69233
H	7.32705	-0.09449	2.15657
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H	3.53551	1.77631	1.31448
C	3.84661	-0.22283	0.53984
C	-0.92322	2.72849	-2.49652
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H	-1.14841	3.64355	-3.04765
H	-0.79009	1.8813	-3.17648
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B	1.81839	3.38667	-2.87498
H	2.81087	1.42723	-1.97773
H	1.72738	3.15087	-4.0481
H	2.52497	4.27064	-2.4792
N	1.76487	5.49385	-4.59883
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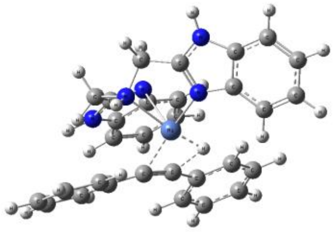
TS1′:



TS1′	
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SCF done for solvent	**-1601.224506**
Thermal correction to Gibbs Free Energy	**0.440622**
Temperature	**328.15 K**

Coordinates

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H	3.73686	2.00472	1.46243
N	-1.6566	-0.74769	0.73588
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C	1.04444	1.89339	2.1246
H	0.99322	2.23676	3.16925
H	1.34472	2.7466	1.50788
C	2.06252	0.8007	1.95146
C	3.99216	-0.12349	1.40609
C	5.2872	-0.44987	0.99892
H	6.0441	0.30771	0.8255
C	5.55675	-1.79845	0.83112
H	6.54712	-2.1041	0.5109
C	4.5786	-2.78533	1.06868
H	4.8362	-3.82788	0.91687
C	3.30079	-2.45262	1.48252
H	2.54218	-3.20723	1.65878
C	3.00376	-1.09525	1.64712
C	-0.8894	0.53759	2.67151
H	-0.08617	-0.03427	3.14252
H	-1.41528	1.11816	3.44441
C	-1.81403	-0.42272	1.99547
C	-3.47809	-1.81596	1.55849
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H	-5.21477	-2.78107	2.43936
C	-4.93236	-3.22308	0.34186
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C	-4.15538	-3.02026	-0.81466
H	-4.45503	-3.5004	-1.73973
C	-3.02587	-2.21883	-0.79943
H	-2.43178	-2.0347	-1.68854
C	-2.68944	-1.61721	0.41438
H	-0.15713	-0.86379	-1.18608
C	1.33599	4.672	-1.2657
C	0.92956	3.33992	-1.2791
C	1.8821	2.31856	-1.16845

C	3.2453	2.64901	-1.08598
C	3.64043	3.9814	-1.07224
C	2.68556	4.99611	-1.15057
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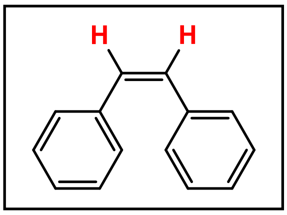
H	-0.11721	3.07121	-1.39475
H	3.97848	1.84806	-1.03599
H	4.69508	4.23099	-1.01501
H	2.99745	6.03512	-1.14258
C	1.49485	0.92639	-1.15095
C	1.5622	-0.30702	-1.31482
C	2.14935	-1.59689	-1.61259
C	1.49219	-2.8094	-1.38145
C	3.46247	-1.59904	-2.10499
C	2.1367	-4.00963	-1.65629
H	0.48605	-2.80404	-0.97279
C	4.09745	-2.80303	-2.37836
H	3.97333	-0.65521	-2.26814
C	3.43607	-4.00985	-2.15716
H	1.62282	-4.9481	-1.47696
H	5.1122	-2.79915	-2.76209
H	3.93498	-4.94914	-2.37178
H	-0.88056	2.21596	1.47005

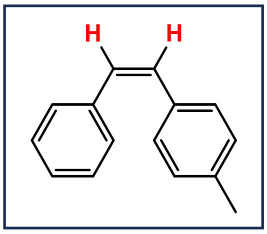
11. Spectral Data for alkynes and chalcones

(*Z*)-1,2-diphenylethene (1b):[1]



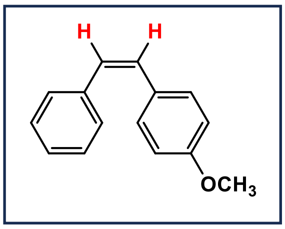
Purified by column chromatography using silica gel and hexane as eluent 89% (80.1mg) isolated yield; colourless oil. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.29 – 7.19 (m, 10H), 6.62 (s, 2H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ 137.4, 130.4, 129.0, 128.3, 127.2.

(*Z*)-1-methyl-4-styrylbenzene (2b):[14]



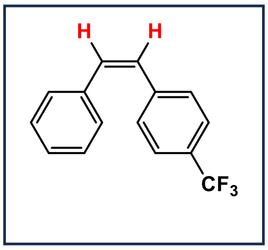
Purified by column chromatography using silica gel and hexane as eluent 95% (92.15 mg) isolated yield; colourless oil. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.30 – 7.18 (m, 5H), 7.15 (d, J = 8.2 Hz, 2H), 7.03 (d, J = 7.8 Hz, 2H), 6.56 (s, 2H), 2.32 (s, 3H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ 137.6, 136.9, 134.4, 130.3, 129.6, 129.0, 128.9, 128.9, 128.3, 127.0, 21.3.

(*Z*)-1-methoxy-4-styrylbenzene (3b):[15]



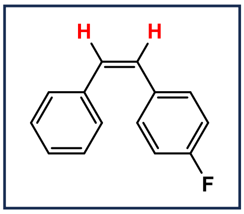
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 92% (96.6 mg) isolated yield; yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.33 – 7.25 (m, 4H), 7.25 – 7.19 (m, 3H), 6.81 – 6.77 (m, 2H), 6.56 (s, 2H), 3.82 (s, 3H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ 158.8, 137.8, 130.3, 129.9, 129.0, 128.9, 128.4, 127.0, 113.7, 55.3.

(*Z*)-1-styryl-4-(trifluoromethyl)benzene (4b):[16]



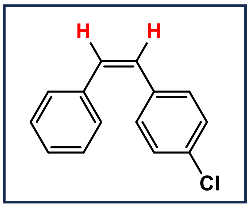
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 80% (99.3 mg) isolated yield; yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.46 (d, J = 7.9 Hz, 2H), 7.32 (d, J = 8.1 Hz, 2H), 7.27 – 7.17 (m, 5H), 6.71 (d, J = 12.2 Hz, 1H), 6.58 (d, J = 12.1 Hz, 1H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ 141.0, 136.7, 132.4, 129.3, 129.0, 128.9, 128.6, 128.5 (q, $J_{C,F}$ = 22.9 Hz), 127.7, 125.3 (q, $J_{C,F}$ = 3.8 Hz), 124.3 (q, $J_{C,F}$ = 271.6 Hz). **^{19}F{^{1}H} NMR** (470 MHz, $CDCl_3$): δ –62.4.

(*Z*)-1-fluoro-4-styrylbenzene (5b):[15]



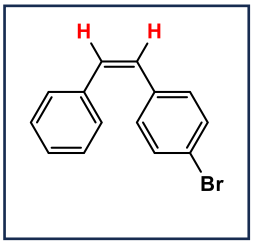
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 74% (73.4 mg) isolated yield; colourless oil. **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.26 – 7.16 (m, 7H), 6.91 (t, J = 8.7 Hz, 2H), 6.60 (d, J = 12.2 Hz, 1H), 6.55 (d, J = 12.2 Hz, 1H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ 161.9 (d, $J_{C,F}$ = 245 Hz), 137.2, 133.3 (d, $J_{C,F}$ = 3.7 Hz), 130.6 (d, $J_{C,F}$ = 8.3 Hz), 130.4, 129.2, 129.0, 128.4, 127.3, 115.3 (d, $J_{C,F}$ = 21.2 Hz). **^{19}F{^{1}H} NMR** (470 MHz, $CDCl_3$): δ –114.6.

(*Z*)-1-chloro-4-styrylbenzene (6b):[15]



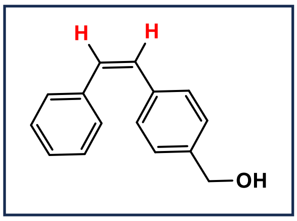
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 82% (88.1 mg) isolated yield; colourless oil. **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.35 – 7.14 (m, 9H), 6.64 (d, J = 12.2 Hz, 1H), 6.54 (d, J = 12.2 Hz, 1H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ 137.0, 135.8, 132.9, 131.1, 129.1, 128.9, 128.5, 128.5, 127.5, 126.8.

(*Z*)-1-bromo-4-styrylbenzene (7b):[15]



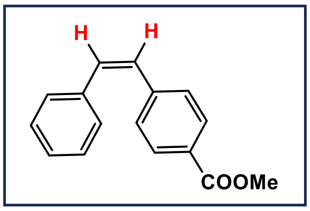
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 77% (99.8 mg) isolated yield; yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.35 (s, 2H), 7.26 – 7.21 (m, 5H), 7.11 (d, J = 8.5 Hz, 2H), 6.64 (d, J = 12.2 Hz, 1H), 6.51 (d, J = 12.2 Hz, 1H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ 136.3, 131.5, 131.2, 130.7, 129.1, 128.9, 128.5, 127.5, 121.1.

(*Z*)-(4-styrylphenyl)methanol (8b):[15]



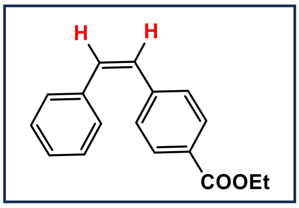
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 81% (85.1 mg) isolated yield; brown oil. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.33 – 7.09 (m, 9H), 6.61 (d, J = 12.2 Hz, 1H), 6.58 (d, J = 12.2 Hz, 1H), 4.65 (s, 2H), 1.71 (s, 1H).**^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ 139.8, 137.3, 136.8, 130.5, 130.0, 129.2, 129.0, 128.4, 127.3, 127.0, 65.3.

methyl (*Z*)-4-styrylbenzoate (9b):[1]



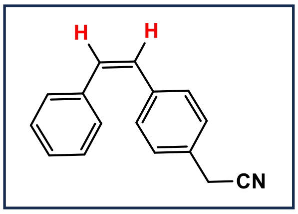
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 79% (94.1 mg) isolated yield; yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.92 – 7.87 (m, 2H), 7.31 (d, J = 8.2 Hz, 2H), 7.25 – 7.19 (m, 5H), 6.71 (d, J = 12.2 Hz, 1H), 6.61 (d, J = 12.2 Hz, 1H), 3.90 (s, 3H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ 167.0, 142.2, 136.8, 132.4, 129.7, 129.4, 129.0, 128.7, 128.5, 127.6, 52.2.

ethyl (*Z*)-4-styrylbenzoate (10b):[17]



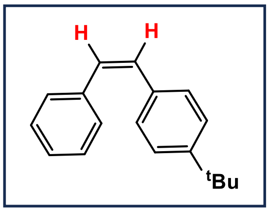
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 76% (95.8 mg) isolated yield; yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.90 (d, J = 8.4 Hz, 2H), 7.30 (d, J = 8.1 Hz, 2H), 7.22 (s, 5H), 6.71 (d, J = 12.2 Hz, 1H), 6.61 (d, J = 12.2 Hz, 1H), 4.36 (q, J = 7.1 Hz, 2H), 1.38 (t, J = 7.3 Hz, 3H).**^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ 166.6, 142.1, 136.8, 132.3, 129.6, 129.4, 129.0, 129.0, 128.5, 127.6, 61.0, 14.5.

(*Z*)-2-(4-styrylphenyl)acetonitrile (11b):[18]



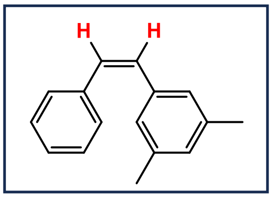
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 70% (76.7 mg) isolated yield; yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.29 – 7.20 (m, 7H), 7.18 (d, J = 8.2 Hz, 2H), 6.65 (d, J = 12.2 Hz, 1H), 6.57 (d, J = 12.2 Hz, 1H), 3.71 (s, 2H).**^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ 137.3, 137.1, 131.2, 129.8, 129.4, 128.9, 128.6, 128.5, 128.0, 127.5, 118.0, 23.5.

(*Z*)-1-(tert-butyl)-4-styrylbenzene (12b):[15]



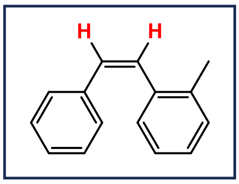
Purified by column chromatography using silica gel and hexane as eluent 83% (98.1 mg) isolated yield; colourless oil. **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.35 – 7.18 (m, 9H), 6.57 (s, 2H), 1.31 (s, 9H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ 150.3, 137.8, 134.3, 130.3, 129.7, 129.0, 128.7, 128.4, 127.1, 125.2, 34.7, 31.4.

(*Z*)-1,3-dimethyl-5-styrylbenzene (13b):[15]



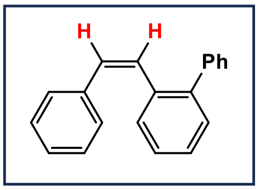
Purified by column chromatography using silica gel and hexane as eluent 82% (85.4 mg) isolated yield; colourless oil. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.29 – 7.23 (m, 3H), 7.21 (d, J = 8.3 Hz, 2H), 6.88 (s, 2H), 6.84 (s, 1H), 6.55 (s, 2H), 2.21 (s, 6H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ 137.8, 137.3, 130.6, 130.0, 129.0, 128.9, 128.2, 127.2, 126.7, 21.3.

(*Z*)-1-methyl-2-styrylbenzene (14b):[15]



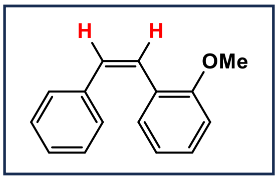
Purified by column chromatography using silica gel and hexane as eluent 89% (86.4 mg) isolated yield; colourless oil. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.21 – 7.02 (m, 9H), 6.68 – 6.59 (m, 2H), 2.28 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ 137.2, 136.2, 131.7, 130.6, 130.2, 129.7, 129.1, 129.0, 128.2, 127.4, 127.2, 125.8, 20.0.

(*Z*)-2-styryl-1,1'-biphenyl (15b):[18]



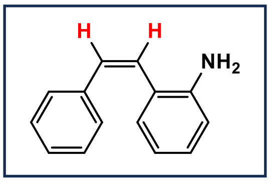
Purified by column chromatography using silica gel and hexane as eluent 78% (99.9 mg) isolated yield; colourless oil. **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.47 – 7.44 (m, 2H), 7.40 – 7.27 (m, 8H), 7.23 – 7.14 (m, 4H), 6.52 (d, J = 12.2 Hz, 1H), 6.43 (d, J = 12.1 Hz, 1H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ 141.3, 137.2, 135.9, 131.7, 130.6, 130.1, 130.1, 129.6, 129.1, 128.3, 128.2, 127.6, 127.2, 127.2, 77.4, 77.2, 76.9.

(*Z*)-1-methoxy-2-styrylbenzene (16b):[19]



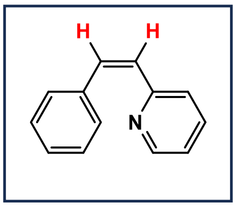
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 90% (94.6 mg) isolated yield; yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.28 – 7.13 (m, 7H), 6.91 (dd, J = 8.4, 1.1 Hz, 1H), 6.77 (td, J = 7.5, 1.1 Hz, 1H), 6.71 (d, J = 12.2 Hz, 1H), 6.65 (d, J = 12.2 Hz, 1H), 3.84 (s, 3H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ 157.4, 137.5, 130.4, 130.3, 129.0, 128.7, 128.6, 128.2, 127.0, 126.0, 120.4, 110.8, 55.6.

(*Z*)-2-styrylaniline (17b):[18]



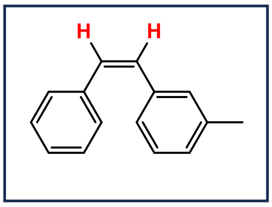
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 83% (81.1 mg) isolated yield; yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.24 – 7.16 (m, 5H), 7.09 (t, J = 7.6 Hz, 2H), 6.70 (dd, J = 7.7, 4.0 Hz, 2H), 6.66 (d, J = 12.2 Hz, 1H), 6.52 (d, J = 12.2 Hz, 1H), 3.70 (s, 2H).**^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ 143.8, 136.8, 131.8, 129.7, 128.9, 128.5, 128.3, 127.6, 126.6, 123.3, 118.6, 115.7.

(*Z*)-2-styrylpyridine (18b):[20]



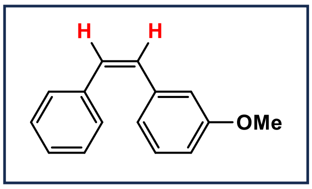
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 81% (73.3 mg) isolated yield; yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$): δ 8.59 (d, J = 4.9 Hz, 1H), 7.44 (td, J = 7.7, 1.7 Hz, 1H), 7.31 – 7.19 (m, 5H), 7.16 (d, J = 7.9 Hz, 1H), 7.09 (ddd, J = 7.5, 4.8, 1.2 Hz, 1H), 6.84 (d, J = 12.2 Hz, 1H), 6.70 (d, J = 12.2 Hz, 1H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ 156.4, 149.6, 136.8, 135.9, 133.5, 130.5, 129.0, 128.4, 127.8, 124.0, 121.9.

(*Z*)-1-methyl-3-styrylbenzene (19b):[1]



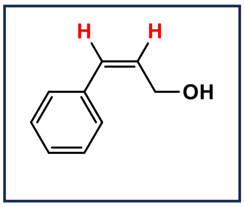
Purified by column chromatography using silica gel and hexane as eluent 90% (87.4 mg) isolated yield; colourless oil. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.28 – 7.18 (m, 5H), 7.09 (dd, J = 12.3, 7.4 Hz, 3H), 7.01 (d, J = 7.3 Hz, 1H), 6.58 (s, 2H), 2.27 (s, 3H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ 137.9, 137.5, 137.3, 130.5, 130.2, 129.7, 129.0, 128.3, 128.2, 128.0, 127.2, 126.0, 77.5, 77.2, 76.8, 21.5.

(*Z*)-1-methoxy-3-styrylbenzene (20b):[20]



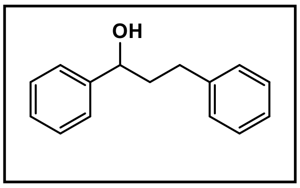
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 91% (95.7 mg) isolated yield; yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.28 – 7.12 (m, 6H), 6.84 (d, J = 7.7 Hz, 1H), 6.79 (t, J = 2.1 Hz, 1H), 6.75 (dd, J = 8.1, 2.7 Hz, 1H), 6.62 (d, J = 12.2 Hz, 1H), 6.57 (d, J = 12.2 Hz, 1H), 3.65 (s, 3H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ 159.5, 138.7, 137.4, 130.6, 130.3, 129.4, 129.1, 128.4, 127.3, 121.7, 113.9, 113.5, 55.2.

(*Z*)-3-phenylprop-2-en-1-ol (21b):[14]



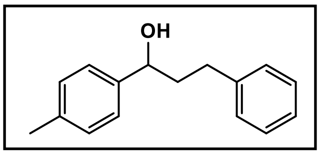
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 68% (45.6 mg) isolated yield; yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.35 (dd, J = 8.2, 6.8 Hz, 2H), 7.30 – 7.25 (m, 1H), 7.22 (dd, J = 7.0, 1.7 Hz, 2H), 6.58 (d, J = 11.7 Hz, 1H), 5.88 (dt, J = 11.7, 6.4 Hz, 1H), 4.44 (dd, J = 6.3, 1.7 Hz, 2H).**^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): 136.7, 131.3, 131.2, 128.9, 128.4, 127.4, 59.8.

1,3-diphenylpropan-1-ol (22d):[2]



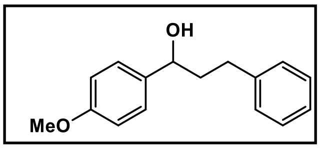
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 88% (93.4 mg) isolated yield; colourless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.35 (d, *J* = 3.7 Hz, 4H), 7.29 (dd, *J* = 9.0, 5.9 Hz, 3H), 7.23 – 7.16 (m, 3H), 4.68 (dd, *J* = 7.9, 5.5 Hz, 1H), 2.77 – 2.64 (m, 2H), 2.16 – 1.99 (m, 3H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ 144.7, 141.9, 128.6, 128.6, 128.5, 127.7, 126.0, 126.0, 74.0, 40.6, 32.2.

3-phenyl-1-(*p*-tolyl)propan-1-ol (23d):[21]



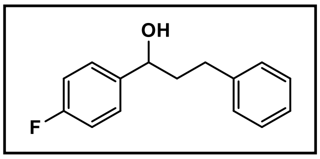
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 86% (97.3 mg) isolated yield; colourless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.27 (t, J = 8.5 Hz, 5H), 7.22–7.17 (m, 4H), 4.67 (t, J = 6.7 Hz, 1H), 2.72 (ddd, J = 25.4, 12.9, 6.5 Hz, 2H), 2.36 (s, 3H), 2.10 (ddd, J = 38.8, 13.1, 6.9 Hz, 3H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ 142.0, 141.7, 137.5, 129.3, 128.6, 128.5, 126.0, 126.0, 73.9, 40.5, 32.2, 21.2.

1-(4-methoxyphenyl)-3-phenylpropan-1-ol (24d):[21]



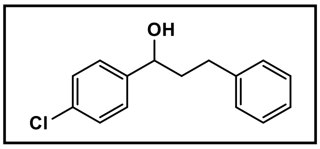
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 81% (98.1 mg) isolated yield; colourless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.29 (dd, J = 8.3, 6.3 Hz, 4H), 7.23–7.15 (m, 3H), 6.94–6.84 (m, 2H), 4.64 (dd, J = 7.7, 5.7 Hz, 1H), 3.82 (s, 3H), 2.76–2.62 (m, 2H), 2.22–1.90 (m, 3H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ 159.2, 142.0, 136.8, 128.6, 128.5, 127.3, 126.0, 114.0, 73.6, 55.4, 40.4, 32.2.

1-(4-fluorophenyl)-3-phenylpropan-1-ol (25d):[22]



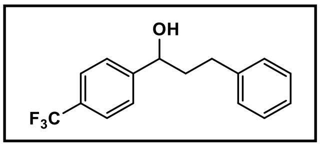
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 89% (102.4 mg) isolated yield; colourless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.31 (dt, J = 14.3, 7.2 Hz, 5H), 7.19 (d, J = 7.4 Hz, 3H), 7.04 (t, J = 8.5 Hz, 2H), 4.69 (t, J = 6.7 Hz, 1H), 2.71 (ddt, J = 23.8, 15.3, 7.7 Hz, 2H), 2.20 – 1.93 (m, 3H).**^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ 162.3 (d, $J_{C,F}$ = 245.5 Hz), 141.7, 140.4 (d, $J_{C,F}$ = 3 Hz), 128.6, 128.5, 127.6 (d, $J_{C,F}$ = 8 Hz), 126.1, 115.4 (d, $J_{C,F}$ = 21.3 Hz), 73.4, 40.7, 32.1.**^{19}F{^{1}H} NMR** (470 MHz, $CDCl_3$): δ –114.9.

1-(4-chlorophenyl)-3-phenylpropan-1-ol (26d):[22]



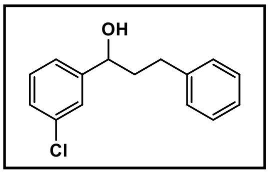
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 88% (108.56 mg) isolated yield; colourless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.31 (dt, *J* = 18.6, 9.6 Hz, 7H), 7.18 (d, *J* = 8.3 Hz, 2H), 4.67 (t, *J* = 7.0 Hz, 1H), 2.69 (td, *J* = 14.8, 7.5 Hz, 2H), 2.27–1.92 (m, 3H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ 143.2, 141.6, 133.4, 128.8, 128.6, 128.6, 127.4, 126.1, 73.3, 40.6, 32.1.

3-phenyl-1-(4-(trifluoromethyl)phenyl)propan-1-ol (27d):[2]



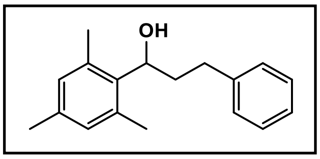
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 92% (128.9 mg) isolated yield; colourless oil. **^{1}H NMR** (400 MHz, $CDCl_3$). δ 7.62 (d, J = 8.0 Hz, 2H), 7.47 (d, J = 8.0 Hz, 2H), 7.34 – 7.27 (m, 2H), 7.20 (d, J = 7.6 Hz, 3H), 4.77 (dd, J = 7.9, 5.0 Hz, 1H), 2.81–2.67 (m, 2H), 2.18 – 1.97 (m, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ 148.7, 141.5, 130.8 (q, $J_{C,F}$ = 32.6 Hz), 128.6, 128.5, 128.3, 126.2, 125.6 (q, $J_{C,F}$ = 3.8 Hz), 124.1 (q, $J_{C,F}$ = 271.4 Hz), 73.3, 40.7, 32.0. **^{19}F{^{1}H} NMR** (470 MHz, $CDCl_3$): δ –62.3.

1-(3-chlorophenyl)-3-phenylpropan-1-ol (28d):[23]



Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 80% (98.7 mg) isolated yield; colourless oil. **^{1}H NMR** (400 MHz, $CDCl_3$). δ 7.36 (s, 1H), 7.29 (dd, J = 13.1, 6.9 Hz, 4H), 7.20 (d, J = 8.1 Hz, 4H), 4.67 (s, 1H), 2.73 (tt, J = 14.6, 7.2 Hz, 2H), 2.05 (ddq, J = 29.1, 13.8, 6.7 Hz, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ 146.8, 141.6, 134.5, 129.9, 128.6, 127.8, 126.2, 126.1, 124.2, 73.3, 40.6, 32.0.

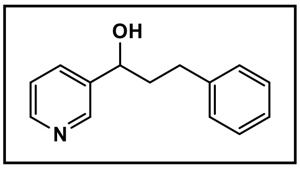
1-mesityl-3-phenylpropan-1-ol (29d):[2]



Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 79% (100 mg) isolated yield; colourless oil. **^{1}H NMR** (500 MHz, $CDCl_3$). δ 7.33–7.28 (m, 2H), 7.26–7.18 (m, 3H), 6.82 (s, 2H), 5.14 (dd, J = 9.3, 4.7 Hz, 1H), 2.91 (ddd, J = 14.3, 9.6, 5.0 Hz, 1H), 2.70 (ddd, J = 13.8, 9.3, 7.3 Hz, 1H), 2.41–2.37 (m, 1H), 2.35 (s, 6H), 2.26 (s, 3H), 2.02–1.95 (m, 1H), 1.73

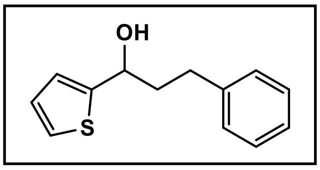
(s, 1H).**^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ 142.0, 136.9, 136.1, 130.3, 128.6, 128.5, 126.0, 70.7, 37.2, 32.9, 20.8, 20.7.

3-phenyl-1-(pyridin-3-yl)propan-1-ol (30d):[2]



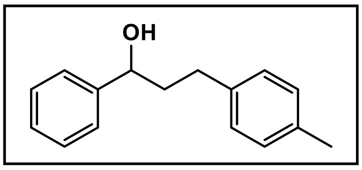
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 83% (88.5 mg) isolated yield; colourless oil. **^{1}H NMR** (400 MHz, $CDCl_3$). δ 8.38 (s, 1H), 8.34 (d, J = 4.9 Hz, 1H), 7.70 (d, J = 7.6 Hz, 1H), 7.30 – 7.14 (m, 6H), 4.68 (dd, J = 8.2, 5.2 Hz, 1H), 4.42 (s, 1H), 2.71 (dddd, J = 20.8, 14.1, 9.8, 5.8 Hz, 2H), 2.12 (ddd, J = 16.7, 8.2, 4.0 Hz, 1H), 1.99 (ddd, J = 14.4, 9.6, 5.2 Hz, 1H).**^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ 148.3, 147.6, 141.5, 140.7, 134.1, 128.5, 128.5, 126.0, 123.7, 71.0, 40.6, 32.0.

3-phenyl-1-(thiophen-2-yl)propan-1-ol (31d):[24]



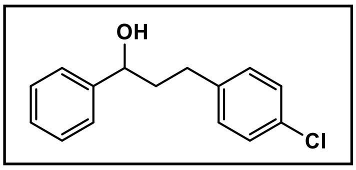
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 80% (87.3 mg) isolated yield; colourless oil. **^{1}H NMR** (400 MHz, $CDCl_3$). δ 7.34–7.28 (m, 3H), 7.21 (d, J = 6.9 Hz, 4H), 7.11 (d, J = 5.0 Hz, 1H), 4.80 (t, J = 6.6 Hz, 1H), 2.84–2.67 (m, 2H), 2.20–2.06 (m, 2H), 1.87 (s, 1H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ 146.1, 141.8, 128.6, 128.6, 126.4, 126.0, 125.8, 121.1, 70.0, 39.9, 32.1.

1-phenyl-3-(p-tolyl)propan-1-ol (32d):[23]



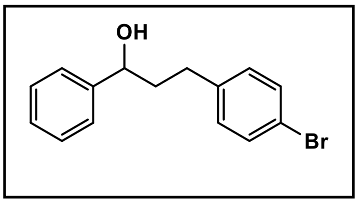
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 84% (95.1 mg) isolated yield; colourless oil. **^{1}H NMR** (400 MHz, $CDCl_3$). δ 7.37 (d, J = 4.3 Hz, 4H), 7.31–7.28 (m, 1H), 7.10 (s, 4H), 4.70 (dd, J = 7.8, 5.4 Hz, 1H), 2.69 (ddd, J = 18.3, 9.3, 6.0 Hz, 2H), 2.33 (m, 3H), 2.21 – 1.91 (m, 3H).**^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ 144.7, 138.8, 135.4, 129.2, 128.6, 128.4, 127.8, 126.1, 74.1, 40.7, 31.7, 21.1.

3-(4-chlorophenyl)-1-phenylpropan-1-ol (33d):[24]



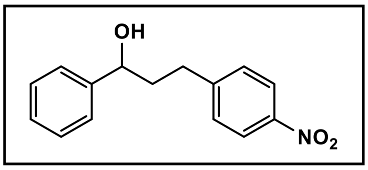
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 83% (102 mg) isolated yield; colourless oil. **^{1}H NMR** (400 MHz, $CDCl_3$). δ 7.36 (s, 4H), 7.30 (s, 1H), 7.26 (d, J = 8.9 Hz, 2H), 7.13 (d, J = 8.1 Hz, 2H), 4.68 (t, J = 7.0 Hz, 1H), 2.71 (dt, J = 25.6, 8.2 Hz, 2H), 2.06 (dp, J = 38.1, 7.2 Hz, 3H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ 144.5, 140.4, 131.7, 129.9, 128.7, 128.7, 128.6, 127.9, 126.0, 73.9, 40.5, 31.5.

3-(4-bromophenyl)-1-phenylpropan-1-ol (34d):[24]



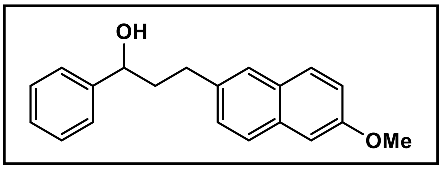
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 78% (113.1 mg) isolated yield; colourless oil. **^{1}H NMR** (400 MHz, $CDCl_3$). δ 7.47 – 7.28 (m, 7H), 7.07 (d, J = 8.0 Hz, 2H), 4.67 (dd, J = 7.8, 5.3 Hz, 1H), 2.67 (ddd, J = 16.6, 9.4, 6.1 Hz, 2H), 2.19 – 1.85 (m, 3H). **$^{13}C\{^1H\}$ NMR** (125 MHz, $CDCl_3$): δ 144.5, 140.9, 131.6, 128.7, 128.5, 127.9, 126.0, 119.7, 73.8, 40.4, 31.6.

3-(4-nitrophenyl)-1-phenylpropan-1-ol (35d):[2]



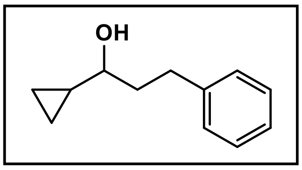
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 78% (99 mg) isolated yield; colourless oil. **^1H NMR** (500 MHz, $CDCl_3$). δ 8.15 (d, J = 8.5 Hz, 2H), 7.39 – 7.31 (m, 7H), 4.71 (dd, J = 8.1, 5.2 Hz, 1H), 2.88 (td, J = 9.9, 9.3, 4.8 Hz, 1H), 2.83 – 2.78 (m, 1H), 2.19 – 2.13 (m, 1H), 2.08 – 2.03 (m, 1H), 1.91 (s, 1H). **$^{13}C\{^1H\}$ NMR** (125 MHz, $CDCl_3$): δ 144.3, 129.4, 128.8, 128.1, 126.0, 123.8, 73.8, 40.0, 32.1.

3-(6-methoxynaphthalen-2-yl)-1-phenylpropan-1-ol (36d):[24]



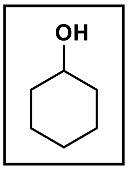
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 75% (109.5 mg) isolated yield; colourless oil. **^1H NMR** (500 MHz, $CDCl_3$). δ 7.67 (dd, J = 8.4, 2.3 Hz, 2H), 7.57 (s, 1H), 7.37 (d, J = 4.2 Hz, 4H), 7.31 (td, J = 7.4, 6.4, 3.0 Hz, 2H), 7.15–7.11 (m, 2H), 4.72 (t, J = 6.8 Hz, 1H), 3.92 (s, 3H), 2.92–2.80 (m, 2H), 2.25–2.19 (m, 1H), 2.11 (ddd, J = 20.3, 9.6, 6.0 Hz, 1H), 1.95 (d, J = 3.1 Hz, 1H). **$^{13}C\{^1H\}$ NMR** (100 MHz, $CDCl_3$): δ 157.3, 144.7, 137.0, 133.1, 129.2, 129.0, 128.7, 127.9, 127.8, 127.0, 126.5, 126.1, 118.8, 105.8, 74.0, 55.4, 40.6, 32.1.

1-cyclopropyl-3-phenylpropan-1-ol (37d):[21]



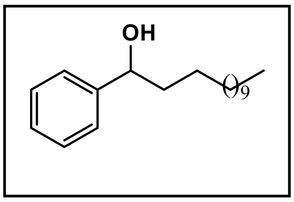
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 81% (71.3 mg) isolated yield; colourless oil. **^1H NMR** (400 MHz, $CDCl_3$). δ 7.36 – 7.13 (m, 5H), 2.99 – 2.63 (m, 3H), 1.92 (q, J = 7.3 Hz, 2H), 1.63 (s, 2H), 0.93 (dq, J = 8.1, 4.3, 3.5 Hz, 1H), 0.51 (qt, J = 11.8, 5.9 Hz, 2H), 0.22 (ddq, J = 22.3, 8.2, 4.1 Hz, 2H). **$^{13}C\{^1H\}$ NMR** (125 MHz, $CDCl_3$): δ 142.4, 128.5, 128.5, 125.9, 76.3, 38.8, 32.2, 18.2, 2.9, 2.7.

cyclohexanol (38d):[21]



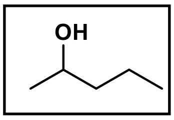
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 78% (38.5 mg) isolated yield; colourless oil. **^1H NMR** (400 MHz, $CDCl_3$). δ 3.57 (hept, J = 4.1 Hz, 1H), 1.87 (td, J = 11.4, 10.9, 6.2 Hz, 3H), 1.70 (dd, J = 8.9, 4.5 Hz, 2H), 1.56 – 1.45 (m, 1H), 1.32–1.11 (m, 5H). **$^{13}C\{^1H\}$ NMR** (100 MHz, $CDCl_3$): δ 70.4, 35.6, 25.5, 24.2.

1-phenylpentan-1-ol (39d):[2]



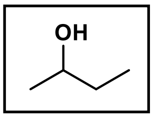
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 73% (59.9 mg) isolated yield; colourless oil. **^1H NMR** (500 MHz, $CDCl_3$). δ 7.36 (d, J = 4.6 Hz, 4H), 7.31 – 7.27 (m, 1H), 4.70 – 4.65 (m, 1H), 1.77 (ddd, J = 37.6, 9.2, 4.4 Hz, 2H), 1.43 (dd, J = 13.0, 6.8 Hz, 1H), 1.27 (s, 20H), 0.90 (t, J = 6.8 Hz, 3H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ 145.1, 128.6, 127.6, 126.0, 74.9, 39.3, 32.1, 29.8, 29.7, 29.5, 26.0, 22.8, 14.3.

pentan-2-ol (40d)[25]



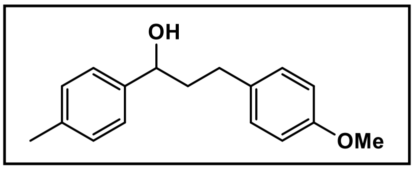
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 78% NMR yield; colourless liquid. **^{1}H NMR** (400 MHz, $CDCl_3$). δ 3.81 (td, *J* = 6.4, 4.3 Hz, 1H), 1.42 (tdd, *J* = 14.0, 6.7, 4.0 Hz, 4H), 1.19 (d, *J* = 6.1 Hz, 3H), 0.97 – 0.89 (m, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ 68.1, 41.7, 23.6, 19.1, 14.2.

butan-2-ol (41d)[25]



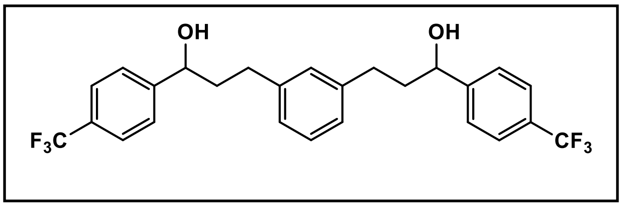
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 71% NMR yield; colourless liquid. **^{1}H NMR** (400 MHz, $CDCl_3$). δ 3.72 (h, *J* = 6.1 Hz, 1H), 1.53 – 1.40 (m, 2H), 1.18 (d, *J* = 5.9 Hz, 3H), 0.92 (t, *J* = 7.5 Hz, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): 69.6, 32.1, 23.0, 10.1.

3-(4-methoxyphenyl)-1-(p-tolyl)propan-1-ol (42d):[2]



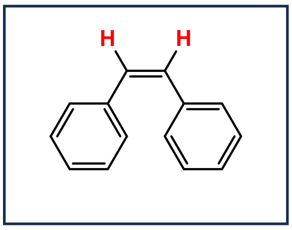
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 76% (97.4 mg) isolated yield; colourless oil. **^{1}H NMR** (500 MHz, $CDCl_3$). δ 7.26 (d, J = 7.7 Hz, 2H), 7.19 (d, J = 7.8 Hz, 2H), 7.14 (d, J = 8.6 Hz, 2H), 6.86 (d, J = 9.0 Hz, 2H), 4.65 (dd, J = 7.7, 5.4 Hz, 1H), 3.81 (s, 3H), 2.72 – 2.60 (m, 2H), 2.38 (s, 3H), 2.15 – 1.97 (m, 3H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ 157.8, 137.3, 134.0, 129.4, 129.2, 126.0, 113.9, 73.7, 31.2, 21.2.

3,3'-(1,3-phenylene)bis(1-(4-(trifluoromethyl)phenyl)propan-1-ol) (43d):[2]

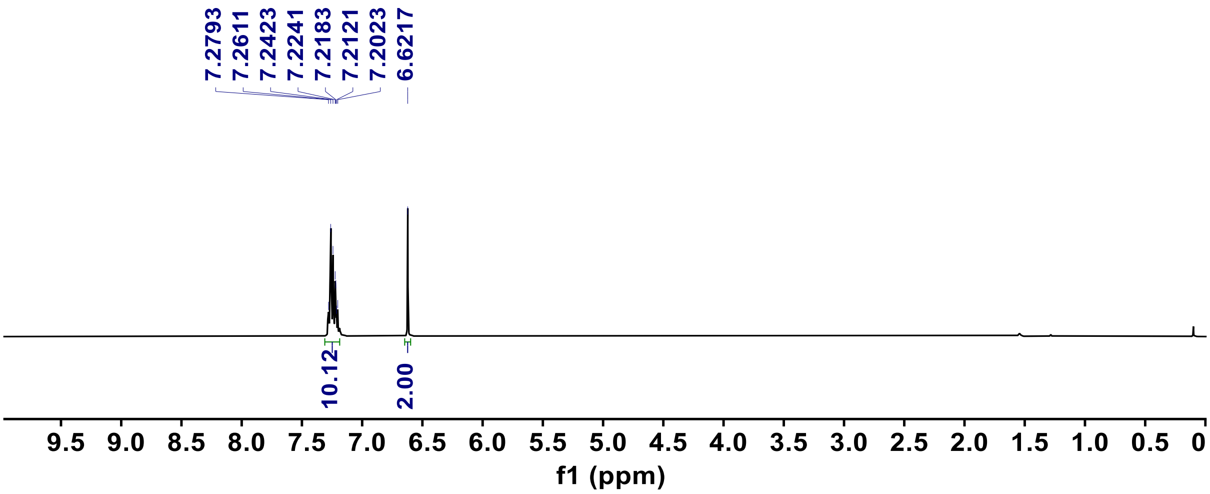


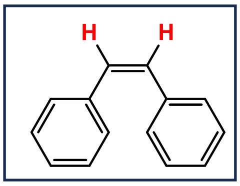
Purified by column chromatography using silica gel and ethyl acetate-hexane as eluent 80% (192 mg) isolated yield; colourless oil. **^{1}H NMR** (500 MHz, $CDCl_3$). δ 7.55 (s, 2H), 7.40 – 7.37 (m, 2H), 7.37 (d, *J* = 1.6 Hz, 4H), 7.31 (d, *J* = 7.8 Hz, 4H), 4.69 (dd, *J* = 7.7, 5.3 Hz, 2H), 2.83 (ddd, *J* = 15.1, 9.8, 5.6 Hz, 2H), 2.78 – 2.70 (m, 2H), 2.19 – 2.11 (m, 2H), 2.05 (ddd, *J* = 14.2, 10.1, 5.0 Hz, 2H), 2.00 (d, *J* = 9.9 Hz, 2H). **^{13}C{^{1}H} NMR** (125 MHz, $CDCl_3$): δ 146.1, 144.4, 128.8 (q, $J_{C,F}$ = 32.2 Hz), 128.0, 126.0, 125.4 (q, $J_{C,F}$ = 5 Hz), 124.5 (q, $J_{C,F}$ = 271.9 Hz), 73.8, 40.2, 32.0.**^{19}F{^{1}H} NMR** (470 MHz, $CDCl_3$): δ –62.3.

12. Copies of ^{1}H and ^{13}C NMR Spectra of Products

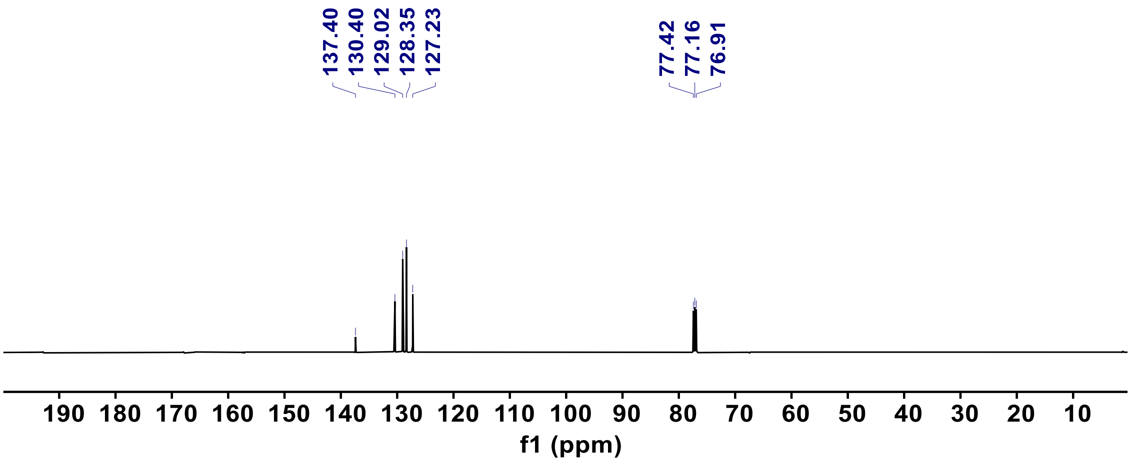


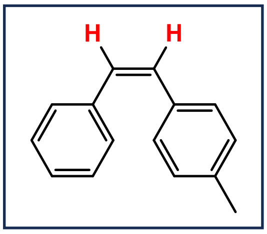
^{1}H NMR ($CDCl_3$, 400 MHz), **1b**



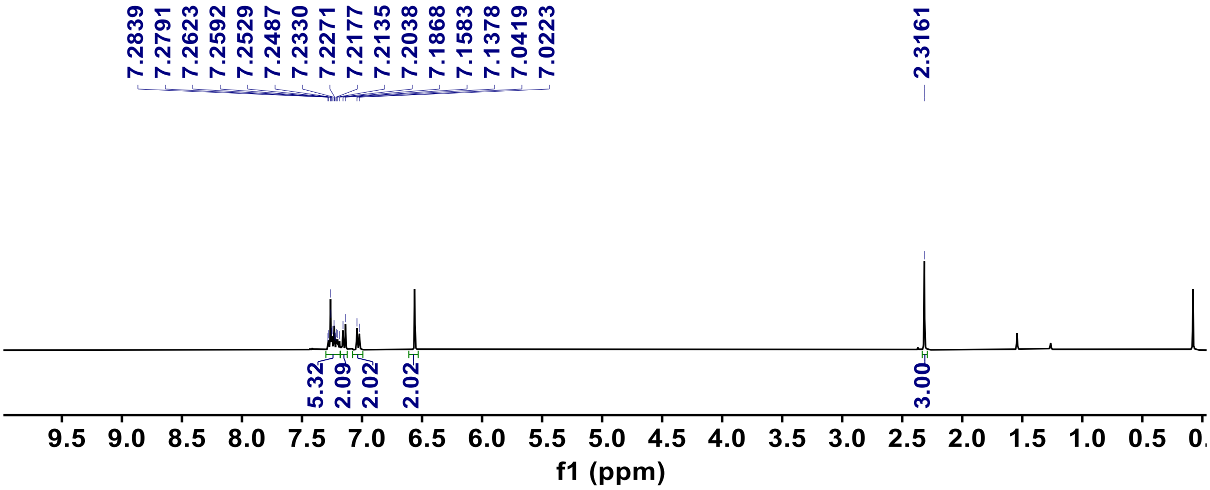


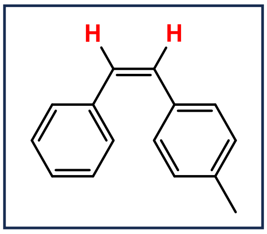
^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$), **1b**



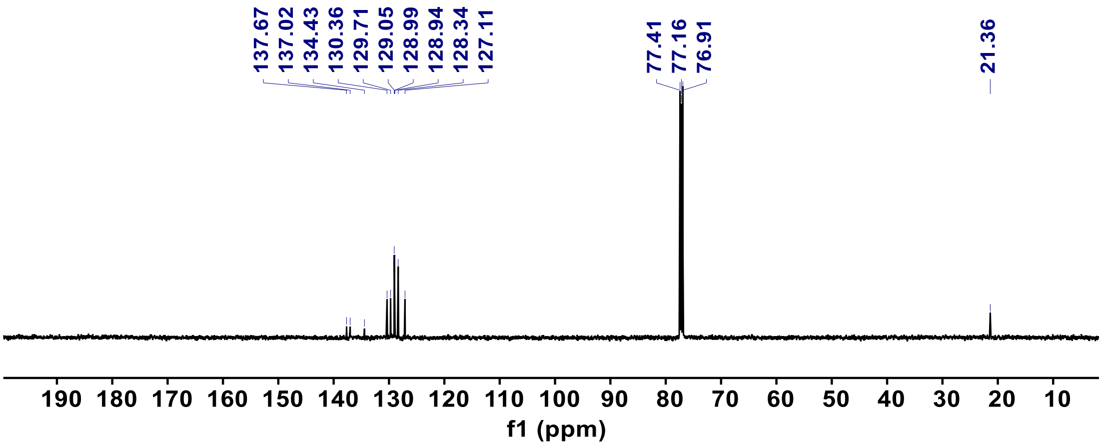


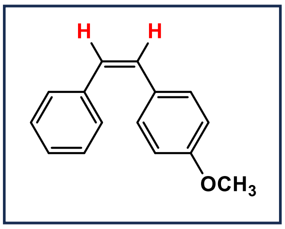
^{1}**H NMR** (CDCl$_3$, 400 MHz), **2b**



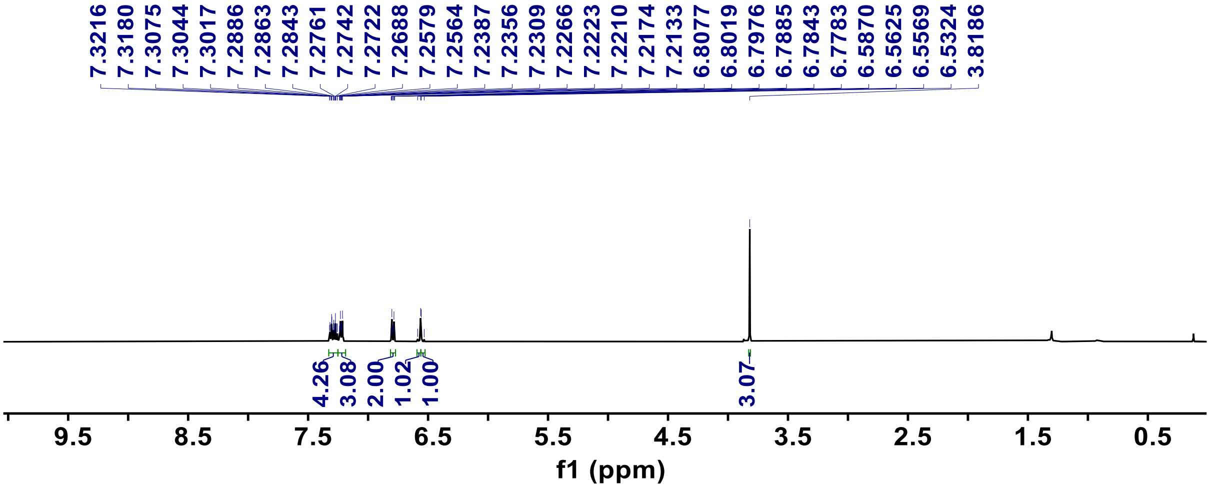


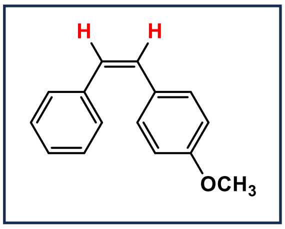
^{13}**C{^{1}H} NMR** (125 MHz, CDCl$_3$), **2b**



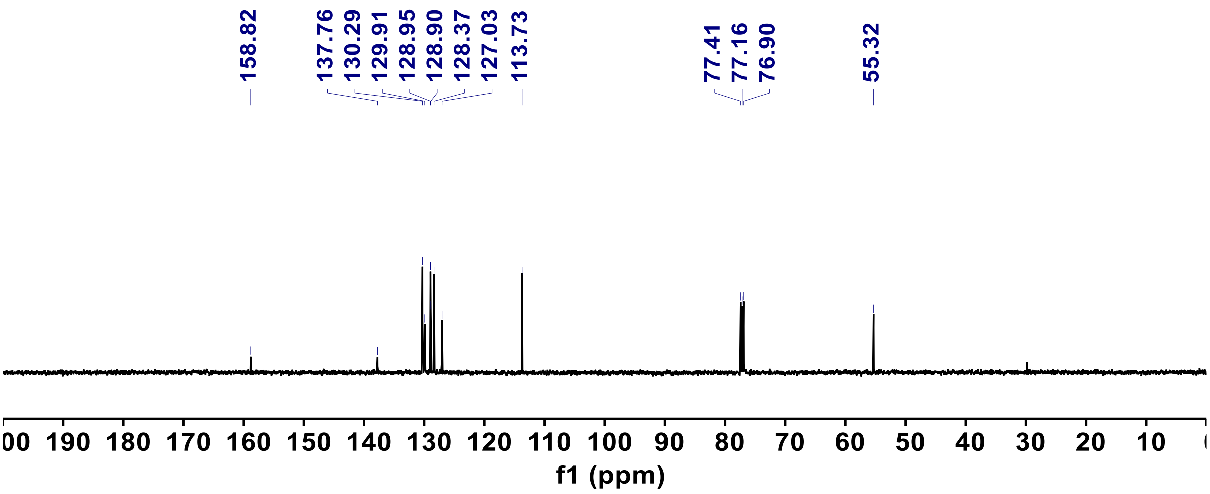


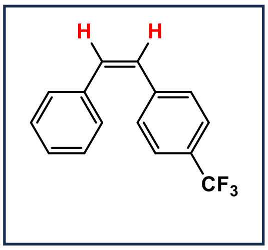
[1]H NMR ($CDCl_3$, 500 MHz), **3b**



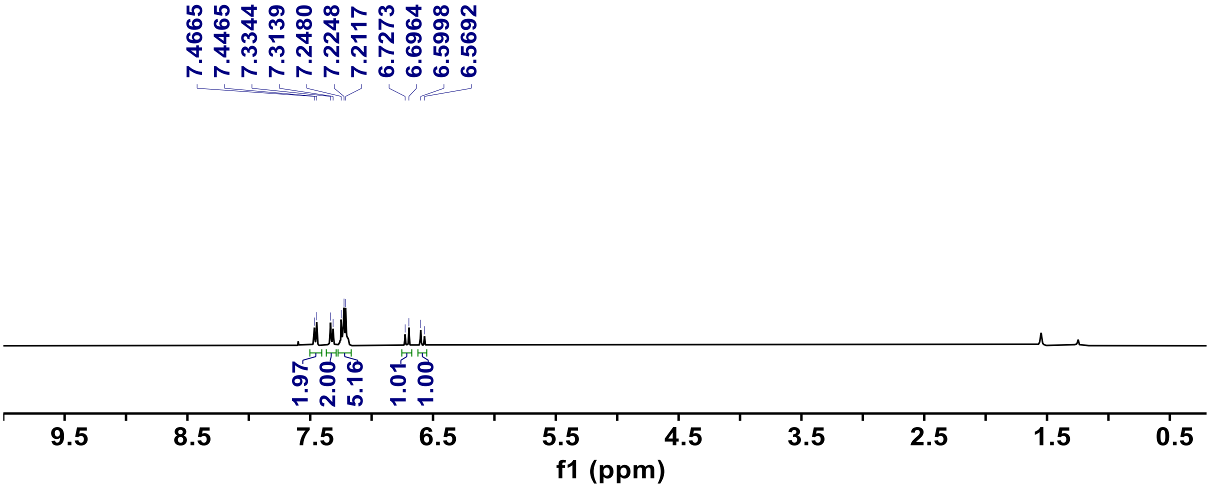


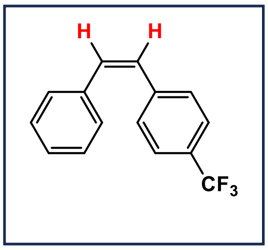
[13]C{[1]H} NMR (125 MHz, $CDCl_3$), **3b**



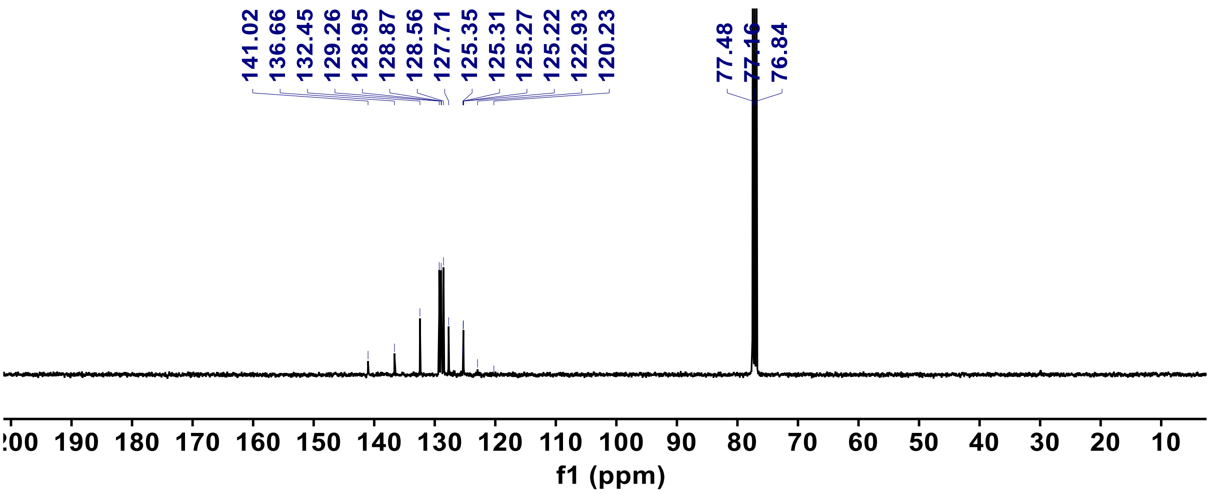


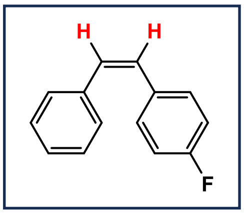
[1]H NMR (CDCl3, 400 MHz), **4b**



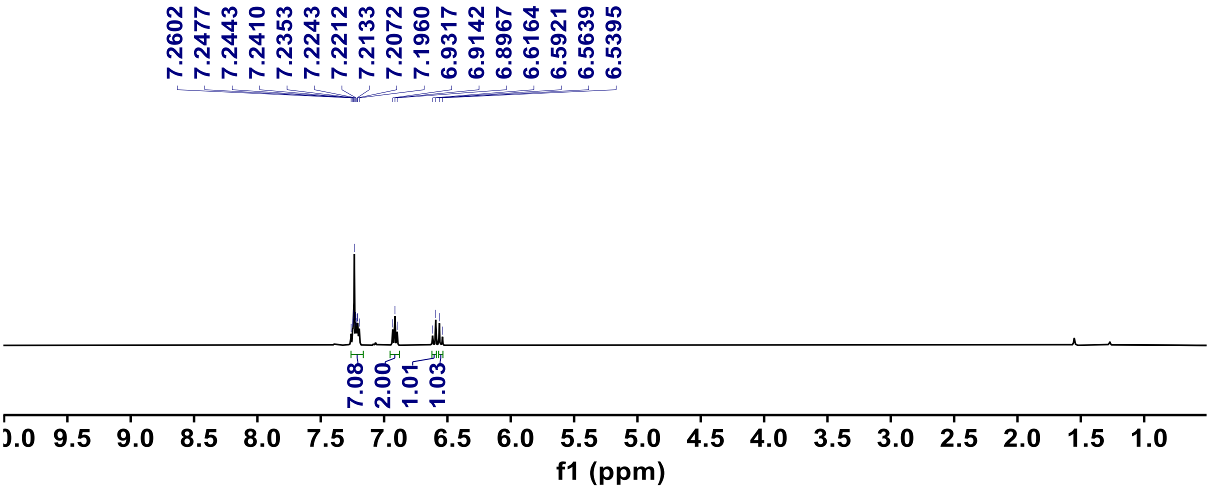


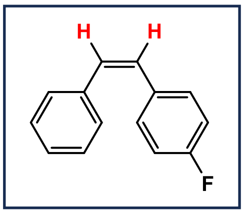
[13]C{[1]H} NMR (100 MHz, CDCl3), **4b**



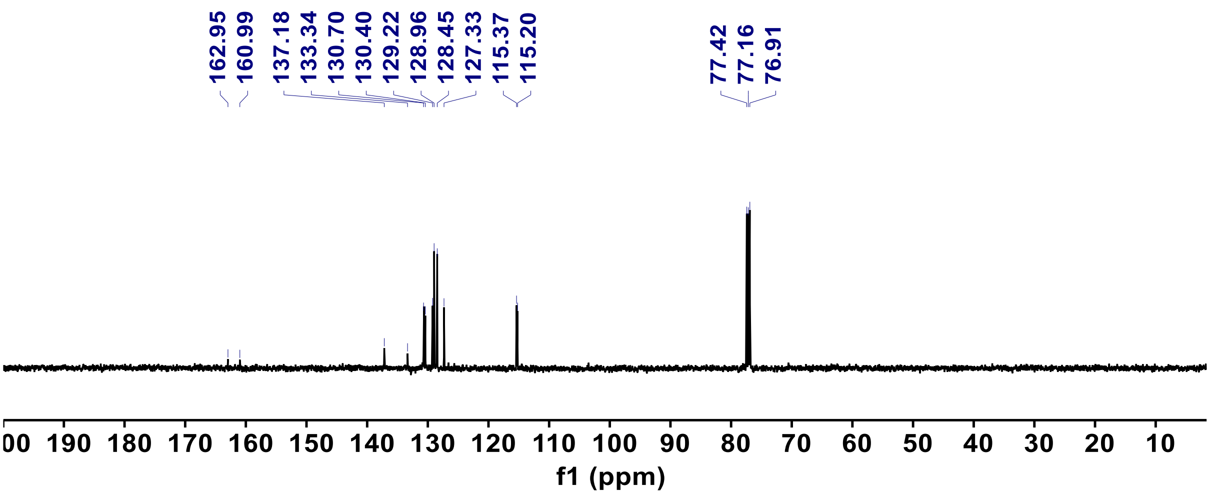


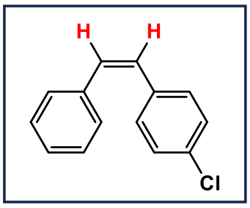
^{1}**H NMR** (CDCl$_3$, 500 MHz), **5b**



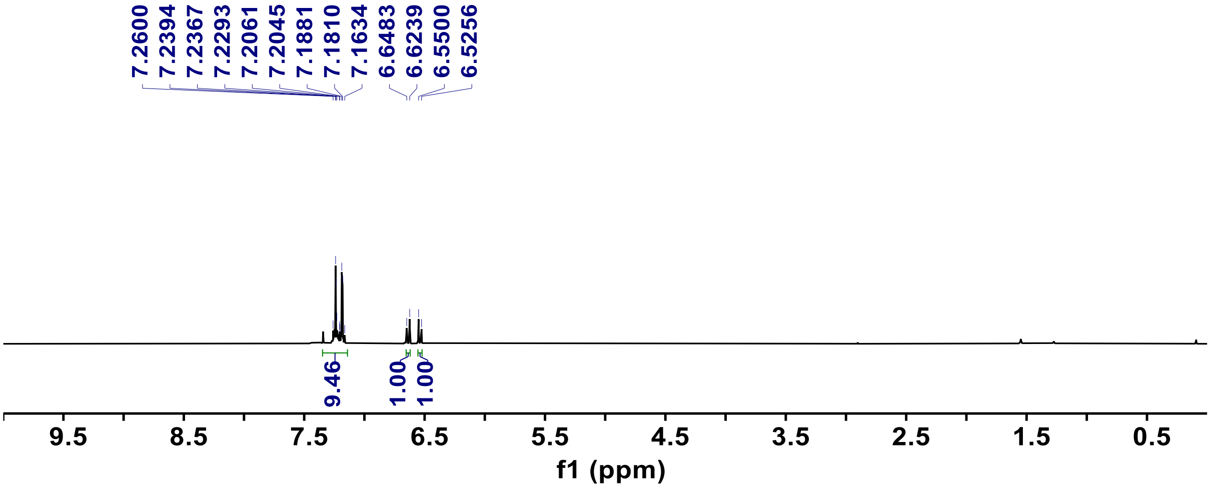


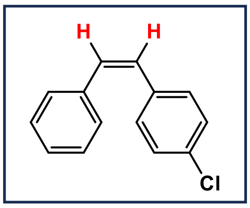
^{13}**C{^{1}H} NMR** (125 MHz, CDCl$_3$), **5b**



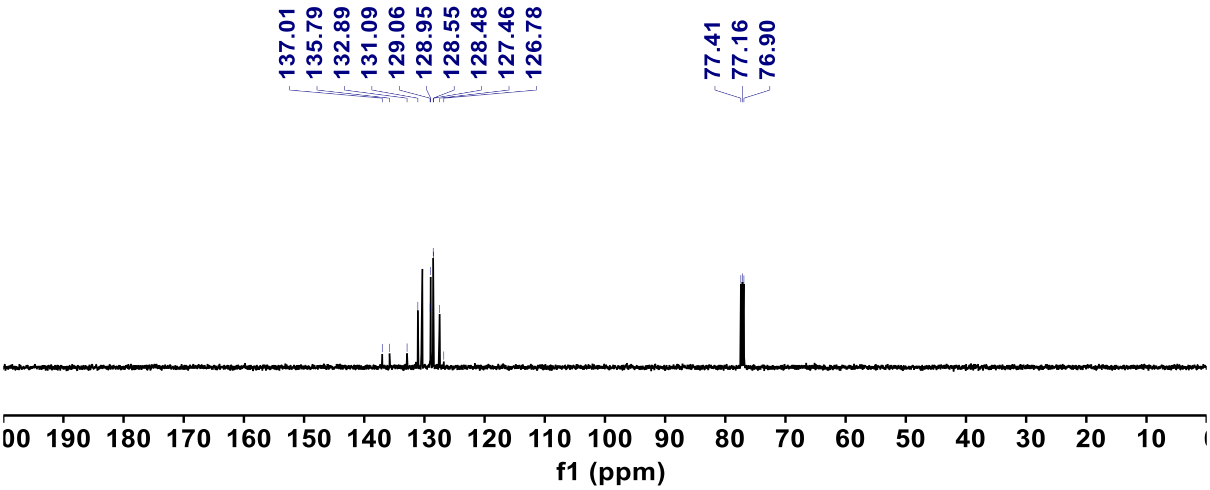


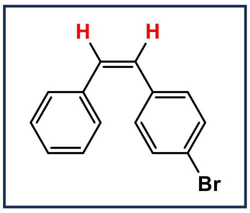
^{1}H NMR ($CDCl_3$, 500 MHz), **6b**



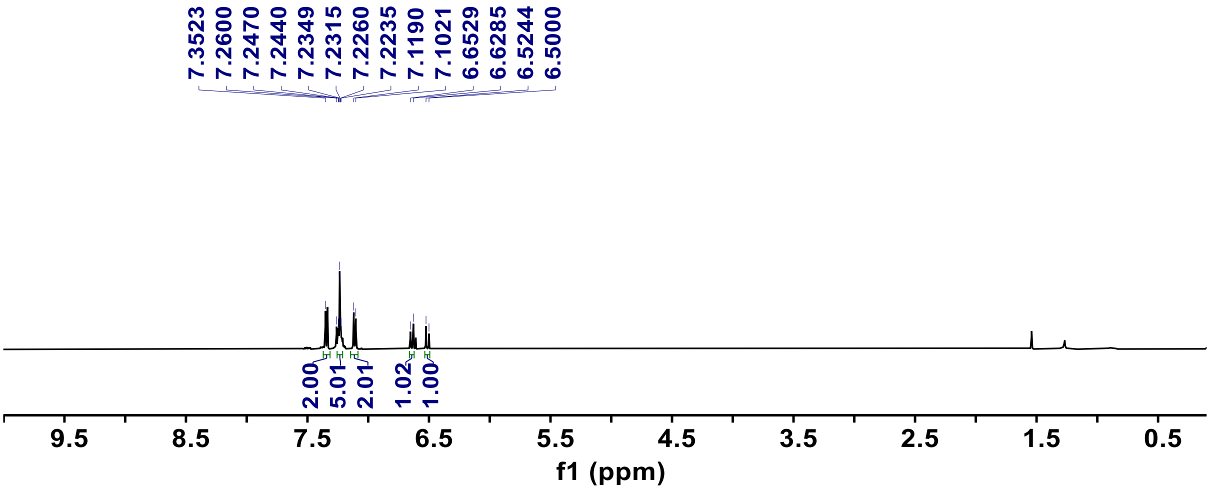


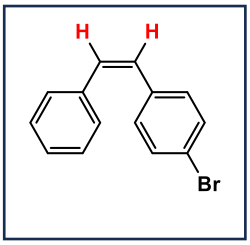
^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$), **6b**



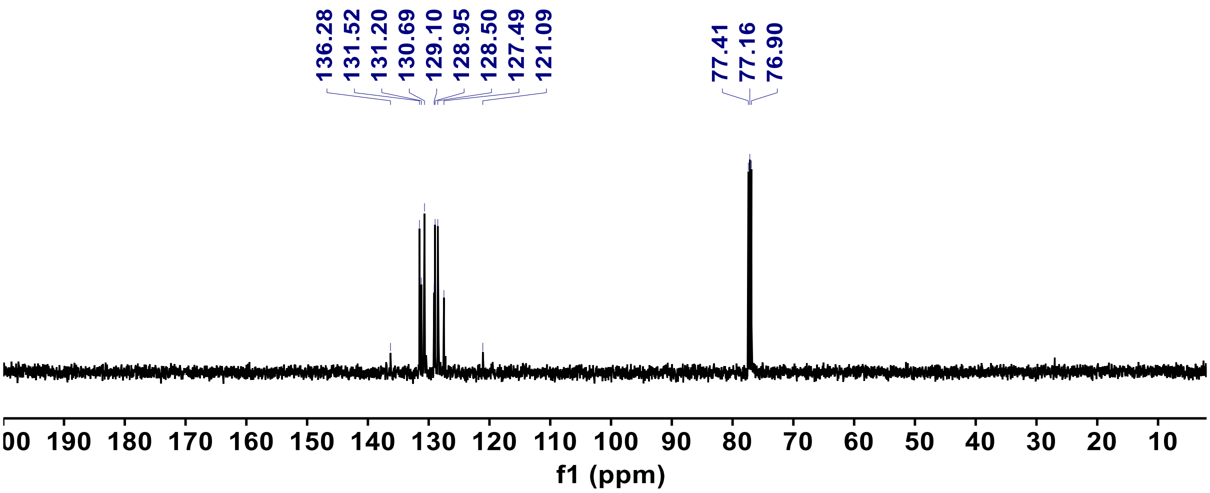


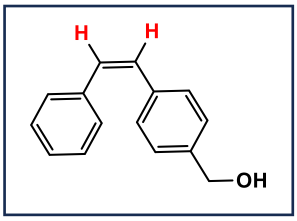
^{1}H NMR ($CDCl_3$, 500 MHz), **7b**



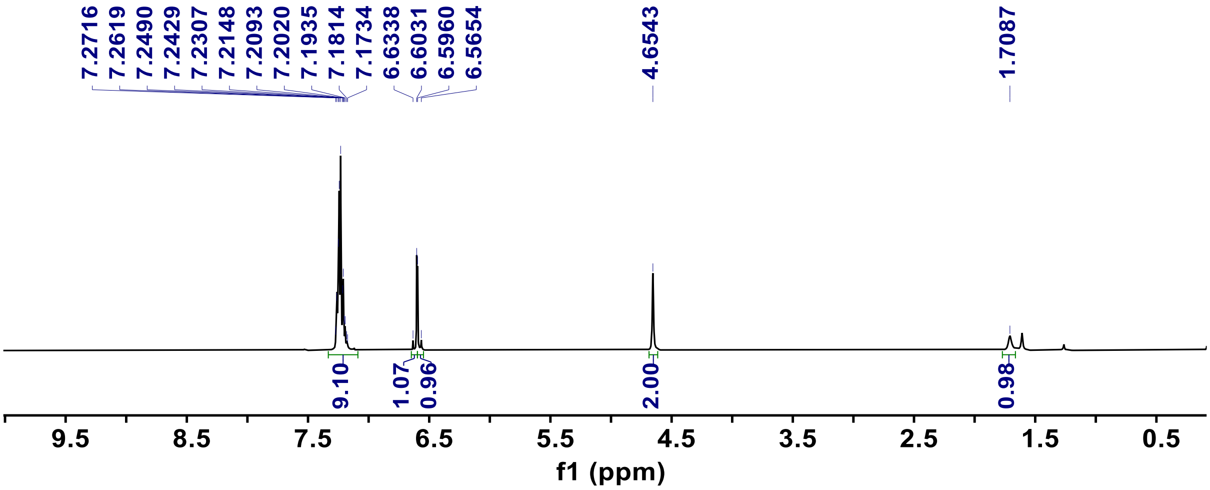


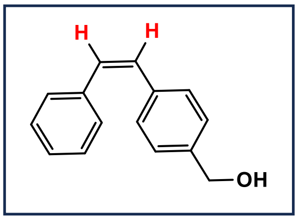
^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$), **7b**



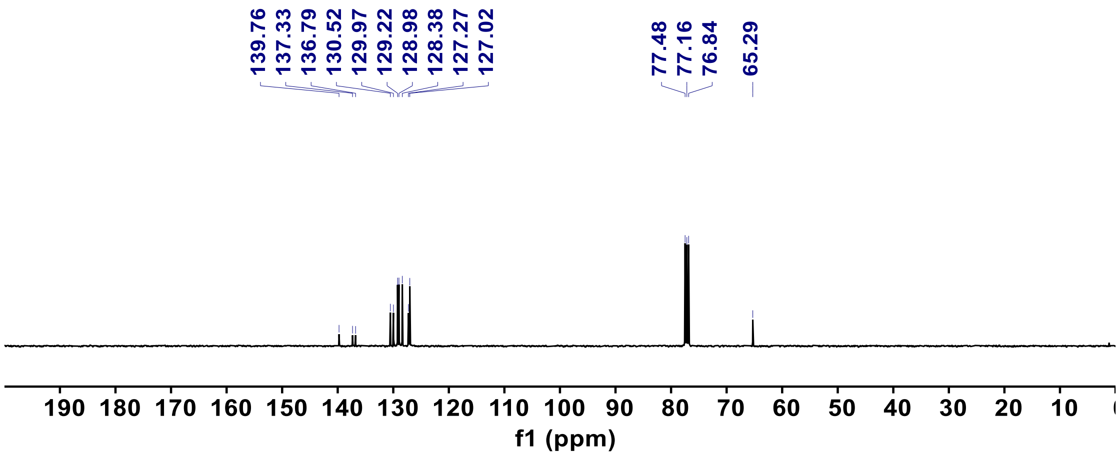


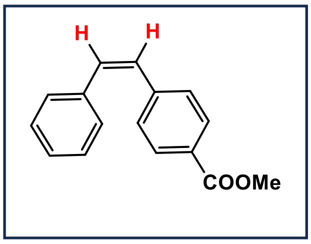
^{1}H NMR (CDCl$_3$, 400 MHz), **8b**



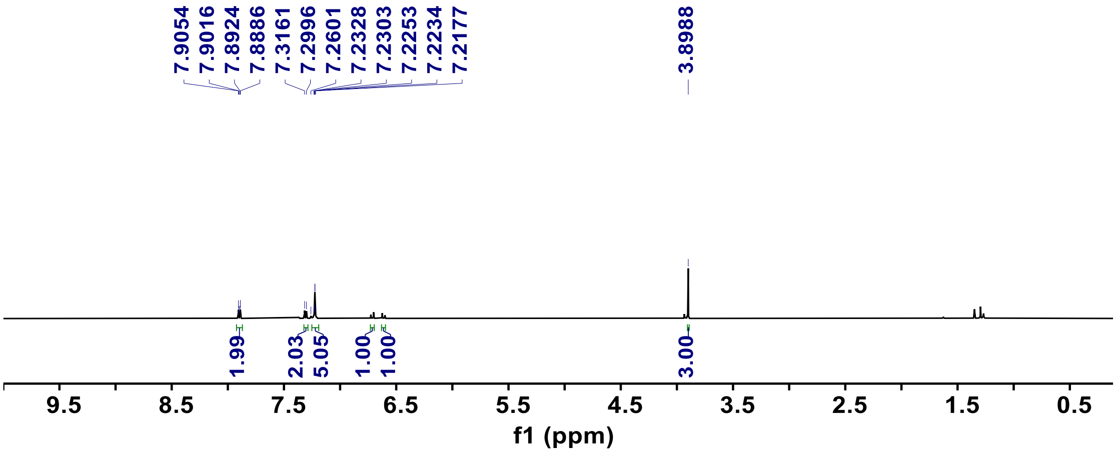


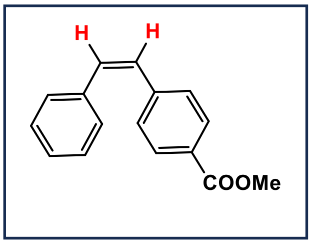
^{13}C{^{1}H} NMR (100 MHz, CDCl$_3$), **8b**



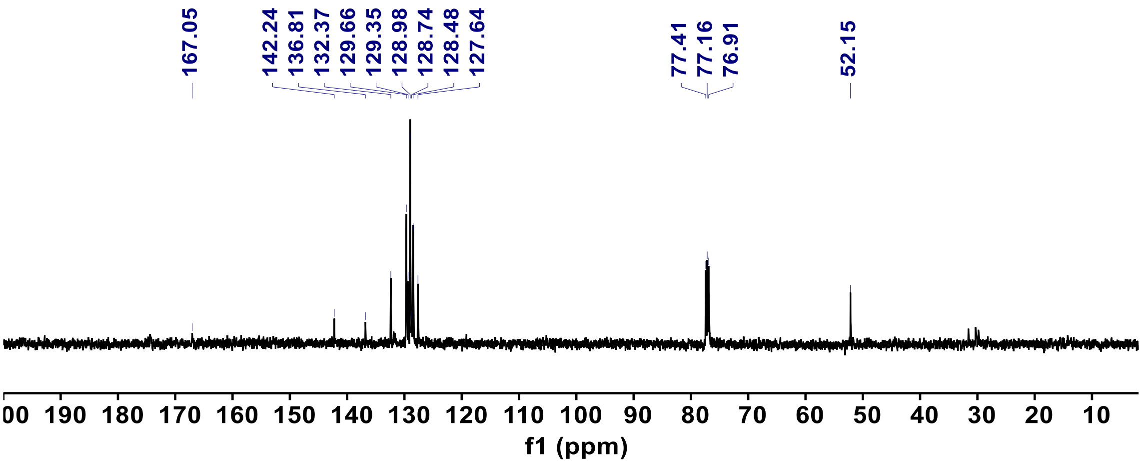


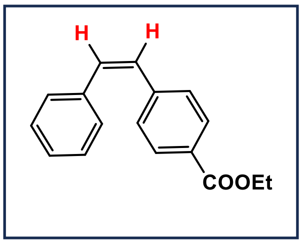
^{1}H NMR ($CDCl_3$, 400 MHz), **9b**



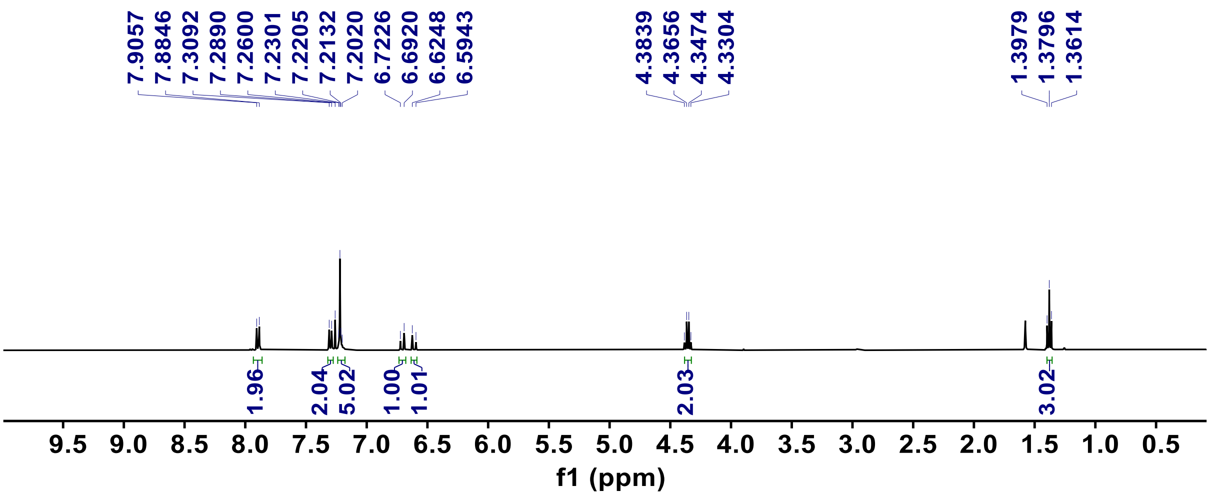


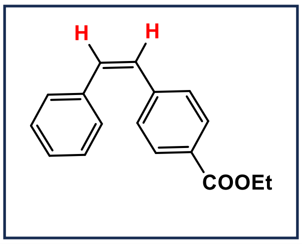
$^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$), **9b**



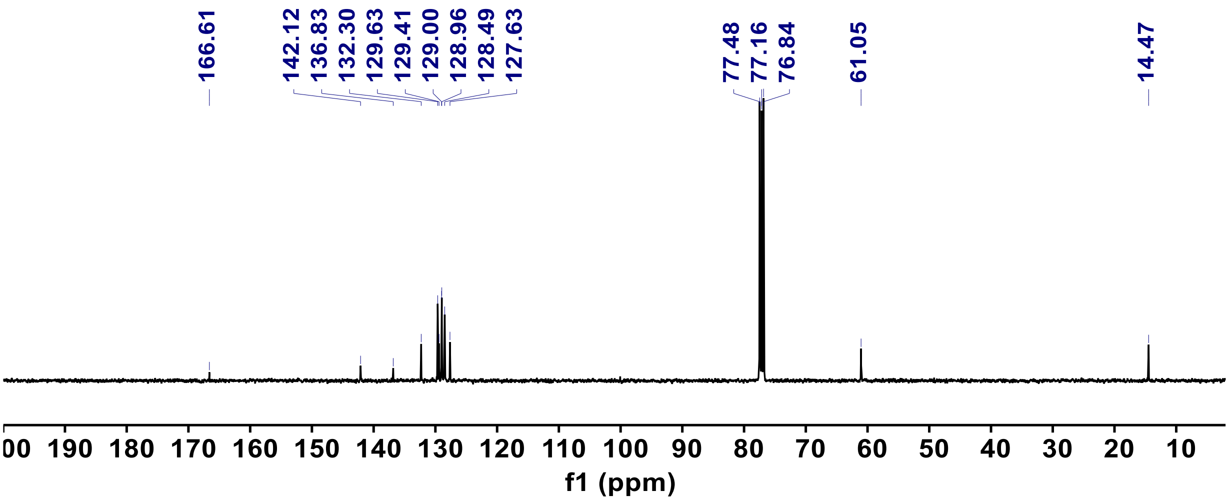


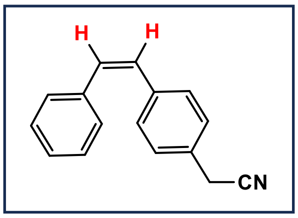
^{1}**H NMR** ($CDCl_3$, 400 MHz), **10b**



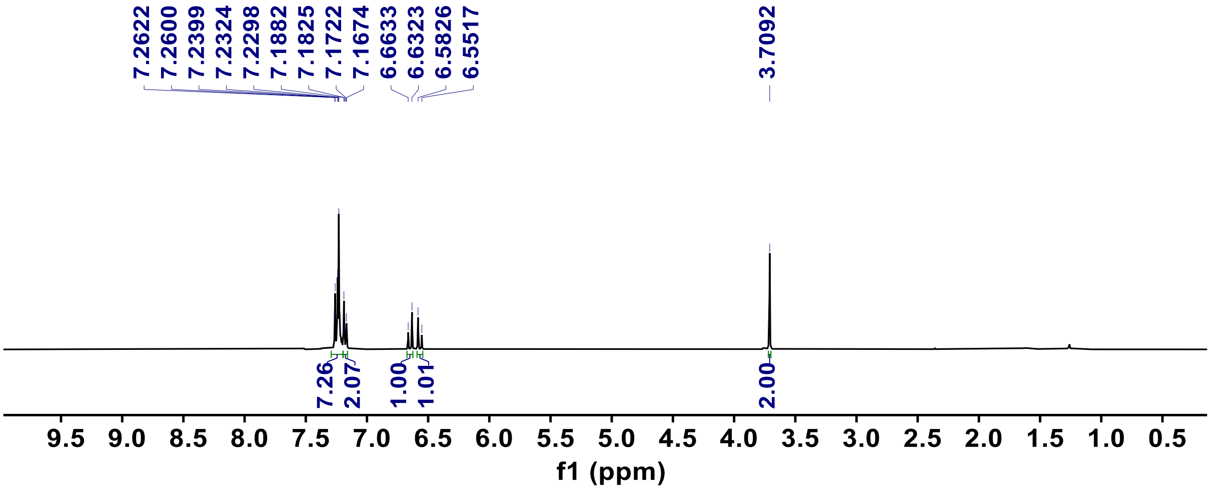


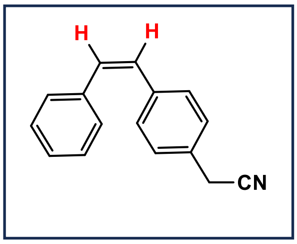
^{13}**C{^{1}H} NMR** (100 MHz, $CDCl_3$), **10b**



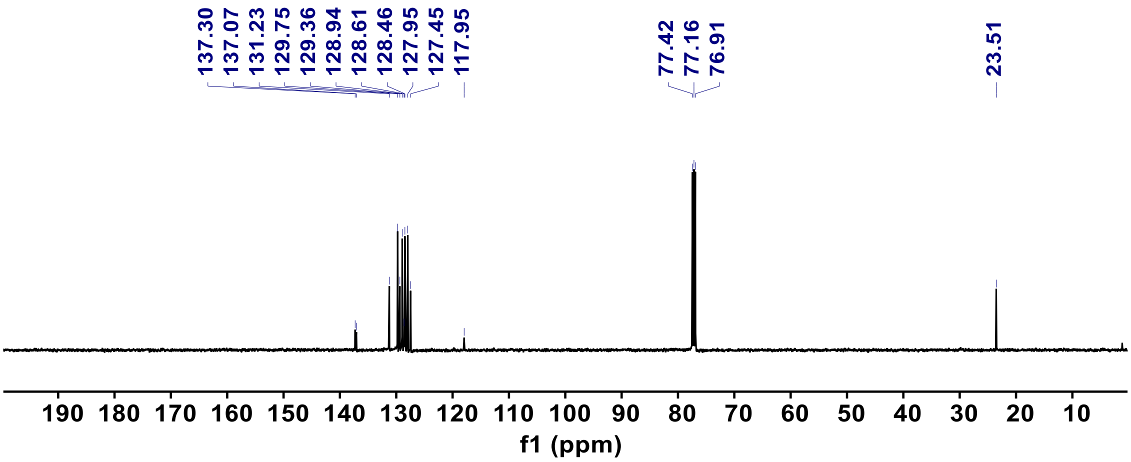


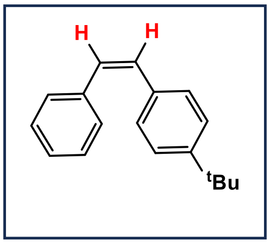
[1]H NMR ($CDCl_3$, 400 MHz), **11b**



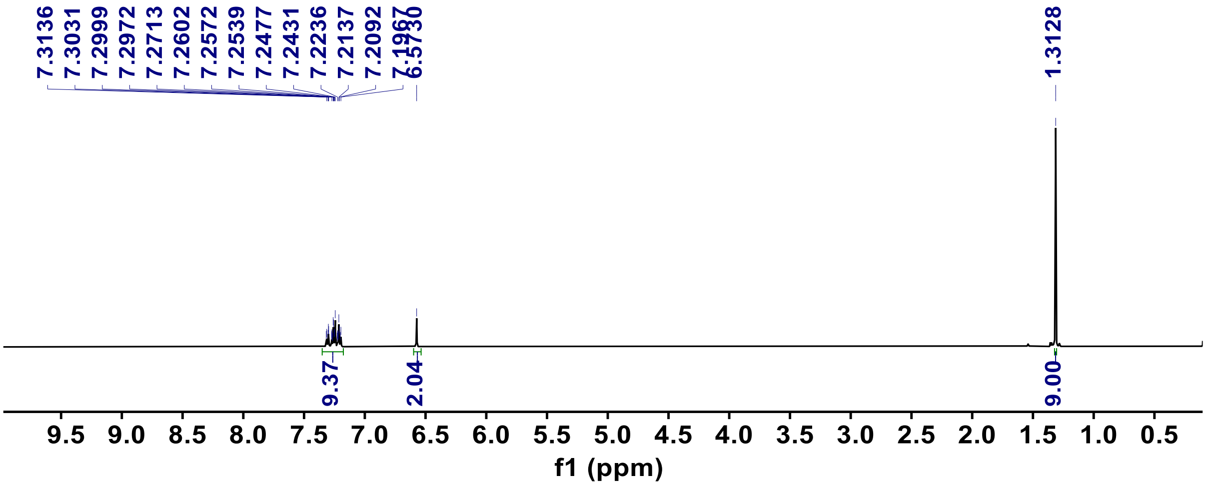


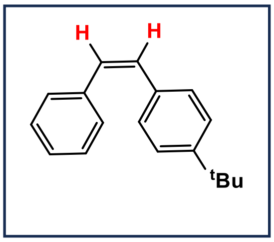
[13]C{[1]H} NMR (125 MHz, $CDCl_3$), **11b**



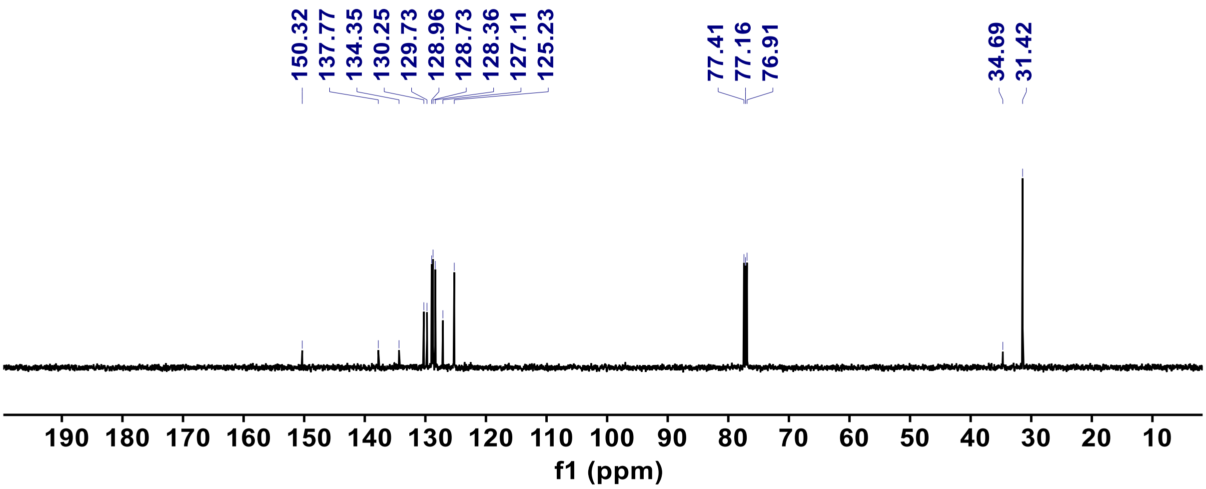


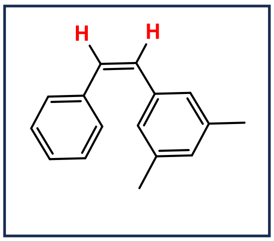
^{1}H NMR (CDCl$_3$, 500 MHz), **12b**



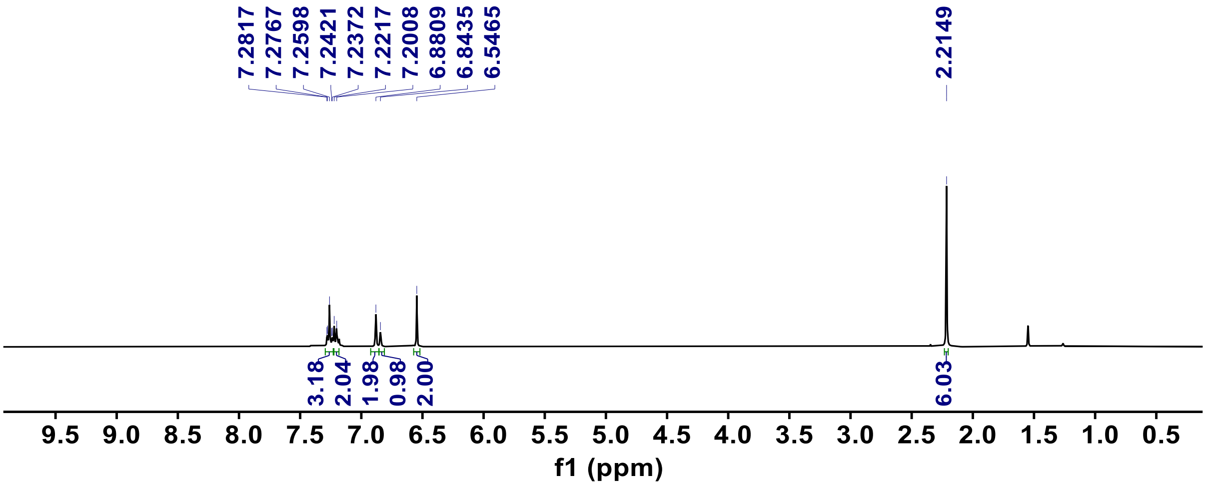


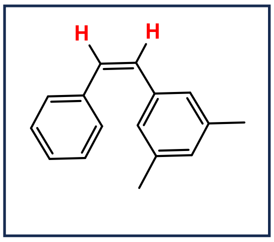
^{13}C{^{1}H} NMR (125 MHz, CDCl$_3$), **12b**



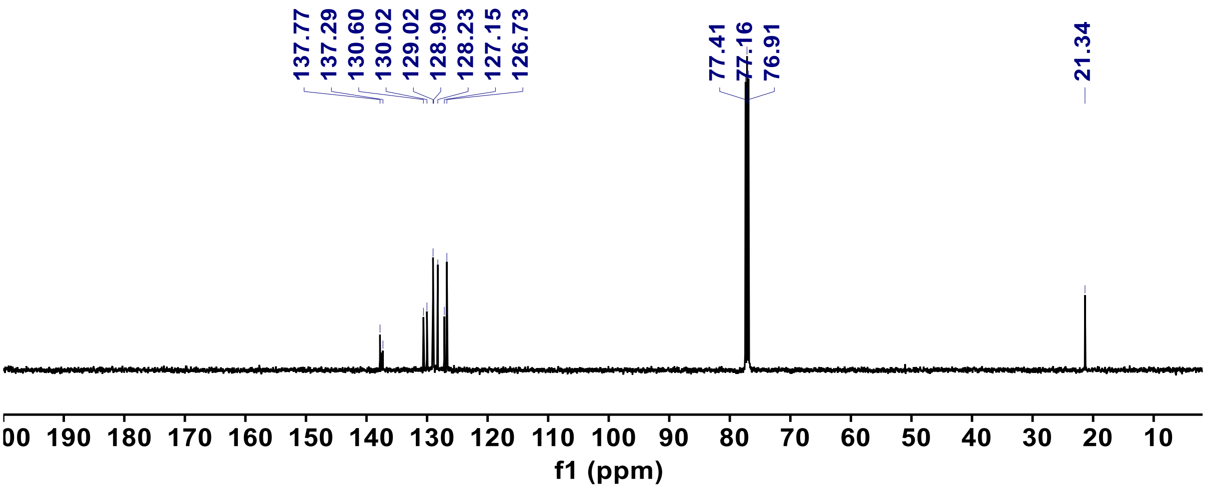


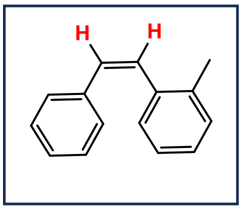
¹H NMR (CDCl$_3$, 400 MHz), **13b**



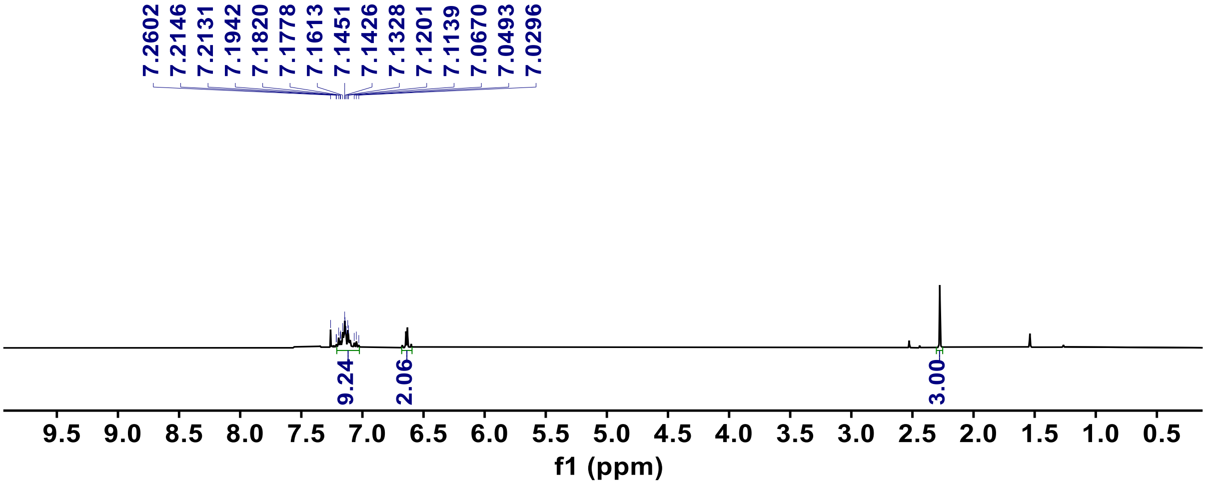


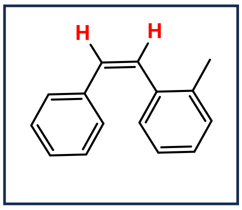
¹³C{¹H} NMR (125 MHz, CDCl$_3$), **13b**



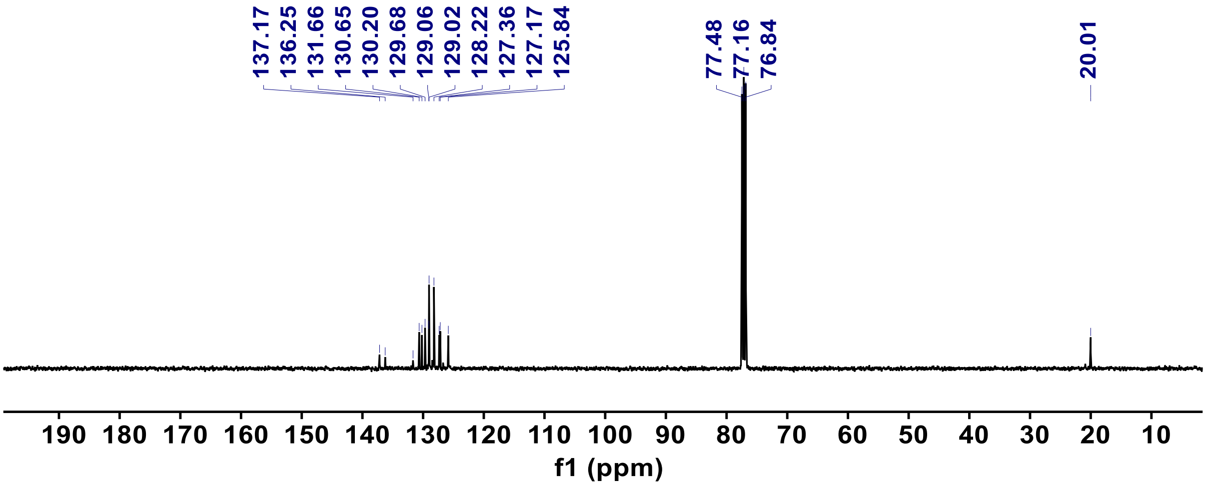


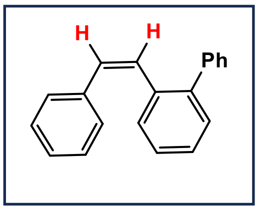
¹H NMR (CDCl$_3$, 400 MHz), **14b**



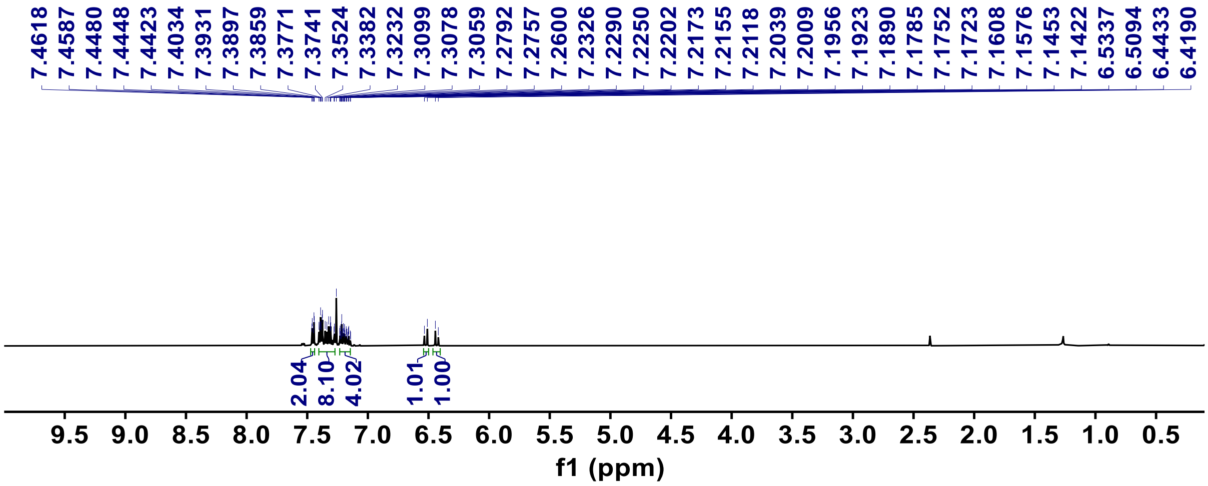


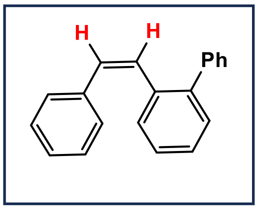
^{13}C{^{1}H} NMR (100 MHz, CDCl$_3$), **14b**



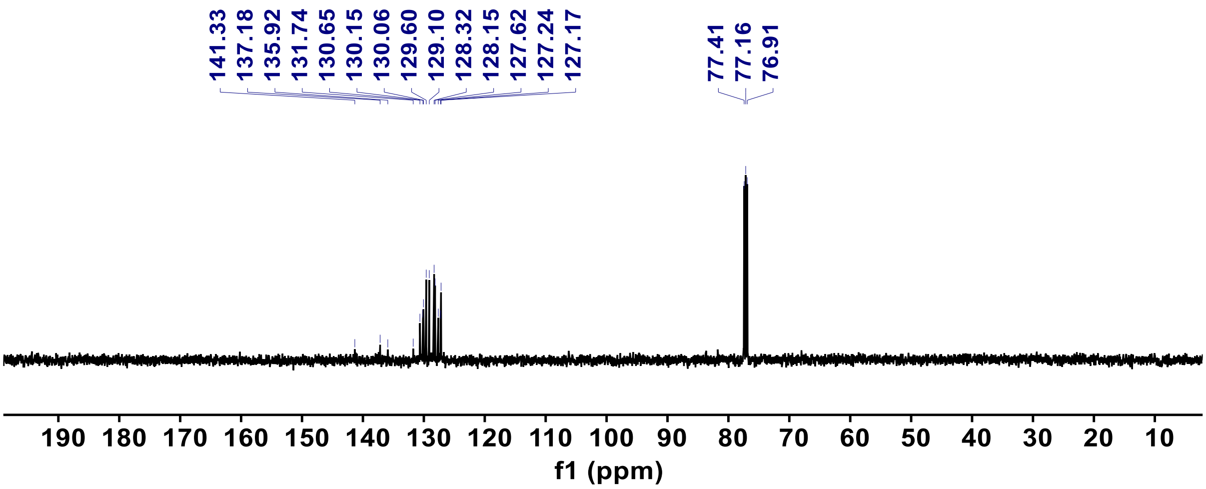


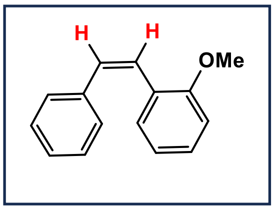
[1]H NMR (CDCl$_3$, 500 MHz), **15b**



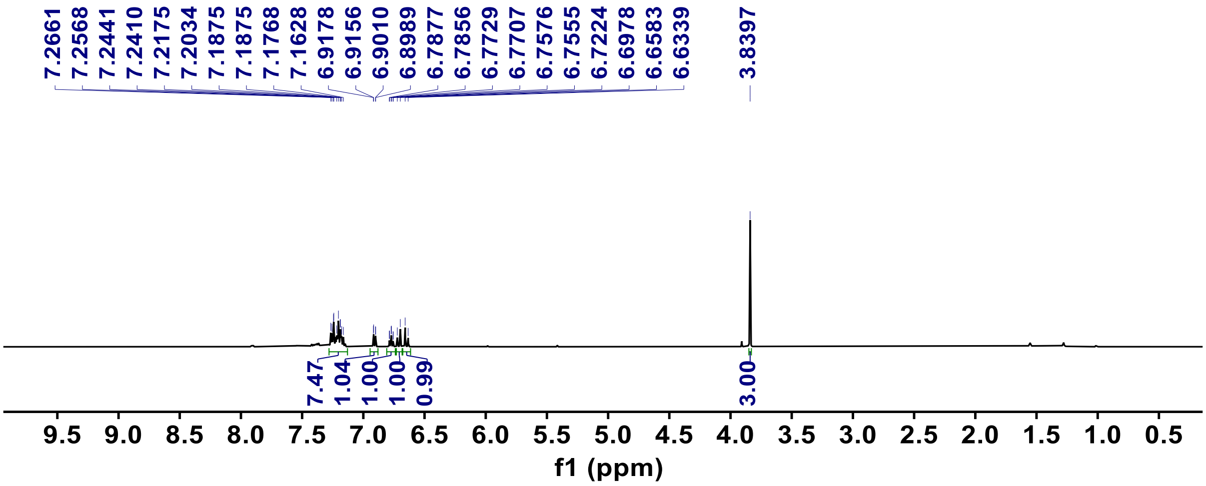


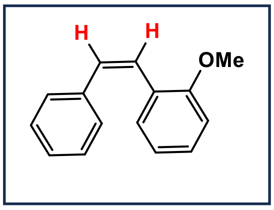
[13]C{[1]H} NMR (125 MHz, CDCl$_3$), **15b**



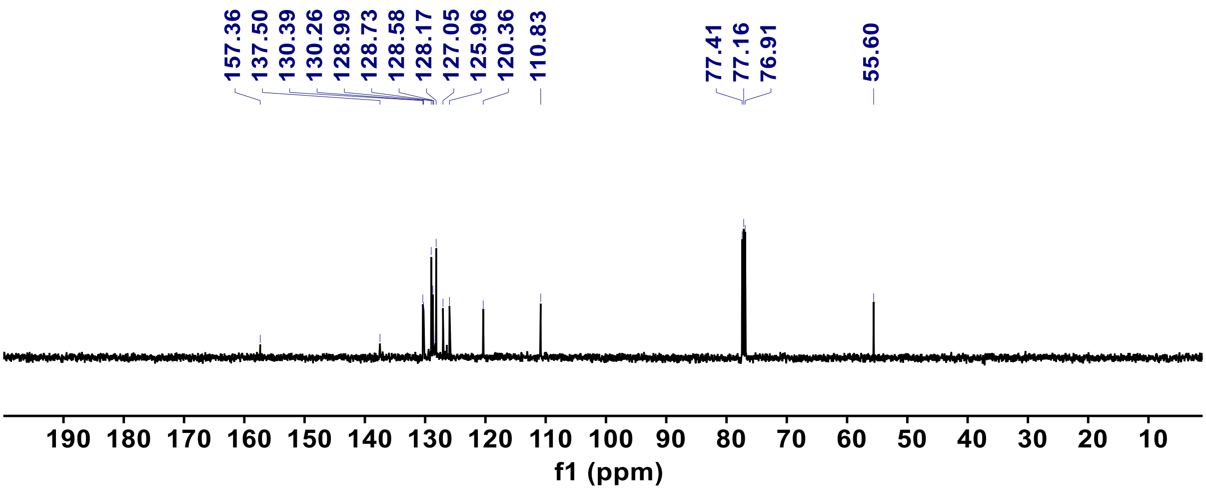


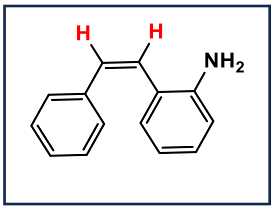
¹H NMR (CDCl₃, 500 MHz), **16b**



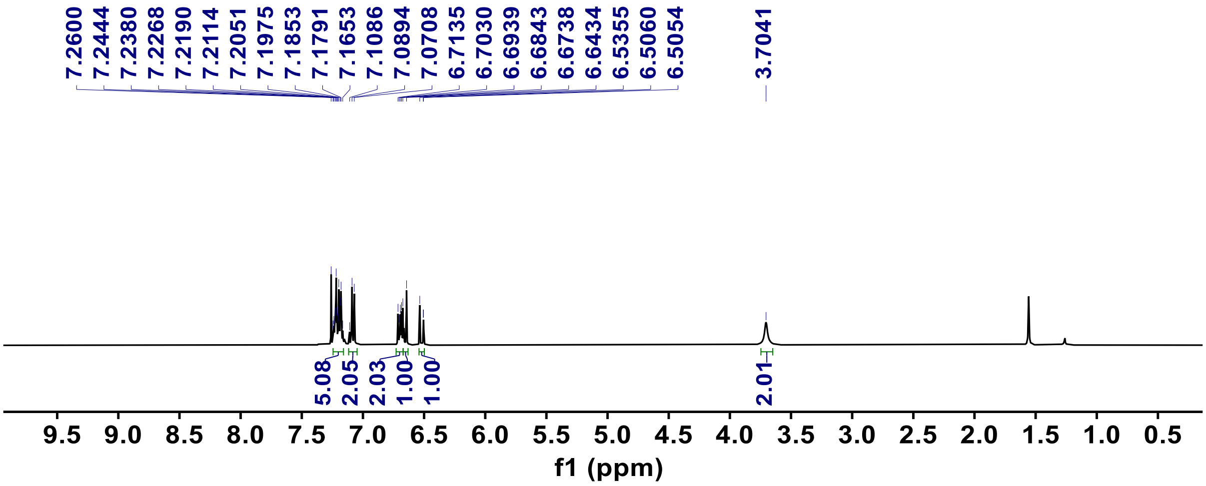


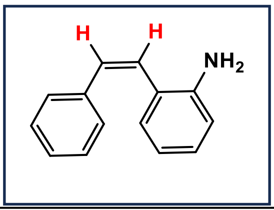
^{13}C{^{1}H} NMR (125 MHz, CDCl₃), **16b**



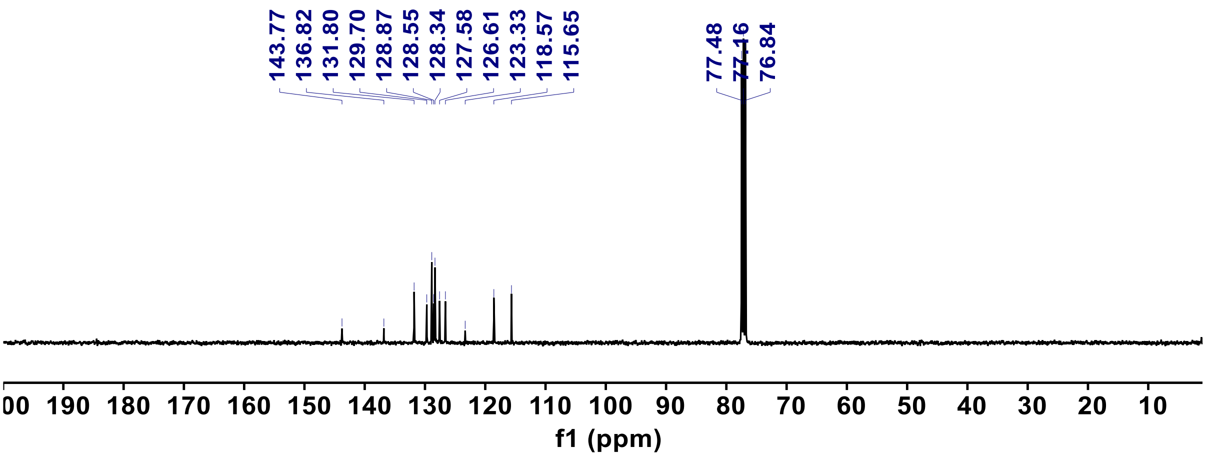


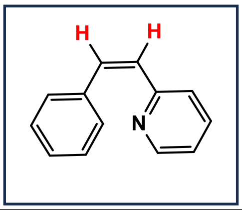
[1]H NMR ($CDCl_3$, 400 MHz), **17b**



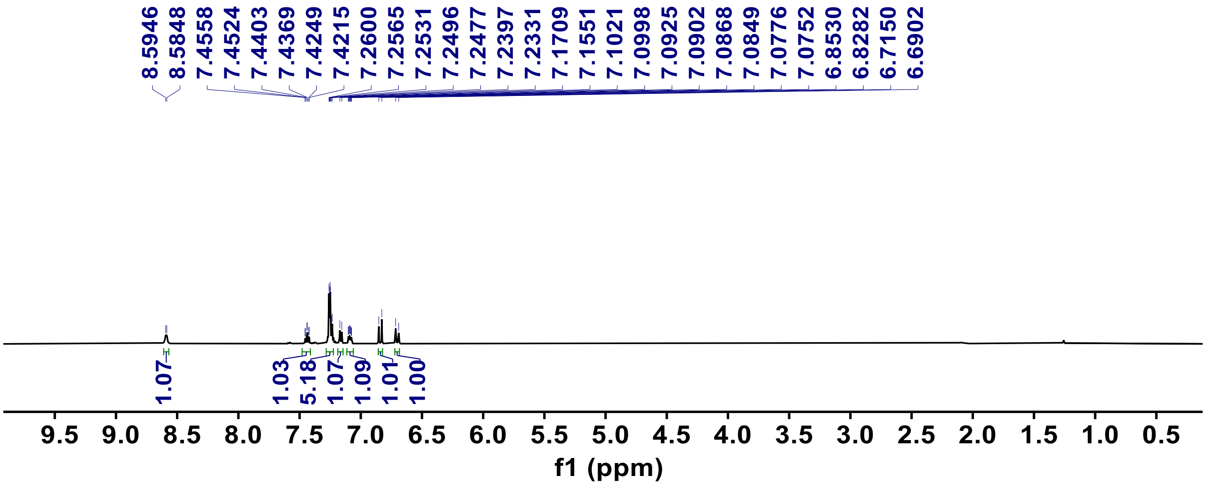


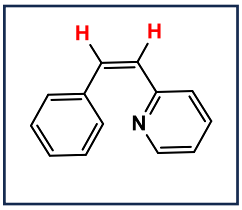
[13]C{[1]H} NMR (100 MHz, $CDCl_3$), **17b**



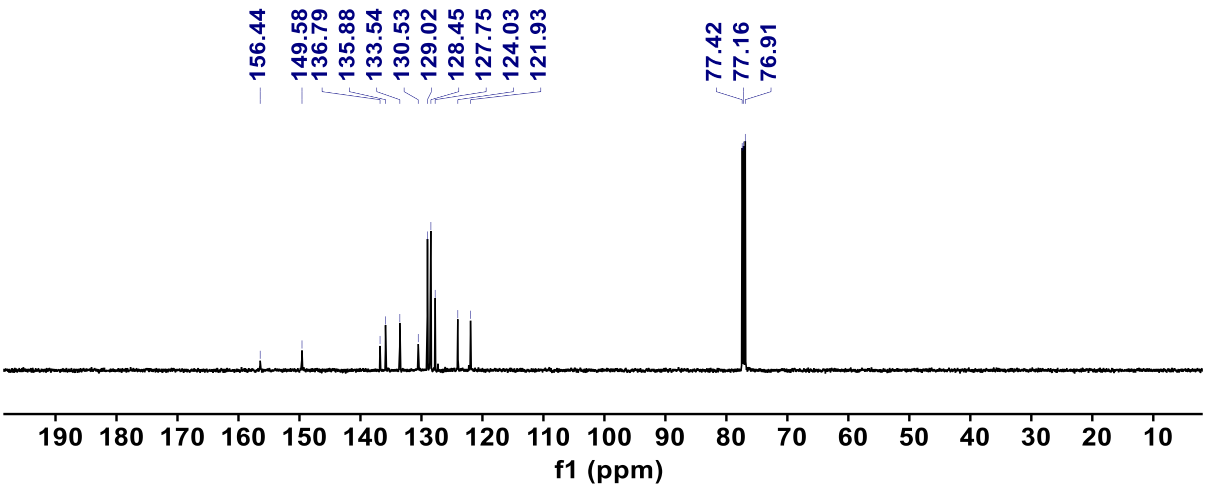


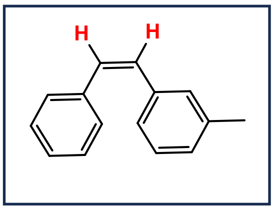
^{1}H NMR (CDCl$_3$, 500 MHz), **18b**



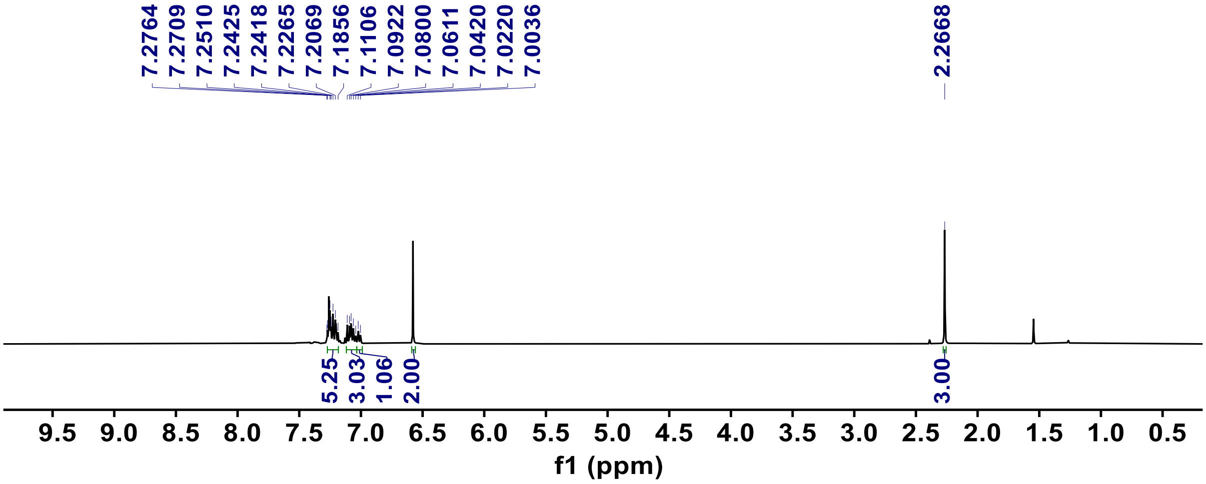


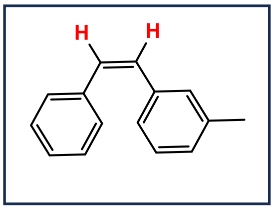
^{13}C{^{1}H} NMR (125 MHz, CDCl$_3$), **18b**



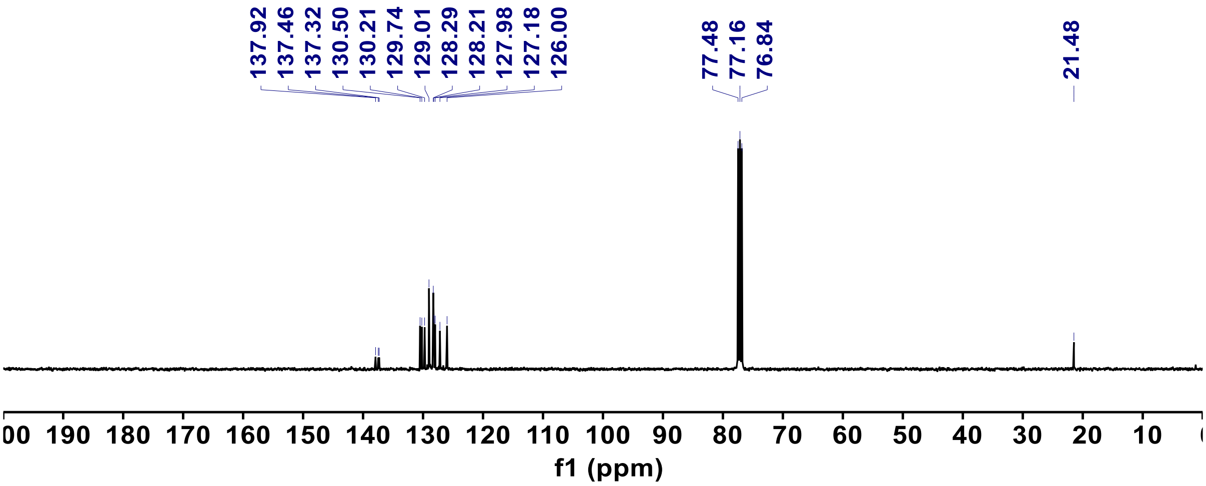


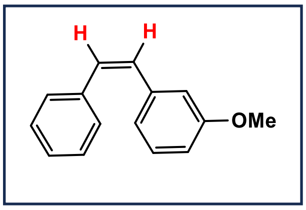
^{1}H NMR ($CDCl_3$, 400 MHz), **19b**



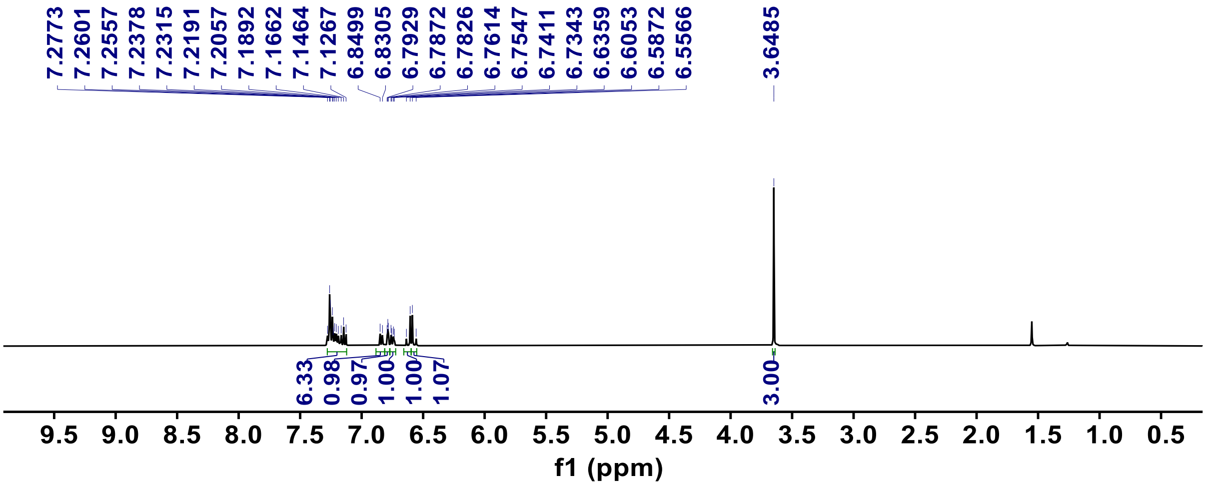


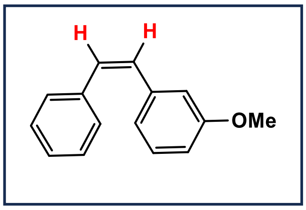
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$), **19b**



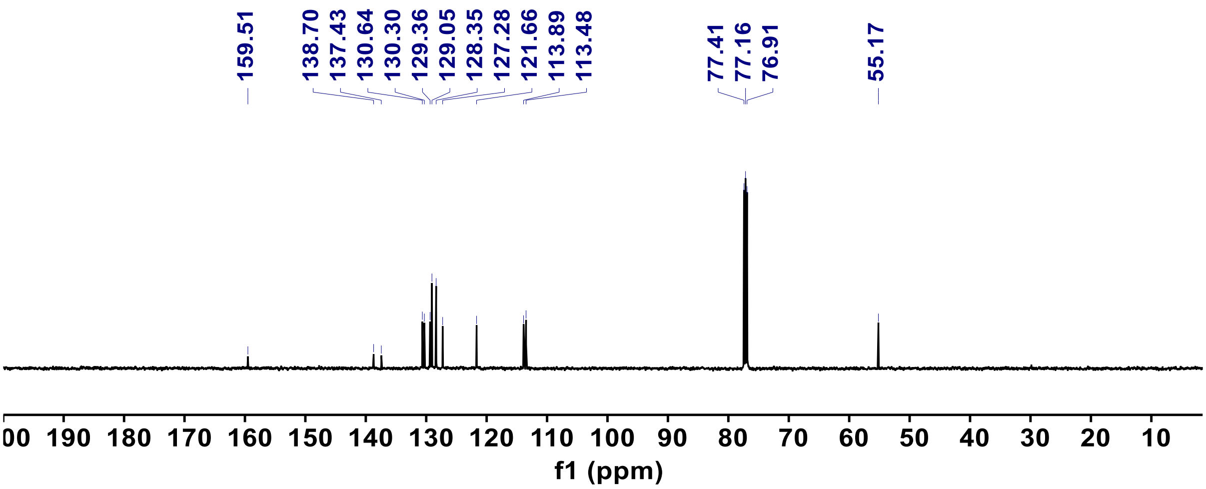


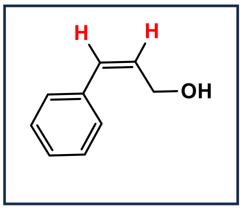
^{1}**H NMR** ($CDCl_3$, 400 MHz), **20b**



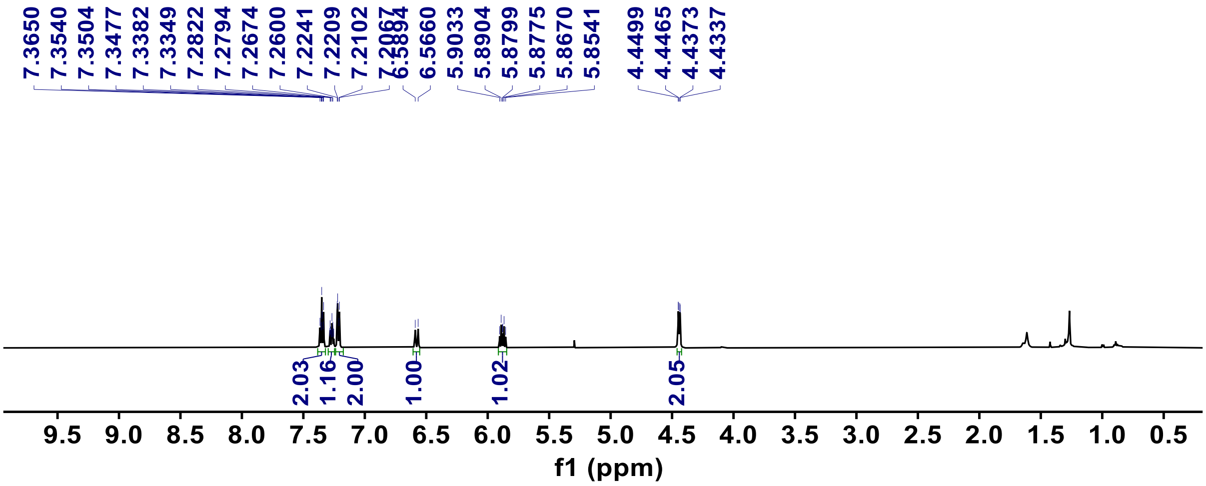


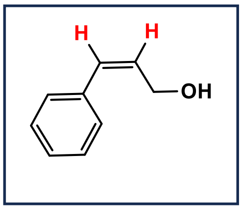
^{13}**C{^{1}H} NMR** (125 MHz, $CDCl_3$), **20b**



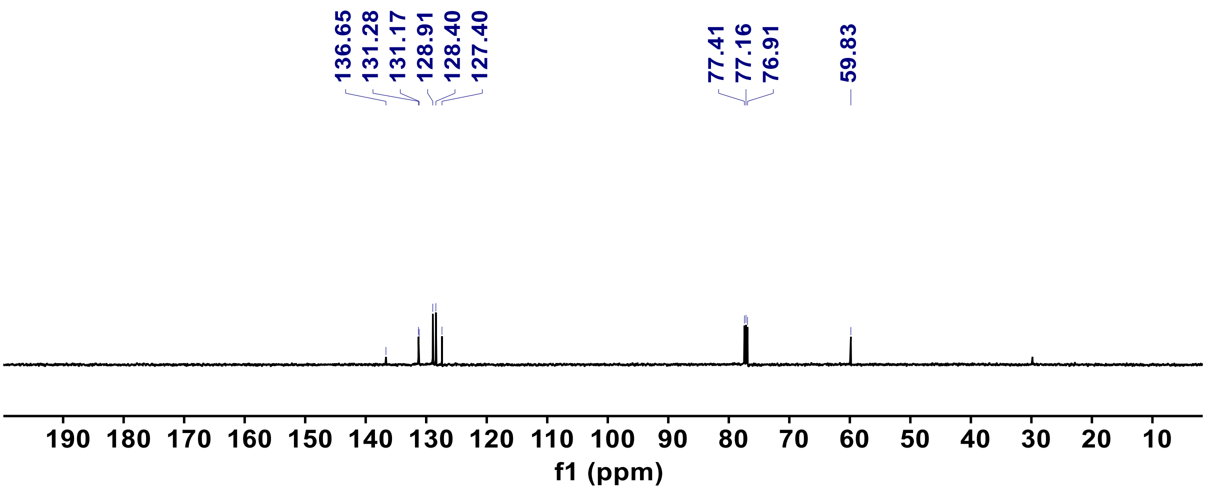


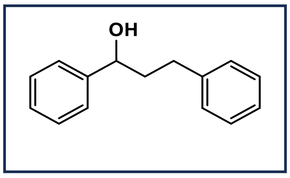
[1]H NMR (CDCl3, 500 MHz), **21b**



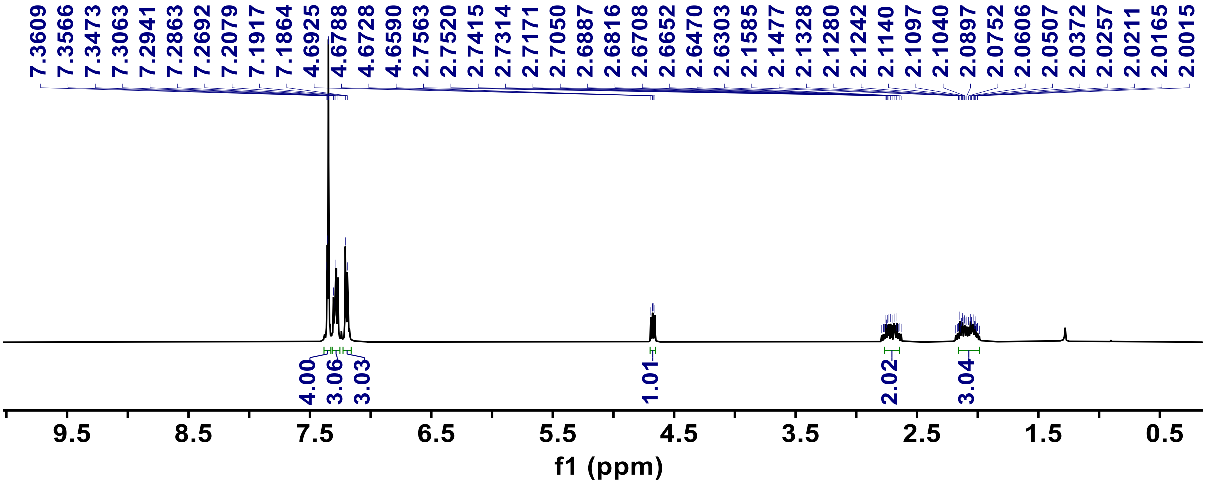


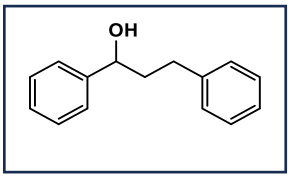
[13]C{[1]H} NMR (125 MHz, CDCl3), **21b**



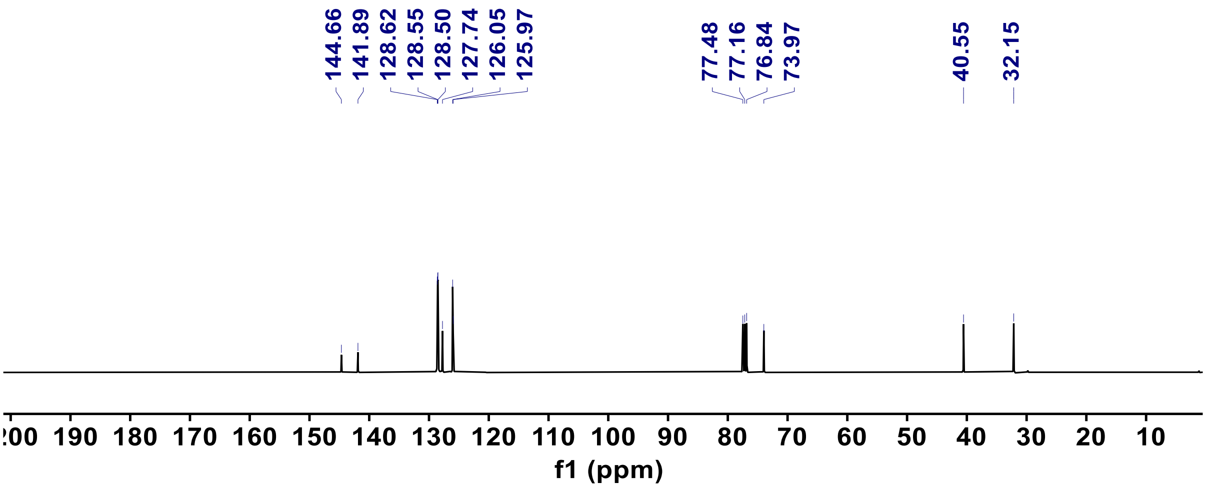


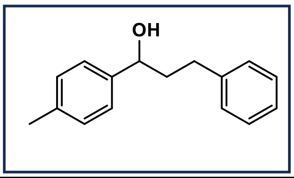
^{1}H NMR (400 MHz, $CDCl_3$), **22d**



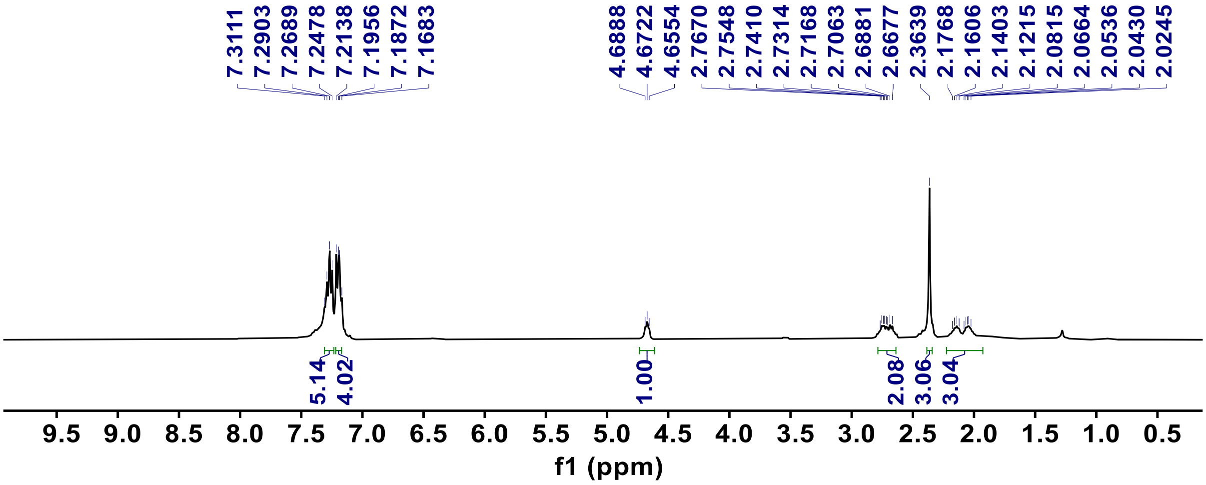


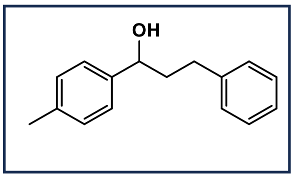
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$), **22d**



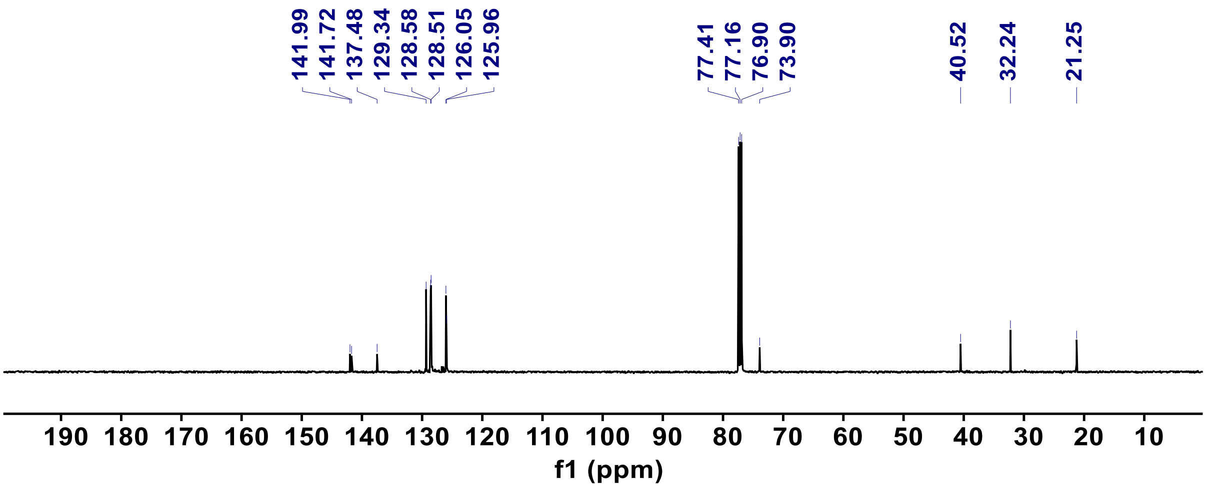


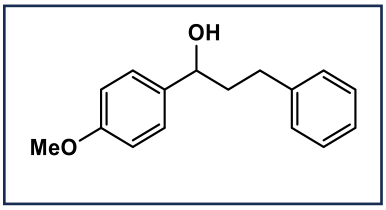
^{1}**H NMR** (400 MHz, $CDCl_3$), **23d**



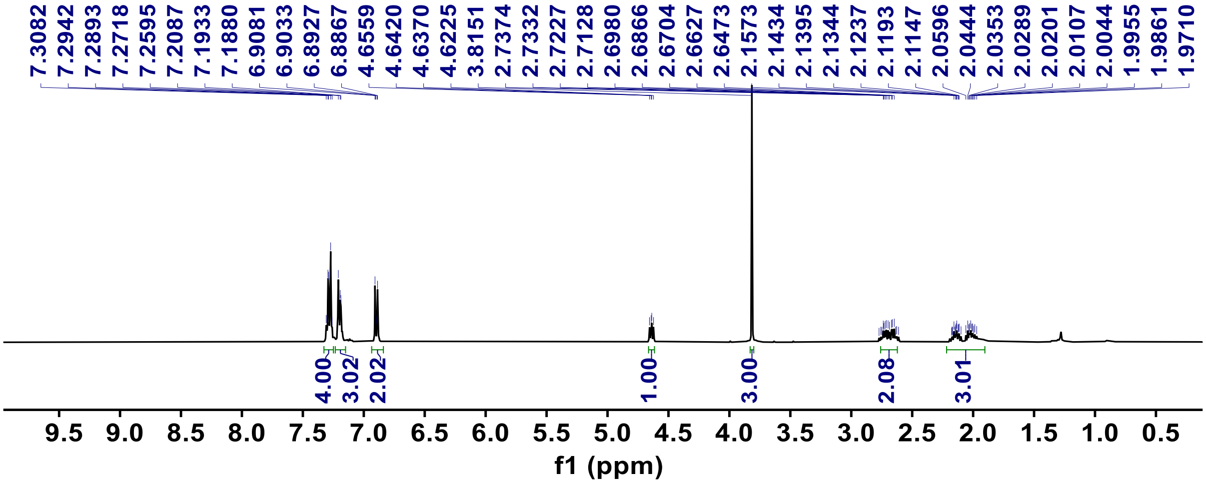


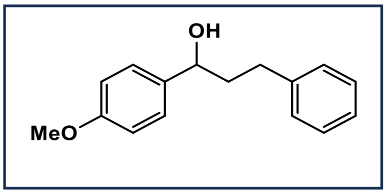
^{13}**C{^{1}H} NMR** (125 MHz, $CDCl_3$), **23d**



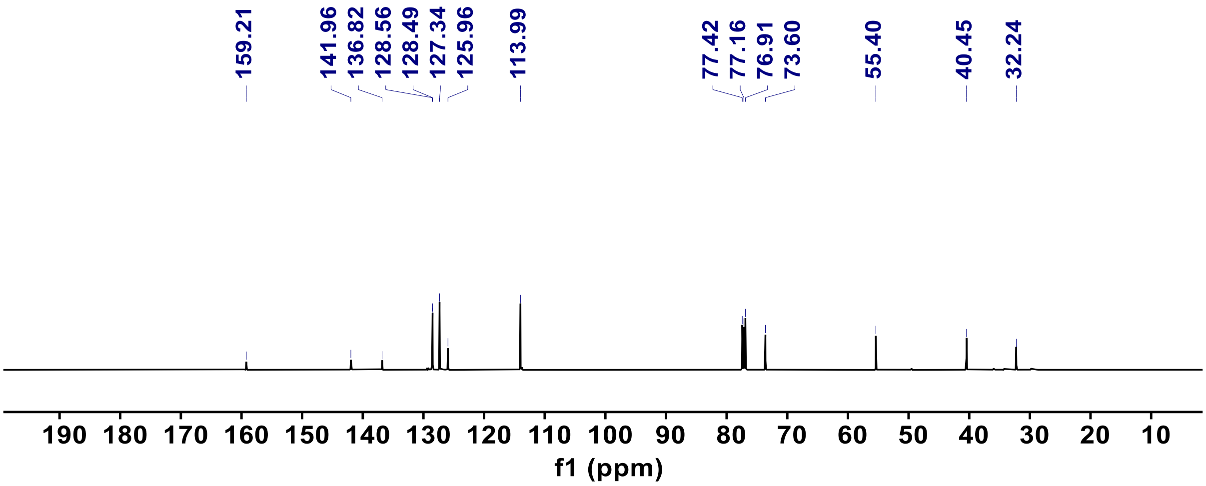


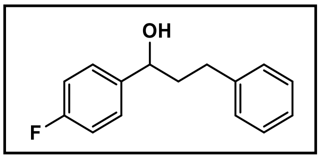
^{1}**H NMR** (400 MHz, $CDCl_3$), **24d**



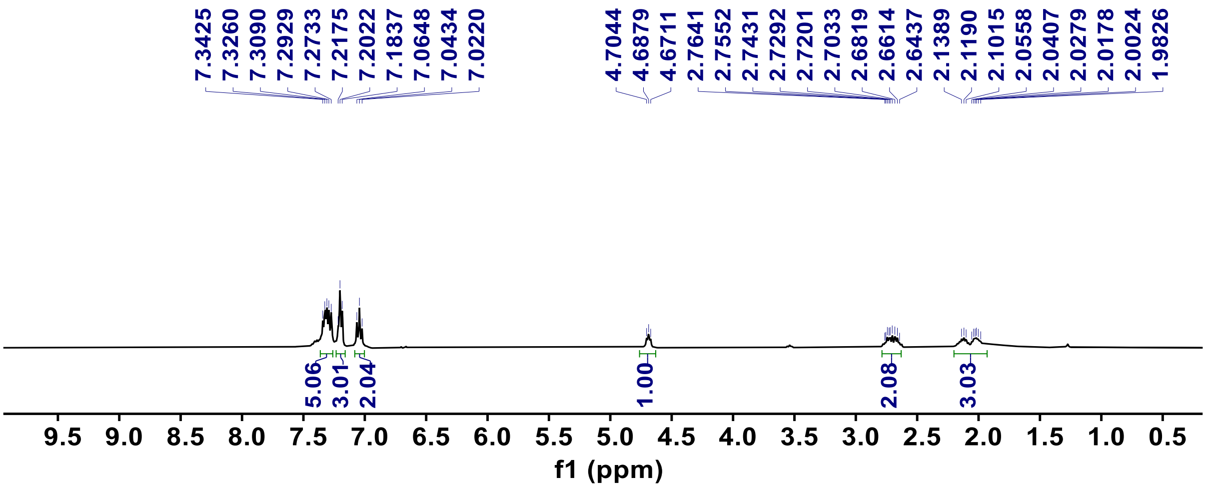


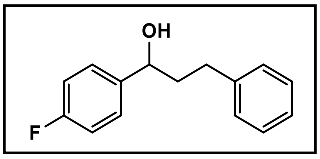
^{13}**C{^{1}H} NMR** (125 MHz, $CDCl_3$), **24d**



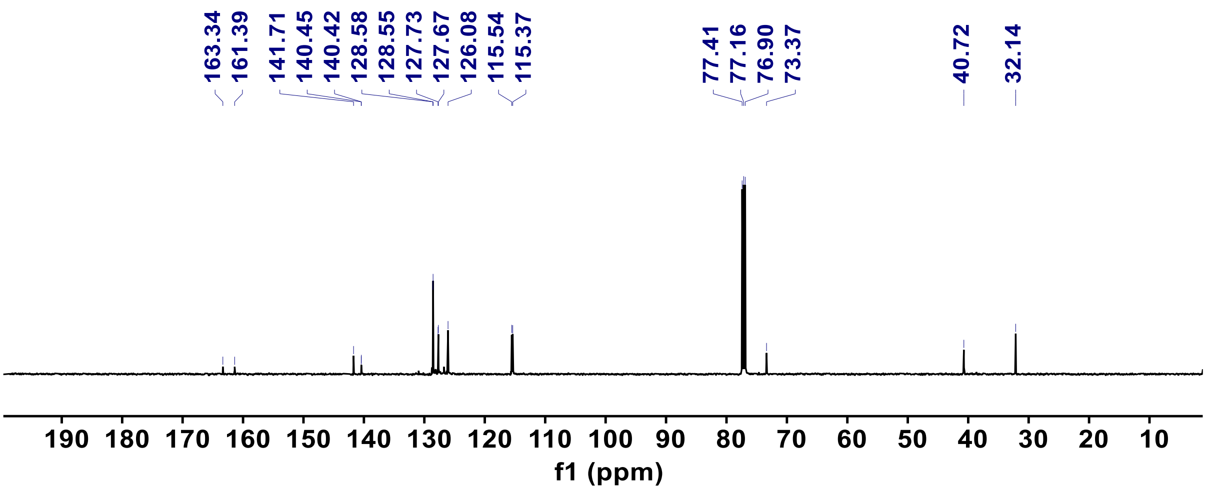


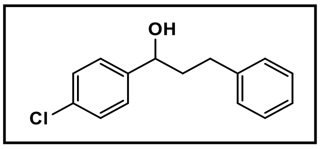
^{1}**H NMR** (400 MHz, $CDCl_3$), **25d**



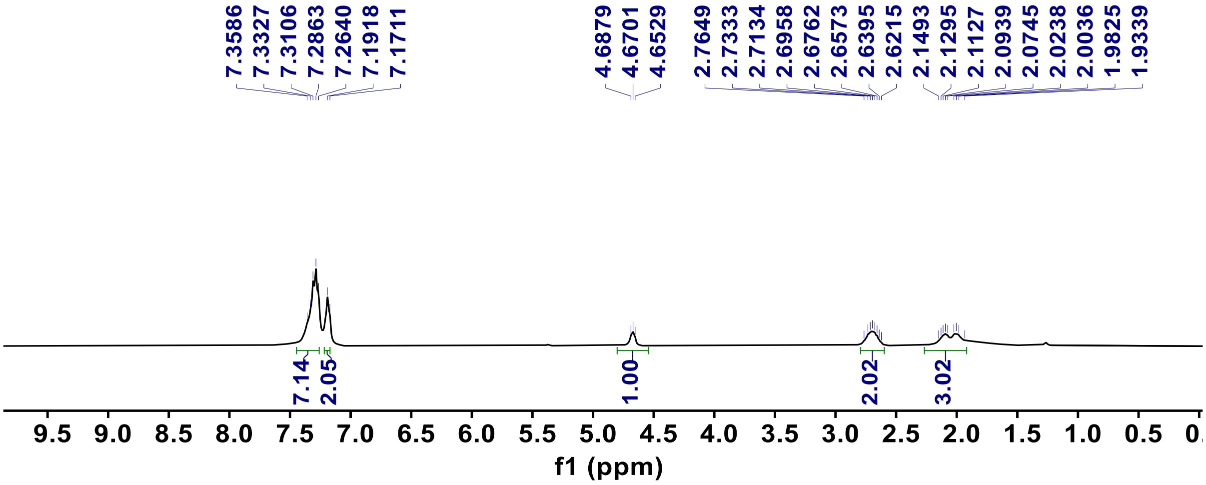


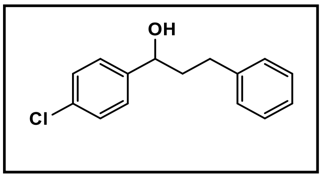
^{13}**C{^{1}H} NMR** (125 MHz, $CDCl_3$), **25d**



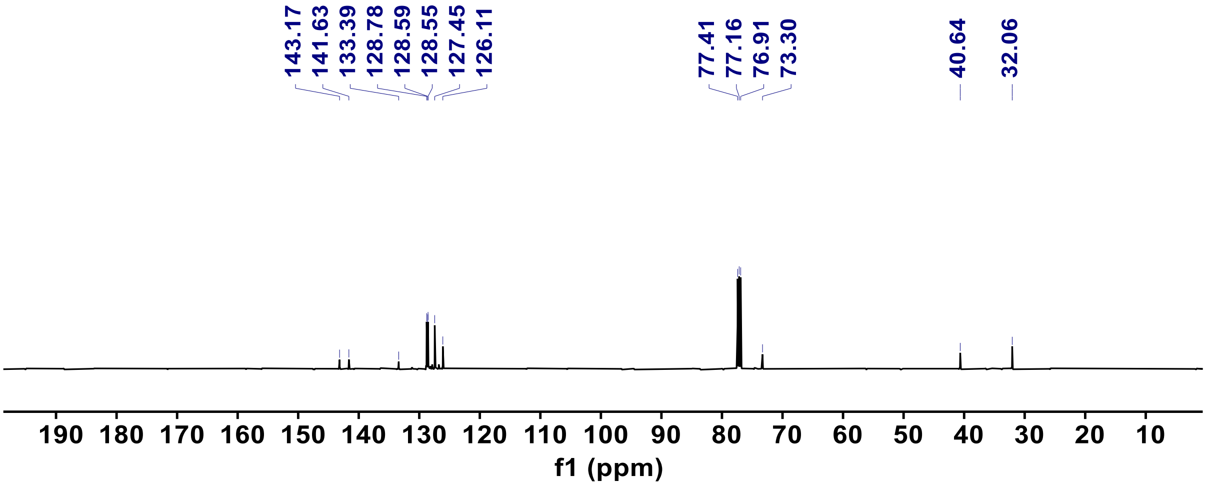


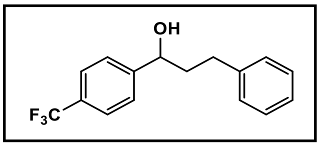
^{1}H NMR (400 MHz, $CDCl_3$), **26d**



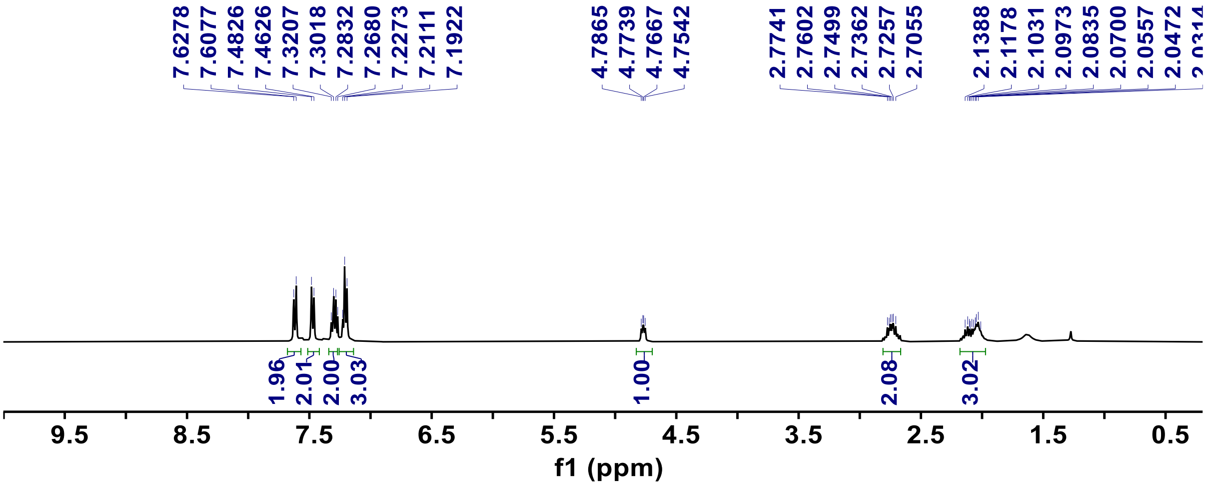


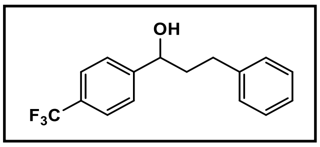
^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$), **26d**



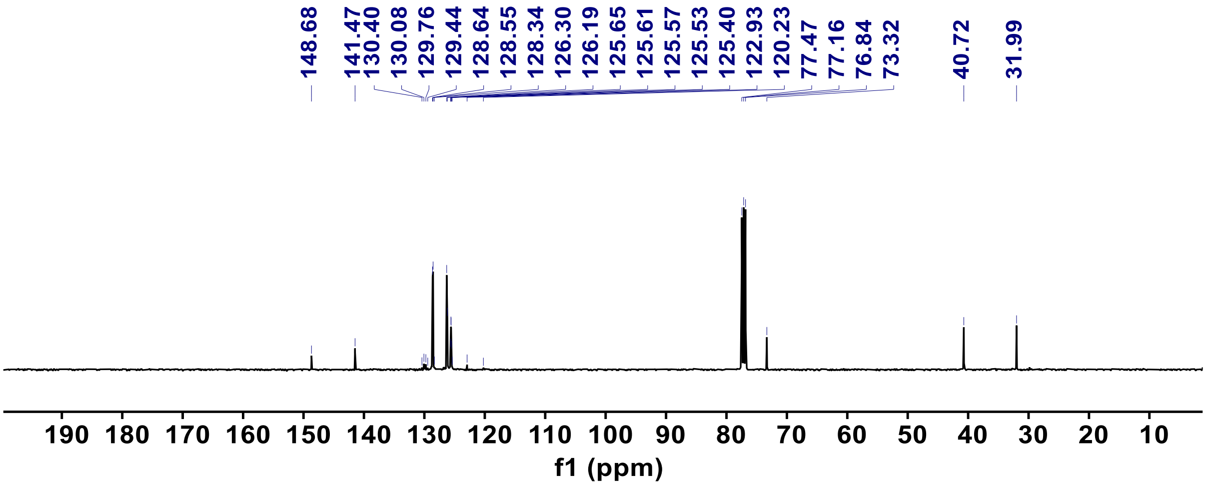


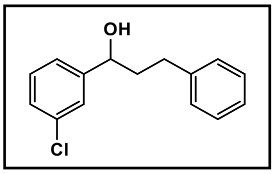
[1]H NMR (400 MHz, CDCl3), **27d**



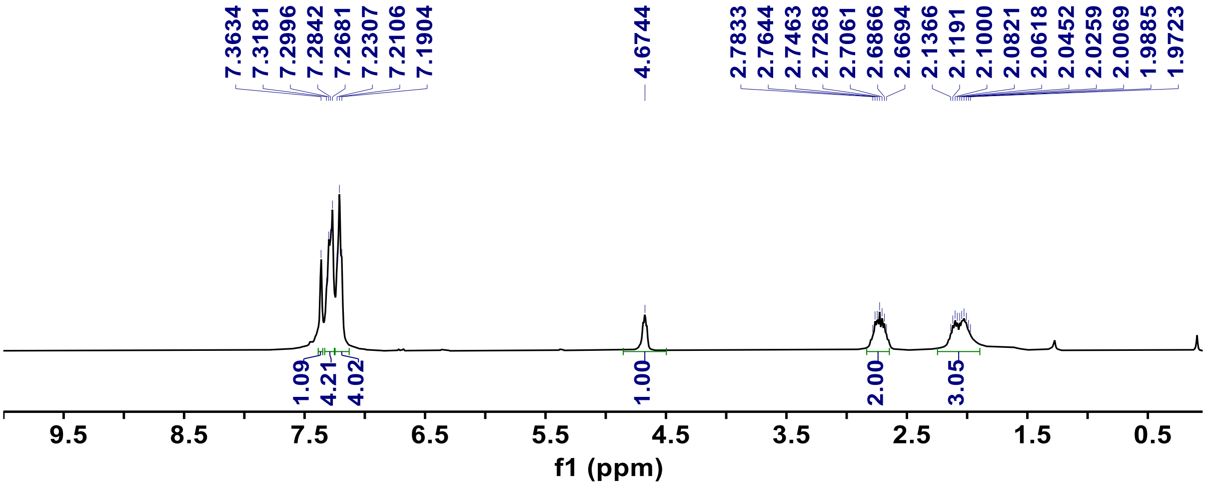


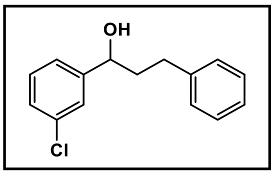
[13]C{[1]H} NMR (100 MHz, CDCl3), **27d**



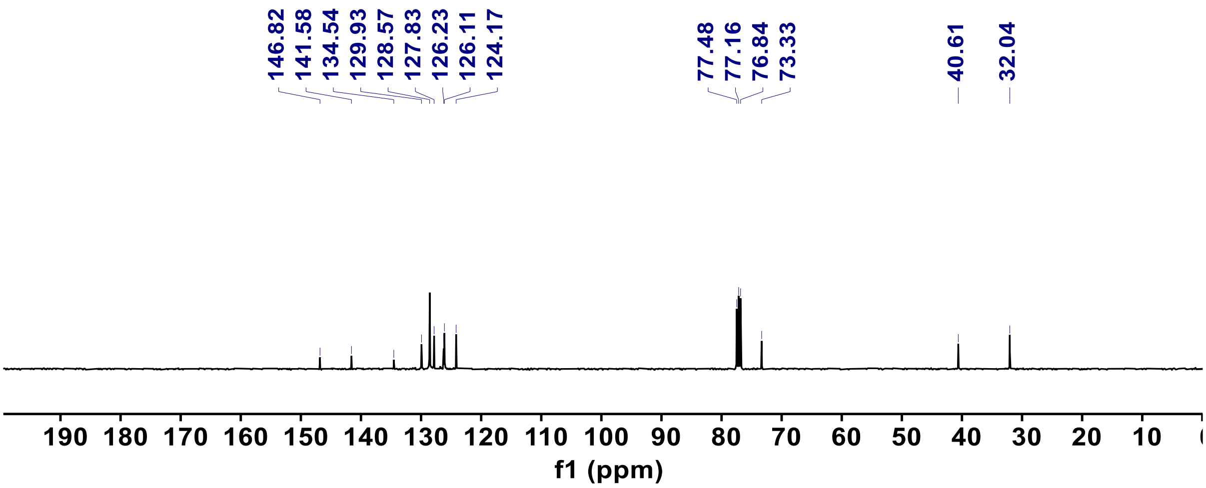


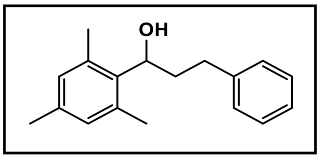
^{1}H NMR (400 MHz, $CDCl_3$), **28d**



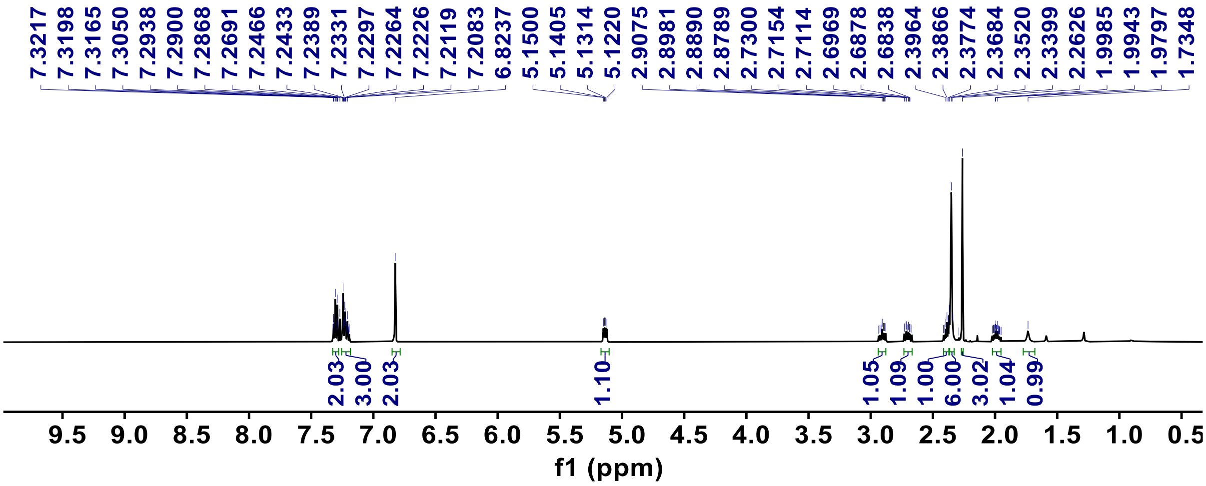


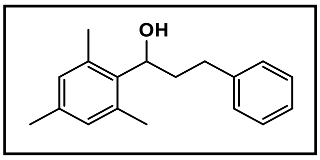
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$), **28d**



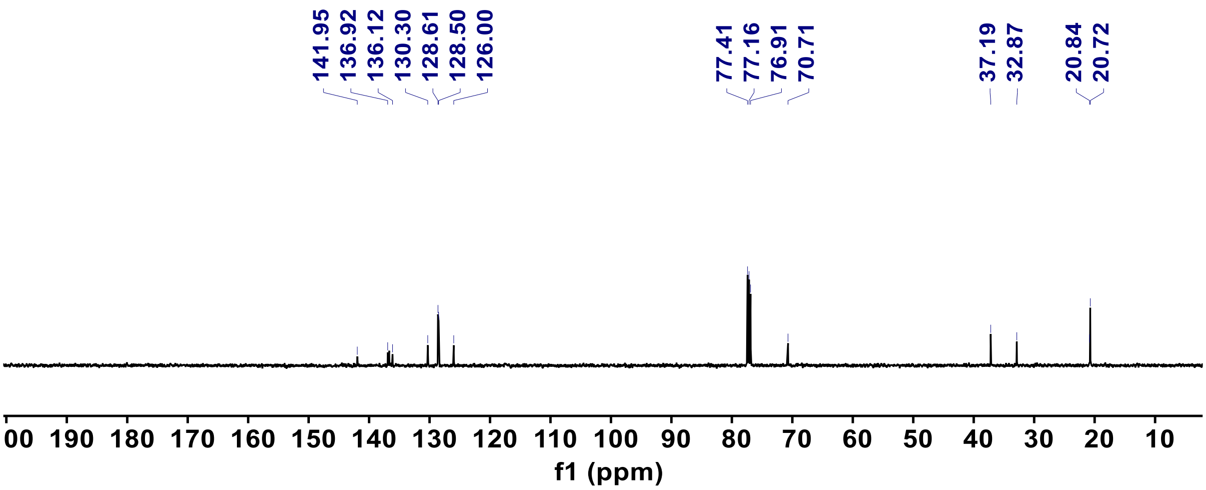


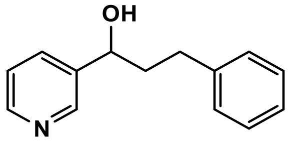
^{1}H NMR (500 MHz, $CDCl_3$), **29d**



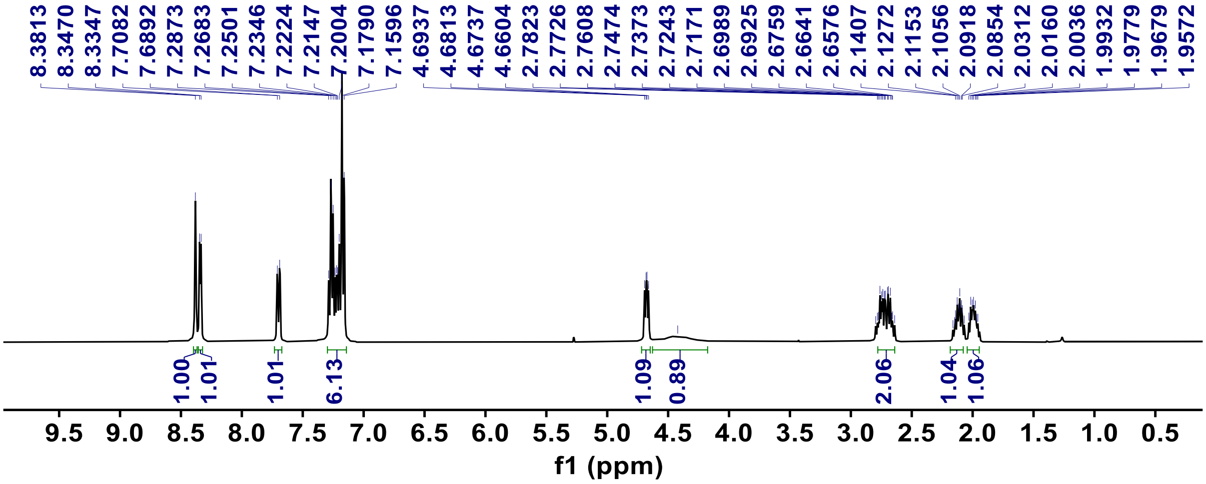


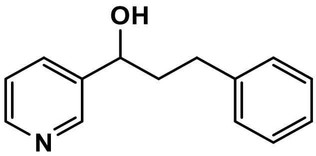
^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$), **29d**



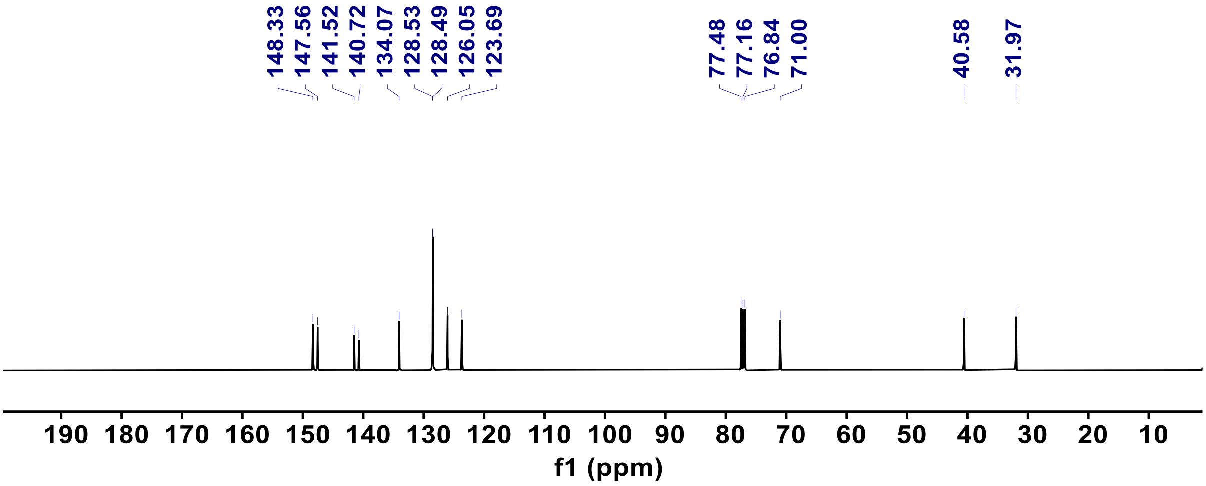


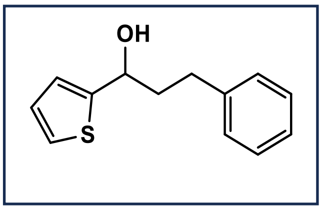
^{1}H NMR (400 MHz, $CDCl_3$), **30d**



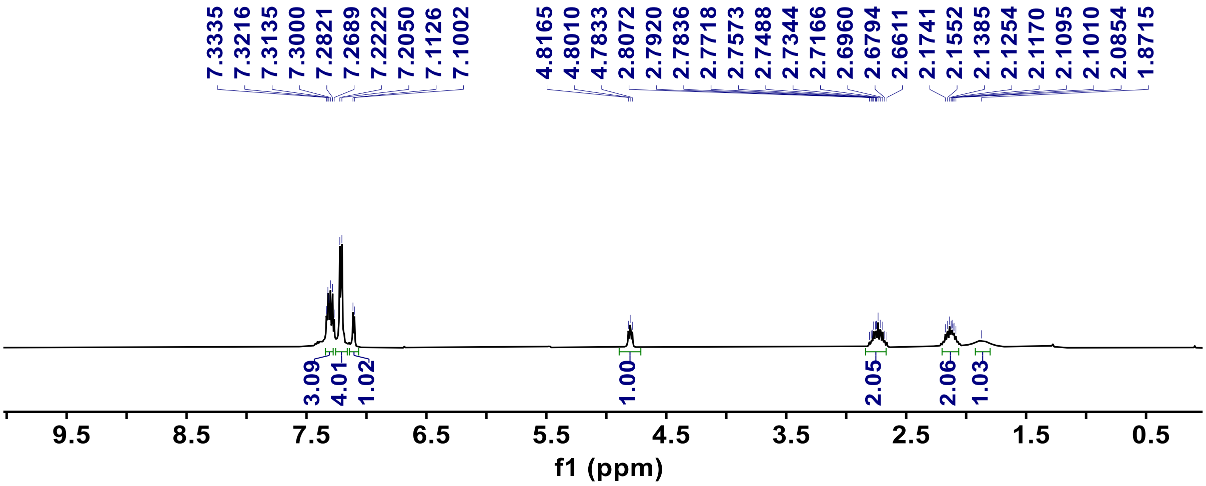


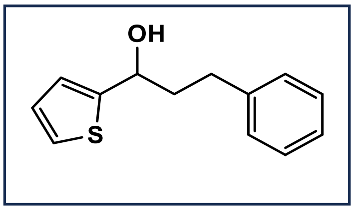
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$), **30d**



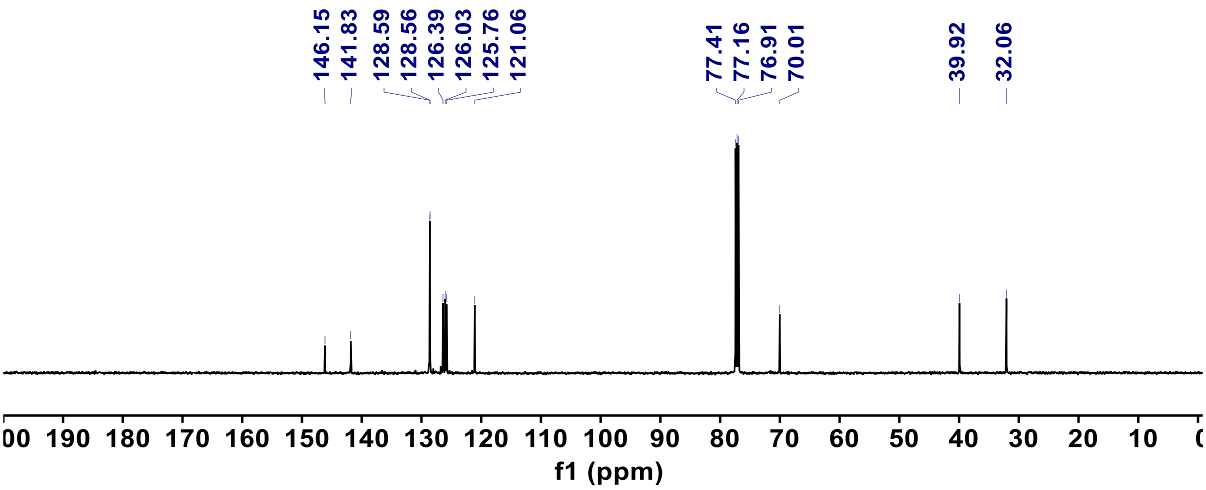


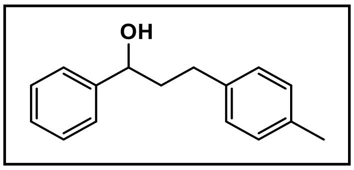
^{1}H NMR (400 MHz, $CDCl_3$), **31d**



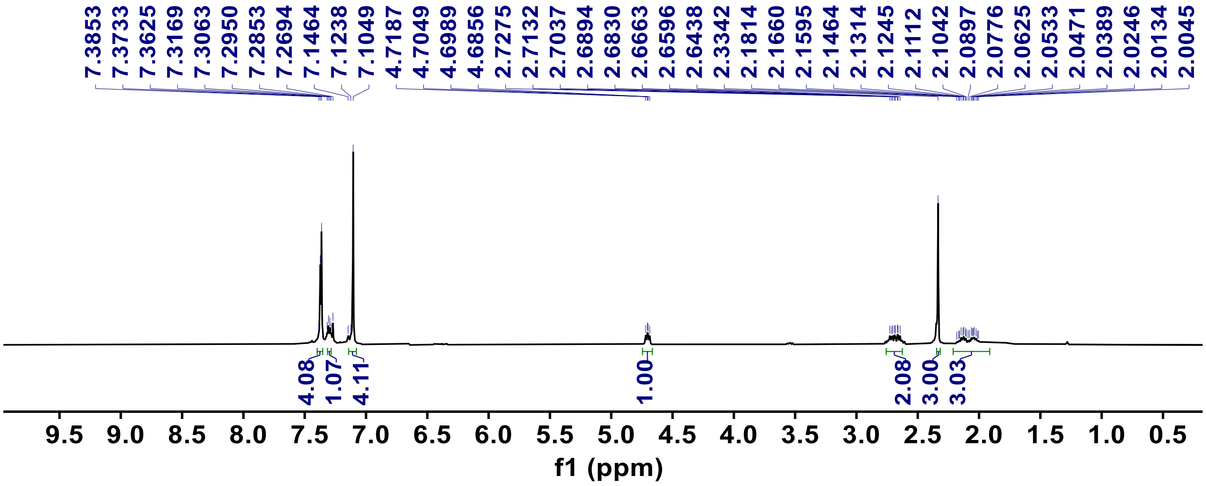


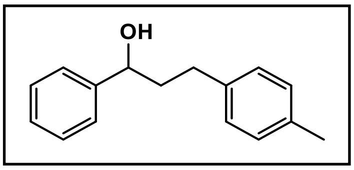
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$), **31d**



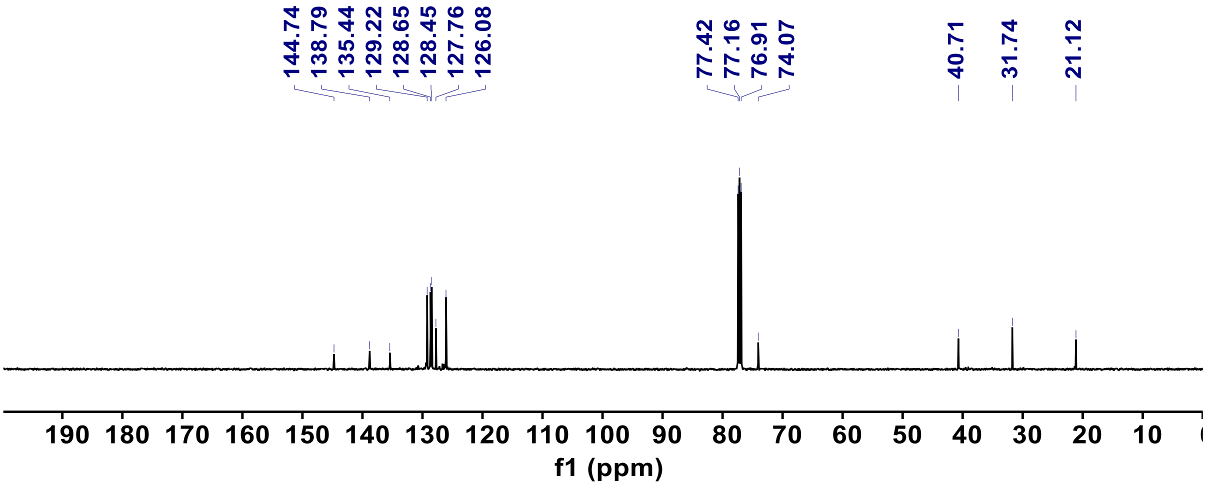


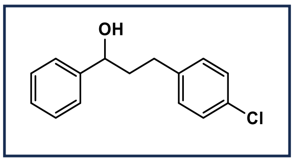
[1]H NMR (400 MHz, $CDCl_3$), **32d**



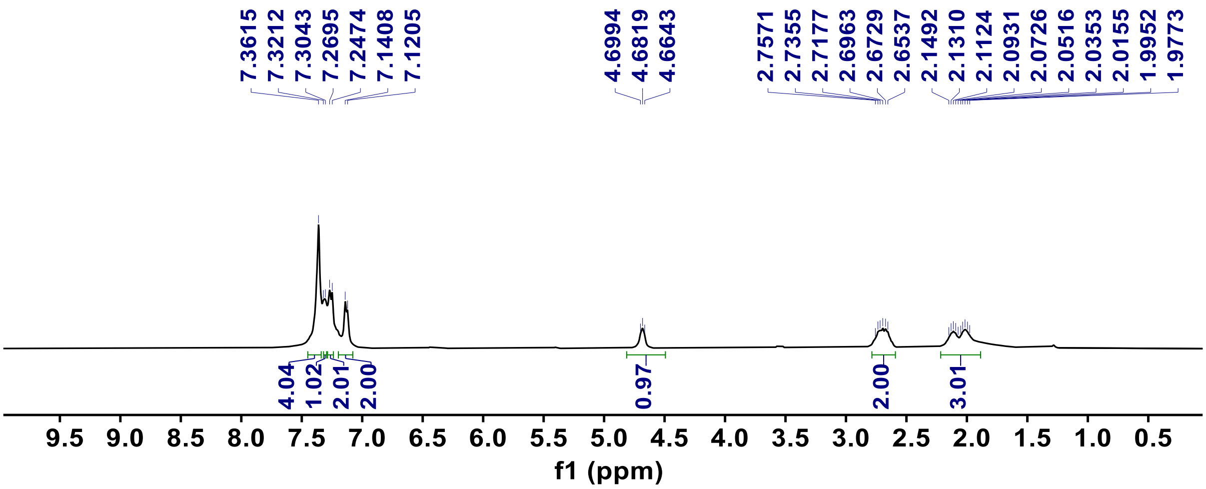


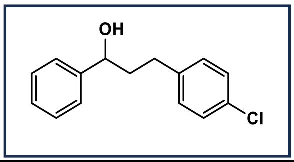
[13]C{[1]H} NMR (125 MHz, $CDCl_3$), **32d**



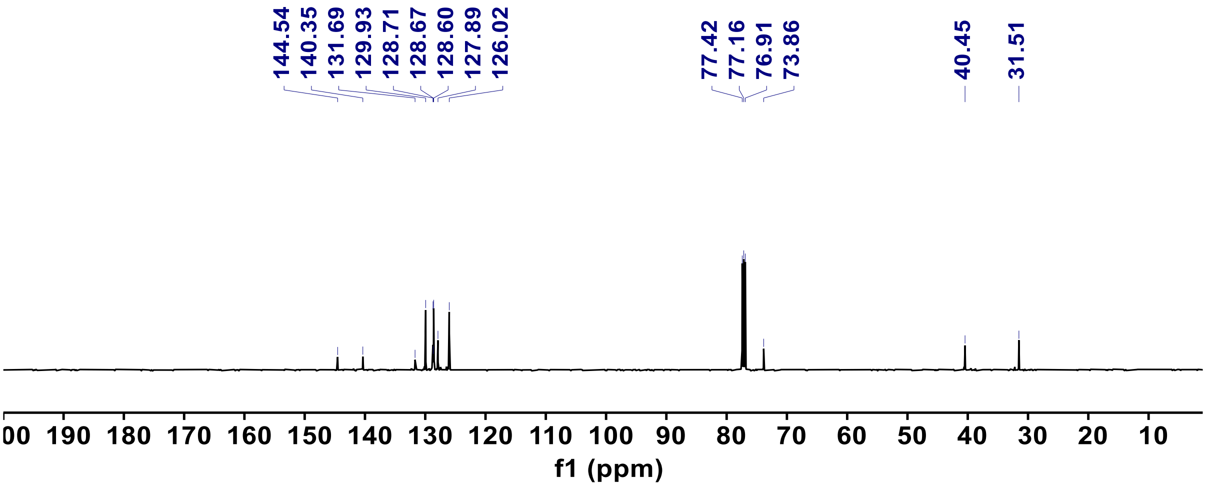


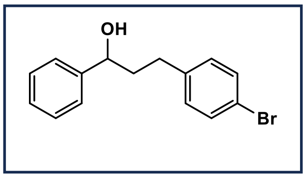
^{1}**H NMR** (400 MHz, $CDCl_3$), **33d**



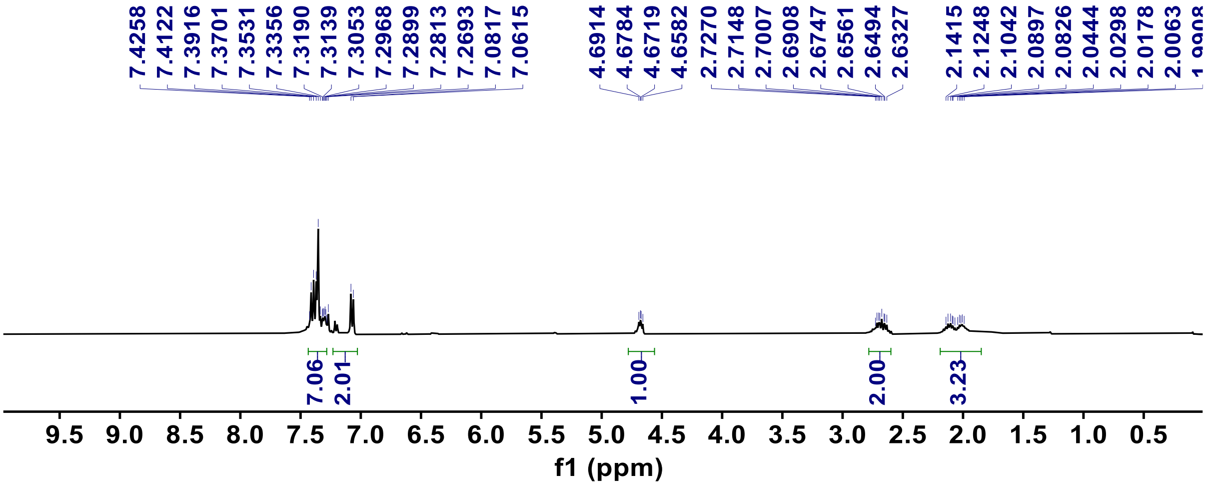


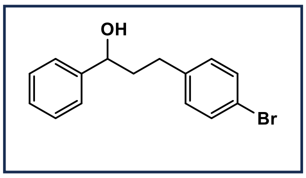
^{13}**C{^{1}H} NMR** (125 MHz, $CDCl_3$), **33d**



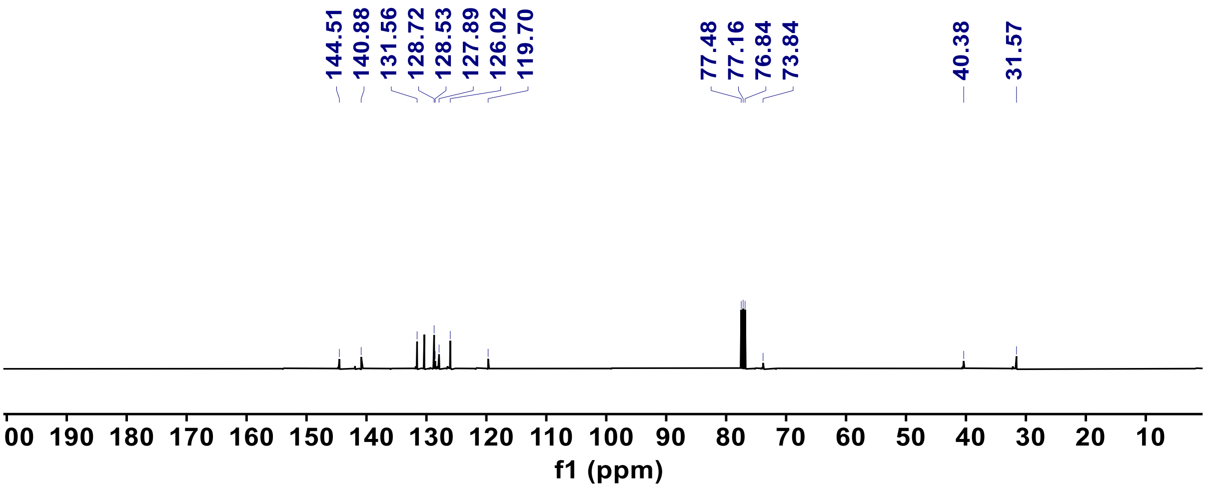


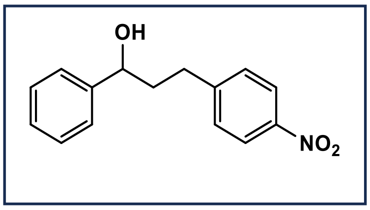
^{1}**H NMR** (400 MHz, $CDCl_3$), **34d**



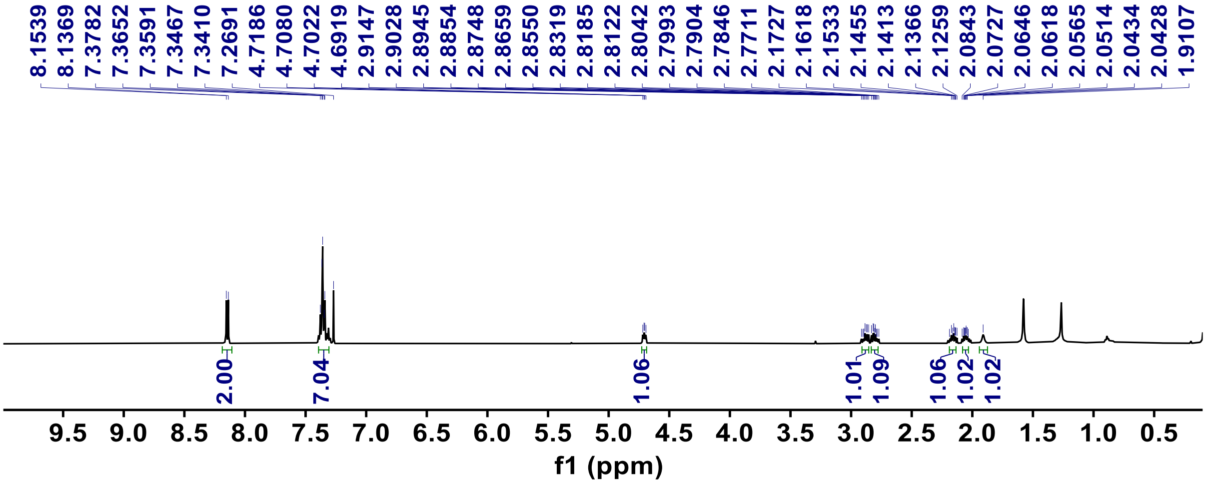


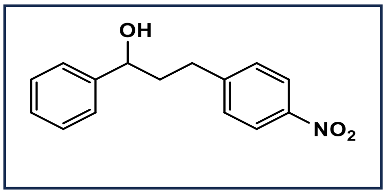
^{13}**C{^{1}H} NMR** (100 MHz, $CDCl_3$), **34d**



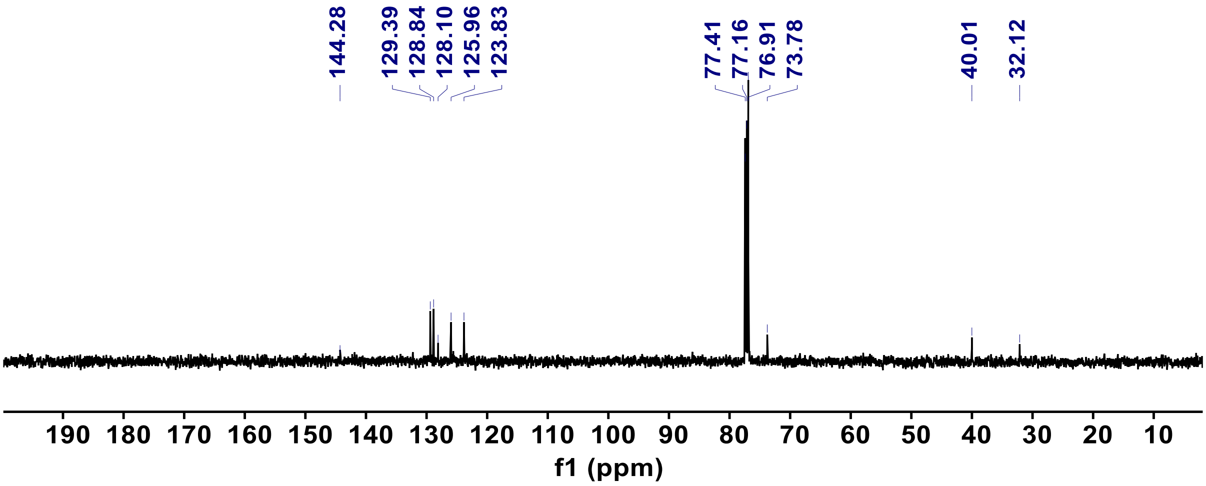


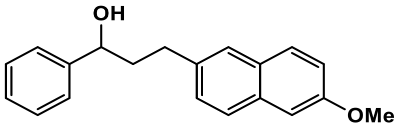
^{1}**H NMR** (500 MHz, $CDCl_3$), **35d**



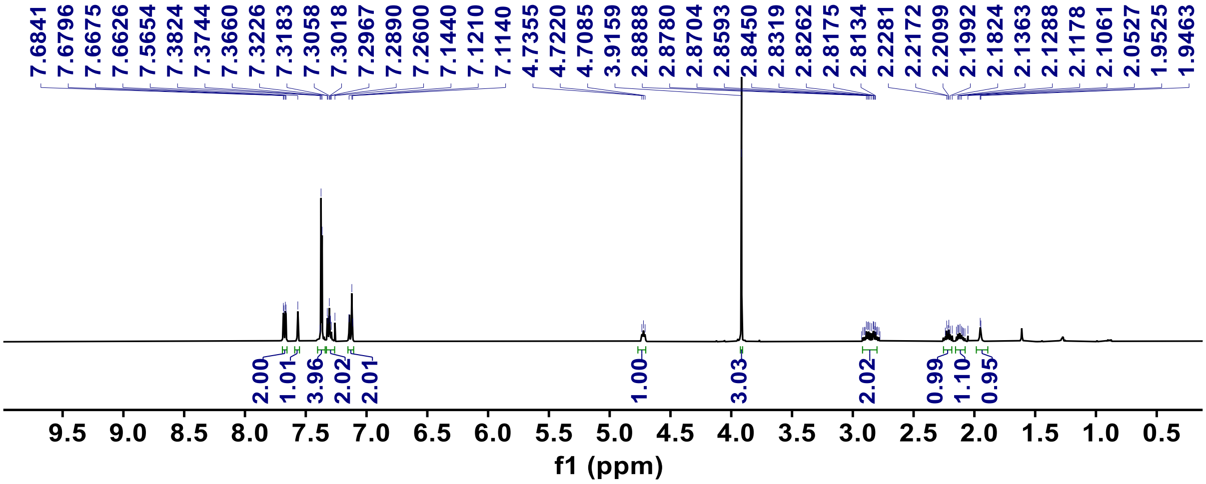


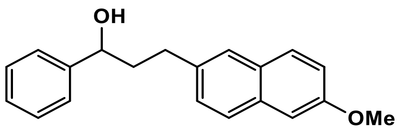
^{13}**C{^{1}H} NMR** (125 MHz, $CDCl_3$), **35d**



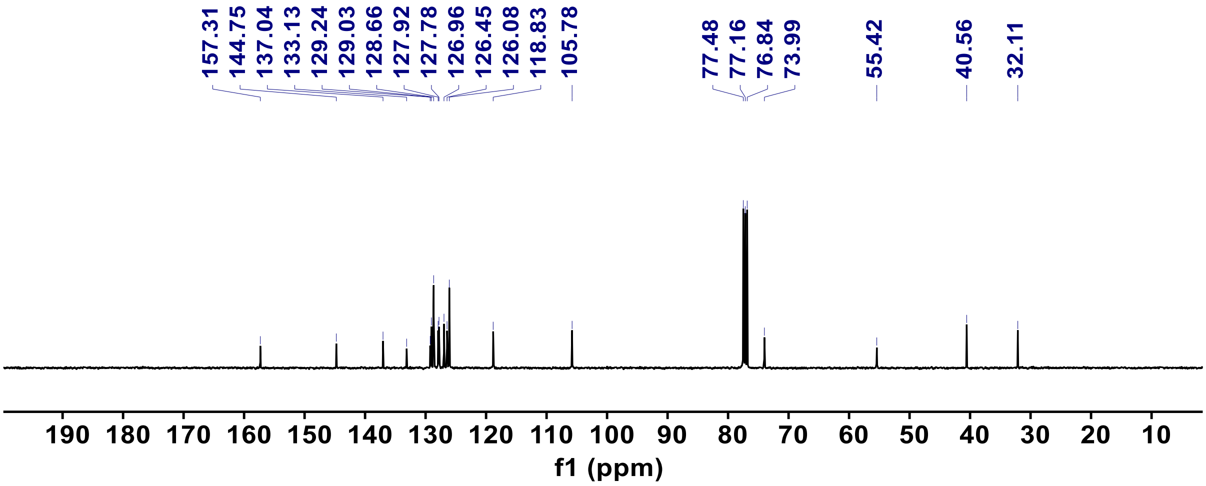


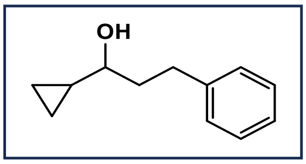
^{1}H NMR (500 MHz, $CDCl_3$), **36d**



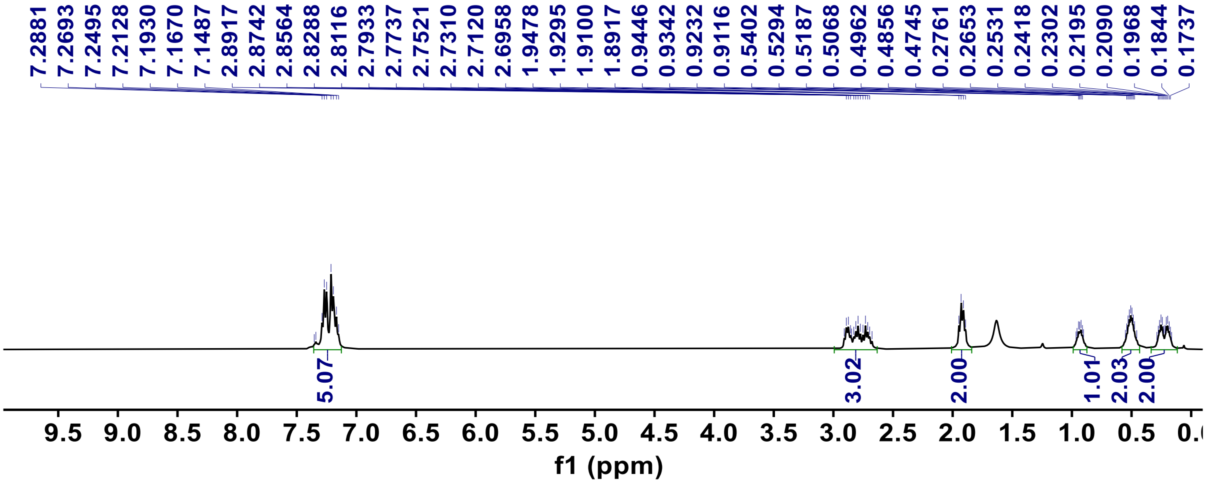


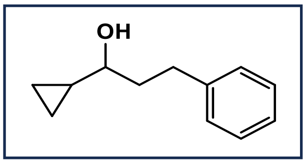
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$), **36d**



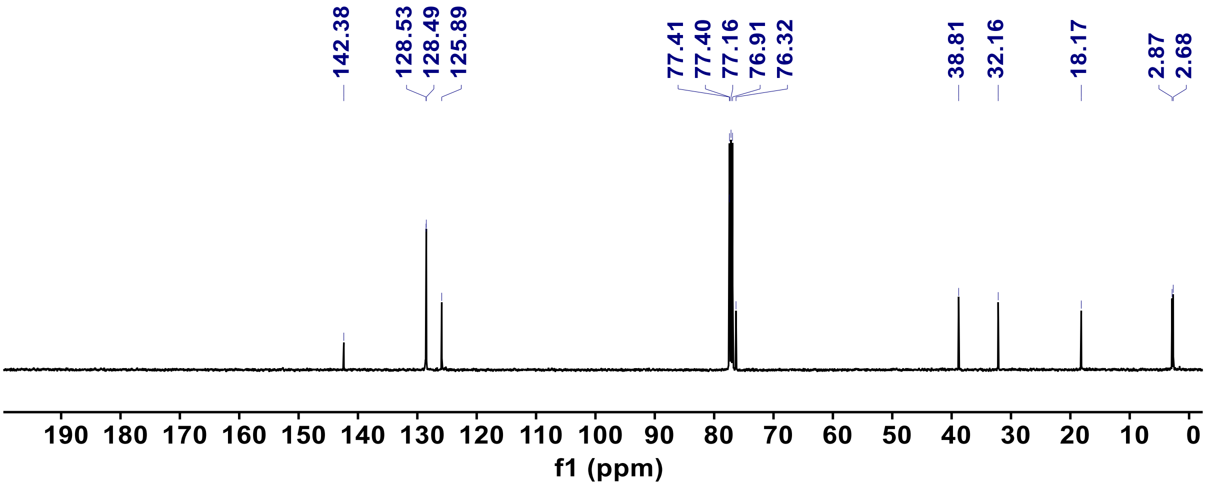


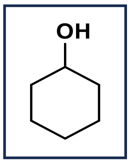
[1]H NMR (400 MHz, $CDCl_3$), **37d**



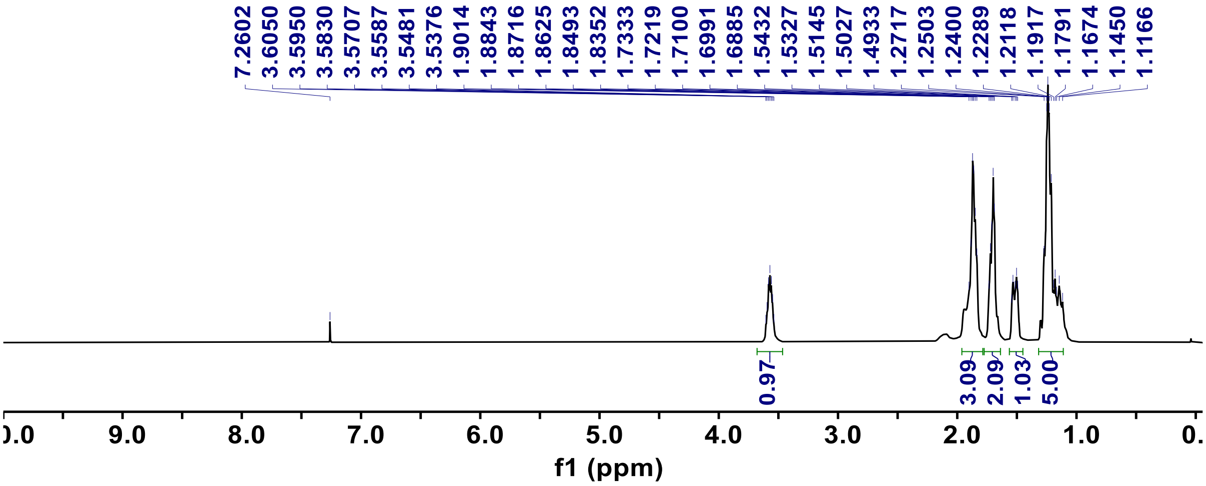


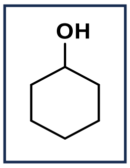
[13]C{[1]H} NMR (125 MHz, $CDCl_3$), **37d**



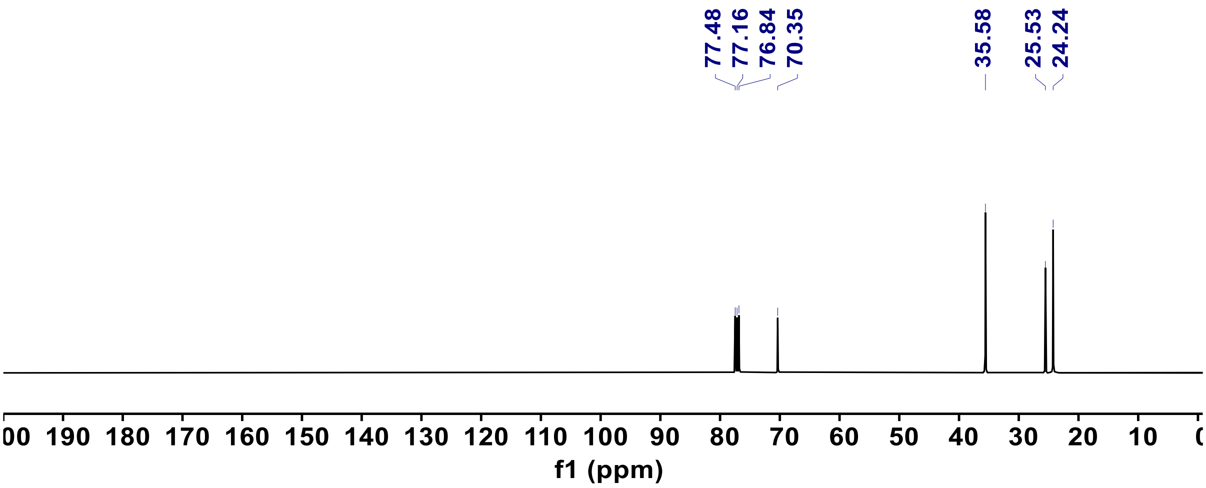


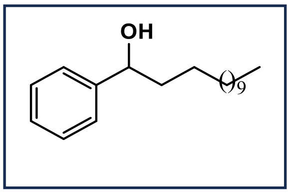
[1]H NMR (400 MHz, $CDCl_3$), **38d**



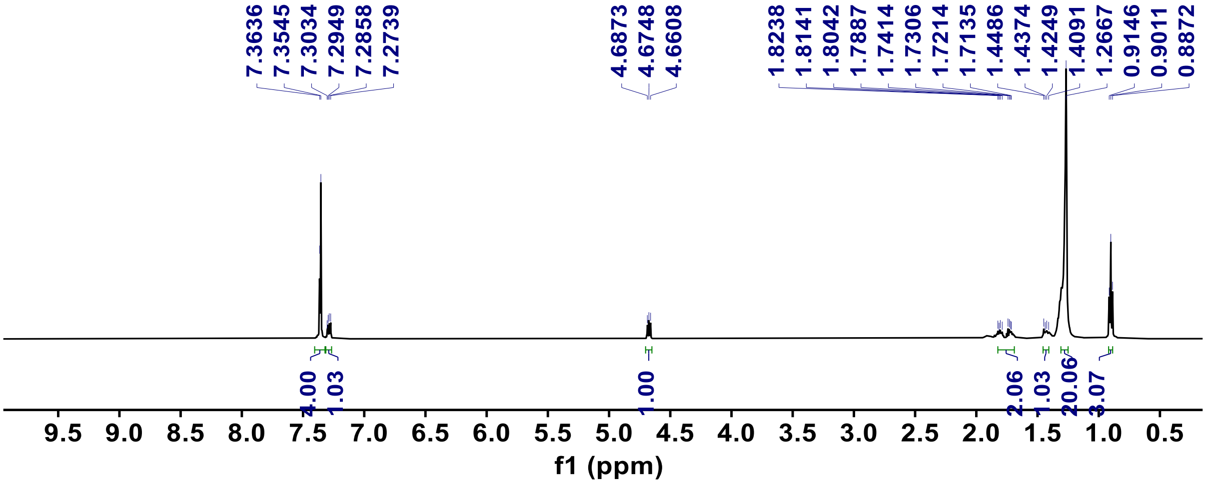


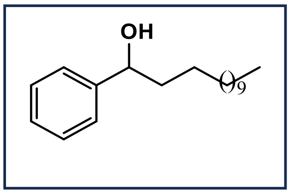
[13]C{[1]H} NMR (100 MHz, $CDCl_3$), **38d**



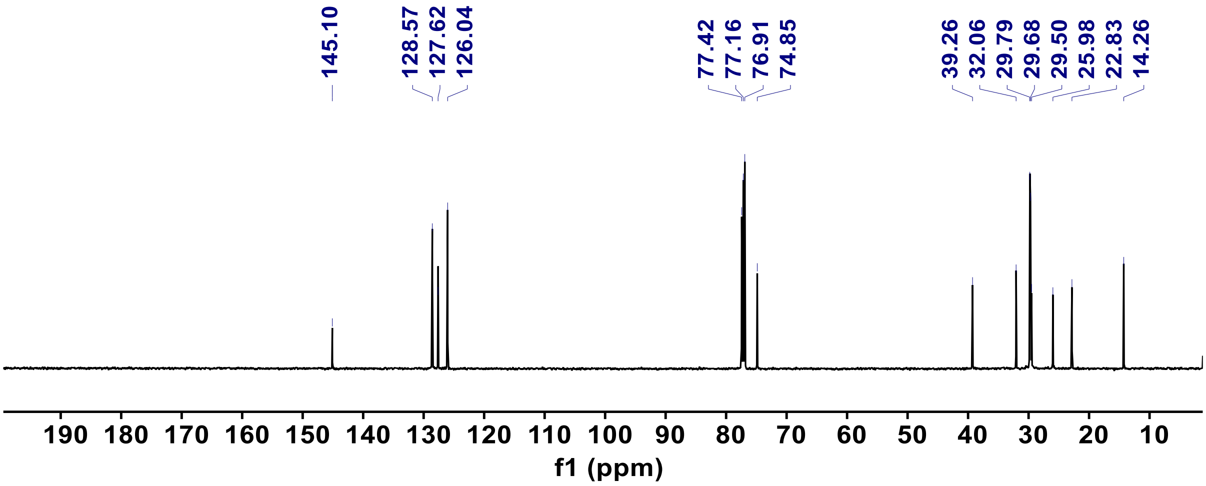


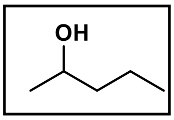
^{1}**H NMR** (500 MHz, $CDCl_3$), **39d**



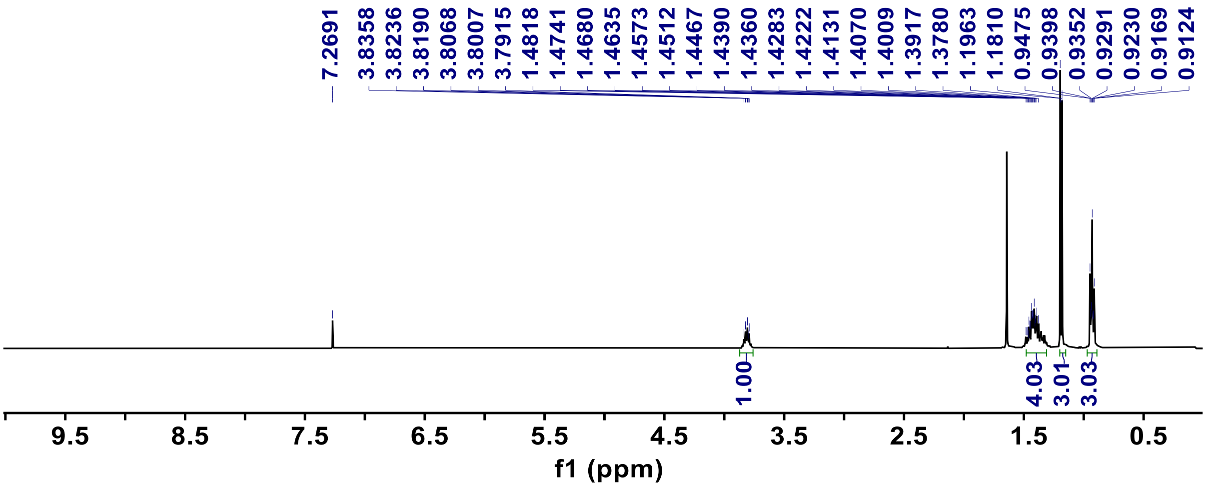


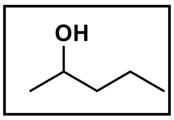
^{13}**C{^{1}H} NMR** (100 MHz, $CDCl_3$), **39d**



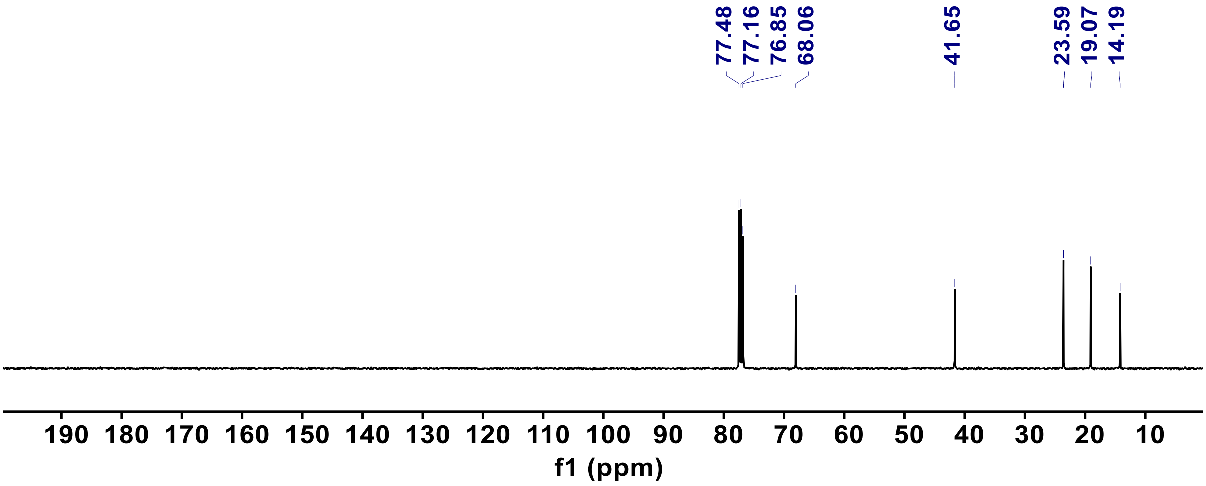


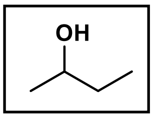
^{1}**H NMR** (400 MHz, $CDCl_3$), **40d**



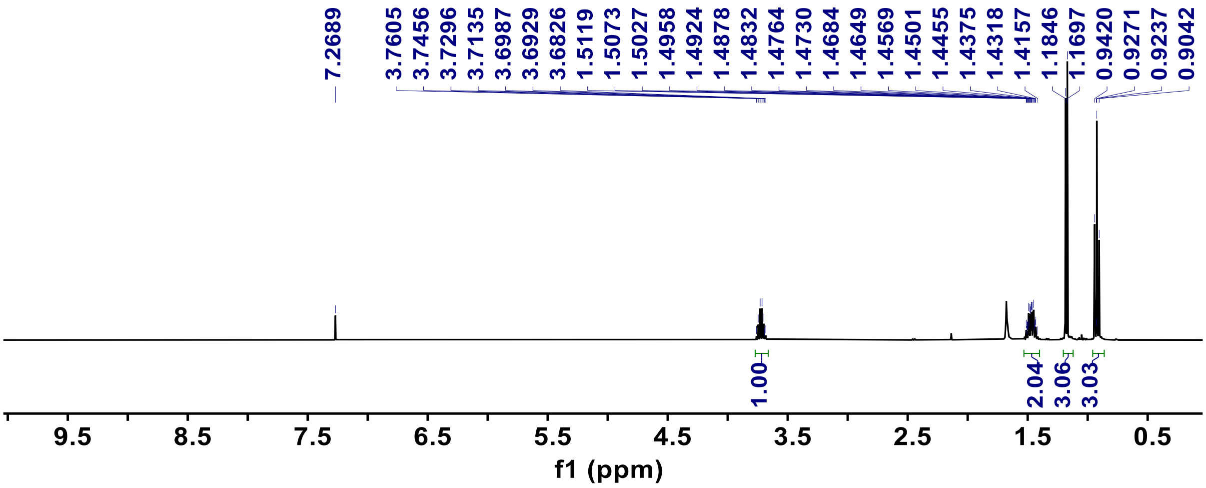


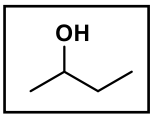
^{13}**C{^{1}H} NMR** (100 MHz, $CDCl_3$), **40d**



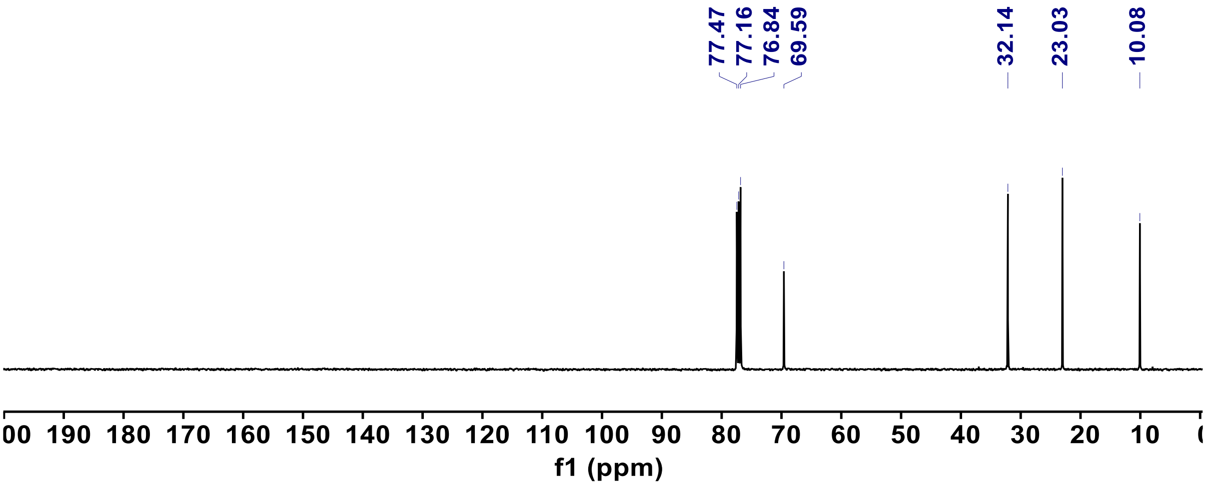


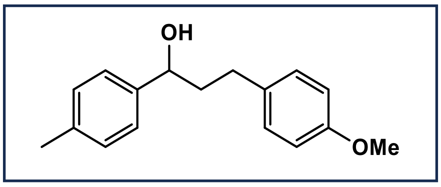
^{1}H NMR (400 MHz, $CDCl_3$), **41d**



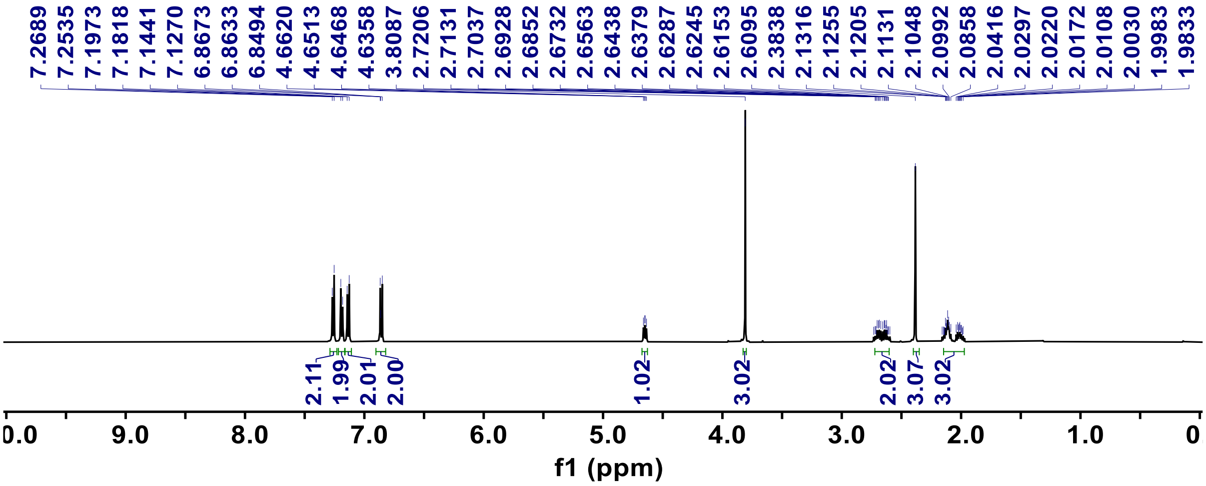


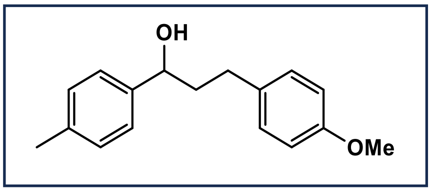
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$), **41d**



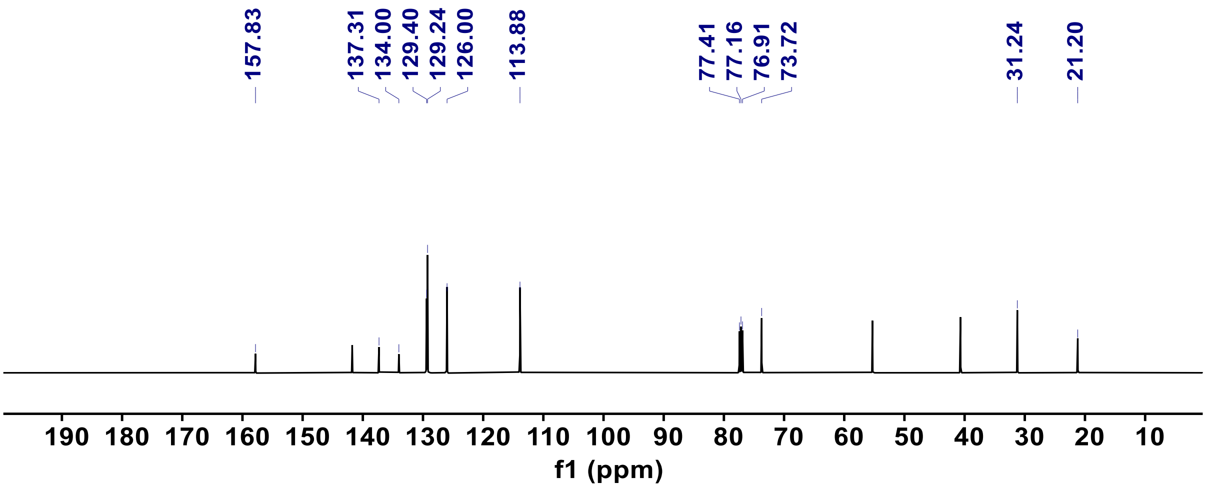


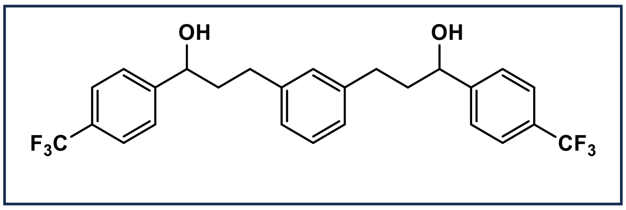
^{1}H NMR (500 MHz, $CDCl_3$), **42d**



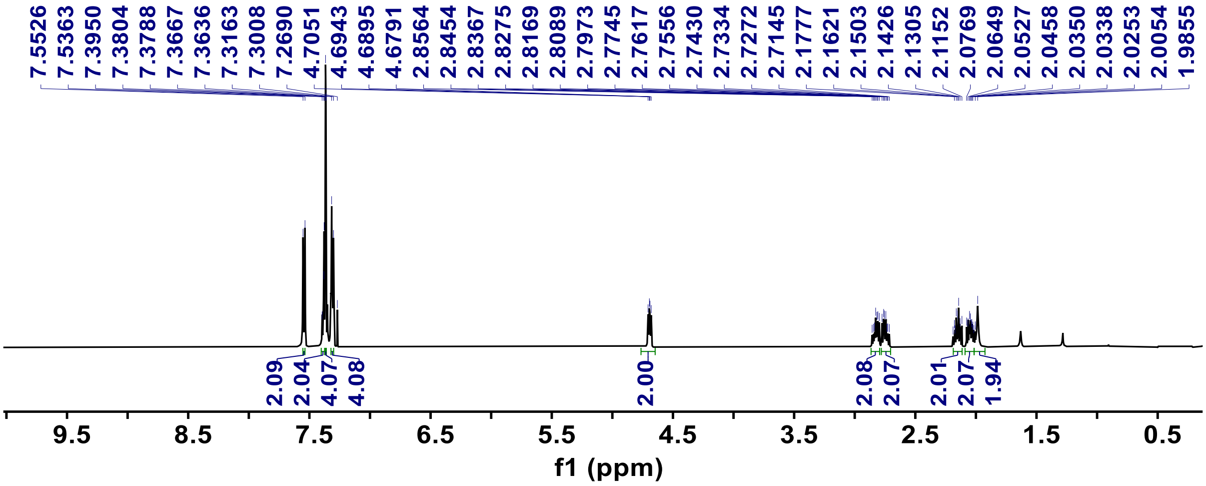


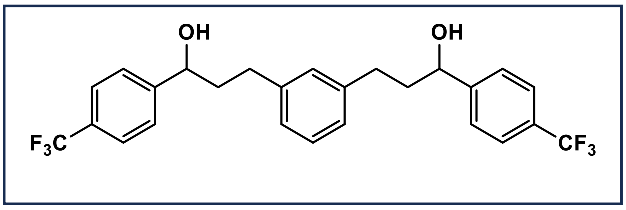
^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$), **42d**



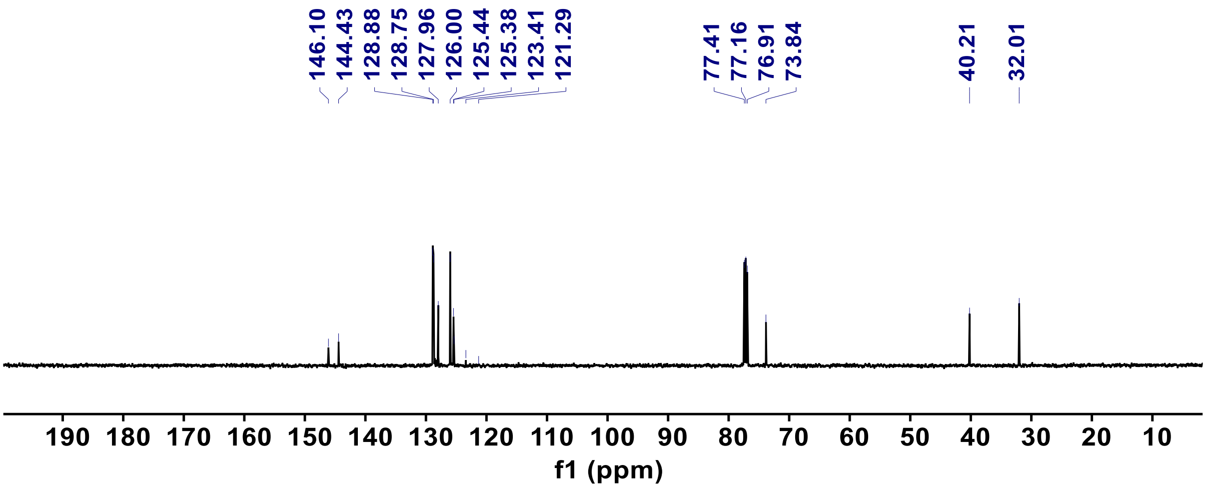


¹H NMR (500 MHz, CDCl₃), **43d**

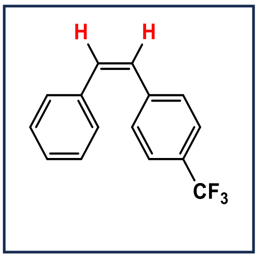




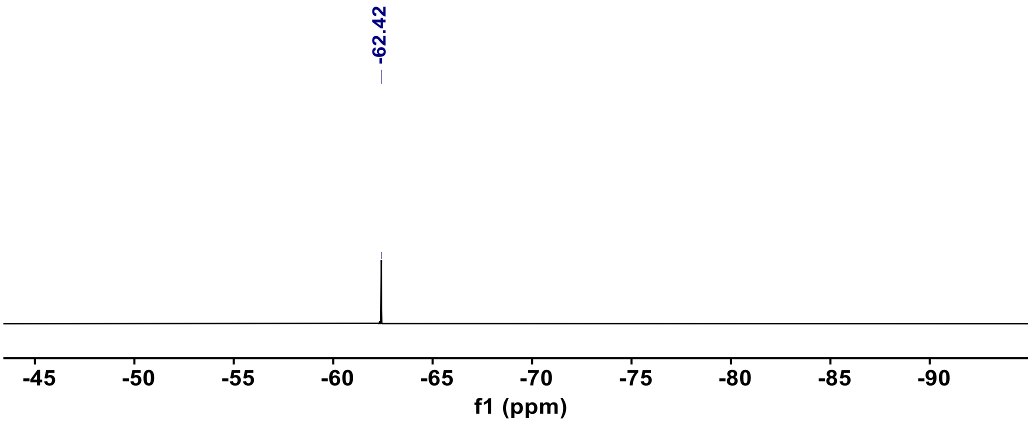
¹³C{¹H} NMR (125 MHz, CDCl₃), **43d**

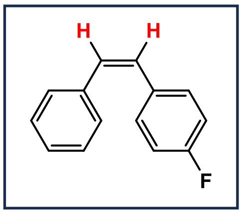


13. Copies of ^{19}F NMR Spectra of Products

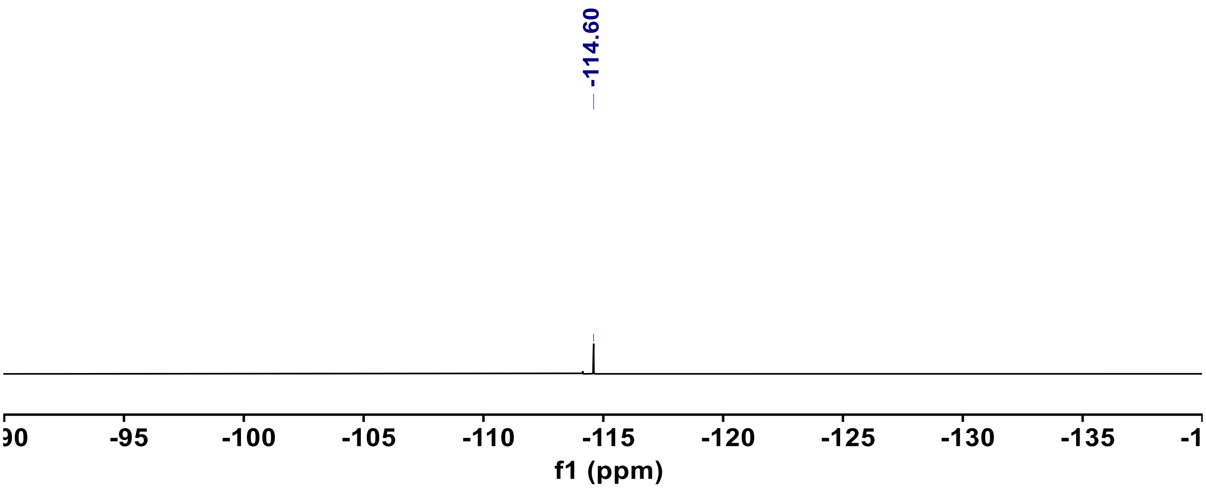


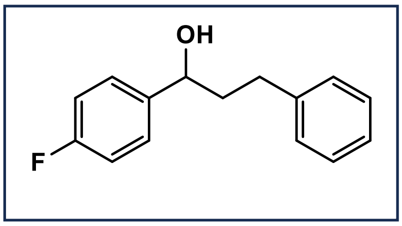
^{19}F{^{1}H} NMR (470 MHz, $CDCl_3$), **4b**



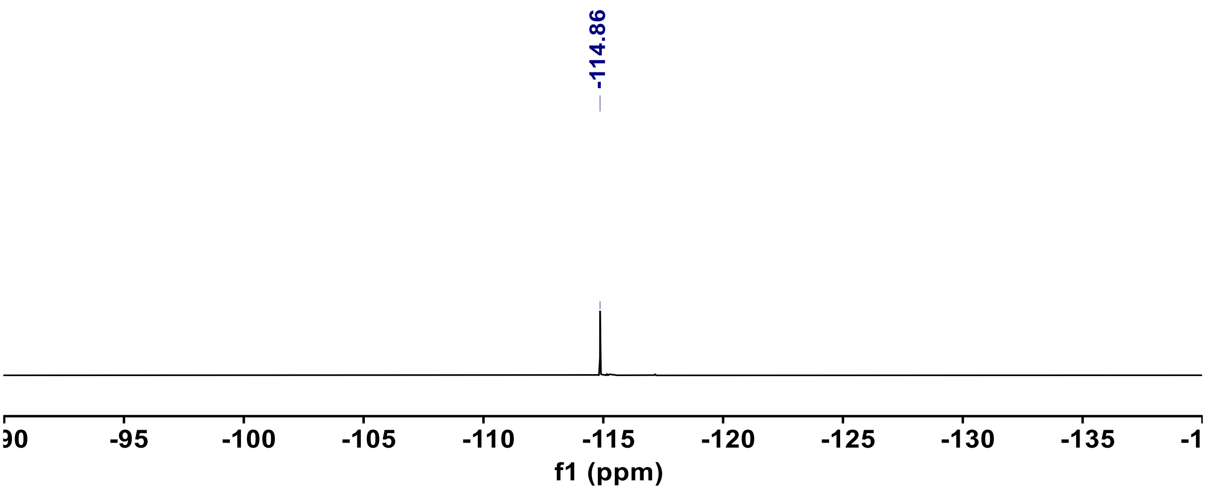


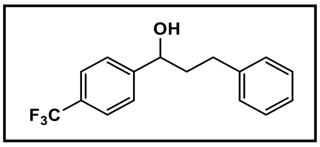
^{19}F{^{1}H} NMR (470 MHz, $CDCl_3$), **5b**



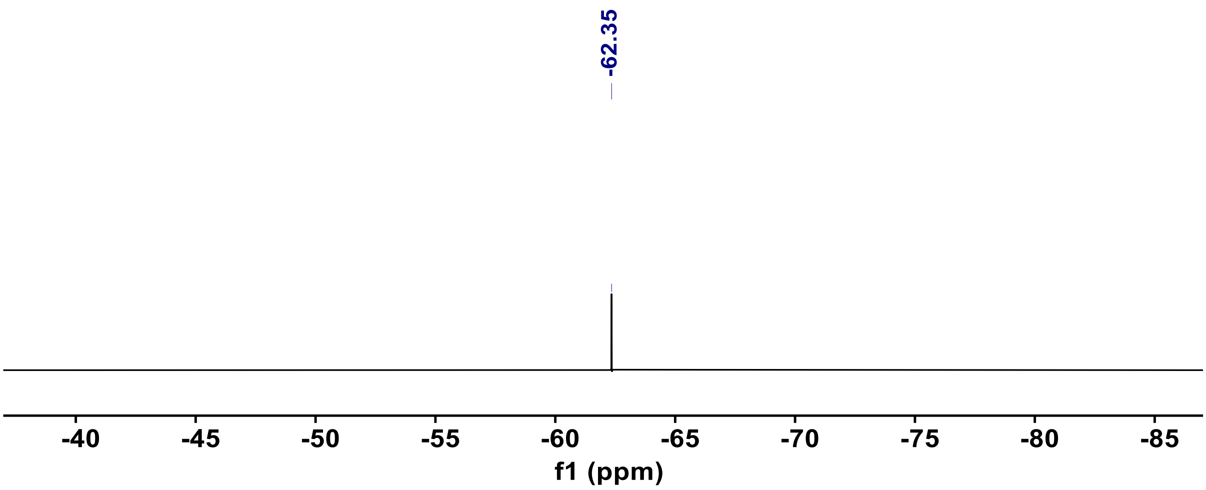


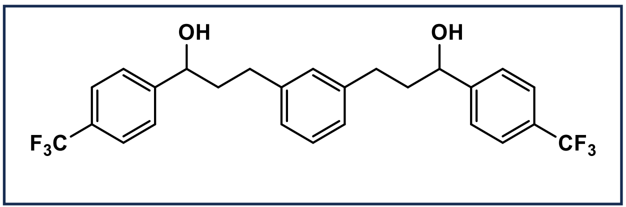
^{19}**F{^{1}H} NMR** (470 MHz, $CDCl_3$), **25d**



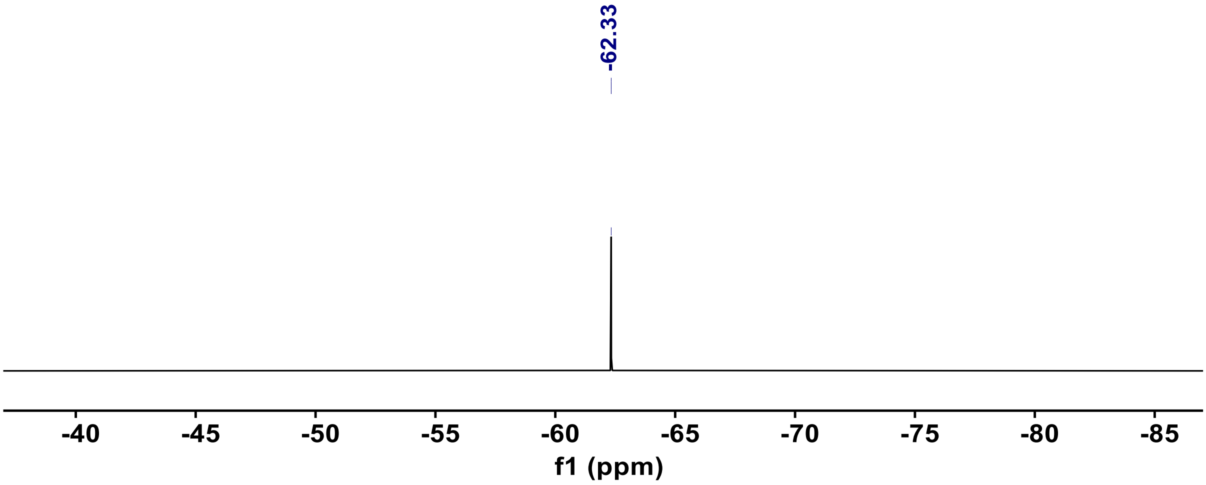


^{19}**F{^{1}H} NMR** (470 MHz, $CDCl_3$), **27d**





$^{19}F\{^{1}H\}$ NMR (470 MHz, $CDCl_3$), **43d**



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