

Supporting Information

Room temperature chemoselective hydrogenation of C=C, C=O and C=N bonds by using a well-defined mixed donor Mn(I) pincer catalyst

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Contents

	Page #
1. General Experimental	S3
2. Synthesis of Ligand and Manganese Complexes	S3
3. Synthesis of Starting Compound	S7
4. Detailed Optimization Study	S8
5. Representative Procedure for Hydrogenation	S9
6. Characterization Data of Hydrogenated Compounds	S10
7. Mechanistic Experiments	S32
8. DFT Calculations	S38
9. X-ray Structural Data	S39
10. References	S45
11. ^1H , $^{13}\text{C}\{^1\text{H}\}$ -NMR and $^{31}\text{P}\{^1\text{H}\}$ -NMR, Mass and IR Spectra of Complexes	S47
12. ^1H and $^{13}\text{C}\{^1\text{H}\}$ -NMR Spectra of Starting Compound	S62
13. ^1H and $^{13}\text{C}\{^1\text{H}\}$ -NMR Spectra of Hydrogenated Compounds	S63

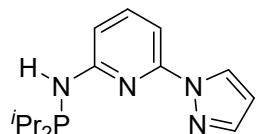
1. General Experimental

All the manipulations were conducted under an argon atmosphere either in a glove box or using standard Schlenk techniques in pre-dried glasswares. The catalytic reactions were performed in flame-dried glass vials with magnetic bar by placing them in the pressure reactor. Solvents were dried over Na/benzophenone or Mg and distilled prior to use. Liquid reagents were flushed with argon prior to use. The ligand precursor 6-(1*H*-pyrazol-1-yl)pyridin-2-amine,¹ ligands **L1**² and **L3**^{1,3} were prepared according to the previously described procedures. The Mn(CO)₅Br was prepared by treating the Mn(CO)₁₀ with Br₂. All other chemicals were obtained from commercial sources and were used without further purification. Infrared (IR) spectra were recorded on a FT-IR Bruker Alpha II spectrometer as solution of chloroform, THF or methanol. High resolution mass spectrometry (HRMS) mass spectra were recorded on a Thermo Scientific Q-Exactive, Accela 1250 pump. NMR: (¹H and ¹³C{¹H}) spectra were recorded at 200, 400 or 500 MHz (¹H), 100 or 125 MHz (¹³C{¹H}), DEPT (distortionless enhancement by polarization transfer), 377 MHz (¹⁹F), 162 MHz (³¹P{¹H}) respectively, in CDCl₃ solutions, if not otherwise specified; chemical shifts (δ) are given in ppm. The ¹H and ¹³C{¹H} NMR spectra are referenced to residual solvent signals (CDCl₃: δ H = 7.26 ppm, δ C = 77.2 ppm; DMSO-*d*₆: δ H = 2.50 ppm, δ C = 39.5 ppm; acetone-*d*₃: δ H = 2.05 ppm).

GC Method. Gas Chromatography analyses were performed using a Shimadzu GC2010 gas chromatograph equipped with a Shimadzu AOC-20s auto sampler and a Restek RTX-5 capillary column (30 m x 0.25 mm x 0.25 μ m). The instrument was set to an injection volume of 1 μ L, an inlet split ratio of 10:1, and inlet and detector temperatures of 250 and 320 °C, respectively. UHP-grade nitrogen was used as carrier gas with a flow rate of 30 mL/min. The temperature program used for all the analyses is as follows: 80 °C, 1 min; 30 °C/min to 200 °C, 2 min; 30 °C/min to 260 °C, 3 min; 30 °C/min to 300 °C, 15 min.

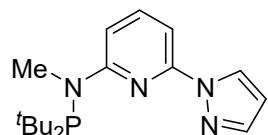
2. Synthesis of Ligand and Manganese Complexes

Synthesis of *N*-(di-*iso*-propylphosphaneyl)-6-(1*H*-pyrazol-1-yl)pyridin-2-amine (L2):



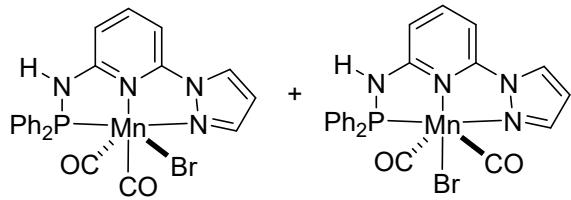
In a 50 mL oven dried Schlenk flask, 6-(1*H*-pyrazol-1-yl)pyridin-2-amine (0.20 g, 1.25 mmol) was dissolved in THF (10 mL) followed by the addition of freshly distilled Et₃N (0.21

mL, 1.5 mmol) under inert atmosphere. The reaction mixture was cooled to 0 °C and chlorodiisopropylphosphine (0.21 g, 1.37 mmol) was added dropwise. The reaction mixture was allowed to room temperature and stirred for 1 h. Further the reaction mixture was cooled to -78 °C and *n*-BuLi (0.94 mL, 1.5 mmol; 1.6 M in THF) was added dropwise resulting in a colorless solution. Then the reaction was allowed to room temperature and stirred for 1 h, followed by heating at 60 °C for 16 h. The volatiles were evaporated under vacuum and 30 mL of toluene was added into it. The filtration and evaporation of toluene extract gave *N*-(di-*iso*-propylphosphaneyl)-6-(1*H*-pyrazol-1-yl)pyridin-2-amine (**L2**; 0.27 g, 78%) as colorless liquid. ¹H-NMR (500 MHz, C₆D₆): δ = 8.65 (d, *J* = 2.1 Hz, 1H, Ar-H), 7.68-7.66 (m, 2H, Ar-H), 7.13 (t, *J* = 8.1 Hz, 1H, Ar-H), 6.95 (dd, *J* = 7.9, 2.2 Hz, 1H, Ar-H), 6.14 (dd, *J* = 2.4, 1.5 Hz, 1H), 4.55 (br s, 1H, NH), 1.41 (d sept, *J* = 6.9, 1.7 Hz, 2H, CH), 0.90 (dd, *J* = 16.2, 7.3 Hz, 6H, CH₃), 0.86 (dd, *J* = 11.0, 7.0 Hz, 6H, CH₃). ¹³C{¹H}-NMR (125 MHz, C₆D₆): δ = 160.4 (d, *J* = 20.0 Hz, C_q), 151.4 (C_q), 142.2 (CH), 140.6 (CH), 127.0 (CH), 107.7 (CH), 106.4 (d, *J* = 17.2 Hz, CH), 103.0 (CH), 26.8 (d, *J* = 12.4 Hz, 2C, CH), 19.2 (CH₃), 19.0 (CH₃), 17.5 (CH₃), 17.4 (CH₃). ³¹P{¹H}-NMR (162 MHz, C₆D₆): 48.6 (s).

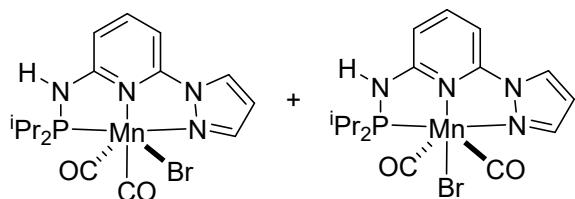


***N*-(Di-*tert*-butylphosphaneyl)-*N*-methyl-6-(1*H*-pyrazol-1-yl)pyridin-2-amine**

(**L3^{Me}**): In a 50 mL round bottom flask, *N*-(di-*tert*-butylphosphaneyl)-6-(1*H*-pyrazol-1-yl)pyridin-2-amine (0.10 g, 0.33 mmol) in THF (5 mL) was cooled to -20 °C and *n*-BuLi (0.25 mL, 0.40 mmol; 1.6 M in hexane) was added followed by the addition of MeI (0.055 g, 0.39 mmol). The reaction mixture was allowed to the room temperature and stirred for overnight. The volatiles were evaporated under vacuo and 20 mL of water was added. The organic layer was extracted in EtOAc and the crude product was subjected to the column chromatography on silica gel (petroleum ether/EtOAc:10/1) to yield **L3^{Me}** (0.071 g, 68%) as white solid. ¹H-NMR (500 MHz, CDCl₃): δ = 8.30 (d, *J* = 2.4 Hz, 1H, Ar-H), 7.66 (s, 1H, Ar-H), 7.36 (dt, *J* = 7.9, 2.1 Hz, 1H, Ar-H), 7.04 (d, *J* = 7.5 Hz, 1H, Ar-H), 6.51 (d, *J* = 8.1 Hz, 1H), 6.37 (t, *J* = 2.1 Hz, 1H, Ar-H), 1.83 (d, *J* = 11.1 Hz, 3H, CH₃), 1.34 (d, *J* = 14.1 Hz, 18H, CH₃). ¹³C{¹H}-NMR (100 MHz, CDCl₃): δ = 164.4 (d, *J* = 9.2 Hz, C_q), 149.8 (C_q), 140.9 (CH), 138.6 (d, *J* = 3.8 Hz, CH), 126.3 (CH), 116.1 (d, *J* = 22.1 Hz, CH), 106.5 (CH), 98.5 (CH), 36.4 (d, *J* = 65.6 Hz, 2C, C_q), 27.2 (6C, CH₃), 5.6 (d, *J* = 42.0 Hz, CH₃). ³¹P{¹H}-NMR (162 MHz, CDCl₃): 36.9 (s).

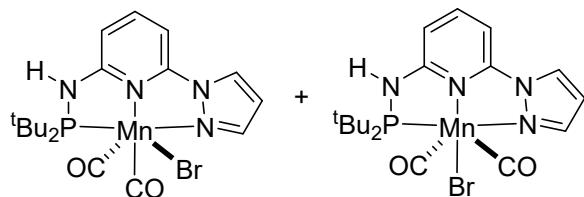


Synthesis and Characterization of Mn-1: In a 25 mL round bottom flask *N*-(diphenylphosphanoyl)-6-(1*H*-pyrazol-1-yl)pyridin-2-amine (**L1**; 0.084 g, 0.244 mmol) and Mn(CO)₅Br (0.067 g, 0.244 mmol) were added inside the glove box. The reaction flask was taken out and THF (3 mL) was added. The reaction mixture was stirred under inert atmosphere at room temperature (27 °C) for 20 h, wherein the desired complex was precipitated out. The solid compound was separated from mother liquor and was washed with *n*-hexane (10 mL x 3). The resulted complex was dried under vacuum to give yellow powder of **Mn-1** (0.090 g, 69%). **FT-IR** (ν_{CO} , cm⁻¹): 1935, 1865, 1857. **¹H-NMR** (500 MHz, DMSO-*d*₆): (*one isomer*): δ = 10.34 (br s, 1H), 9.15 (br s, 1H), 8.57 (br s, 1H), 8.10 (br s, 1H), 7.77-7.42 (m, 11H), 7.28 (br s, 1H), 6.92 (br s, 1H); (*other isomer*): δ = 10.02 (br s, 1H), 8.99 (br s, 1H), 8.22 (br s, 1H), 7.96 (br s, 1H), 7.77-7.42 (m, 11H), 7.16 (br s, 1H), 6.77 (br s, 1H). **¹³C{¹H}-NMR** (125 MHz, DMSO-*d*₆): (*for both isomers*) δ = 229.3, 225.3, 223.8, 160.0, 147.4, 146.1, 144.9, 141.5, 139.9, 136.2, 130.9, 129.8, 129.5, 128.9, 128.1, 127.7, 127.0, 125.7, 110.9, 106.7, 99.3. **³¹P{¹H}-NMR** (162 MHz, DMSO-*d*₆, ppm): 136.9 (s), 134.5 (s). **ESI-MS** (–ve mode): *m/z* [M–H][–] Calcd for [C₂₂H₁₇⁷⁹BrMnN₄O₂P–H] 532.9569, Found 532.9575; *m/z* [M–H][–] Calcd for [C₂₂H₁₇⁸¹BrMnN₄O₂P–H] 534.9549, Found 534.9554.

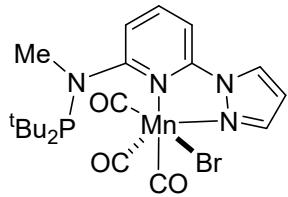


Synthesis and Characterization of Mn-2: This complex was synthesized following the procedure similar to the synthesis of **Mn-1**, using *N*-(di-*iso*-propylphosphanoyl)-6-(1*H*-pyrazol-1-yl)pyridin-2-amine (**L2**; 0.060 g, 0.217 mmol) and Mn(CO)₅Br (0.060 g, 0.218 mmol). The complex **Mn-2** was obtained as an orange powder. Yield: 0.090 g (89%). **FT-IR** (ν_{CO} , cm⁻¹): 1940, 1872, 1857. **¹H-NMR** (400 MHz, DMSO-*d*₆): (*one isomer*): δ = 9.15 (br s, 1H), 8.92 (br s, 1H), 8.49 (br s, 1H), 7.94 (br s, 1H), 7.53 (br s, 1H), 7.03 (br s, 1H), 6.91 (br s, 1H), 1.30-1.18 (m, 14H); (*other isomer*): δ = 9.13 (br s, 1H), 8.80 (br s, 1H), 8.10 (br s, 1H), 7.79 (br s, 1H), 7.40 (br s, 1H), 6.91 (br s, 1H), 6.72 (br s, 1H), 1.18-1.09 (m, 14H).

$^{13}\text{C}\{\text{H}\}$ -NMR (100 MHz, DMSO- d_6): (*one isomer*): δ = 230.2 (d, J = 15.3 Hz, CO), 226.6 (d, J = 22.9 Hz, CO), 161.0 (d, J = 9.5 Hz, C_q), 147.4 (C_q), 146.1 (CH), 141.1 (CH), 130.9 (CH), 111.4 (CH), 106.5 (CH), 98.8 (CH), 29.7, 26.4, 18.1, 17.4; (*other isomer*): δ = 227.0 (d, J = 19.1 Hz, CO), 225.8 (d, J = 22.9 Hz, CO), 160.6 (d, J = 9.5 Hz, C_q), 147.4 (C_q), 144.3 (CH), 139.5 (CH), 129.3 (CH), 110.6 (CH), 105.2 (CH), 98.1 (CH), 26.5, 25.8, 17.3, 16.5. **$^{31}\text{P}\{\text{H}\}$ -NMR** (162 MHz, DMSO- d_6 , ppm): 159.8 (s), 158.4 (s). **ESI-MS** (–ve mode): *m/z* [M–H][–] Calcd for [C₁₆H₂₁⁷⁹BrMnN₄O₂P–H] 464.9882, Found 464.9887; *m/z* [M–H][–] Calcd for [C₁₆H₂₁⁸¹BrMnN₄O₂P–H] 466.9862, Found 466.9866.

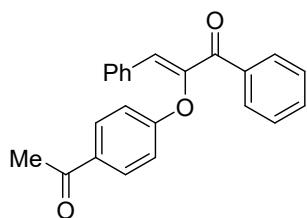


Synthesis and Characterization of Mn-3: In a 25 mL round bottom flask *N*-(di-tert-butylphosphanyl)-6-(1*H*-pyrazol-1-yl)pyridin-2-amine (**L3**; 0.050 g, 0.164 mmol), Mn(CO)₅Br (0.045 g, 0.164 mmol) and THF (10 mL) were added under argon atmosphere. The reaction mixture was stirred under inert atmosphere in dark at room temperature (27 °C) for 48 h. The resulted dark-red reaction mixture was concentrated and hexane was slowly added to precipitate out the orange compound. The mother liquor was separated and the solid compound was washed with hexane (5 mL x 3) and dried under vacuum to give orange solid of **Mn-3** (0.064 g, 79%). Note: The synthesized **Mn-3** is sensitive to light, hence stored in brown colored vial. **FT-IR** (ν_{CO} , cm^{–1}): 2053, 1959, 1930. **$^1\text{H-NMR}$** (200 MHz, CD₃OD): (*one isomer*): δ = 8.53 (br s, 1H, Ar–H), 7.79 (br s, 1H, Ar–H), 7.56 (br s, 1H, Ar–H), 7.07 (br s, 1H, Ar–H), 6.75 (br s, 1H, Ar–H), 6.48 (br s, 1H, Ar–H), 0.99 (d, J = 14.5 Hz, 18H, CH₃); (*other isomer*): δ = 8.39 (br s, 1H, Ar–H), 7.79 (br s, 1H, Ar–H), 7.56 (br s, 1H, Ar–H), 7.07 (br s, 1H, Ar–H), 6.75 (br s, 1H, Ar–H), 6.39 (br s, 1H, Ar–H), 0.93 (d, J = 14.5 Hz, 18H, CH₃). **$^{31}\text{P}\{\text{H}\}$ -NMR** (162 MHz, CD₂Cl₂, ppm): 178.5 (s), 175.3 (s). **$^{31}\text{P}\{\text{H}\}$ -NMR** (162 MHz, CD₃OD, ppm): 176.6 (s), 171.3 (s). **ESI-MS** (–ve mode): *m/z* [M–H][–] Calcd for [C₁₈H₂₅⁷⁹BrMnN₄O₂P–H] 493.0195, Found 493.0197; *m/z* [M–H][–] Calcd for [C₁₈H₂₅⁸¹BrMnN₄O₂P–H] 495.0175, Found 495.0178. **Elem. Anal.** Calcd for C₁₈H₂₅BrMnN₄O₂P: C, 43.66; H, 5.09; N, 11.31. Found: C, 43.37; H, 5.26; N, 11.04.



Synthesis and characterization of Mn-3^{Me}: This complex was synthesized following the procedure similar to the synthesis of **Mn-1**, using *N*-(di-tert-butylphosphanyl)-*N*-methyl-6-(1*H*-pyrazol-1-yl)pyridin-2-amine (0.042 g, 0.132 mmol) and Mn(CO)₅Br (0.036 g, 0.131 mmol), and the reaction mixture was stirred at room temperature (27 °C) for 16 h. The complex **Mn-3^{Me}** was obtained as an orange powder. Yield: 0.060 g (85%). **FT-IR** (ν_{CO} , cm⁻¹): 2018, 1924, 1901. **¹H-NMR** (500 MHz, acetone- d_6): δ = 8.67 (br s, 1H, Ar-H), 8.21 (br s, 1H, Ar-H), 7.45 (br s, 1H, Ar-H), 7.02 (br s, 1H, Ar-H), 6.73 (br s, 1H, Ar-H), 6.63 (br s, 1H, Ar-H), 1.93 (s, 3H, CH₃), 1.43 (d, J = 12.8 Hz, 18H, CH₃). **¹³C{¹H}-NMR** (125 MHz, DMSO- d_6): δ = 224.2 (CO), 223.9 (CO), 223.1 (CO), 164.9 (C_q), 148.3 (C_q), 144.0 (CH), 138.1 (CH), 129.7 (CH), 112.0 (CH), 110.5 (CH), 96.4 (CH), 36.2 (d, J = 63.6 Hz, 2C C_q), 25.8 (d, J = 30.5 Hz, 6C, CH₃), 5.1 (d, J = 42.0 Hz, CH₃). **³¹P{¹H}-NMR** (162 MHz, acetone- d_6): 41.5 (s).

3. Synthesis of Starting Compound

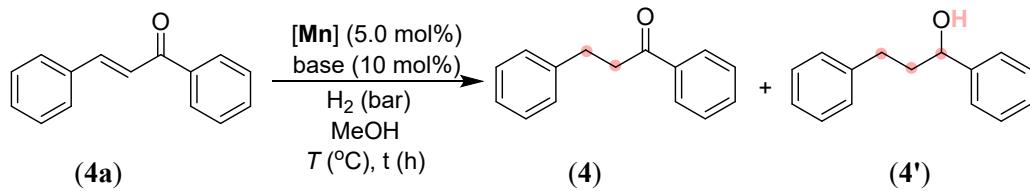


(Z)-2-(4-Acetylphenoxy)-1,3-diphenylprop-2-en-1-one (40a): A mixture of 2-(4-acetylphenoxy)-1-phenylethan-1-one (0.50 g, 1.97 mmol) and benzaldehyde (0.21 g, 1.98 mmol) were dissolved in 20 mL mixture of EtOH:MeOH (4:1) in a round bottom flask followed by dropwise addition of 10% NaOH (10 mL) at 0 °C. The reaction mixture was allowed to the room temperature and stirred for overnight. The volatiles were evaporated under vacuo and 20 mL of water was added. The organic layer was extracted in EtOAc and the crude product was subjected to the column chromatography (silica gel, petroleum ether/EtOAc:30/1) to yield (Z)-2-(4-acetylphenoxy)-1,3-diphenylprop-2-en-1-one (**40a**) (0.41 g, 61%) as yellow solid. **¹H-NMR** (400 MHz, CDCl₃): δ = 7.87 (d, J = 8.6 Hz, 4H, Ar-H), 7.72-7.70 (m, 2H, Ar-H), 7.55 (t, J = 7.4 Hz, 1H, Ar-H), 7.44 (t, J = 7.7 Hz, 2H, Ar-H), 7.37-7.36 (m, 3H), 7.12 (s, 1H, CH), 7.05 (d, J = 8.8 Hz, 2H, Ar-H), 2.51 (s, 3H, CH₃).

¹³C{¹H}-NMR (100 MHz, CDCl₃): δ = 196.8 (CO), 191.5 (CO), 160.1 (C_q), 147.3 (C_q), 136.9 (C_q), 133.0 (CH), 132.5 (C_q), 132.3 (C_q), 130.9 (2C, CH), 130.8 (2C, CH), 130.3 (CH), 129.9 (CH), 129.5 (2C, CH), 129.1 (2C, CH), 128.6 (2C, CH), 115.9 (2C, CH), 26.6 (CH₃). HRMS (ESI): *m/z* Calcd for C₂₃H₁₈O₃ + H⁺ [M + H]⁺ 343.1329; Found 343.1321.

4. Detailed Optimization Study

Table S1. Detailed Optimization of Reaction Parameters.^a



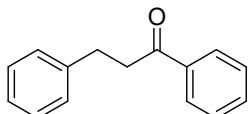
Entry	[Mn]	base	H ₂ (bar)	T (°C)/t (h)	Conv (%) ^b	4 (%) ^b	4' (%) ^b
1	Mn-1	KO ^t Bu	30	50/20	75	65	10
2 ^c	Mn-2	KO ^t Bu	30	50/20	100	--	80
3	Mn-3	KO ^t Bu	30	50/20	100	63 (60)	37
4	Mn-3	KO ^t Bu	30	27/20	100	81 (79)	19
5	Mn-3	KO ^t Bu	20	27/20	100	86	14
6	Mn-3	KO ^t Bu	10	27/20	100	91 (88)	9
7	Mn-3	NaO ^t Bu	10	27/20	40	39	trace
8	Mn-3	LiO ^t Bu	10	27/20	74	73	trace
9	Mn-3	K ₂ CO ₃	10	27/20	100	74	26
10	Mn-3	KOAc	10	27/20	20	19	trace
11	Mn-3	K ₃ PO ₄	10	27/20	100	88	12
12	Mn-3	K ₃ PO ₄	10	27/8	100	95	5
13	Mn-3	K ₃ PO ₄	10	27/1	99	95	4
14	Mn-3	K₃PO₄	5	27/1	100	98 (96)	2
15	Mn-3	K ₃ PO ₄	2	27/1	53	53	--
16 ^d	Mn-3	K ₃ PO ₄	5	27/1	50	49	1
17 ^e	Mn-3	K ₃ PO ₄	5	27/1	68	68	trace
18 ^f	Mn-3	K ₃ PO ₄	5	27/1	45	44	1
19	Mn-1	K ₃ PO ₄	5	27/1	trace	trace	--
20	Mn-2	K ₃ PO ₄	5	27/1	23	19	--
21	Mn(CO) ₅ Br/L3	K ₃ PO ₄	5	27/1	39	39	--

22	MnBr ₂ / L3	K ₃ PO ₄	5	27/1	--	--	--
23	MnCl ₂ / L3	K ₃ PO ₄	5	27/1	--	--	--
24	Mn(CO) ₅ Br/bpy	K ₃ PO ₄	5	27/1	--	--	--
25	Mn(CO) ₅ Br/phen	K ₃ PO ₄	5	27/1	--	--	--
26	Mn(CO) ₅ Br/dppf	K ₃ PO ₄	5	27/1	--	--	--
27	Mn(CO) ₅ Br/dppbz	K ₃ PO ₄	5	27/1	--	--	--
28	--	K ₃ PO ₄	5	27/1	--	--	--
29	Mn-3	--	5	27/1	--	--	--
30	Mn-3	K ₃ PO ₄	--	27/1	--	--	--

(Mn-1) **(Mn-2)** **(Mn-3)**

^a Reaction Conditions: **4a** (0.042 g, 0.20 mmol), base (0.02 mmol), [Mn] catalyst (0.01 mmol, 5 mol %), solvent (1.0 mL). ^bGC conversion, isolated yield is given in parentheses. ^c20% allylic alcohol was observed. ^d Using 6.0 mol% K₃PO₄. ^e Using 3 mol% of **Mn-3**. ^f Using 3 mol% of **Mn-3** and 6 mol% of K₃PO₄. bpy = 2,2'-bipyridine, phen = 1,10-phenanthroline, dppf = 1,1'-bis(diphenylphosphino)ferrocene, dppbz = 1,2-bis(diphenylphosphino)benzene. All three manganese complexes contain mixture of two geometrical isomers.

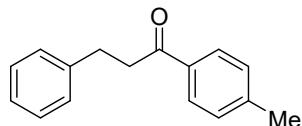
5. Representative Procedure for Hydrogenation



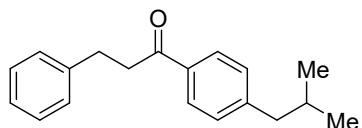
Synthesis of 1,3-diphenylpropan-1-one (4): To a dry vial with magnetic bar was introduced **Mn-3** (0.005 g, 0.01 mmol), K₃PO₄ (0.0043 g, 0.02 mmol), and (*E*)-chalcone (**4a**; 0.042 g, 0.202 mmol) inside the glove box. The reaction vial was transferred to an autoclave under argon atmosphere. Then MeOH (1.0 mL) was added and the autoclave was pressurized with H₂ (5 bar) and vented for five times. Finally, the autoclave was pressurized with 5 bar H₂ and stirred (700 rpm) at room temperature (27 °C) for 1 h. After reaction time, the reaction mixture was concentrated and subjected to column chromatography on silica gel (petroleum ether/EtOAc: 70/1) to yield **4** (0.041 g, 96%) as white solid. ¹H-NMR (500 MHz, CDCl₃): δ =

7.95 (d, $J = 7.4$ Hz, 2H, Ar–H), 7.54 (t, $J = 7.4$ Hz, 1H, Ar–H), 7.44 (t, $J = 7.6$ Hz, 2H, Ar–H), 7.31–7.18 (m, 5H, Ar–H), 3.29 (t, $J = 7.7$ Hz, 2H, CH₂), 3.06 (t, $J = 7.7$ Hz, 2H, CH₂). ¹³C{¹H}-NMR (125 MHz, CDCl₃): δ = 199.4 (CO), 144.4 (C_q), 137.0 (C_q), 133.2 (CH), 128.8 (2C, CH), 128.7 (2C, CH), 128.6 (2C, CH), 128.2 (2C, CH), 126.3 (CH), 40.6 (CH₂), 30.3 (CH₂). HRMS (ESI): *m/z* Calcd for C₁₅H₁₄O + H⁺ [M + H]⁺ 211.1117; Found 211.1115. The ¹H and ¹³C{¹H} spectra are consistent with those reported in the literature.⁴

6. Characterization Data of Hydrogenated Compounds

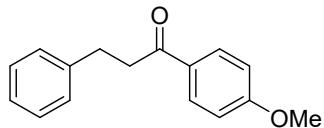


3-Phenyl-1-(*p*-tolyl)propan-1-one (5): The representative procedure was followed, using substrate **5a** (0.045 g, 0.202 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 3 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 50/1) yielded **5** (0.040 g, 88%) as brown solid. ¹H-NMR (400 MHz, CDCl₃): δ = 7.85 (d, $J = 8.3$ Hz, 2H, Ar–H), 7.30–7.27 (m, 2H, Ar–H), 7.25–7.17 (m, 5H, Ar–H), 3.26 (t, $J = 7.8$ Hz, 2H, CH₂), 3.05 (t, $J = 7.7$ Hz, 2H, CH₂), 2.39 (s, 3H, CH₃). ¹³C{¹H}-NMR (100 MHz, CDCl₃): δ = 199.0 (CO), 143.9 (C_q), 141.5 (C_q), 134.5 (C_q), 129.4 (2C, CH), 128.6 (2C, CH), 128.6 (2C, CH), 128.3 (2C, CH), 126.2 (CH), 40.5 (CH₂), 30.4 (CH₂), 21.8 (CH₃). HRMS (ESI): *m/z* Calcd for C₁₆H₁₆O + H⁺ [M + H]⁺ 225.1274; Found 225.1272. The ¹H and ¹³C{¹H} spectra are consistent with those reported in the literature.⁵

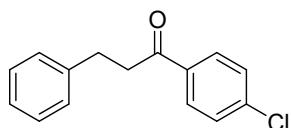


1-(4-Isobutylphenyl)-3-phenylpropan-1-one (6): The representative procedure was followed, using substrate **6a** (0.053 g, 0.20 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 5 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 50/1) yielded **6** (0.037 g, 70%) as yellow oil. ¹H-NMR (500 MHz, CDCl₃): δ = 7.88 (d, $J = 8.1$ Hz, 2H, Ar–H), 7.31–7.28 (m, 2H, Ar–H), 7.26–7.18 (m, 5H, Ar–H), 3.28 (t, $J = 7.7$ Hz, 2H, CH₂), 3.06 (t, $J = 7.8$ Hz, 2H, CH₂), 2.52 (d, $J = 7.1$ Hz, 2H, CH₂), 1.90–1.88 (m, 1H, CH), 0.90 (d, $J = 6.6$ Hz, 6H, CH₃). ¹³C{¹H}-NMR (125 MHz, CDCl₃): δ = 199.1 (CO), 147.7 (C_q), 141.6 (C_q), 134.8 (C_q), 129.5 (2C, CH), 128.7 (2C, CH), 128.6 (2C, CH), 128.2 (2C, CH), 126.3 (CH), 45.6 (CH₂), 40.5 (CH₂), 30.4 (CH₂), 30.3 (CH),

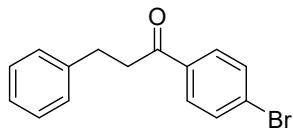
22.5 (2C, CH₃). HRMS (ESI): *m/z* Calcd for C₁₉H₂₂O + H⁺ [M + H]⁺ 267.1743; Found 276.1740. The ¹H and ¹³C{¹H} spectra are consistent with those reported in the literature.⁶



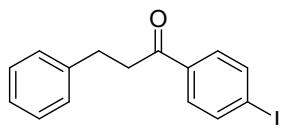
1-(4-Methoxyphenyl)-3-phenylpropan-1-one (7): The representative procedure was followed, using substrate **7a** (0.048 g, 0.201 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 3 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 30/1) yielded **7** (0.043 g, 89%) as white solid. ¹H-NMR (400 MHz, CDCl₃): δ = 7.94 (d, *J* = 9.0 Hz, 2H, Ar–H), 7.32–7.24 (m, 4H, Ar–H), 7.20 (t, *J* = 7.0 Hz, 1H, Ar–H), 6.92 (d, *J* = 9.0 Hz, 2H, Ar–H), 3.85 (s, 3H, CH₃), 3.25 (t, *J* = 7.8 Hz, 2H, CH₂), 3.06 (t, *J* = 7.8 Hz, 2H, CH₂). ¹³C{¹H}-NMR (100 MHz, CDCl₃): δ = 198.0 (CO), 163.6 (C_q), 141.6 (C_q), 130.4 (2C, CH), 130.1 (C_q), 128.6 (2C, CH), 128.6 (2C, CH), 126.2 (CH), 113.9 (2C, CH), 55.6 (CH₃), 40.2 (CH₂), 30.5 (CH₂). HRMS (ESI): *m/z* Calcd for C₁₆H₁₆O₂ + H⁺ [M + H]⁺ 241.1223; Found 241.1220. The ¹H and ¹³C{¹H} spectra are consistent with those reported in the literature.⁵



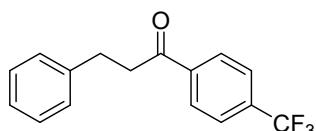
1-(4-Chlorophenyl)-3-phenylpropan-1-one (8): The representative procedure was followed, using substrate **8a** (0.049 g, 0.202 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 2 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 50/1) yielded **8** (0.040 g, 81%) as white solid. ¹H-NMR (400 MHz, CDCl₃): δ = 7.88 (d, *J* = 8.6 Hz, 2H, Ar–H), 7.41 (d, *J* = 8.6 Hz, 2H, Ar–H), 7.31–7.27 (m, 2H, Ar–H), 7.24–7.18 (m, 3H, Ar–H), 3.26 (t, *J* = 7.7 Hz, 2H, CH₂), 3.05 (t, *J* = 7.7 Hz, 2H, CH₂). ¹³C{¹H}-NMR (100 MHz, CDCl₃): δ = 198.1 (CO), 141.2 (C_q), 139.6 (C_q), 135.3 (C_q), 129.6 (2C, CH), 129.1 (2C, CH), 128.7 (2C, CH), 128.6 (2C, CH), 126.4 (CH), 40.6 (CH₂), 30.2 (CH₂). HRMS (ESI): *m/z* Calcd for C₁₅H₁₃ClO + H⁺ [M + H]⁺ 245.0728; Found 245.0726. The ¹H and ¹³C{¹H} spectra are consistent with those reported in the literature.⁷



1-(4-Bromophenyl)-3-phenylpropan-1-one (9): The representative procedure was followed, using substrate **9a** (0.058 g, 0.202 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 2 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 100/1) yielded **9** (0.042 g, 72%) as white solid. ¹H-NMR (400 MHz, CDCl₃): δ = 7.80 (d, *J* = 8.6 Hz, 2H, Ar–H), 7.58 (d, *J* = 8.6 Hz, 2H, Ar–H), 7.31–7.18 (m, 5H, Ar–H), 3.25 (t, *J* = 7.6 Hz, 2H, CH₂), 3.05 (t, *J* = 7.6 Hz, 2H, CH₂). ¹³C{¹H}-NMR (100 MHz, CDCl₃): δ = 198.3 (CO), 141.2 (C_q), 135.7 (C_q), 132.1 (2C, CH), 129.7 (2C, CH), 128.7 (2C, CH), 128.6 (2C, CH), 128.4 (C_q), 126.4 (CH), 40.6 (CH₂), 30.2 (CH₂). HRMS (ESI): *m/z* Calcd for C₁₅H₁₃BrO + H⁺ [M + H]⁺ 289.0223, 291.0208; Found 289.0216, 291.0197. The ¹H and ¹³C{¹H} spectra are consistent with those reported in the literature.⁸

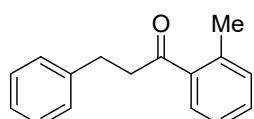


1-(4-Iodophenyl)-3-phenylpropan-1-one (10): The representative procedure was followed, using substrate **10a** (0.067 g, 0.201 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 2 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 50/1) yielded **10** (0.055 g, 81%) as white solid. ¹H-NMR (400 MHz, CDCl₃): δ = 7.80 (d, *J* = 8.4 Hz, 2H, Ar–H), 7.64 (d, *J* = 8.4 Hz, 2H, Ar–H), 7.29 (t, *J* = 7.4 Hz, 2H, Ar–H), 7.24–7.18 (m, 3H, Ar–H), 3.24 (t, *J* = 7.6 Hz, 2H, CH₂), 2.93 (t, *J* = 7.6 Hz, 2H, CH₂). ¹³C{¹H}-NMR (100 MHz, CDCl₃): δ = 198.6 (CO), 141.2 (C_q), 138.1 (2C, CH), 136.2 (C_q), 129.6 (2C, CH), 128.7 (2C, CH), 128.6 (2C, CH), 126.4 (CH), 101.2 (C_q), 40.5 (CH₂), 30.2 (CH₂). HRMS (ESI): *m/z* Calcd for C₁₅H₁₃IO + H⁺ [M + H]⁺ 337.0084; Found 337.0080. The ¹H and ¹³C{¹H} spectra are consistent with those reported in the literature.⁹

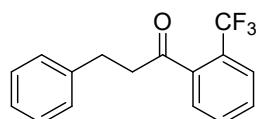


3-Phenyl-1-(4-(trifluoromethyl)phenyl)propan-1-one (11): The representative procedure was followed, using substrate **11a** (0.056 g, 0.203 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 2 h. Purification by column chromatography on silica gel

(petroleum ether/EtOAc: 100/1) yielded **11** (0.044 g, 78%) as yellow oil. ^1H -NMR (500 MHz, CDCl_3): δ = 8.04 (d, J = 8.2 Hz, 2H, Ar–H), 7.71 (d, J = 8.2 Hz, 2H, Ar–H), 7.33–7.28 (m, 2H, Ar–H), 7.26–7.20 (m, 3H, Ar–H), 3.33 (t, J = 7.6 Hz, 2H, CH_2), 3.08 (t, J = 7.6 Hz, 2H, CH_2). $^{13}\text{C}\{\text{H}\}$ -NMR (125 MHz, CDCl_3): δ = 198.4 (CO), 141.0 (C_q), 139.7 (C_q), 134.5 (q, $^2J_{\text{C}-\text{F}}$ = 32.8 Hz, C_q), 128.8 (2C, CH), 128.6 (2C, CH), 128.5 (2C, CH), 126.5 (CH), 125.9 (q, $^3J_{\text{C}-\text{F}}$ = 3.8 Hz, 2C, CH), 123.8 (q, $^1J_{\text{C}-\text{F}}$ = 272.6 Hz, C_q), 40.9 (CH_2), 30.1 (CH_2). ^{19}F -NMR (377 MHz, CDCl_3): δ = –63.1 (s). HRMS (ESI): m/z Calcd for $\text{C}_{16}\text{H}_{13}\text{F}_3\text{O} + \text{H}^+$ [M + H]⁺ 279.0991; Found 279.0988. The ^1H and $^{13}\text{C}\{\text{H}\}$ spectra are consistent with those reported in the literature.⁷

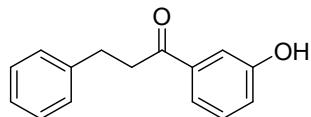


3-Phenyl-1-(o-tolyl)propan-1-one (12): The representative procedure was followed, using substrate **12a** (0.045 g, 0.202 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 3 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 50/1) yielded **12** (0.035 g, 77%) as yellow oil. ^1H -NMR (400 MHz, CDCl_3): δ = 7.59 (d, J = 7.9 Hz, 1H, Ar–H), 7.35 (t, J = 7.4 Hz, 1H, Ar–H), 7.28 (t, J = 7.4 Hz, 2H, Ar–H), 7.24–7.17 (m, 5H, Ar–H), 3.22 (t, J = 7.7 Hz, 2H, Ar–H), 3.04 (t, J = 7.6 Hz, 2H, CH_2), 2.46 (s, 3H, CH_3). $^{13}\text{C}\{\text{H}\}$ -NMR (100 MHz, CDCl_3): δ = 203.6 (CO), 141.4 (C_q), 138.3 (C_q), 138.1 (C_q), 132.1 (CH), 131.4 (CH), 128.7 (2C, CH), 128.6 (2C, CH), 128.5 (CH), 126.3 (CH), 125.8 (CH), 43.4 (CH_2), 30.5 (CH_2), 21.4 (CH_3). HRMS (ESI): m/z Calcd for $\text{C}_{16}\text{H}_{16}\text{O} + \text{H}^+$ [M + H]⁺ 225.1274; Found 225.1271. The ^1H and $^{13}\text{C}\{\text{H}\}$ spectra are consistent with those reported in the literature.¹⁰

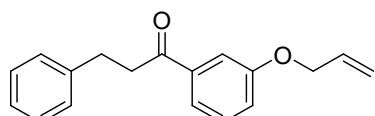


3-Phenyl-1-(2-(trifluoromethyl)phenyl)propan-1-one (13): The representative procedure was followed, using substrate **13a** (0.056 g, 0.203 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 2 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 50/1) yielded **13** (0.048 g, 85%) as yellow oil. ^1H -NMR (400 MHz, CDCl_3): δ = 7.69 (d, J = 7.8 Hz, 1H, Ar–H), 7.57–7.50 (m, 2H, Ar–H), 7.31–7.27 (m, 3H, Ar–H), 7.24–7.18 (m, 3H, Ar–H), 3.16 (t, J = 7.6 Hz, 2H, CH_2), 3.05 (t, J = 7.4 Hz, 2H, CH_2).

¹³C{¹H}-NMR (100 MHz, CDCl₃): δ = 203.6 (CO), 140.8 (C_q), 140.5 (q, ³J_{C-F} = 1.9 Hz, C_q), 132.0 (CH), 130.2 (CH), 128.7 (2C, CH), 128.5 (2C, CH), 127.1 (q, ²J_{C-F} = 32.1 Hz, C_q), 127.0 (CH), 126.9 (q, ³J_{C-F} = 5.0 Hz, CH), 126.4 (CH), 122.4 (q, ¹J_{C-F} = 273.9 Hz, C_q), 45.0 (q, ⁵J_{C-F} = 1.5 Hz, CH₂), 30.0 (CH₂). ¹⁹F-NMR (377 MHz, CDCl₃): δ = -58.1 (s). HRMS (ESI): *m/z* Calcd for C₁₆H₁₃F₃O + H⁺ [M + H]⁺ 279.0991; Found 279.0986. The ¹H and ¹³C{¹H} spectra are consistent with those reported in the literature.¹⁰

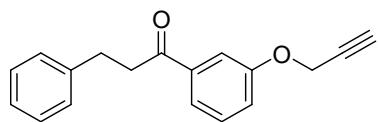


1-(3-Hydroxyphenyl)-3-phenylpropan-1-one (14): The representative procedure was followed, using substrate **14a** (0.045 g, 0.201 mmol) and the reaction mixture was stirred at 50 °C for 24 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 10/1) yielded **14** (0.015 g, 33%) as a white solid. ¹H-NMR (400 MHz, CDCl₃): δ = 7.53 (s, 1H, Ar–H), 7.50 (d, *J* = 7.9 Hz, 1H, Ar–H), 7.34-7.27 (m, 3H, Ar–H), 7.24-7.18 (m, 3H, Ar–H), 7.07 (d, *J* = 7.9 Hz, 1H, Ar–H), 6.21-6.09 (br s, 1H, OH), 3.28 (t, *J* = 7.3 Hz, 2H, CH₂), 3.05 (t, *J* = 7.3 Hz, 2H, CH₂). ¹³C{¹H}-NMR (100 MHz, CDCl₃): δ = 200.0 (CO), 156.4 (C_q), 141.3 (C_q), 138.4 (C_q), 130.1 (CH), 128.7 (2C, CH), 128.6 (2C, CH), 126.4 (CH), 120.9 (CH), 120.8 (CH), 114.7 (CH), 40.8 (CH₂), 30.3 (CH₂). HRMS (ESI): *m/z* Calcd for C₁₅H₁₄O₂ + H⁺ [M + H]⁺ 227.1067; Found 227.1065.¹¹

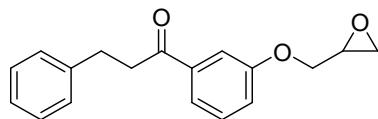


1-(3-(Allyloxy)phenyl)-3-phenylpropan-1-one (15): The representative procedure was followed, using substrate **15a** (0.053 g, 0.201 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 3 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 50/1) yielded **15** (0.039 g, 73%) as yellow oil. ¹H-NMR (400 MHz, CDCl₃): δ = 7.54 (d, *J* = 7.8 Hz, 1H, Ar–H), 7.51-7.50 (m, 1H, Ar–H), 7.35 (t, *J* = 7.9 Hz, 1H, Ar–H), 7.30 (t, *J* = 7.3 Hz, 2H, Ar–H), 7.26-7.19 (m, 3H, Ar–H), 7.12 (dd, *J* = 8.3, 2.0 Hz, 1H, Ar–H), 6.10-6.01 (m, 1H, CH), 5.43 (dd, *J* = 17.3, 1.5 Hz, 1H, CH), 5.31 (dd, *J* = 10.6, 1.4 Hz, 1H, CH), 4.57 (d, *J* = 5.3 Hz, 2H, CH₂), 3.28 (t, *J* = 7.7 Hz, 2H, CH₂), 3.06 (t, *J* = 7.6 Hz, 2H, CH₂). ¹³C{¹H}-NMR (100 MHz, CDCl₃): δ = 199.4 (CO), 159.3 (C_q), 141.7 (C_q), 138.7 (C_q), 133.3 (CH), 130.1 (CH), 129.0 (2C, CH), 129.0 (2C, CH), 126.6 (CH),

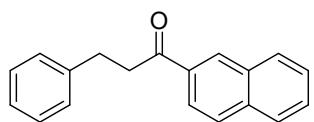
121.3 (CH), 120.6 (CH), 118.4 (CH₂), 113.8 (CH), 69.4 (CH₂), 41.0 (CH₂), 30.6 (CH₂). HRMS (ESI): *m/z* Calcd for C₁₈H₁₈O₂ + H⁺ [M + H]⁺ 267.1380; Found 267.1373.



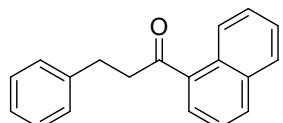
3-Phenyl-1-(3-(prop-2-yn-1-yloxy)phenyl)propan-1-one (16): The representative procedure was followed, using substrate **16a** (0.053 g, 0.202 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 3 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 50/1) yielded **16** (0.037 g, 69%) as yellow oil. ¹H-NMR (400 MHz, CDCl₃): δ = 7.57 (d, *J* = 8.1 Hz, 2H, Ar-H), 7.38 (t, *J* = 7.9 Hz, 1H, Ar-H), 7.30 (t, *J* = 7.4 Hz, 2H, Ar-H), 7.26-7.16 (m, 4H, Ar-H), 4.73 (d, *J* = 2.3 Hz, 2H, CH₂), 3.28 (t, *J* = 7.7 Hz, 2H, CH₂), 3.06 (t, *J* = 7.6 Hz, 2H, CH₂), 2.53 (t, *J* = 2.2 Hz, 1H, CH). ¹³C{¹H}-NMR (100 MHz, CDCl₃): δ = 198.9 (CO), 157.9 (C_q), 141.4 (C_q), 138.4 (C_q), 129.8 (CH), 128.7 (2C, CH), 128.6 (2C, CH), 126.3 (CH), 121.6 (CH), 120.4 (CH), 113.7 (CH), 78.2 (C_q), 76.1 (CH), 56.1 (CH₂), 40.7 (CH₂), 30.3 (CH₂). HRMS (ESI): *m/z* Calcd for C₁₈H₁₆O₂ + H⁺ [M + H]⁺ 265.1223; Found 265.1217.



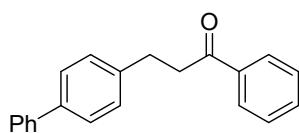
1-(3-(Oxiran-2-ylmethoxy)phenyl)-3-phenylpropan-1-one (17): The representative procedure was followed, using substrate **17a** (0.057 g, 0.203 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 4 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 30/1) yielded **17** (0.039 g, 68%) as yellow oil. ¹H-NMR (400 MHz, CDCl₃): δ = 7.56 (d, *J* = 7.8 Hz, 1H, Ar-H), 7.50 (t, *J* = 1.9 Hz, 1H, Ar-H), 7.36 (t, *J* = 7.9 Hz, 1H, Ar-H), 7.30 (t, *J* = 7.3 Hz, 2H, Ar-H), 7.26-7.19 (m, 3H, Ar-H), 7.14 (dd, *J* = 2.5, 0.6 Hz, 1H, Ar-H), 4.30 (dd, *J* = 11.0, 2.9 Hz, 1H, CH), 3.97 (dd, *J* = 11.0, 5.9 Hz, 1H, CH), 3.39-3.35 (m, 1H, CH), 3.29 (t, *J* = 7.6 Hz, 2H, CH₂), 3.06 (t, *J* = 7.6 Hz, 2H, CH₂), 2.92 (t, *J* = 4.5 Hz, 1H, CH₂), 2.67 (dd, *J* = 4.9 Hz, 2.63 Hz, 1H, CH₂). ¹³C{¹H}-NMR (100 MHz, CDCl₃): δ = 199.1 (CO), 158.9 (C_q), 141.4 (C_q), 138.4 (C_q), 129.9 (CH), 128.7 (2C, CH), 128.6 (2C, CH), 126.3 (CH), 121.4 (CH), 120.3 (CH), 113.2 (CH), 69.1 (CH₂), 50.2 (CH), 44.7 (CH₂), 40.7 (CH₂), 30.3 (CH₂). HRMS (ESI): *m/z* Calcd for C₁₈H₁₈O₃ + H⁺ [M + H]⁺ 283.1329; Found 283.1223.



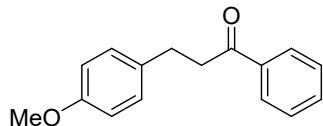
1-(Naphthalen-2-yl)-3-phenylpropan-1-one (18): The representative procedure was followed, using substrate **18a** (0.052 g, 0.201 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 3 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 50/1) yielded **18** (0.037 g, 71%) as brown solid. ¹H-NMR (500 MHz, CDCl₃): δ = 8.44 (s, 1H, Ar–H), 8.02 (dd, *J* = 8.6, 1.6 Hz, 1H, Ar–H), 7.92–7.84 (m, 3H, Ar–H), 7.59–7.50 (m, 2H, Ar–H), 7.33–7.19 (m, 5H, Ar–H), 3.42 (t, *J* = 7.8 Hz, 2H, CH₂), 3.12 (t, *J* = 7.7 Hz, 2H, CH₂). ¹³C{¹H}-NMR (125 MHz, CDCl₃): δ = 199.3 (CO), 141.5 (C_q), 135.7 (C_q), 134.3 (C_q), 132.7 (C_q), 129.8 (CH), 129.7 (CH), 128.7 (2C, CH), 128.6 (2C, CH), 128.6 (CH), 128.6 (CH), 127.9 (CH), 126.9 (CH), 126.3 (CH), 124.0 (CH), 40.7 (CH₂), 30.4 (CH₂). HRMS (ESI): *m/z* Calcd for C₁₉H₁₆O + H⁺ [M + H]⁺ 261.1274; Found 261.1270. The ¹H and ¹³C{¹H} spectra are consistent with those reported in the literature.¹²



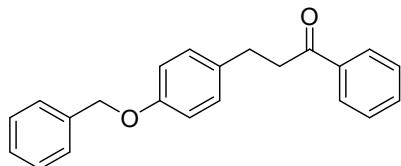
1-(Naphthalen-1-yl)-3-phenylpropan-1-one (19): The representative procedure was followed, using substrate **19a** (0.052 g, 0.201 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 3 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 50/1) yielded **19** (0.049 g, 94%) as white solid. ¹H-NMR (400 MHz, CDCl₃): δ = 8.54 (d, *J* = 8.5 Hz, 1H, Ar–H), 7.94 (d, *J* = 8.3 Hz, 1H, Ar–H), 7.85 (d, *J* = 8.3 Hz, 1H, Ar–H), 7.79 (dd, *J* = 7.1, 0.9 Hz, 1H, Ar–H), 7.58–7.49 (m, 2H, Ar–H), 7.44 (t, *J* = 7.7 Hz, 1H, Ar–H), 7.30–7.17 (m, 5H, Ar–H), 3.36 (t, *J* = 7.7 Hz, 2H, CH₂), 3.12 (t, *J* = 7.6 Hz, 2H, CH₂). ¹³C{¹H}-NMR (100 MHz, CDCl₃): δ = 203.7 (CO), 141.3 (C_q), 136.1 (C_q), 134.1 (C_q), 132.7 (CH), 130.3 (C_q), 128.7 (2C, CH), 128.6 (2C, CH), 128.6 (CH), 128.0 (CH), 127.6 (CH), 126.6 (CH), 126.3 (CH), 125.9 (CH), 124.5 (CH), 44.0 (CH₂), 30.7 (CH₂). HRMS (ESI): *m/z* Calcd for C₁₉H₁₆O + H⁺ [M + H]⁺ 261.1274; Found 261.1270. The ¹H and ¹³C{¹H} spectra are consistent with those reported in the literature.⁷



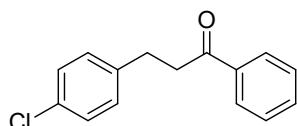
3-((1,1'-Biphenyl)-4-yl)-1-phenylpropan-1-one (20): The representative procedure was followed, using substrate **20a** (0.057 g, 0.20 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 2 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 50/1) yielded **20** (0.051 g, 89%) as yellow solid. ¹H-NMR (500 MHz, CDCl₃): δ = 8.01 (d, *J* = 7.1 Hz, 2H, Ar–H), 7.63–7.56 (m, 5H, Ar–H), 7.50–7.44 (m, 4H, Ar–H), 7.38–7.34 (m, 3H, Ar–H), 3.37 (t, *J* = 7.7 Hz, 2H, CH₂), 3.15 (t, *J* = 7.6 Hz, 2H, CH₂). ¹³C{¹H}-NMR (125 MHz, CDCl₃): δ = 199.3 (CO), 141.1 (C_q), 140.6 (C_q), 139.3 (C_q), 137.0 (C_q), 133.2 (CH), 129.0 (2C, CH), 128.9 (2C, CH), 128.8 (2C, CH), 128.2 (2C, CH), 127.4 (2C, CH), 127.3 (CH), 127.1 (2C, CH), 40.5 (CH₂), 29.9 (CH₂). HRMS (ESI): *m/z* Calcd for C₂₁H₁₈O + H⁺ [M + H]⁺ 287.1430; Found 287.1425. The ¹H and ¹³C{¹H} spectra are consistent with those reported in the literature.⁵



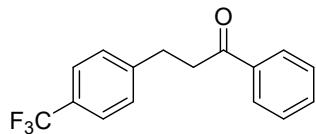
3-(4-Methoxyphenyl)-1-phenylpropan-1-one (21): The representative procedure was followed, using substrate **21a** (0.048 g, 0.201 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 3 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 30/1) yielded **21** (0.044 g, 91%) as yellow solid. ¹H-NMR (400 MHz, CDCl₃): δ = 7.98–7.95 (m, 2H, Ar–H), 7.56 (vt, *J* = 7.4 Hz, 1H, Ar–H), 7.48–7.43 (m, 2H, Ar–H), 7.18 (d, *J* = 8.8 Hz, 2H, Ar–H), 6.85 (d, *J* = 8.8 Hz, 2H, Ar–H), 3.79 (s, 3H, CH₃), 3.28 (t, *J* = 7.7 Hz, 2H, CH₂), 3.02 (t, *J* = 7.6 Hz, 2H, CH₂). ¹³C{¹H}-NMR (100 MHz, CDCl₃): δ = 199.5 (CO), 158.1 (C_q), 137.0 (C_q), 133.5 (C_q), 133.2 (CH), 129.5 (2C, CH), 128.7 (2C, CH), 128.2 (2C, CH), 114.1 (2C, CH), 55.4 (CH₃), 40.9 (CH₂), 29.4 (CH₂). HRMS (ESI): *m/z* Calcd for C₁₆H₁₆O₂ + H⁺ [M + H]⁺ 241.1223; Found 241.1218. The ¹H and ¹³C{¹H} spectra are consistent with those reported in the literature.⁵



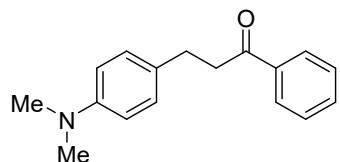
3-(4-(Benzyl)phenyl)-1-phenylpropan-1-one (22): The representative procedure was followed, using substrate **22a** (0.063 g, 0.20 mmol), 1.0 mL of MeOH:DCM (4:1) and the reaction mixture was stirred at room temperature (27 °C) for 5 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 30/1) yielded **22** (0.046 g, 73%) as yellow oil. ¹H-NMR (400 MHz, CDCl₃): δ = 7.96 (d, *J* = 7.7 Hz, 2H, Ar–H), 7.56 (vt, *J* = 7.4 Hz, 1H, Ar–H), 7.48–7.31 (m, 7H, Ar–H), 7.18 (d, *J* = 8.8 Hz, 2H, Ar–H), 6.92 (d, *J* = 8.6 Hz, 2H, Ar–H), 5.05 (s, 2H, CH₂), 3.28 (t, *J* = 7.6 Hz, 2H, CH₂), 3.02 (t, *J* = 7.7 Hz, 2H, CH₂). ¹³C{¹H}-NMR (100 MHz, CDCl₃): δ = 199.6 (CO), 157.4 (C_q), 137.3 (C_q), 137.1 (C_q), 133.8 (C_q), 133.2 (CH), 129.6 (2C, CH), 128.8 (2C, CH), 128.7 (2C, CH), 128.2 (2C, CH), 128.1 (CH), 127.6 (2C, CH), 115.1 (2C, CH), 70.2 (CH₂), 40.9 (CH₂), 29.5 (CH₂). HRMS (ESI): *m/z* Calcd for C₂₂H₂₀O₂ + H⁺ [M + H]⁺ 317.1536; Found 317.1531. The ¹H and ¹³C{¹H} spectra are consistent with those reported in the literature.¹³



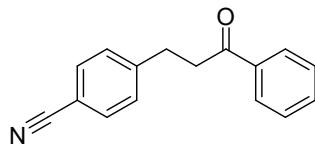
3-(4-Chlorophenyl)-1-phenylpropan-1-one (23): The representative procedure was followed, using substrate **23a** (0.049 g, 0.20 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 2 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 50/1) yielded **23** (0.039 g, 80%) as yellow solid. ¹H-NMR (400 MHz, CDCl₃): δ = 7.94 (d, *J* = 7.4 Hz, 2H, Ar–H), 7.55 (t, *J* = 7.4 Hz, 1H, Ar–H), 7.45 (t, *J* = 7.6 Hz, 2H, Ar–H), 7.25 (d, *J* = 8.4 Hz, 2H, Ar–H), 7.17 (d, *J* = 8.4 Hz, 2H, Ar–H), 3.27 (t, *J* = 7.6 Hz, 2H, CH₂), 3.03 (t, *J* = 7.6 Hz, 2H, CH₂). ¹³C{¹H}-NMR (100 MHz, CDCl₃): δ = 199.0 (CO), 139.9 (C_q), 136.9 (C_q), 133.3 (CH), 132.0 (C_q), 130.0 (2C, CH), 128.8 (2C, CH), 128.7 (2C, CH), 128.2 (2C, CH), 40.3 (CH₂), 29.5 (CH₂). HRMS (ESI): *m/z* Calcd for C₁₅H₁₃ClO – H⁺ [M – H]⁺ 243.0571; Found 243.0570. The ¹H and ¹³C{¹H} spectra are consistent with those reported in the literature.¹⁰



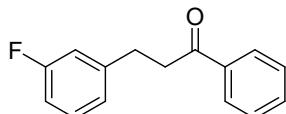
1-Phenyl-3-(4-(trifluoromethyl)phenyl)propan-1-one (24): The representative procedure was followed, using substrate **24a** (0.056 g, 0.203 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 2 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 50/1) yielded **24** (0.054 g, 96%) as a white solid. ¹H-NMR (500 MHz, CDCl₃): δ = 7.96 (d, *J* = 7.8 Hz, 2H, Ar–H), 7.59–7.54 (m, 3H, Ar–H), 7.46 (t, *J* = 7.6 Hz, 2H, Ar–H), 7.38 (d, *J* = 8.0 Hz, 2H, Ar–H), 3.33 (t, *J* = 7.6 Hz, 2H, CH₂), 3.14 (t, *J* = 7.5 Hz, 2H, CH₂). ¹³C{¹H}-NMR (125 MHz, CDCl₃): δ = 198.7 (CO), 145.6 (q, ⁵J_{C–F} = 1.5 Hz, C_q), 136.8 (C_q), 133.4 (CH), 129.0 (2C, CH), 128.8 (2C, CH), 128.7 (q, ²J_{C–F} = 32.1 Hz, C_q), 128.2 (2C, CH), 125.6 (q, ³J_{C–F} = 3.8 Hz, 2C, CH), 124.5 (q, ¹J_{C–F} = 271.1 Hz, CF₃), 40.0 (CH₂), 29.9 (CH₂). ¹⁹F-NMR (377 MHz, CDCl₃): δ = –62.4 (s). HRMS (ESI): *m/z* Calcd for C₁₆H₁₃F₃O + H⁺ [M + H]⁺ 279.0991; Found 279.0985. The ¹H and ¹³C{¹H} spectra are consistent with those reported in the literature.⁵



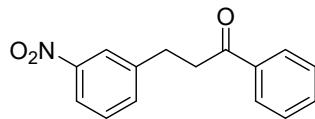
3-(4-(Dimethylamino)phenyl)-1-phenylpropan-1-one (25): The representative procedure was followed, using substrate **25a** (0.051 g, 0.203 mmol), 1.0 mL of MeOH:DCM (4:1) and the reaction mixture was stirred at room temperature (27 °C) for 5 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 30/1) yielded **25** (0.041 g, 80%) as yellow oil. ¹H-NMR (400 MHz, CDCl₃): δ = 7.97 (d, *J* = 7.8 Hz, 2H, Ar–H), 7.56 (t, *J* = 7.3 Hz, 1H, Ar–H), 7.46 (t, *J* = 7.6 Hz, 2H, Ar–H), 7.15 (d, *J* = 8.63 Hz, 2H, Ar–H), 6.72 (d, *J* = 8.8 Hz, 2H, Ar–H), 3.27 (t, *J* = 7.8 Hz, 2H, CH₂), 2.99 (t, *J* = 7.8 Hz, 2H, CH₂), 2.93 (s, 6H, CH₃). ¹³C{¹H}-NMR (100 MHz, CDCl₃): δ = 199.9 (CO), 149.4 (C_q), 137.1 (C_q), 133.1 (CH), 129.4 (C_q), 129.2 (2C, CH), 128.7 (2C, CH), 128.2 (2C, CH), 113.2 (2C, CH), 41.1 (CH₂), 41.0 (CH₃), 29.4 (CH₂). HRMS (ESI): *m/z* Calcd for C₁₇H₁₉NO + H⁺ [M + H]⁺ 254.1539; Found 254.1536. The ¹H and ¹³C{¹H} spectra are consistent with those reported in the literature.⁸



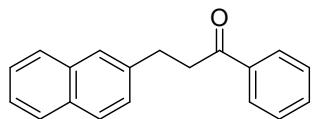
4-(3-Oxo-3-phenylpropyl)benzonitrile (26): The representative procedure was followed, using substrate **26a** (0.047 g, 0.201 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 2 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 30/1) yielded **26** (0.042 g, 89%) as white solid. ¹H-NMR (500 MHz, CDCl₃): δ = 7.94 (d, *J* = 7.2 Hz, 2H, Ar–H), 7.54–7.58 (m, 3H, Ar–H), 7.54 (t, *J* = 7.7 Hz, 2H, Ar–H), 7.36 (d, *J* = 8.3 Hz, 2H, Ar–H), 3.32 (t, *J* = 7.4 Hz, 2H, CH₂), 3.13 (t, *J* = 7.4 Hz, 2H, CH₂). ¹³C{¹H}-NMR (125 MHz, CDCl₃): δ = 198.4 (CO), 147.1 (C_q), 136.7 (C_q), 133.5 (CH), 132.4 (2C, CH), 129.5 (2C, CH), 128.8 (2C, CH), 128.1 (2C, CH), 119.1 (C_q), 110.2 (C_q), 39.5 (CH₂), 30.1 (CH₂). HRMS (ESI): *m/z* Calcd for C₁₆H₁₃NO + H⁺ [M + H]⁺ 236.1070; Found 236.1067. The ¹H and ¹³C{¹H} spectra are consistent with those reported in the literature.¹⁴



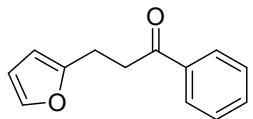
3-(3-Fluorophenyl)-1-phenylpropan-1-one (27): The representative procedure was followed, using substrate **27a** (0.046 g, 0.203 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 3 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 50/1) yielded **27** (0.038 g, 82%) as yellow solid. ¹H-NMR (400 MHz, CDCl₃): δ = 7.96 (d, *J* = 7.8 Hz, 2H, Ar–H), 7.57 (tt, *J* = 7.4, 1.9 Hz, 1H, Ar–H), 7.46 (t, *J* = 7.6 Hz, 2H, Ar–H), 7.28–7.23 (m, 1H, Ar–H), 7.03 (d, *J* = 7.6 Hz, 1H, Ar–H), 6.98–6.95 (m, 1H, Ar–H), 6.90 (td, *J* = 8.5, 2.4 Hz, 1H, Ar–H), 3.31 (t, *J* = 7.6 Hz, 2H, CH₂), 3.08 (t, *J* = 7.6 Hz, 2H, CH₂). ¹³C{¹H}-NMR (100 MHz, CDCl₃): δ = 198.9 (CO), 163.1 (d, ¹J_{C-F} = 245.4 Hz, C_q), 144.0 (d, ³J_{C-F} = 6.9 Hz, C_q), 136.9 (C_q), 133.3 (CH), 130.1 (d, ³J_{C-F} = 8.4 Hz, CH), 128.8 (2C, CH), 128.2 (2C, CH), 124.2 (d, ⁴J_{C-F} = 3.1 Hz, CH), 115.5 (d, ²J_{C-F} = 20.6 Hz, CH), 113.2 (d, ²J_{C-F} = 21.4 Hz, CH), 40.1 (CH₂), 29.9 (d, ⁴J_{C-F} = 1.5 Hz, CH₂). ¹⁹F-NMR (377 MHz, CDCl₃): δ = -113.5 (s). HRMS (ESI): *m/z* Calcd for C₁₅H₁₃FO + H⁺ [M + H]⁺ 229.1023; Found 229.1021. The ¹H and ¹³C{¹H} spectra are consistent with those reported in the literature.¹⁵



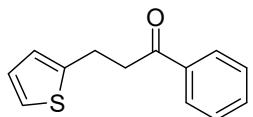
3-(3-Nitrophenyl)-1-phenylpropan-1-one (28): The representative procedure was followed, using substrate **28a** (0.051 g, 0.201 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 5 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 50/1) yielded **28** (0.045 g, 88%) as a white solid. ¹H-NMR (400 MHz, CDCl₃): δ = 8.12 (s, 1H, Ar–H), 8.05 (d, *J* = 8.1 Hz, 1H, Ar–H), 7.95 (d, *J* = 7.8 Hz, 2H, Ar–H), 7.61 (d, *J* = 7.8 Hz, 1H, Ar–H), 7.57 (t, *J* = 7.4 Hz, 1H, Ar–H), 7.48-7.43 (m, 3H, Ar–H), 3.37 (t, 7.4 Hz, 2H, CH₂), 3.19 (t, *J* = 7.3 Hz, 2H, CH₂). ¹³C{¹H}-NMR (100 MHz, CDCl₃): δ = 198.4 (CO), 148.5 (C_q), 143.5 (C_q), 136.7 (C_q), 135.1 (CH), 133.5 (CH), 129.5 (CH), 128.9 (2C, CH), 128.1 (2C, CH), 123.4 (CH), 121.5 (CH), 39.7 (CH₂), 29.6 (CH₂). HRMS (ESI): *m/z* Calcd for C₁₅H₁₃NO₃ + H⁺ [M + H]⁺ 256.0973; Found 256.0961. The ¹H and ¹³C{¹H} spectra are consistent with those reported in the literature.¹⁶



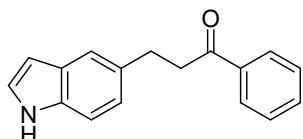
3-(Naphthalen-2-yl)-1-phenylpropan-1-one (29): The representative procedure was followed, using substrate **29a** (0.052 g, 0.201 mmol), 1.0 mL of MeOH:DCM (4:1)] and the reaction mixture was stirred at room temperature (27 °C) for 5 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 50/1) yielded **29** (0.050 g, 96%) as a white solid. ¹H-NMR (400 MHz, CDCl₃): δ = 7.99 (d, *J* = 8.3 Hz, 2H, Ar–H), 7.81 (t, *J* = 7.8 Hz, 3H, Ar–H), 7.70 (s, 1H, Ar–H), 7.56 (t, *J* = 7.4 Hz, 1H, Ar–H), 7.49-7.39 (m, 5H, Ar–H), 3.40 (t, *J* = 7.7 Hz, 2H, CH₂), 3.25 (t, *J* = 7.7 Hz, 2H, CH₂). ¹³C{¹H}-NMR (100 MHz, CDCl₃): δ = 199.4 (CO), 139.0 (C_q), 137.0 (C_q), 133.8 (C_q), 133.3 (CH), 132.3 (C_q), 128.8 (2C, CH), 128.3 (CH), 128.2 (2C, CH), 127.8 (CH), 127.6 (CH), 127.4 (CH), 126.7 (CH), 126.2 (CH), 125.5 (CH), 40.5 (CH₂), 30.4 (CH₂). HRMS (ESI): *m/z* Calcd for C₁₉H₁₆O + H⁺ [M + H]⁺ 261.1274; Found 261.1270. The ¹H and ¹³C{¹H} spectra are consistent with those reported in the literature.⁷



3-(Furan-2-yl)-1-phenylpropan-1-one (30): The representative procedure was followed, using substrate **30a** (0.040 g, 0.202 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 2 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 30/1) yielded **30** (0.035 g, 87%) as yellow oil. ¹H-NMR (400 MHz, CDCl₃): δ = 7.98 (d, *J* = 7.8 Hz, 2H, Ar–H), 7.56 (tt, *J* = 7.4, 1.9 Hz, 1H, Ar–H), 7.46 (t, *J* = 7.6 Hz, 2H, Ar–H), 7.31 (d, *J* = 1.8 Hz, 1H, Ar–H), 6.29 (dd, *J* = 3.1, 1.9 Hz, 1H, Ar–H), 6.05 (dd, *J* = 3.1, 0.8 Hz, 1H, Ar–H), 3.34 (t, *J* = 7.4 Hz, 2H, CH₂), 3.10 (t, *J* = 7.5 Hz, 2H, CH₂). ¹³C{¹H}-NMR (100 MHz, CDCl₃): δ = 198.8 (CO), 154.9 (C_q), 141.2 (CH), 136.9 (C_q), 133.3 (CH), 128.8 (2C, CH), 128.2 (2C, CH), 110.4 (CH), 105.5 (CH), 37.1 (CH₂), 22.6 (CH₂). HRMS (ESI): *m/z* Calcd for C₁₃H₁₂O₂ + H⁺ [M + H]⁺ 201.0910; Found 201.0908. The ¹H and ¹³C{¹H} spectra are consistent with those reported in the literature.⁴

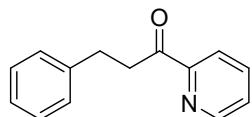


1-Phenyl-3-(thiophen-2-yl)propan-1-one (31): The representative procedure was followed, using substrate **31a** (0.043 g, 0.201 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 3 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 30/1) yielded **31** (0.035 g, 81%) as green oil. ¹H-NMR (400 MHz, CDCl₃): δ = 7.96 (d, *J* = 7.4 Hz, 2H, Ar–H), 7.56 (t, *J* = 7.4 Hz, 1H, Ar–H), 7.45 (t, *J* = 7.7 Hz, 2H, Ar–H), 7.11 (d, *J* = 5.1 Hz, 1H, Ar–H), 6.91 (dd, *J* = 5.0, 3.5 Hz, 1H, Ar–H), 6.86 (d, *J* = 3.3 Hz, 1H, Ar–H), 3.38-3.34 (m, 2H, CH₂), 3.31-3.27 (m, 2H, CH₂). ¹³C{¹H}-NMR (100 MHz, CDCl₃): δ = 198.7 (CO) 144.0 (C_q), 136.9 (C_q), 133.3 (CH), 128.8 (2C, CH), 128.2 (2C, CH), 127.0 (CH), 124.8 (CH), 123.5 (CH), 40.7 (CH₂), 24.4 (CH₂). The ¹H and ¹³C{¹H} spectra are consistent with those reported in the literature.⁵

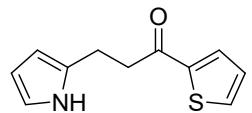


3-(1H-Indol-5-yl)-1-phenylpropan-1-one (32): The representative procedure was followed, using substrate **32a** (0.050 g, 0.202 mmol), 1.0 mL of MeOH:DCM (4:1) and the reaction

mixture was stirred at room temperature (27 °C) for 5 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 20/1) yielded **32** (0.036 g, 72%) as a yellow solid. ¹H-NMR (400 MHz, CDCl₃): δ = 8.19 (br s, 1H, NH), 7.99 (d, *J* = 7.4 Hz, 2H, Ar–H), 7.58-7.53 (m, 2H, Ar–H), 7.46 (t, *J* = 7.6 Hz, 2H, Ar–H), 7.33 (d, *J* = 8.4 Hz, 1H, Ar–H), 7.19 (t, *J* = 2.8 Hz, 1H, Ar–H), 7.11 (dd, *J* = 8.4, 1.6 Hz, 1H, Ar–H), 6.51 (t, *J* = 8.4 Hz, 1H, Ar–H), 3.36 (d, *J* = 7.8 Hz, 2H, CH₂), 3.18 (t, *J* = 7.7 Hz, 2H, CH₂). ¹³C{¹H}-NMR (100 MHz, CDCl₃): δ = 200.0 (CO), 137.1 (C_q), 134.7 (C_q), 133.1 (CH), 132.7 (C_q), 128.7 (2C, CH), 128.3 (C_q), 128.2 (2C, CH), 124.7 (CH), 123.0 (CH), 120.0 (CH), 111.2 (CH), 102.4 (CH), 41.7 (CH₂), 30.5 (CH₂). HRMS (ESI): *m/z* Calcd for C₁₇H₁₅NO + H⁺ [M + H]⁺ 250.1226; Found 250.1225.

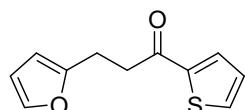


3-Phenyl-1-(pyridin-2-yl)propan-1-one (33): The representative procedure was followed, using substrate **33a** (0.042 g, 0.201 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 2 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 30/1) yielded **33** (0.026 g, 61%) as a green oil. ¹H-NMR (400 MHz, CDCl₃): δ = 8.66 (d, *J* = 4.6 Hz, 1H, Ar–H), 8.05 (d, *J* = 7.8 Hz, 1H, Ar–H), 7.83 (td, *J* = 7.8, 1.7 Hz, 1H, Ar–H), 7.47-7.44 (m, 1H, Ar–H), 7.28 (d, *J* = 4.5 Hz, 4H, Ar–H), 7.21-7.17 (m, 1H, Ar–H), 3.58 (t, *J* = 7.7 Hz, 2H, CH₂), 3.08 (t, *J* = 7.7 Hz, 2H, CH₂). ¹³C{¹H}-NMR (100 MHz, CDCl₃): δ = 201.2 (CO), 153.5 (C_q), 149.1 (CH), 141.6 (C_q), 137.0 (CH), 128.6 (2C, CH), 128.6 (2C, CH), 127.3 (CH), 126.1 (CH), 122.0 (CH), 39.6 (CH₂), 30.0 (CH₂). HRMS (ESI): *m/z* Calcd for C₁₄H₁₃NO + H⁺ [M + H]⁺ 212.1070; Found 212.1068. The ¹H and ¹³C{¹H} spectra are consistent with those reported in the literature.¹⁷

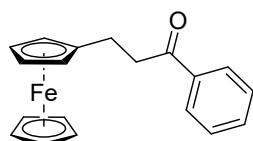


3-(1H-Pyrrol-2-yl)-1-(thiophen-2-yl)propan-1-one (34): The representative procedure was followed, using substrate **34a** (0.041 g, 0.202 mmol), 1.0 mL of MeOH:DCM (4:1) and the reaction mixture was stirred at room temperature (27 °C) for 12 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 20/1) yielded **34** (0.025 g, 60%) as brown solid. ¹H-NMR (400 MHz, CDCl₃): δ = 8.65 (br s, 1H, NH), 7.72 (dd, *J* = 3.8, 0.8 Hz, 1H, Ar–H), 7.65 (dd, *J* = 4.9, 0.8 Hz, 1H, Ar–H), 7.13 (dd, *J* = 4.8, 4.0 Hz, 1H, Ar–H), 6.68-

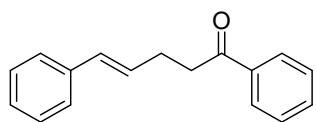
6.67 (m, 1H, Ar–H), 6.12–6.09 (m, 1H, Ar–H), 5.96 (s, 1H, Ar–H), 3.29 (t, J = 6.4 Hz, 2H, CH₂), 3.05 (t, J = 6.4 Hz, 2H, CH₂). ¹³C{¹H}-NMR (100 MHz, CDCl₃): δ = 193.6 (CO), 144.0 (C_q), 134.0 (CH), 132.3 (CH), 131.5 (C_q), 128.4 (CH), 117.0 (CH), 108.0 (CH), 105.6 (CH), 40.1 (CH₂), 21.8 (CH₂). HRMS (ESI): *m/z* Calcd for C₁₁H₁₁NOS + H⁺ [M + H]⁺ 206.0634; Found 206.0630.



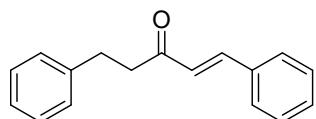
3-(Furan-2-yl)-1-(thiophen-2-yl)propan-1-one (35): The representative procedure was followed, using substrate **35a** (0.041 g, 0.201 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 2 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 30/1) yielded **35** (0.037 g, 89%) as brown liquid. ¹H-NMR (400 MHz, CDCl₃): δ = 7.71 (d, J = 3.9 Hz, 1H, Ar–H), 7.63 (d, J = 5.0 Hz, 1H, Ar–H), 7.30 (d, J = 1.1 Hz, 1H, Ar–H), 7.12 (dd, J = 4.9, 3.9 Hz, 1H, Ar–H), 6.27 (dd, J = 2.9, 2.0 Hz, 1H, Ar–H), 6.05 (d, J = 3.0 Hz, 1H, Ar–H), 3.26 (t, J = 7.5 Hz, 2H, CH₂), 3.08 (t, J = 7.5 Hz, CH₂). ¹³C{¹H}-NMR (100 MHz, CDCl₃): δ = 191.7 (CO), 154.6 (C_q), 144.1 (C_q), 141.3 (CH), 133.8 (CH), 132.0 (CH), 128.3 (CH), 110.4 (CH), 105.6 (CH), 37.7 (CH₂), 22.8 (CH₂). HRMS (ESI): *m/z* Calcd for C₁₁H₁₀O₂S + H⁺ [M + H]⁺ 207.0474; Found 207.0470.



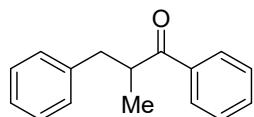
3-Ferrocenyl-1-phenylpropan-1-one (36): The representative procedure was followed, using substrate **36a** (0.064 g, 0.202 mmol), 1.0 mL of MeOH:DCM (4:1) and the reaction mixture was stirred at room temperature (27 °C) for 5 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 30/1) yielded **36** (0.046 g, 72%) as a yellow solid. ¹H-NMR (400 MHz, CDCl₃): δ = 7.97 (d, J = 7.8 Hz, 2H, Ar–H), 7.57 (t, J = 7.4 Hz, 1H, Ar–H), 7.47 (t, J = 7.6 Hz, 2H, Ar–H), 4.14 (s, 5H, Ar–H), 4.13 (s, 2H, Ar–H), 4.08 (s, 2H, Ar–H), 3.20 (t, J = 7.7 Hz, 2H, CH₂) 2.79 (t, J = 7.7 Hz, 2H, CH₂). ¹³C{¹H}-NMR (100 MHz, CDCl₃): δ = 199.7 (CO), 137.1 (C_q), 133.2 (CH), 128.8 (2C, CH), 128.2 (2C, CH), 88.2 (C_q), 68.8 (5C, CH), 68.3 (2C, CH), 67.6 (2C, CH), 40.5 (CH₂), 24.3 (CH₂). HRMS (ESI): *m/z* Calcd for C₁₉H₁₈FeO + H⁺ [M + H]⁺ 318.0702; Found 318.0699. The ¹H and ¹³C{¹H} spectra are consistent with those reported in the literature.⁸



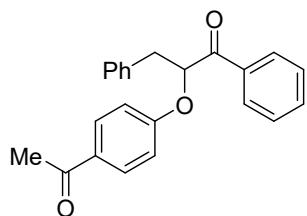
(E)-1,5-Diphenylpent-4-en-1-one (37): The representative procedure was followed, using substrate **37a** (0.047 g, 0.201 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 2 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 50/1) yielded **37** (0.037 g, 78%) as brown solid. ¹H-NMR (400 MHz, CDCl₃): δ = 8.01 (d, *J* = 7.8 Hz, 2H, Ar–H), 7.58 (t, *J* = 7.3 Hz, 1H, Ar–H), 7.48 (t, *J* = 7.6 Hz, 2H, Ar–H), 7.36 (d, *J* = 7.3 Hz, 2H, Ar–H), 7.30 (t, *J* = 7.6 Hz, 2H, Ar–H), 7.21 (t, *J* = 7.1 Hz, 1H, Ar–H), 6.48 (d, *J* = 15.8 Hz, 1H, CH), 6.31 (dt, *J* = 15.9, 6.8 Hz, 1H, CH) 3.17 (t, *J* = 7.4 Hz, 2H, CH₂), 2.68 (q, *J* = 6.9 Hz, 2H, CH₂). ¹³C{¹H}-NMR (100 MHz, CDCl₃): δ = 199.5 (CO), 137.6 (C_q), 137.1 (C_q), 133.2 (CH), 130.9 (CH), 129.3 (CH), 128.8 (2C, CH), 128.7 (2C, CH), 128.2 (2C, CH), 127.2 (CH), 126.2 (2C, CH), 38.4 (CH₂), 27.7 (CH₂). HRMS (ESI): *m/z* Calcd for C₁₇H₁₆O + H⁺ [M + H]⁺ 237.1274; Found 237.1271. The ¹H and ¹³C{¹H} spectra are consistent with those reported in the literature.¹⁸



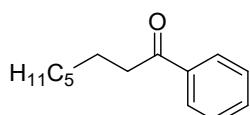
(E)-1,5-Diphenylpent-1-en-3-one (38): The representative procedure was followed, using substrate **38a** (0.047 g, 0.201 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 1 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 50/1) yielded **38** (0.035 g, 74%) as yellow solid. ¹H-NMR (400 MHz, CDCl₃): δ = 7.56-7.51 (m, 3H, Ar–H), 7.39-7.37 (m, 3H, Ar–H), 7.31-7.28 (m, 2H, Ar–H), 7.24-7.18 (m, 3H, Ar–H), 7.73 (d, *J* = 16.3 Hz, 1H, Ar–H), 3.00 (br s, 4H, CH₂). ¹³C{¹H}-NMR (100 MHz, CDCl₃): δ = 199.5 (CO), 142.9 (CH), 131.4 (C_q), 134.6 (C_q), 130.6 (CH), 129.1 (2C, CH), 128.7 (2C, CH), 128.6 (2C, CH), 128.4 (2C, CH), 126.3 (CH), 126.3 (CH), 42.6 (CH₂), 30.3 (CH₂). HRMS (ESI): *m/z* Calcd for C₁₇H₁₆O + H⁺ [M + H]⁺ 237.1274; Found 237.1273. The ¹H and ¹³C{¹H} spectra are consistent with those reported in the literature.¹⁹



2-Methyl-1,3-diphenylpropan-1-one (39): The representative procedure was followed, using substrate **39a** (0.045 g, 0.202 mmol), 10 bar H₂ and the reaction mixture was stirred at 50 °C for 20 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 50/1) yielded **39** (0.028 g, 62%) as colorless oil. ¹H-NMR (400 MHz, CDCl₃): δ = 7.94-7.91 (m, 2H, Ar-H), 7.55-7.51 (m, 1H, Ar-H), 7.43 (vt, *J* = 7.5 Hz, 2H, Ar-H), 7.28-7.24 (m, 2H, Ar-H), 7.20-7.15 (m, 3H, Ar-H), 3.79-3.70 (m, 1H, CH), 3.17 (dd, *J* = 13.7, 6.3 Hz, 1H, CH₂), 2.69 (dd, *J* = 13.7, 7.8 Hz, 1H, CH₂), 1.20 (d, *J* = 6.9 Hz, 3H, CH₃). ¹³C{¹H}-NMR (100 MHz, CDCl₃): δ = 203.9 (CO), 140.1 (C_q), 136.6 (C_q), 133.1 (CH), 129.3 (2C, CH), 128.8 (2C, CH), 128.5 (2C, CH), 128.5 (2C, CH), 126.4 (CH), 42.9 (CH), 39.5 (CH₂), 17.6 (CH₃). HRMS (ESI): *m/z* Calcd for C₁₆H₁₆O + H⁺ [M + H]⁺ 225.1274; Found 225.1268. The ¹H and ¹³C{¹H} spectra are consistent with those reported in the literature.²⁰

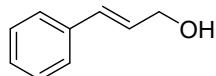


2-(4-Acetylphenoxy)-1,3-diphenylpropan-1-one (40): The representative procedure was followed, using substrate **40a** (0.069 g, 0.202 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 3 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 30/1) yielded **40** (0.040 g, 57%) as a yellow solid. ¹H-NMR (500 MHz, CDCl₃): δ = 8.04 (d, *J* = 7.9 Hz, 2H, Ar-H), 7.82 (d, *J* = 8.8 Hz, 2H, Ar-H), 7.61 (t, *J* = 7.4 Hz, 1H, Ar-H), 7.48 (t, *J* = 7.8 Hz, 2H, Ar-H), 7.32-7.23 (m, 5H, Ar-H), 6.84 (d, *J* = 8.9 Hz, 2H, Ar-H), 5.61 (dd, *J* = 7.4, 5.3 Hz, 1H, CH), 3.36-3.34 (m, 2H, CH₂), 2.48 (s, 3H, CH₃). ¹³C{¹H}-NMR (125 MHz, CDCl₃): δ = 197.4 (CO), 196.8 (CO), 161.5 (C_q), 136.6 (C_q), 134.4 (C_q), 134.2 (CH), 131.2 (C_q), 130.8 (2C, CH), 129.5 (2C, CH), 129.1 (2C, CH), 128.9 (2C, CH), 128.8 (2C, CH), 127.3 (CH), 115.1 (2C, CH), 81.8 (CH), 39.4 (CH₂), 26.5 (CH₃). HRMS (ESI): *m/z* Calcd for C₂₃H₂₀O₃ + H⁺ [M + H]⁺ 345.1485; Found 345.1478.

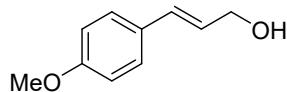


1-Phenyloctan-1-one (41): The representative procedure was followed, using substrate **41a** (0.041 g, 0.203 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 1 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 100/1)

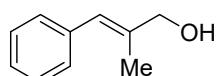
yielded **41** (0.031 g, 75%) as colorless oil. ^1H -NMR (400 MHz, CDCl_3): 7.96 (d, $J = 7.4$ Hz, 2H, Ar–H), 7.55 (t, $J = 7.4$ Hz, 1H, Ar–H), 7.45 (t, $J = 7.6$ Hz, 2H, Ar–H), 2.96 (t, $J = 7.4$ Hz, 2H, CH_2), 1.76–1.69 (m, 2H, CH_2), 1.39–1.23 (m, 8H, CH_2), 0.88 (t, $J = 6.7$ Hz, 3H, CH_3). $^{13}\text{C}\{\text{H}\}$ -NMR (100 MHz, CDCl_3): $\delta = 200.8$ (CO), 137.2 (C_q), 133.0 (CH), 128.7 (2C, CH), 128.2 (2C, CH), 38.8 (CH_2), 31.9 (CH_2), 29.5 (CH_2), 29.3 (CH_2), 24.5 (CH_2), 22.8 (CH_2), 14.3 (CH_3). The ^1H and $^{13}\text{C}\{\text{H}\}$ spectra are consistent with those reported in the literature.²¹



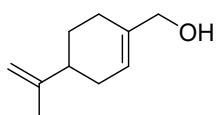
(E)-3-Phenylprop-2-en-1-ol (42): The representative procedure was followed, using substrate **42a** (0.027 g, 0.204 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 1 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 10/1) yielded **42** (0.026 g, 95%) as yellow oil. ^1H -NMR (500 MHz, CDCl_3): $\delta = 7.38$ (d, $J = 7.3$ Hz, 2H, Ar–H), 7.32 (t, $J = 7.4$ Hz, 2H, Ar–H), 7.24 (t, $J = 7.2$ Hz, 1H, Ar–H), 6.61 (d, $J = 16.0$ Hz, 1H, CH), 6.35 (dt, $J = 15.8, 5.8$ Hz, 1H, CH), 4.31 (dd, $J = 5.8, 1.5$ Hz, 2H, CH_2), 2.01 (br s, 1H, OH). $^{13}\text{C}\{\text{H}\}$ -NMR (125 MHz, CDCl_3): $\delta = 136.8$ (C_q), 131.2 (CH), 128.7 (2C, CH), 128.7 (CH), 127.8 (CH), 126.6 (2C, CH), 63.8 (CH_2). The ^1H and $^{13}\text{C}\{\text{H}\}$ spectra are consistent with those reported in the literature.²²



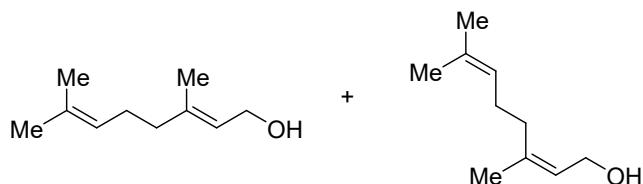
(E)-3-(4-Methoxyphenyl)prop-2-en-1-ol (43): The representative procedure was followed, using substrate **43a** (0.033 g, 0.203 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 3 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 10/1) yielded **43** (0.033 g, 99%) as a white solid. ^1H -NMR (400 MHz, CDCl_3): $\delta = 7.31$ (d, $J = 8.6$ Hz, 2H, Ar–H), 6.85 (d, $J = 8.8$ Hz, 2H, Ar–H), 6.54 (d, $J = 15.9$ Hz, 1H, CH), 6.22 (dt, $J = 15.9, 5.9$ Hz, 1H, CH), 4.28 (dd, $J = 4.9, 1.4$ Hz, 2H, CH_2), 3.80 (s, 3H, CH_3), 1.88 (br s, 1H, OH). $^{13}\text{C}\{\text{H}\}$ -NMR (100 MHz, CDCl_3): $\delta = 159.4$ (C_q), 131.0 (CH), 129.6 (C_q), 127.8 (2C, CH), 126.4 (CH), 114.1 (2C, CH), 64.0 (CH_2), 55.4 (CH_3). HRMS (ESI): m/z Calcd for $\text{C}_{10}\text{H}_{12}\text{O}_2 + \text{H}^+ [\text{M} + \text{H}]^+$ 165.0910; Found 165.0908. The ^1H and $^{13}\text{C}\{\text{H}\}$ spectra are consistent with those reported in the literature.²²



(E)-2-Methyl-3-phenylprop-2-en-1-ol (44): The representative procedure was followed, using substrate **44a** (0.030 g, 0.205 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 3 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 10/1) yielded **44** (0.026 g, 86%) as colorless liquid. ¹H-NMR (400 MHz, CDCl₃): δ = 7.33 (t, *J* = 7.4 Hz, 2H, Ar-H), 7.27 (d, *J* = 7.1 Hz, 2H, Ar-H), 7.21 (t, *J* = 7.13 Hz, 1H, Ar-H), 6.52 (s, 1H, CH), 4.18 (s, 2H, CH₂), 1.90 (s, 3H, CH₃), 1.82 (br s, 1H, OH). ¹³C{¹H}-NMR (100 MHz, CDCl₃): δ = 137.8 (C_q), 137.7 (C_q), 129.0 (2C, CH), 128.3 (2C, CH), 126.6 (CH), 125.2 (CH), 69.1 (CH₂), 15.4 (CH₃). The ¹H and ¹³C{¹H} spectra are consistent with those reported in the literature.²³

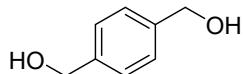


(4-(Prop-1-en-2-yl)cyclohex-1-en-1-yl)methanol (45): The representative procedure was followed, using substrate **45a** (0.031 g, 0.206 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 3 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 20/1) yielded **45** (0.024 g, 77%) as yellow oil. ¹H-NMR (400 MHz, CDCl₃): δ = 5.71-5.67 (m, 1H, CH), 4.73-4.66 (m, 2H, CH₂), 4.01-3.97 (m, 2H, CH₂), 2.19-1.79 (m, 7H, CH), 1.74 (s, 3H, CH₃), 1.37 (br s, 1H, OH). ¹³C{¹H}-NMR (100 MHz, CDCl₃): δ = 150.0 (C_q), 137.4 (C_q), 122.7 (CH), 108.8 (CH₂), 67.5 (CH₂), 41.3 (CH), 30.6 (CH₂), 27.7 (CH₂), 26.3 (CH₂), 21.0 (CH₃). HRMS (ESI): *m/z* Calcd for C₁₀H₁₆O + H⁺ [M + H]⁺ 153.1274; Found 153.11273. The ¹H and ¹³C{¹H} spectra are consistent with those reported in the literature.²⁴

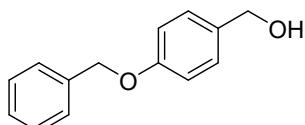


(E/Z)-3-(4-Methoxyphenyl)prop-2-en-1-ol (46): The representative procedure was followed, using isomeric mixture of **46a** (0.031 g, 0.204 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 3 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 10/1) yielded isomeric mixture (3:2) of **46** (0.023 g, 73%) as colorless oil. ¹H-NMR (400 MHz, CDCl₃): δ = 5.45-5.41 (m, 1H, CH), 5.11-5.06 (m, 1H, CH), 4.15-4.07 (m, 2H, CH₂), 2.12-2.00 (m, 4H, CH₂), 1.75-1.67 (m, 6H, CH₃), 1.60 (s, 3H,

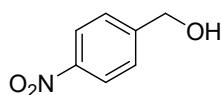
CH_3). $^{13}\text{C}\{\text{H}\}$ -NMR for *E* isomer of **46** (100 MHz, CDCl_3): $\delta = 139.9$ (C_q), 131.9 (C_q), 124.0 (CH), 123.5 (CH), 59.6 (CH_2), 39.7 (CH_2), 26.6 (CH_2), 25.8 (CH_3), 17.8 (CH_3), 16.4 (CH_3). For *Z* isomer of **46**: (100 MHz, CDCl_3): $\delta = 140.1$ (C_q), 132.6 (C_q), 124.6 (CH), 124.0 (CH), 59.1 (CH_2), 32.1 (CH_2), 26.7 (CH_2), 25.8 (CH_3), 23.6 (CH_3), 17.8 (CH_3). HRMS (ESI): m/z Calcd for $\text{C}_{10}\text{H}_{18}\text{O} - \text{H}^+$ [$\text{M} - \text{H}]^+$ 153.1274; Found 153.1273. The ^1H and $^{13}\text{C}\{\text{H}\}$ spectra are consistent with those reported in the literature.²⁵



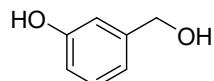
1,4-Phenylenedimethanol (47): The representative procedure was followed, using substrate **47a** (0.027 g, 0.201 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 3 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 10/1) yielded **47** (0.024 g, 86%) as white solid. ^1H -NMR (500 MHz, $\text{DMSO}-d_6$): $\delta = 7.26$ (s, 4H, Ar-H), 5.12 (t, $J = 5.7$ Hz, 2H, OH), 4.48 (d, $J = 5.6$ Hz, 4H, CH_2). $^{13}\text{C}\{\text{H}\}$ -NMR (125 MHz, $\text{DMSO}-d_6$): $\delta = 140.9$ (2C, C_q), 126.2 (4C, CH), 62.8 (2C, CH_2). The ^1H and $^{13}\text{C}\{\text{H}\}$ spectra are consistent with those reported in the literature.²⁶



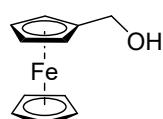
(4-(Benzylxy)phenyl)methanol (48): The representative procedure was followed, using substrate **48a** (0.043 g, 0.203 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 3 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 10/1) yielded **48** (0.043 g, 99%) as a white solid. ^1H -NMR (400 MHz, CDCl_3): $\delta = 7.41$ (d, $J = 7.3$ Hz, 2H, Ar-H), 7.36 (t, $J = 7.3$ Hz, 2H, Ar-H), 7.30 (t, $J = 7.1$ Hz, 1H, Ar-H), 7.25 (d, $J = 8.6$ Hz, 2H, Ar-H), 6.94 (d, $J = 8.6$ Hz, 2H, Ar-H), 5.04 (s, 2H, CH_2), 4.56 (s, 2H, CH_2), 1.91 (s, 1H, OH). $^{13}\text{C}\{\text{H}\}$ -NMR (100 MHz, CDCl_3): $\delta = 158.5$ (C_q), 137.1 (C_q), 133.6 (C_q), 128.8 (2C, CH), 128.7 (2C, CH), 128.1 (CH), 127.6 (2C, CH), 115.1 (2C, CH), 70.2 (CH_2), 65.1 (CH_2). HRMS (ESI): m/z Calcd for $\text{C}_{14}\text{H}_{14}\text{O}_2 - \text{H}^+$ [$\text{M} - \text{H}]^+$ 213.0910; Found 213.0907. The ^1H and $^{13}\text{C}\{\text{H}\}$ spectra are consistent with those reported in the literature.²⁵



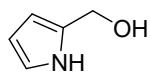
(4-Nitrophenyl)methanol (49): The representative procedure was followed, using substrate **49a** (0.031 g, 0.205 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 3 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 10/1) yielded **49** (0.029 g, 92%) as yellow solid. ¹H-NMR (400 MHz, CDCl₃): δ = 8.18 (d, *J* = 8.8 Hz, 2H, Ar–H), 7.51 (d, *J* = 8.9 Hz, 2H, Ar–H), 4.82 (s, 2H, CH₂), 2.28 (s, 1H, OH). ¹³C{¹H}-NMR (100 MHz, CDCl₃): δ = 148.4 (C_q), 147.4 (C_q), 127.2 (2C, CH), 123.9 (2C, CH), 64.1 (CH₂). The ¹H and ¹³C{¹H} spectra are consistent with those reported in the literature.²⁷



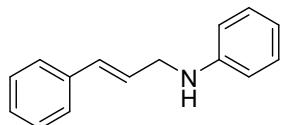
3-(Hydroxymethyl)phenol (50): The representative procedure was followed, using substrate **50a** (0.025 g, 0.205 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 3 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 10/1) yielded **50** (0.021 g, 83%) as white solid. ¹H-NMR (400 MHz, DMSO-d₆): δ = 9.30 (s, 1H, OH), 7.13 (t, *J* = 7.8 Hz, 1H, Ar–H), 6.78 (s, 1H, Ar–H), 6.75 (d, *J* = 7.5 Hz, 1H, Ar–H), 6.65 (dd, *J* = 8.0, 2.0 Hz, 1H, Ar–H), 5.12 (t, *J* = 5.8 Hz, 1H, OH), 4.45 (d, *J* = 5.8 Hz, 2H, CH₂). ¹³C{¹H}-NMR (100 MHz, DMSO-d₆): δ = 158.2 (C_q), 145.0 (C_q), 129.9 (CH), 117.8 (CH), 114.4 (CH), 114.2 (CH), 63.8 (CH₂). The ¹H and ¹³C{¹H} spectra are consistent with those reported in the literature.²⁸



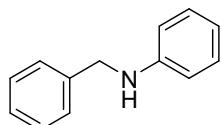
Ferrocenylmethanol (51): The representative procedure was followed, using substrate **51a** (0.043 g, 0.201 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 3 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 10/1) yielded **51** (0.042 g, 97%) as a yellow solid. ¹H-NMR (400 MHz, CDCl₃): δ = 4.32 (s, 2H, CH₂), 4.24 (t, *J* = 1.6 Hz, 2H, Ar–H), 4.19–4.17 (m, 7H, Ar–H), 1.71 (s, 1H, OH). ¹³C{¹H}-NMR (100 MHz, CDCl₃): δ = 88.5 (C_q), 68.5 (7C, CH), 68.1 (2C, CH), 60.9 (CH₂). HRMS (ESI): *m/z* Calcd for C₁₁H₁₂FeO + H⁺ [M + H]⁺ 217.0312; Found 217.0311. The ¹H and ¹³C{¹H} spectra are consistent with those reported in the literature.²⁵



(1*H*-Pyrrol-2-yl)methanol (52): The representative procedure was followed, using substrate **52a** (0.019 g, 0.20 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 3 h. Purification by column chromatography on neutral alumina (petroleum ether/EtOAc: 20/1) yielded **52** (0.018 g, 93%) as a colorless liquid. After purification the isolated product was stored in in refrigerator to avoid polymerization at room temperature. ¹H-NMR (400 MHz, CDCl₃): δ = 8.62 (br s, 1H, NH), 6.73 (s, 1H, Ar–H), 6.13 (d, J = 15.3 Hz, 2H, Ar–H), 4.54 (s, 2H, CH₂), 2.66 (br s, 1H, OH). ¹³C{¹H}-NMR (100 MHz, CDCl₃): δ = 131.1 (C_q), 118.8 (CH), 108.4 (CH), 107.3 (CH), 58.0 (CH₂).



N-Cinnamylaniline (53): The representative procedure was followed, using substrate **53a** (0.042 g, 0.203 mmol) and the reaction mixture was stirred at room temperature (27 °C) for 4 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 50/1) yielded mixture of **53** and *N*-(3-phenylpropyl)aniline (0.038 g, 89%) as a yellow oil. For compound **53**: ¹H-NMR (400 MHz, CDCl₃): δ = 7.35 (d, J = 7.1 Hz, 2H, Ar–H), 7.29 (t, J = 7.3 Hz, 2H, Ar–H), 7.23-7.16 (m, 3H, Ar–H), 6.71 (t, J = 7.3 Hz, 1H, Ar–H), 6.65 (d, J = 7.9 Hz, 2H, Ar–H), 6.58-6.55 (m, 1H, CH), 6.31 (dt, J = 15.9, 5.7 Hz, 1H, CH), 3.92 (d, J = 5.4 Hz, 2H, CH₂), 3.68 (br s, 1H, NH). ¹³C{¹H}-NMR (100 MHz, CDCl₃): δ = 148.2 (C_q), 137.0 (C_q), 131.7 (CH), 129.4 (2C, CH), 128.7 (2C, CH), 127.7 (CH), 127.2 (CH), 126.5 (2C, CH), 117.8 (CH), 113.2 (2C, CH), 46.4 (CH₂). HRMS (ESI): *m/z* Calcd for C₁₅H₁₅N – H⁺ [M – H]⁺ 208.1121; Found 208.1120. The ¹H and ¹³C{¹H} spectra are consistent with those reported in the literature.²²



N-benzyylaniline (54): The representative procedure was followed, using substrate **54a** (0.037 g, 0.204 mmol) and the reaction mixture was stirred at 50 °C for 20 h. Purification by column chromatography on silica gel (petroleum ether/EtOAc: 30/1) yielded **54** (0.034 g, 91%) as

yellow oil. ^1H -NMR (400 MHz, CDCl_3): δ = 7.38-7.31 (m, 4H, Ar-H), 7.28-7.24 (m, 1H, Ar-H), 7.16 (dd, J = 8.6, 7.4 Hz, 2H, Ar-H), 6.71 (t, J = 7.3 Hz, 1H, Ar-H), 6.62 (dd, J = 8.6, 0.9 Hz, 2H, Ar-H), 4.31 (s, 2H, CH_2), 4.00 (br s, 1H, NH). $^{13}\text{C}\{\text{H}\}$ -NMR (100 MHz, CDCl_3): δ = 148.3 (C_q), 139.6 (C_q), 129.4 (2C, CH), 128.8 (2C, CH), 127.7 (2C, CH), 127.4 (CH), 117.7 (CH), 113.0 (2C, CH), 48.5 (CH_2). HRMS (ESI): m/z Calcd for $\text{C}_{13}\text{H}_{13}\text{N} + \text{H}^+$ [M + H] $^+$ 184.1121; Found 184.1120. The ^1H and $^{13}\text{C}\{\text{H}\}$ spectra are consistent with those reported in the literature.²²

7. Mechanistic Experiments

Procedure for Deuterium Labelling Experiment. A standard catalytic hydrogenation reaction was performed using CD_3OD as a solvent. After completion of reaction time, the reaction mixture was evaporated under vacuo. Purification by column chromatography provided the semi-hydrogenated product **4-[D]** with 92% deuterium incorporation (Figure S1).

This finding suggests that one of the hydrogen sources for hydrogenation is the methanol, and incorporation of two D at α -position supports the reversible protonation of substrate.



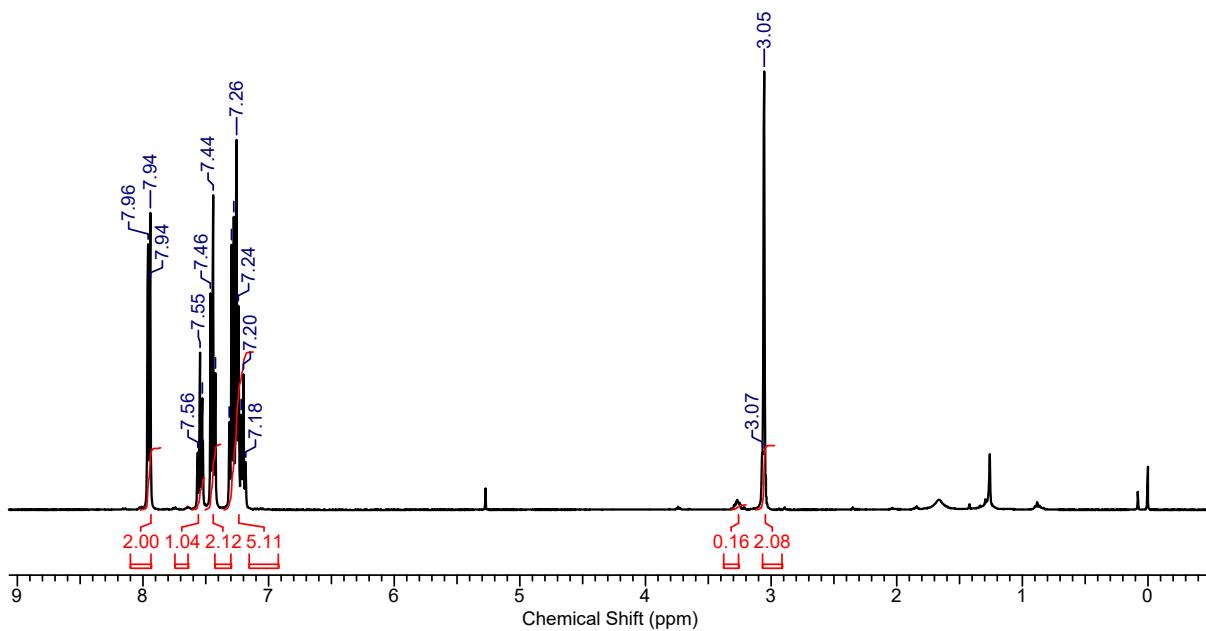


Figure S1. ^1H NMR of Compound 4-[D].

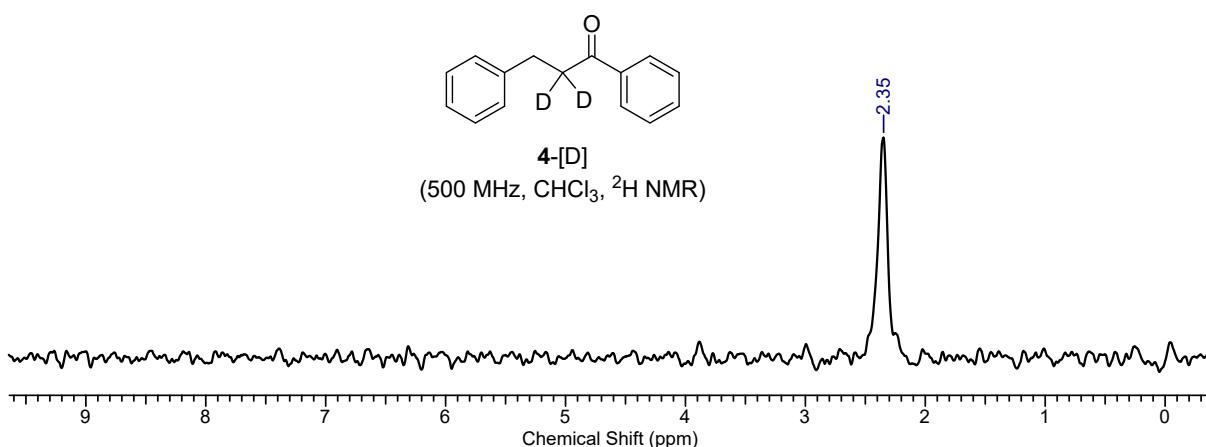


Figure S2. ^2H NMR of 4-[D] in CHCl_3 .

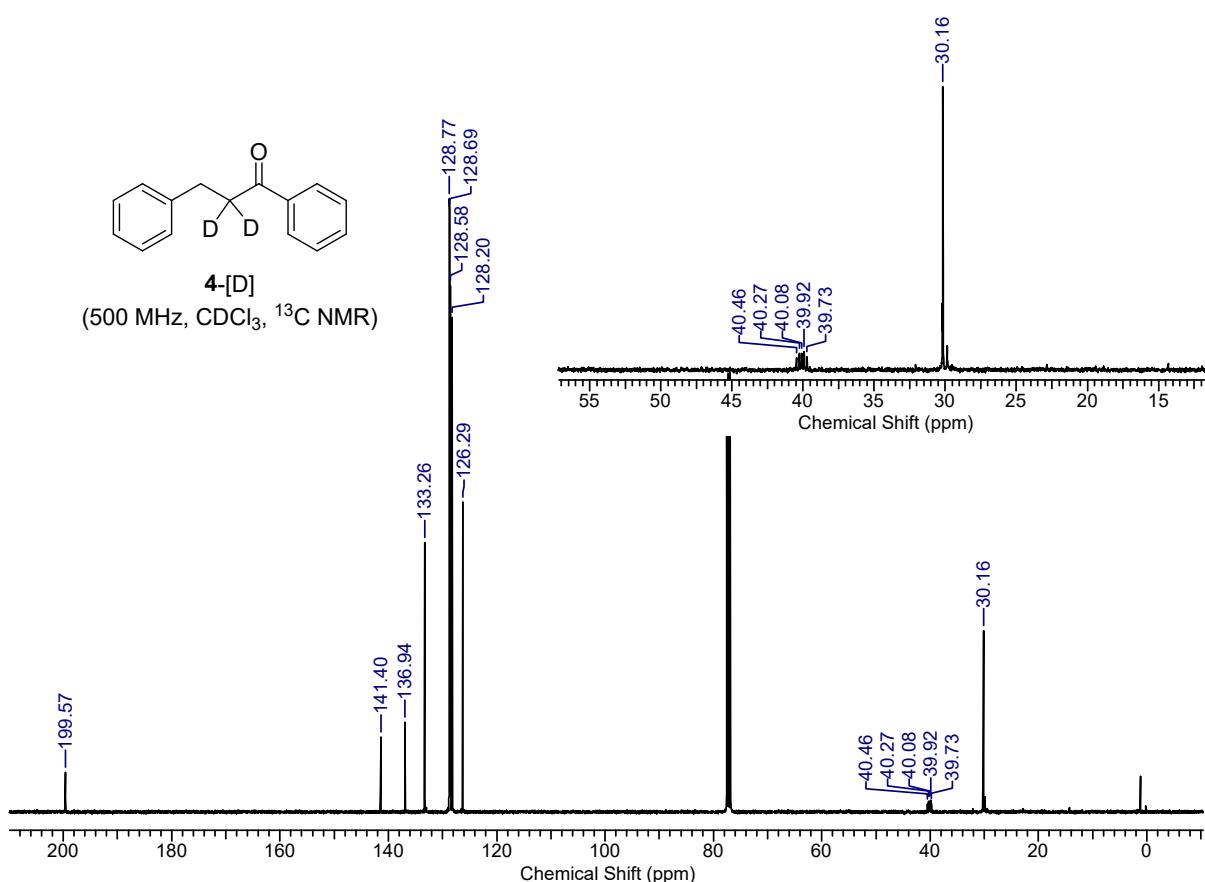
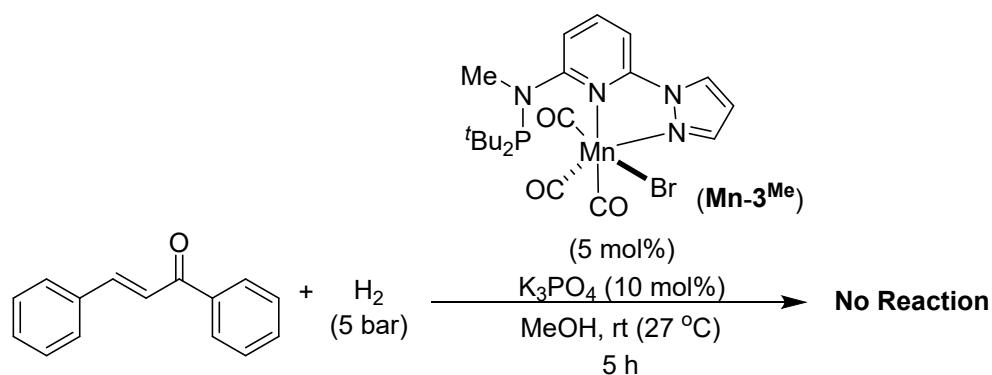


Figure S3. $^{13}\text{C}\{^1\text{H}\}$ -NMR of **4-[D]** in CDCl_3 .

Experiment to Understand Non-innocent Behaviour of Ligand *NH*.

a) **Reaction with Catalytic Mn-3^{Me} :** A standard hydrogenation reaction was performed using **Mn-3^{Me}** as catalyst. After 5 h of the reaction time, the reaction mixture was analysed by GC that ensured no formation of hydrogenated product. This experiment suggests the *NH* moiety in the manganese catalyst is necessary to generate active de-aromatized catalyst in the presence of base (K_3PO_4) that would activate the H_2 molecule.



b) Synthesis of Dearomatized Active Complex (A): In a dry J-Young NMR tube, **Mn-3** (0.02 mmol) and KO*t*Bu (0.04 mmol) was added inside the glove box. To this, 0.6 mL THF was added and the tube was agitated to make a homogeneous mixture. Within few seconds orange to brown color change was noticed. Reaction was analysed by $^{31}\text{P}\{\text{H}\}$ -NMR in different time intervals. After 1 h of reaction time two new peaks were observed at 174.9 and 161.1 ppm along with some decoordination ligand at 70.8 ppm, and the original peaks for **Mn-3** were disappeared. Further heating the same reaction mixture at 50 °C for 1 h, a sharp singlet was observed at 174.8 ppm (Spectrum 3, Figure S4), which could be tentatively assigned to complex **A**. This experiment suggest that the reaction proceeds *via* metal-ligand cooperation through dearomatization-aromatization while using complex **Mn-3**. In addition, the observed single peak for **A** at 174.8 ppm supports the existence of an isomeric mixtures of precatalyst **Mn-3**.

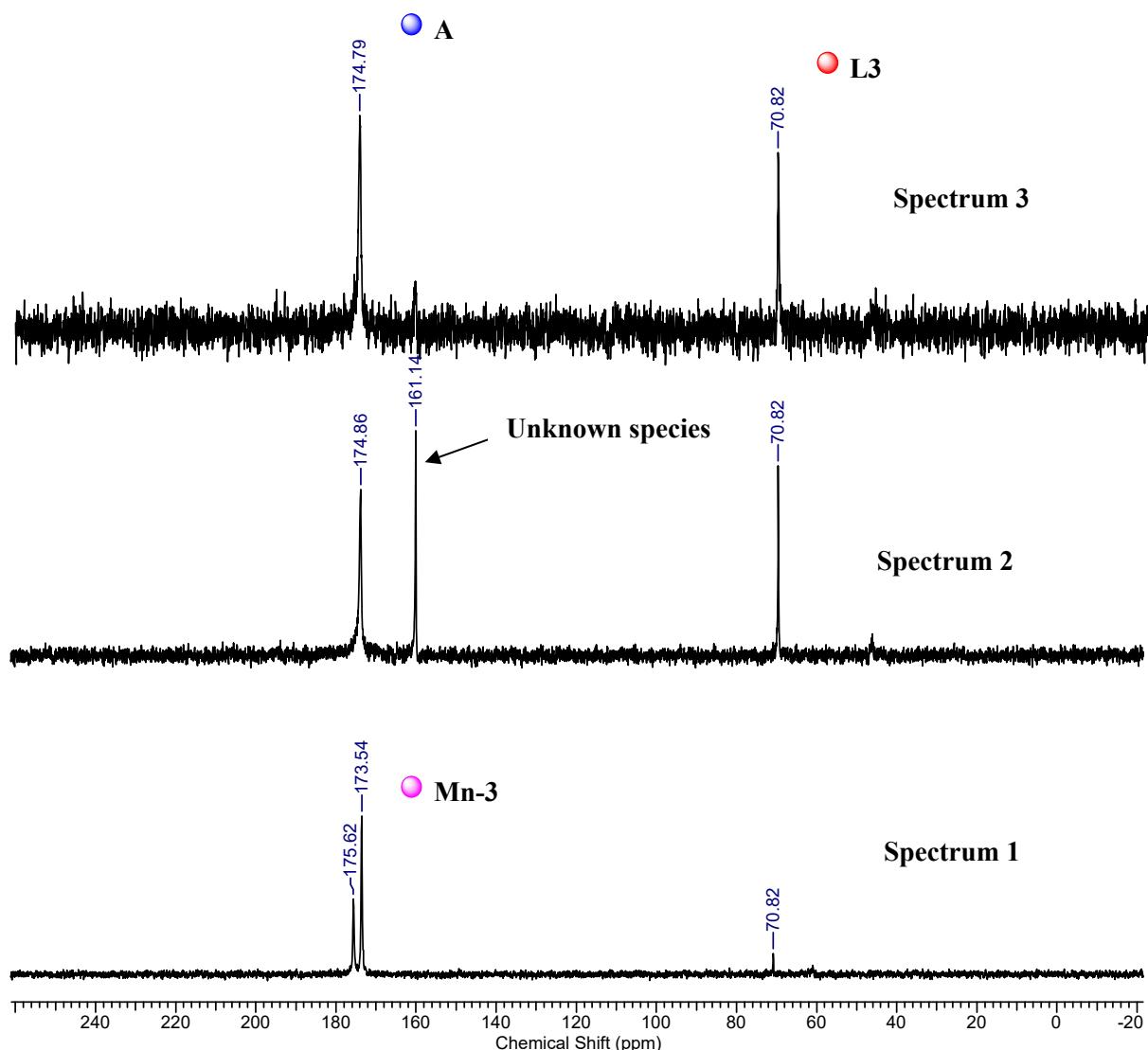
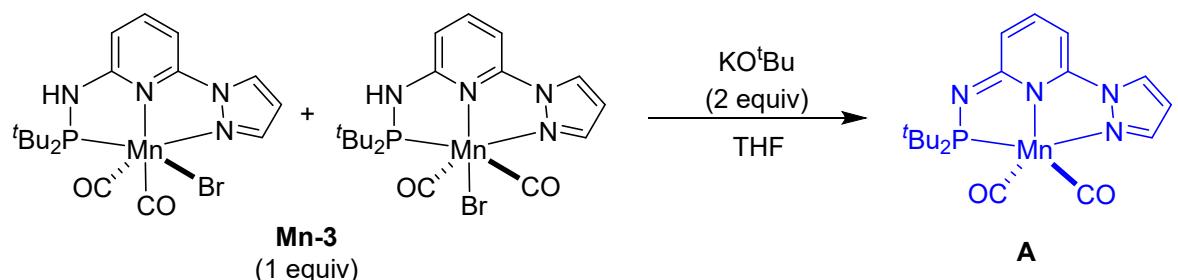
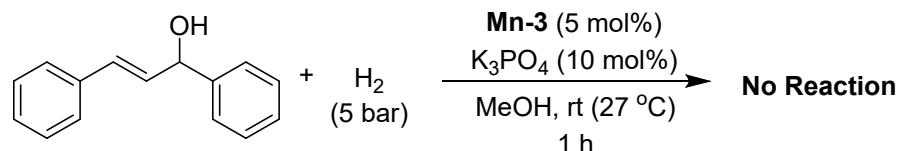


Figure S4. $^{31}\text{P}\{^1\text{H}\}$ NMR spectra for the reaction mixture of **Mn-3** with KO^tBu . **Spectrum 1:** **Mn-3** in THF with trace decoordinated ligand. **Spectrum 2:** After 1 h at room temperature. **Spectrum 3:** After heating at 50°C for 1 h.

Attempted Hydrogenation of (*E*)-1,3-Diphenylprop-2-en-1-ol: Under standard hydrogenation conditions, the compound (*E*)-1,3-diphenylprop-2-en-1-ol was attempted for hydrogenation. The GC analysis of the reaction mixture does not show the formation of alkene hydrogenation product. This experiment suggests that the hydrogenation of (*E*)-chalcone (**4**) does not proceed *via* the 1,2-addition. Hence this reaction proceed *via* the 1,4-addition of hydrogen.



8. DFT Calculations

All the calculations in this study have been performed with density functional theory (DFT), with the aid of the Turbomole 7.5 suite of programs,²⁹ using the PBE functional,³⁰ along with dispersion correction (DFT-D3).³¹ The def2-SVP basis set³² for Mn and the TZVP basis set for all other atoms have been employed. The resolution of identity (RI),³³ along with the multipole accelerated resolution of identity (marij)³⁴ approximations have been employed for an accurate and efficient treatment of the electronic Coulomb term in the DFT calculations. A solvent correction was incorporated with optimization calculations using the COSMO model,³⁵ with methanol ($\epsilon = 32.7$) as the solvent. The values reported are ΔG values, with zero-point energy corrections, internal energy, and entropic contributions included through frequency calculations on the optimized minima, with the temperature taken to be 298.15 K. Harmonic frequency calculations were performed for all stationary points to confirm them as local minima or transition state structures.

Energy span model (ESM)- The Turnover frequency (TOF) of the catalytic cycle can be calculated through the Energetic Span Model (ESM) and put into practical use by Shaik and co-workers.³⁶⁻³⁸ The ESM imparts an easy method to determine the turnover frequencies (TOFs) of catalytic cycles based on their computed energy profiles. In most cases, the TOF is calculated by the TOF-determining transition state (TDTS), the TOF-determining intermediate (TDI), and by the reaction energy, ΔG_r , as shown below

$$TOF = \frac{kBT}{h} e^{-\delta E/RT}$$

where δE is the energy span and is defined as the Gibbs energy difference between the TDTS and the TDI, with the addition of the ΔG_r when the TDTS appears before the TDI. δE is the effective activation energy barrier of the global reaction. The TDTS and TDI are the intermediate and the transition state, respectively, that maximize δE , according to equation 1.

$$\delta E = \begin{cases} TDTS - TDI, & \text{if TDTS appears after TDI} \\ TFTS - TDI + \Delta G_r, & \text{if TDTS appears before TDI} \end{cases} \quad (1)$$

This model has been used to calculate the TOFs (at 298.15 K). The ESM can be applied in a user-friendly way with the recently developed AUTOF computer program.³⁶⁻³⁸

9. X-ray Structural Data

X-ray intensity data measurements of compound **Mn-2** was carried out on a Bruker D8 VENTURE Kappa Duo PHOTON II CPAD diffractometer equipped with Incoatech multilayer mirrors optics. The intensity measurements were carried out with Mo micro-focus sealed tube diffraction source ($\text{MoK}_{\alpha} = 0.71073 \text{ \AA}$) at 100(2) K temperature. The X-ray generator was operated at 50 kV and 1.4 mA. A preliminary set of cell constants and an orientation matrix were calculated from three matrix sets of 36 frames (each matrix run consists of 12 frames). Data were collected with ω scan width of 0.5° at different settings of φ and 2θ with a frame time of 10-20 sec depending on the diffraction power of the crystals keeping the sample-to-detector distance fixed at 5.00 cm. The X-ray data collection was monitored by APEX3 program (Bruker, 2016).³⁹ All the data were corrected for Lorentzian, polarization and absorption effects using SAINT and SADABS programs (Bruker, 2016). Using the APEX3 (Bruker) program suite, the structure was solved with the ShelXS-97 (Sheldrick, 2008)⁴⁰ structure solution program, using direct methods. The model was refined with a version of ShelXL-2018/3 (Sheldrick, 2015)⁴¹ using Least Squares minimization. All the hydrogen atoms were placed in a geometrically idealized position and constrained to ride on their parent atoms. An *ORTEP III*⁴² view of the compounds was drawn with 50% probability displacement ellipsoids, and H atoms are shown as small spheres of arbitrary radii.

Procedure of crystallization: Equimolar ratio of L2 (0.005 g) and Mn(CO)₅Br (0.005 g) was taken in a dry NMR tube and added dry THF (0.5 mL). Then the tube was closed with cap and kept inside the glove box for three days to form orange crystal on the wall of the tube.

Table S2. Crystal Data of Compound **Mn-2**.

Crystal Data	Mn-2
Formula	C ₁₆ H ₂₁ BrMnN ₄ O ₂ P
Molecular weight	467.19
Crystal Size, mm ³	0.240 × 0.260 × 0.360
Temp. (K)	100(2)
Wavelength (Å)	0.71073
Crystal Syst.	orthorhombic
Space Group	<i>Pbca</i>
<i>a</i> /Å	9.1016(5)
<i>b</i> /Å	14.4759(6)
<i>c</i> /Å	28.6257(14)
<i>V</i> /Å ³	3771.5(3)
<i>Z</i>	8
<i>D</i> _{calc} /g cm ⁻³	1.642
μ /mm ⁻¹	2.921
<i>F</i> (000)	1880
<i>Ab. Correct.</i>	multi-scan
<i>T</i> _{min} / <i>T</i> _{max}	0.419/0.541
2 <i>θ</i> _{max}	56
Total reflns.	73416
Unique reflns.	4688
Obs. reflns.	3291
<i>h, k, l</i> (min, max)	(-12, 11), (-19, 19), (-38, 38)
R _{int} / R _{sig}	0.1649/ 0.0655
No. of parameters	230
<i>R</i> 1 [<i>I</i> > 2σ(<i>I</i>)]	0.0494
<i>wR</i> 2[<i>I</i> > 2σ(<i>I</i>)]	0.0889
<i>R</i> 1 [all data]	0.0882
<i>wR</i> 2 [all data]	0.1012
goodness-of-fit	1.051
Δρ _{max} , Δρ _{min} (eÅ ⁻³)	+0.798, -0.589
CCDC No.	2194541

Table S3. Bond Lengths (Å) for Compound **Mn-2**.

Br1-Mn1	2.5916(7)	Mn1-C9	1.773(4)
Mn1-C10	1.797(4)	Mn1-N3	2.011(3)
Mn1-N1	2.012(3)	Mn1-P1	2.2462(12)
P1-N4	1.732(3)	P1-C11	1.846(4)
P1-C14	1.849(4)	O1-C9	1.157(5)
O2-C10	1.149(5)	N1-C1	1.344(5)
N1-C5	1.345(5)	N2-N3	1.362(5)
N2-C6	1.368(6)	N2-C5	1.401(6)
N3-C8	1.323(5)	N4-C1	1.375(5)
N4-H4N	0.88		
C1-C2	1.404(5)	C2-C3	1.376(6)
C2-H2	0.95	C3-C4	1.389(7)
C3-H3	0.95	C4-C5	1.377(6)
C4-H4	0.95	C6-C7	1.356(7)
C6-H6	0.95	C7-C8	1.394(6)
C7-H7	0.95	C8-H8	0.95
C11-C12	1.516(6)	C11-C13	1.530(5)
C11-H11	1.0	C12-H12A	0.98
C12-H12B	0.98	C12-H12C	0.98
C13-H13A	0.98	C13-H13B	0.98
C13-H13C	0.98	C14-C16	1.528(5)
C14-C15	1.535(6)	C14-H14	1.0
C15-H15A	0.98	C15-H15B	0.98
C15-H15C	0.98	C16-H16A	0.98
C16-H16B	0.98	C16-H16C	0.98

Table S4. Bond Angles ($^{\circ}$) for Compound **Mn-2**.

C9-Mn1-C10	87.40(19)	C9-Mn1-N3	91.59(17)
C10-Mn1-N3	99.97(17)	C9-Mn1-N1	96.23(16)
C10-Mn1-N1	175.88(16)	N3-Mn1-N1	78.02(14)
C9-Mn1-P1	92.06(14)	C10-Mn1-P1	99.34(14)
N3-Mn1-P1	160.49(11)	N1-Mn1-P1	82.53(10)
C9-Mn1-Br1	175.54(14)	C10-Mn1-Br1	91.66(13)
N3-Mn1-Br1	84.28(10)	N1-Mn1-Br1	84.57(9)
P1-Mn1-Br1	92.39(3)	N4-P1-C11	103.72(17)
N4-P1-C14	100.77(17)	C11-P1-C14	104.30(19)
N4-P1-Mn1	99.98(12)	C11-P1-Mn1	121.95(14)
C14-P1-Mn1	122.10(14)	C1-N1-C5	119.5(4)
C1-N1-Mn1	122.5(3)	C5-N1-Mn1	117.9(3)
N3-N2-C6	110.9(4)	N3-N2-C5	117.2(3)
C6-N2-C5	131.7(4)	C8-N3-N2	105.3(3)
C8-N3-Mn1	140.2(3)	N2-N3-Mn1	114.5(3)
C1-N4-P1	118.6(3)	N1-C1-N4	116.1(3)
C1-N4-H4N	120.2	P1-N4-H4N	120.2
N1-C1-C2	120.6(4)	N4-C1-C2	123.3(4)
C3-C2-C1	118.4(4)	C3-C2-H2	120.8
C1-C2-H2	120.8	C2-C3-C4	121.3(4)
C2-C3-H3	119.3	C4-C3-H3	119.3
C5-C4-C3	116.6(4)	C5-C4-H4	121.7
C3-C4-H4	121.7	N1-C5-C4	123.5(4)
N1-C5-N2	112.2(4)	C4-C5-N2	124.3(4)
C7-C6-N2	106.6(4)	C7-C6-H6	126.7
N2-C6-H6	126.7	C6-C7-C8	106.1(4)
C6-C7-H7	126.9	C8-C7-H7	126.9
N3-C8-C7	111.1(4)	N3-C8-H8	124.4
C7-C8-H8	124.4	O1-C9-Mn1	175.3(4)
O2-C10-Mn1	176.7(4)	C12-C11-C13	110.5(3)
C12-C11-P1	112.9(3)	C13-C11-P1	111.0(3)

C12-C11-H11	107.4	C13-C11-H11	107.4
P1-C11-H11	107.4	C11-C12-H12A	109.5
C11-C12-H12B	109.5	H12A-C12-H12B	109.5
C11-C12-H12C	109.5	H12A-C12-H12C	109.5
H12B-C12-H12C	109.5	C11-C13-H13A	109.5
C11-C13-H13B	109.5	H13A-C13-H13B	109.5
C11-C13-H13C	109.5	H13A-C13-H13C	109.5
H13B-C13-H13C	109.5	C16-C14-C15	110.5(3)
C16-C14-P1	111.1(3)	C15-C14-P1	114.4(3)
C16-C14-H14	106.8	C15-C14-H14	106.8
P1-C14-H14	106.8	C14-C15-H15A	109.5
C14-C15-H15B	109.5	H15A-C15-H15B	109.5
C14-C15-H15C	109.5	H15A-C15-H15C	109.5
H15B-C15-H15C	109.5	C14-C16-H16A	109.5
C14-C16-H16B	109.5	H16A-C16-H16B	109.5
C14-C16-H16C	109.5	H16A-C16-H16C	109.5
H16B-C16-H16C	109.5		

Table S5. Torsion Angles ($^{\circ}$) for Compound **Mn-2**.

C6-N2-N3-C8	-0.1(5)	C5-N2-N3-C8	-176.5(4)
C6-N2-N3-Mn1	178.5(3)	C5-N2-N3-Mn1	2.1(4)
C11-P1-N4-C1	132.7(3)	C14-P1-N4-C1	-119.5(3)
Mn1-P1-N4-C1	6.2(3)	C5-N1-C1-N4	177.3(3)
Mn1-N1-C1-N4	1.3(5)	C5-N1-C1-C2	-1.1(6)
Mn1-N1-C1-C2	-177.1(3)	P1-N4-C1-N1	-5.4(5)
P1-N4-C1-C2	173.0(3)	N1-C1-C2-C3	1.8(6)
N4-C1-C2-C3	-176.5(4)	C1-C2-C3-C4	-0.1(6)
C2-C3-C4-C5	-2.0(6)	C1-N1-C5-C4	-1.3(6)
Mn1-N1-C5-C4	174.9(3)	C1-N1-C5-N2	179.2(3)
Mn1-N1-C5-N2	-4.6(4)	C3-C4-C5-N1	2.8(6)
C3-C4-C5-N2	-177.7(4)	N3-N2-C5-N1	1.5(5)

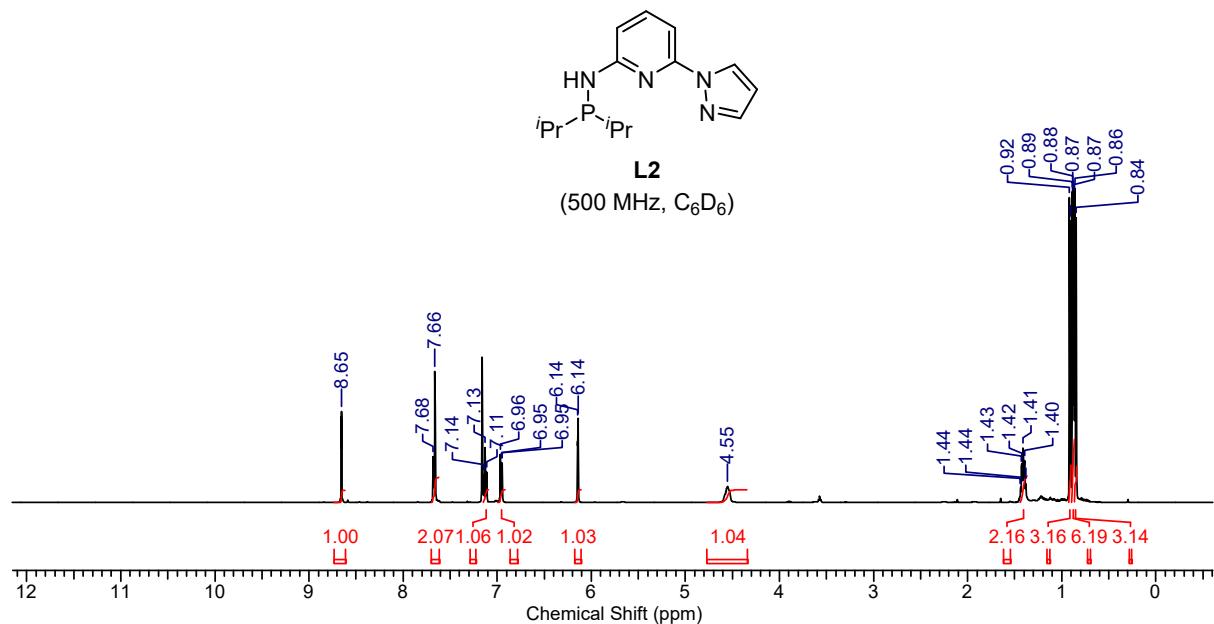
C6-N2-C5-N1	-174.0(4)	N3-N2-C5-C4	-178.0(4)
C6-N2-C5-C4	6.5(7)	N3-N2-C6-C7	0.5(5)
C5-N2-C6-C7	176.2(4)	N2-C6-C7-C8	-0.7(6)
N2-N3-C8-C7	-0.3(5)	Mn1-N3-C8-C7	-178.4(4)
C6-C7-C8-N3	0.7(6)	N4-P1-C11-C12	-37.8(3)
C14-P1-C11-C12	-142.9(3)	Mn1-P1-C11-C12	73.5(3)
N4-P1-C11-C13	-162.5(3)	C14-P1-C11-C13	92.4(3)
Mn1-P1-C11-C13	-51.2(3)	N4-P1-C14-C16	178.5(3)
C11-P1-C14-C16	-74.2(3)	Mn1-P1-C14-C16	69.4(3)
N4-P1-C14-C15	-55.5(3)	C11-P1-C14-C15	51.9(3)
Mn1-P1-C14-C15	-164.6(2)		

10. References

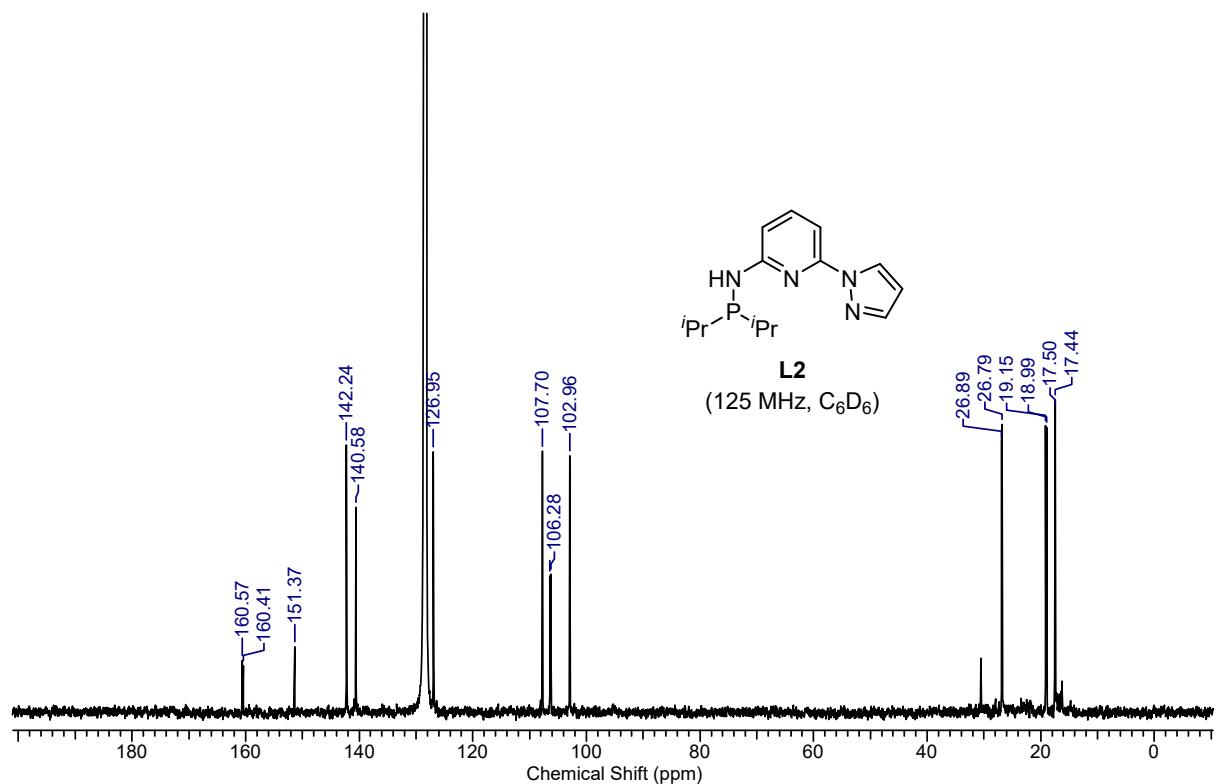
1. D. Gong, W. Liu, T. Chen, Z.-R. Chen and K.-W. Huang, *J. Mol. Catal. A Chem.*, 2014, **395**, 100-107.
2. H. Chen, W. Pan, K.-W. Huang, X. Zhang and D. Gong, *Polym. Chem.*, 2017, **8**, 1805-1814.
3. D. Gong, X. Zhang and K.-W. Huang, *Dalton Trans.*, 2016, **45**, 19399-19407.
4. S. Genç, S. Günnaz, B. Çetinkaya, S. I. Gülcemal and D. Gülcemal, *J. Org. Chem.*, 2018, **83**, 2875-2881.
5. X.-N. Cao, X.-M. Wan, F.-L. Yang, K. Li, X.-Q. Hao, T. Shao, X. Zhu and M.-P. Song, *J. Org. Chem.*, 2018, **83**, 3657-3668.
6. M. Nallagangula, C. Sujatha, V. T. Bhat and K. Namitharan, *Chem. Commun.*, 2019, **55**, 8490-8493.
7. X.-B. Lan, Z. Ye, J. Liu, M. Huang, Y. Shao, X. Cai, Y. Liu and Z. Ke, *ChemSusChem*, 2020, **13**, 2557-2563.
8. S. Genç, S. Gülcemal, S. Günnaz, B. Çetinkaya and D. Gülcemal, *Org. Lett.*, 2021, **23**, 5229-5234.
9. L. Rakers, F. Schäfers and F. Glorius, *Chem. Eur. J.*, 2018, **24**, 15529-15532.
10. X.-B. Lan, Z. Ye, M. Huang, J. Liu, Y. Liu and Z. Ke, *Org. Lett.*, 2019, **21**, 8065-8070.
11. C. Teja and F. R. Nawaz Khan, *ACS Omega*, 2019, **4**, 8046-8055.
12. D. Bhattacharyya, B. K. Sarmah, S. Nandi, H. K. Srivastava and A. Das, *Org. Lett.*, 2021, **23**, 869-875.
13. Z.-C. Ding, C.-Y. Li, J.-J. Chen, J.-H. Zeng, H.-T. Tang, Y.-J. Ding and Z.-P. Zhan, *Adv. Synth. Catal.*, 2017, **359**, 2280-2287.
14. A. Verma, S. Hazra, P. Dolui and A. J. Elias, *Asian J. Org. Chem.*, 2021, **10**, 626-633.
15. N. Luo, Y. Zhong, H. Wen, H. Shui and R. Luo, *Eur. J. Org. Chem.*, 2021, **2021**, 1355-1364.
16. Q. Jiang, T. Guo, Q. Wang, P. Wu and Z. Yu, *Adv. Synth. Catal.*, 2013, **355**, 1874-1880.
17. S. Jung, H. Lee, Y. Moon, H.-Y. Jung and S. Hong, *ACS Catal.*, 2019, **9**, 9891-9896.
18. S. Guven, G. Kundu, A. Weßels, J. S. Ward, K. Rissanen and F. Schoenebeck, *J. Am. Chem. Soc.*, 2021, **143**, 8375-8380.
19. Y.-H. Fu and D. E. Bergbreiter, *ChemCatChem*, 2020, **12**, 6050-6058.
20. A. Alanthadka, S. Bera and D. Banerjee, *J. Org. Chem.*, 2019, **84**, 11676-11686.

21. J. Zhou, M. Jia, M. Song, Z. Huang, A. Steiner, Q. An, J. Ma, Z. Guo, Q. Zhang, H. Sun, C. Robertson, J. Bacsa, J. Xiao and C. Li, *Angew. Chem. Int. Ed.*, 2022, **61**, DOI: 10.1002/anie.202205983.
22. Y.-N. Duan, X. Du, Z. Cui, Y. Zeng, Y. Liu, T. Yang, J. Wen and X. Zhang, *J. Am. Chem. Soc.*, 2019, **141**, 20424-20433.
23. G. Chang, P. Zhang, W. Yang, S. Xie, H. Sun, X. Li, O. Fuhr and D. Fenske, *Dalton Trans.*, 2020, **49**, 9349-9354.
24. S. Elangovan, C. Topf, S. Fischer, H. Jiao, A. Spannenberg, W. Baumann, R. Ludwig, K. Junge and M. Beller, *J. Am. Chem. Soc.*, 2016, **138**, 8809-8814.
25. B. M. Zimmermann, T. T. Ngoc, D.-I. Tzaras, T. Kaicharla and J. F. Teichert, *J. Am. Chem. Soc.*, 2021, **143**, 16865-16873.
26. V. Zubarić, N. Lichtenberger, M. Schelwies, T. Oeser, A. S. K. Hashmi and T. Schaub, *ChemCatChem*, 2022, **14**, e202101443.
27. R. Bhawar, K. S. Patil and S. K. Bose, *New. J. Chem.*, 2021, **45**, 15028-15034.
28. Y. Liu, S. He, Z. Quan, H. Cai, Y. Zhao and B. Wang, *Green Chem.*, 2019, **21**, 830-838.
29. TURBOMOLE 7.5, V., A Development of University of Karlsruhe and Forschungszentrum Karlsruhe GmbH, 1989-2007, TURBOMOLE GmbH, since 2007. 2020.
30. J. P. Perdew, K. Burke and M. Ernzerhof, *Phy. Rev. Lett.*, 1996, **77**, 3865-3868.
31. S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.*, 2010, **132**, 154104-154101 154104-154119.
32. K. Eichkorn, F. Weigend, O. Treutler and R. Ahlrichs, *Theor. Chem. Acta.*, 1997, **97**, 119-124.
33. K. Eichkorn, O. Treutler, H. Öhm, M. Häser and R. Ahlrichs, *Chem. Phys. Lett.*, 1995, **240**, 283-290.
34. M. Sierka, A. Hogekamp and R. Ahlrichs, *J. Chem. Phys.*, 2003, **118**, 9136-9148.
35. A. Klamt and G. Schüürmann, *J. Chem. Soc. Perkin Trans.*, 1993, 799-805.
36. S. Kozuch and S. Shaik, *J. Am. Chem. Soc.*, 2006, **128**, 3355-3365.
37. S. Kozuch and S. Shaik, *J. Phys. Chem. A*, 2008, **112**, 6032-6041.
38. A. Uhe, S. Kozuch and S. Shaik, *J. Comput. Chem.*, 2011, **32**, 978-985.
39. Bruker, APEX3, SAINT and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA., 2016.
40. G. M. Sheldrick, *Acta Crystallogr.*, 2008, **A64**, 112-122.
41. G. M. Sheldrick, *Acta Crystallogr.*, 2015, **C71**, 3-8.
42. L. J. Farrugia, *J. Appl. Crystallogr.*, 2012, **45**, 849-854.

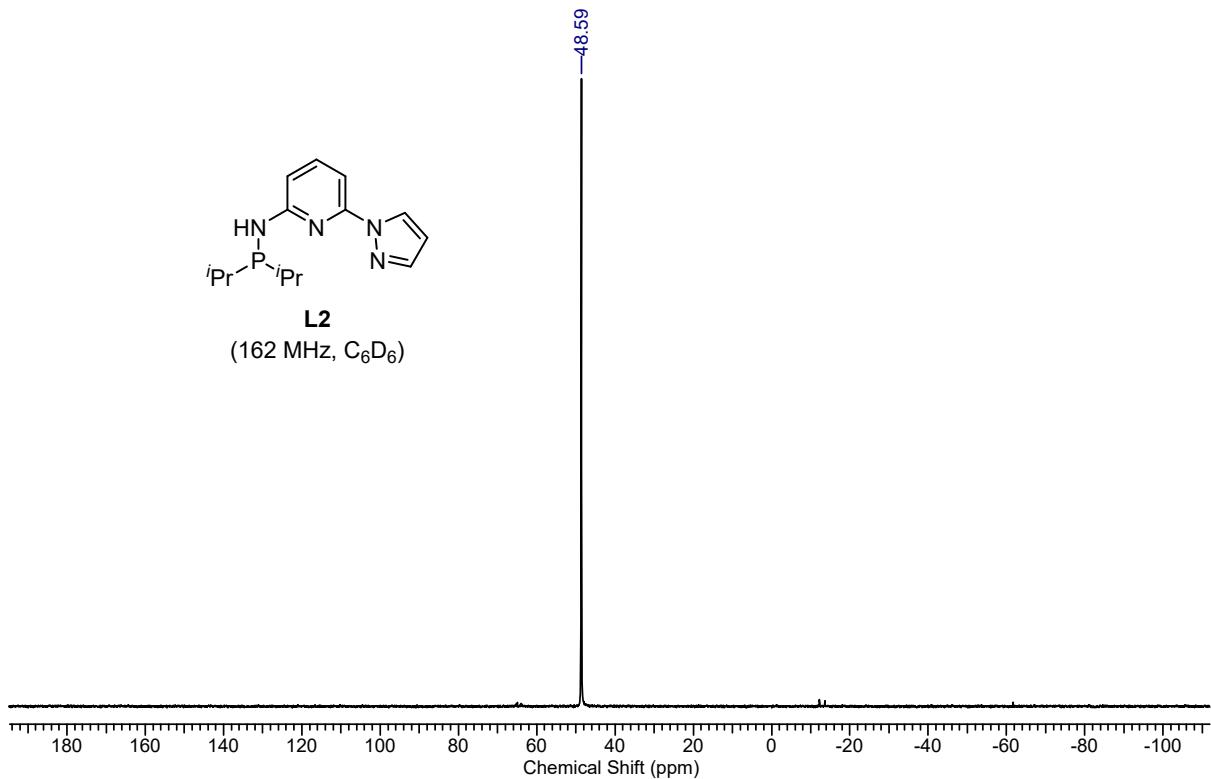
11. ^1H , $^{13}\text{C}\{^1\text{H}\}$, $^{31}\text{P}\{^1\text{H}\}$ -NMR , Mass and IR Spectra of Manganese Complexes



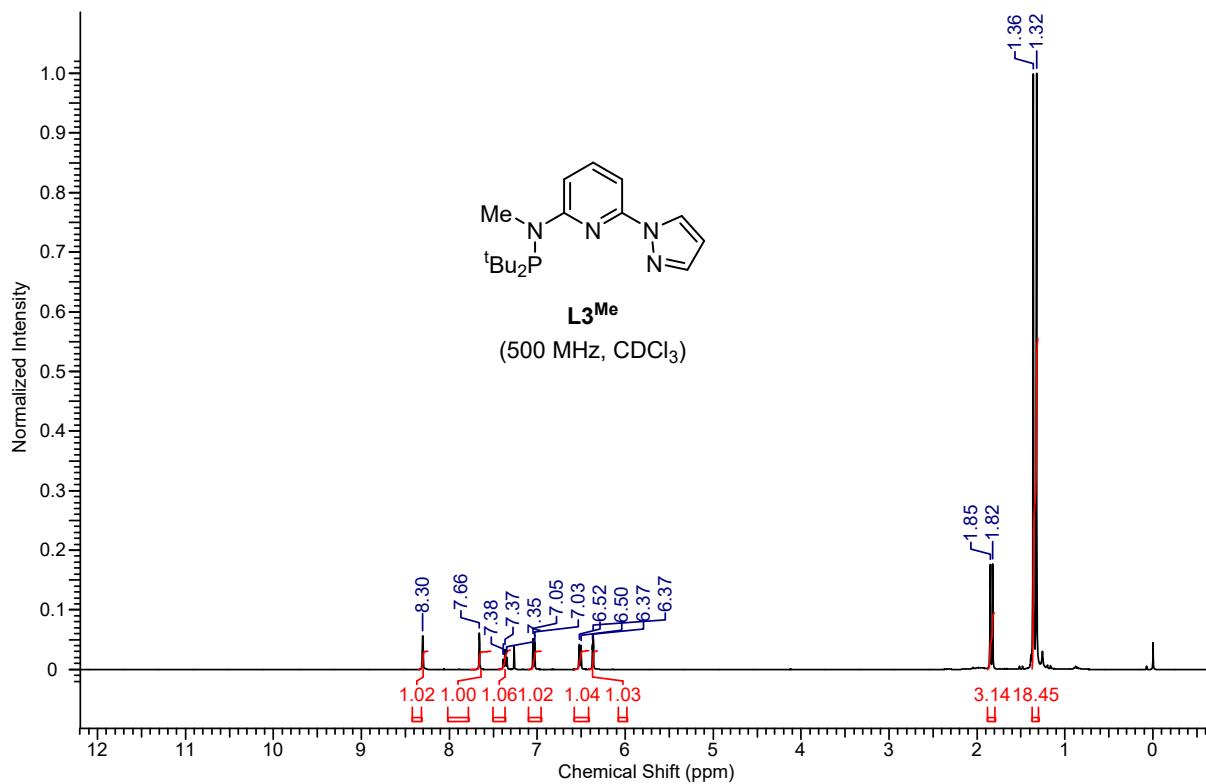
^1H -NMR spectrum of *N*-(diisopropylphosphanoyl)-6-(1*H*-pyrazol-1-yl)pyridin-2-amine (**L2**)



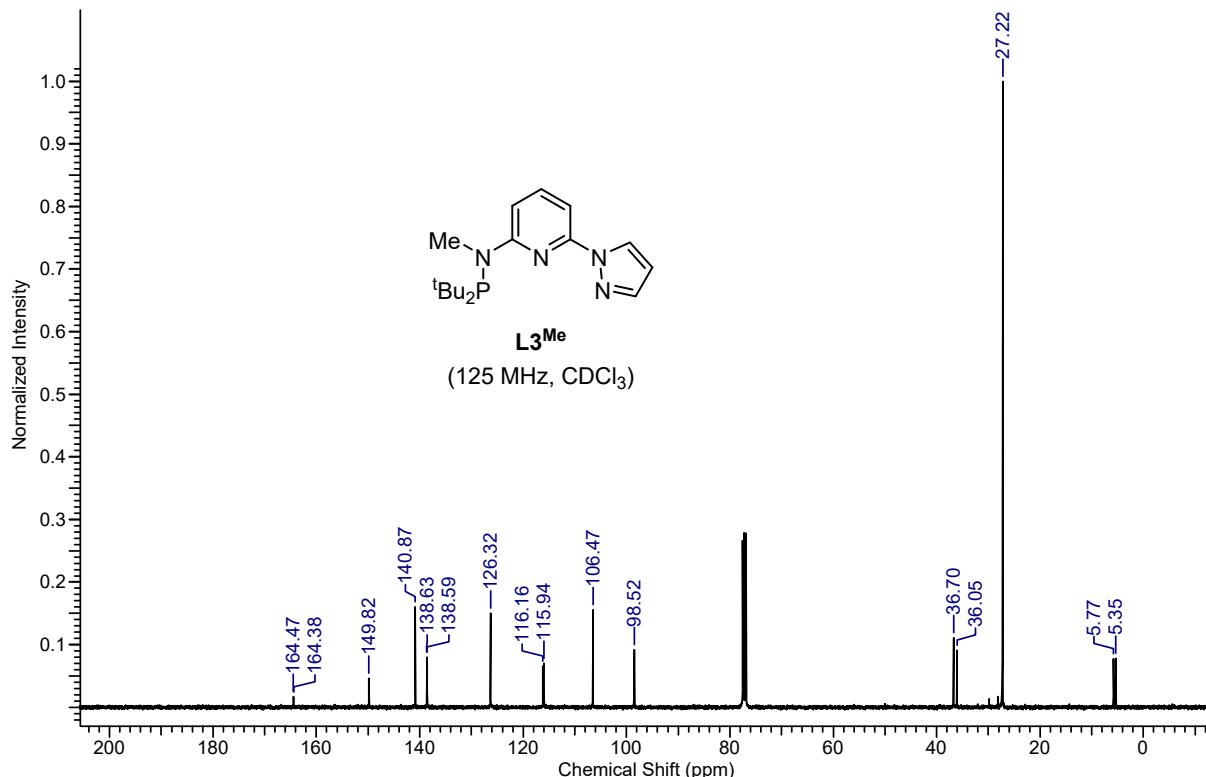
$^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum of *N*-(diisopropylphosphanoyl)-6-(1*H*-pyrazol-1-yl)pyridin-2-amine (**L2**)



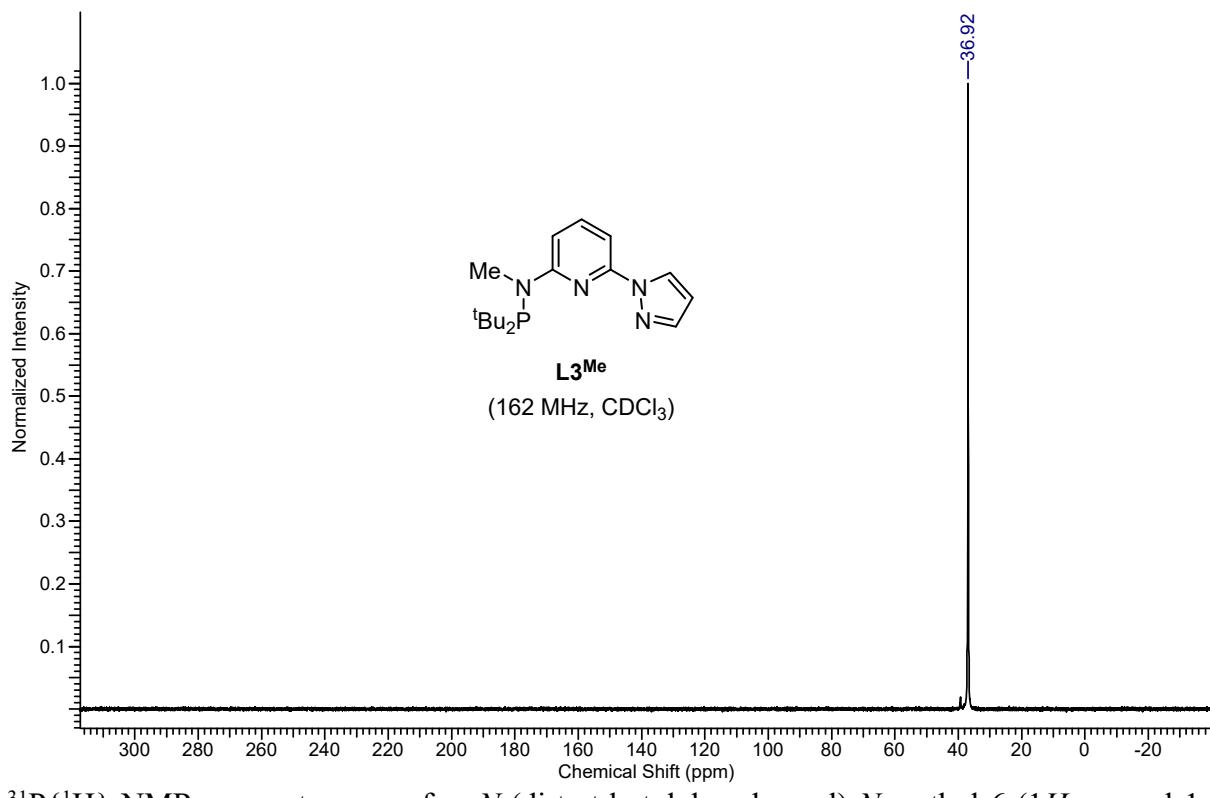
$^{31}\text{P}\{\text{H}\}$ -NMR spectrum of *N*-(diisopropylphosphanoyl)-6-(1*H*-pyrazol-1-yl)pyridin-2-amine (**L2**)



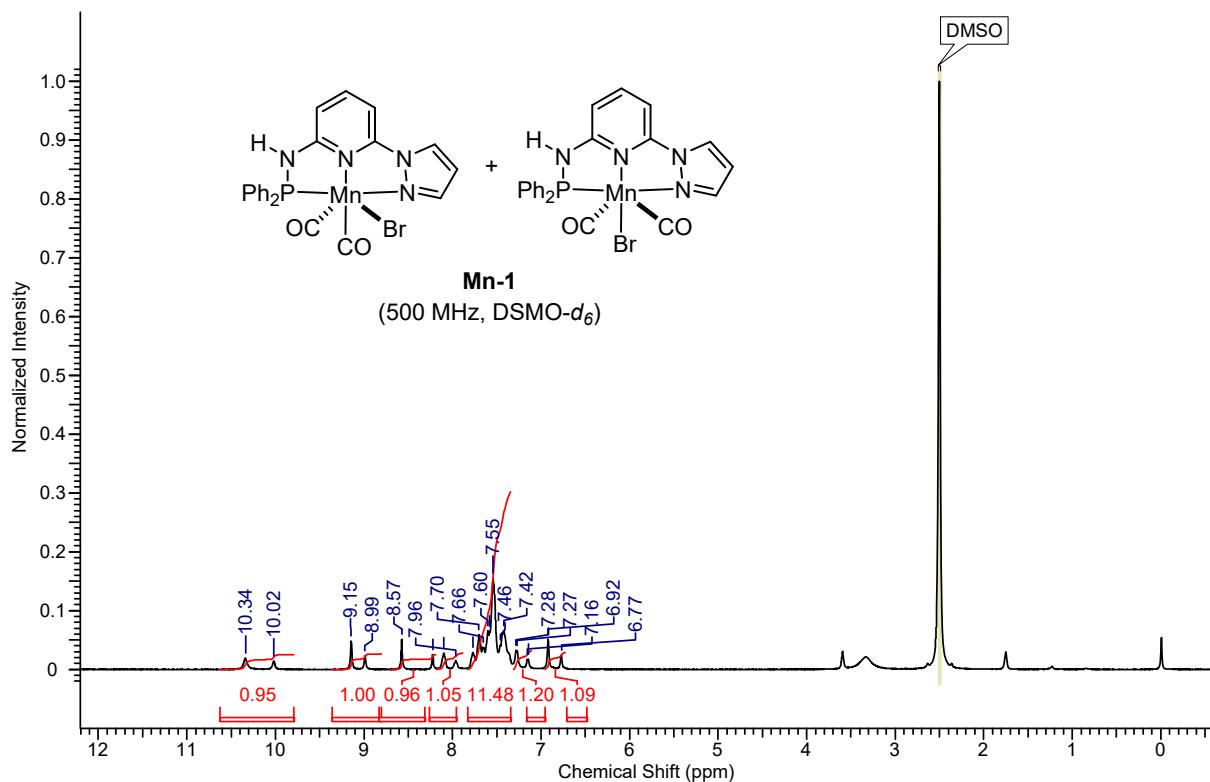
¹H-NMR spectrum of *N*-(di-tert-butylphosphanoyl)-*N*-methyl-6-(1*H*-pyrazol-1-yl)pyridin-2-amine (**L3^{Me}**)



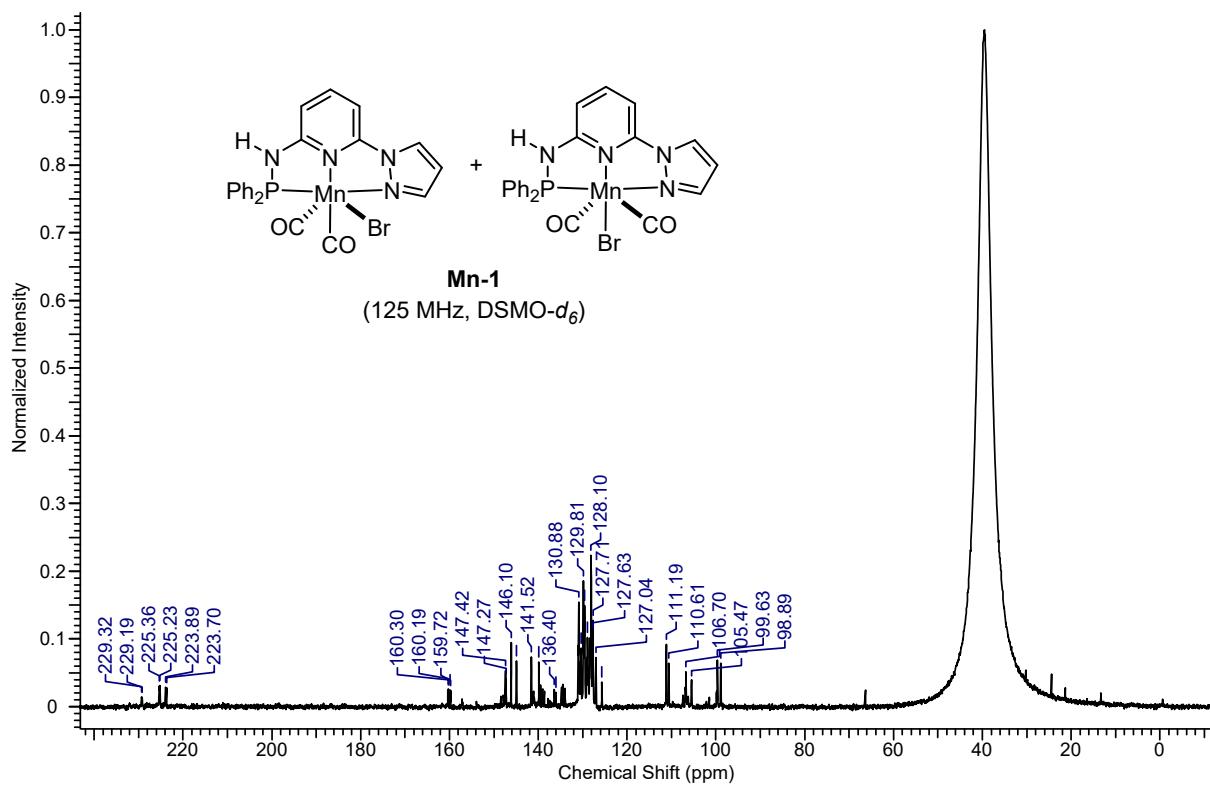
¹³C{¹H}-NMR spectrum of *N*-(di-tert-butylphosphanoyl)-*N*-methyl-6-(1*H*-pyrazol-1-yl)pyridin-2-amine (**L3^{Me}**)



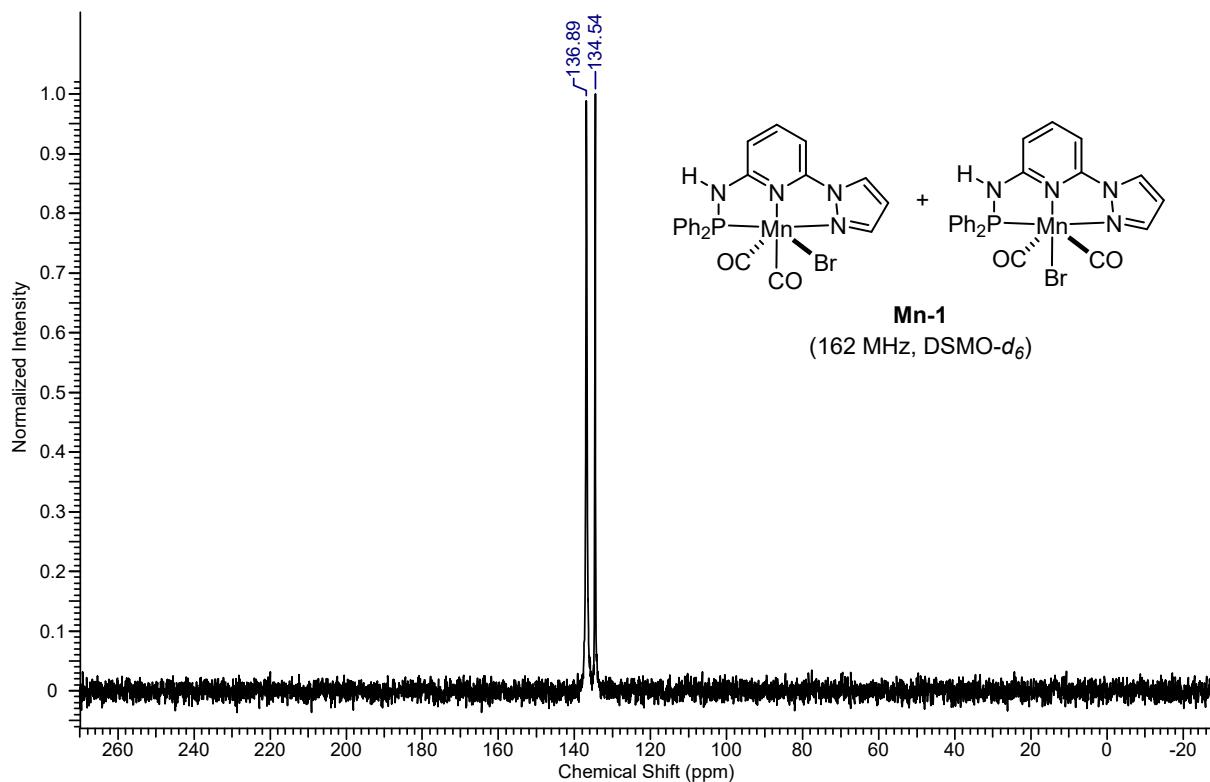
³¹P{¹H}-NMR spectrum of *N*-(di-tert-butylphosphaneyl)-*N*-methyl-6-(1*H*-pyrazol-1-yl)pyridin-2-amine (**L3^{Me}**)



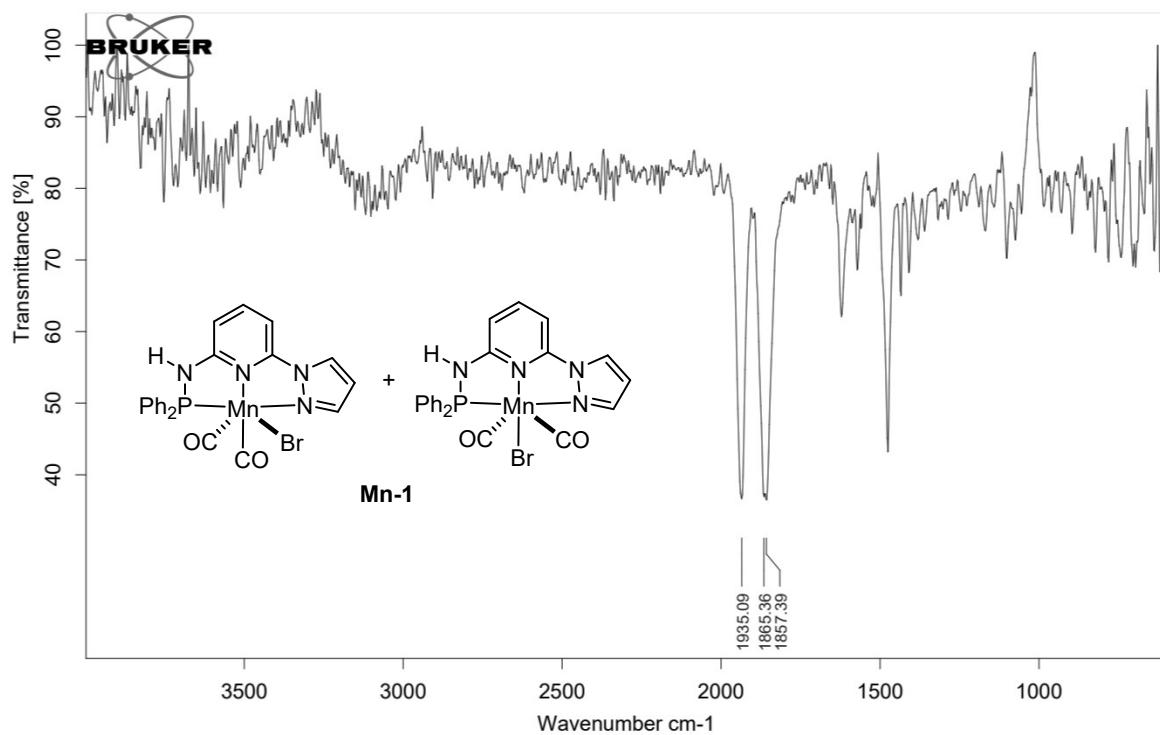
¹H-NMR spectrum of **Mn-1** complex (mixture of two isomers)



¹³C{¹H}-NMR spectrum of **Mn-1** complex (mixture of two isomers)

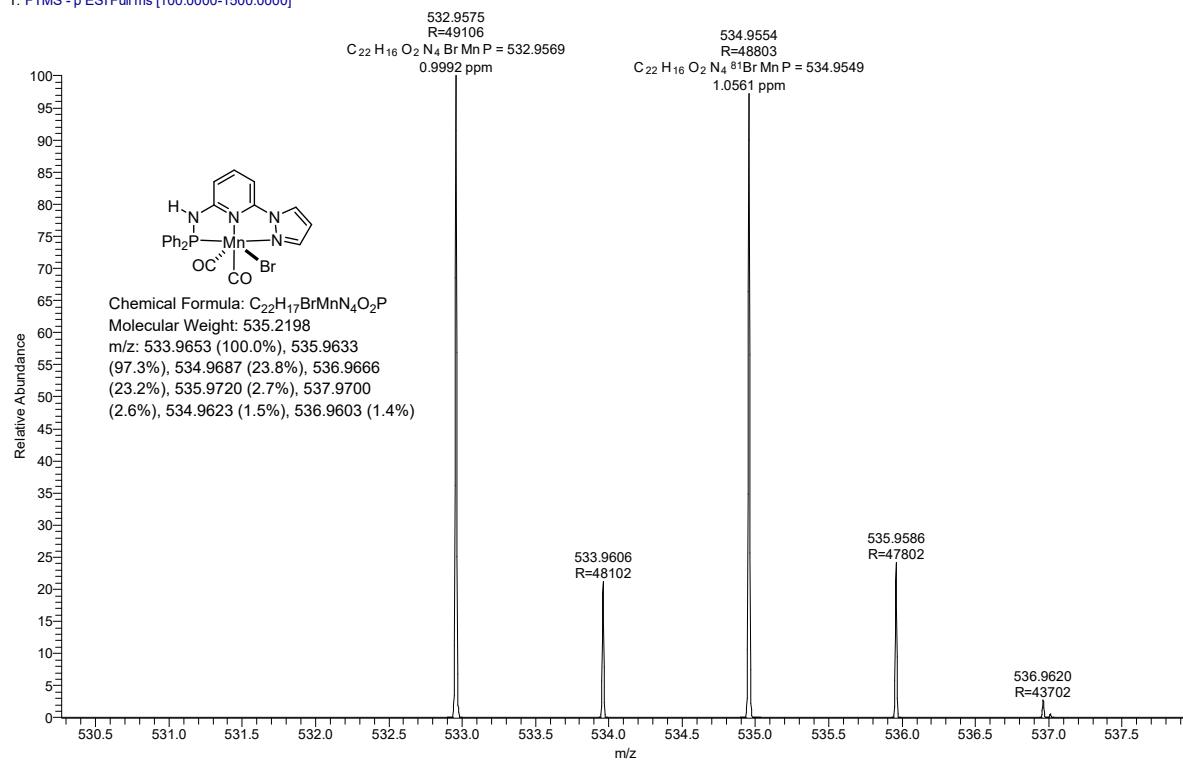


$^{31}\text{P}\{\text{H}\}$ -NMR spectrum of **Mn-1** complex (mixture of two isomers)

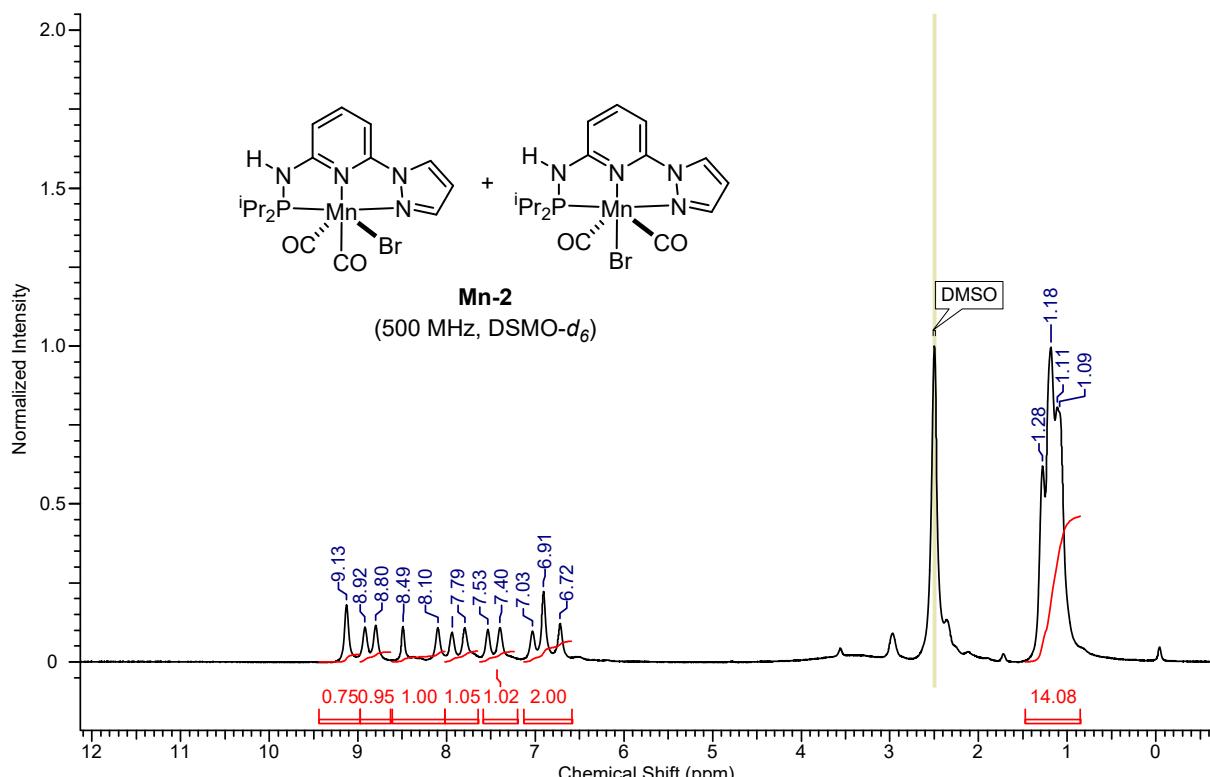


IR spectrum of **Mn-1** complex

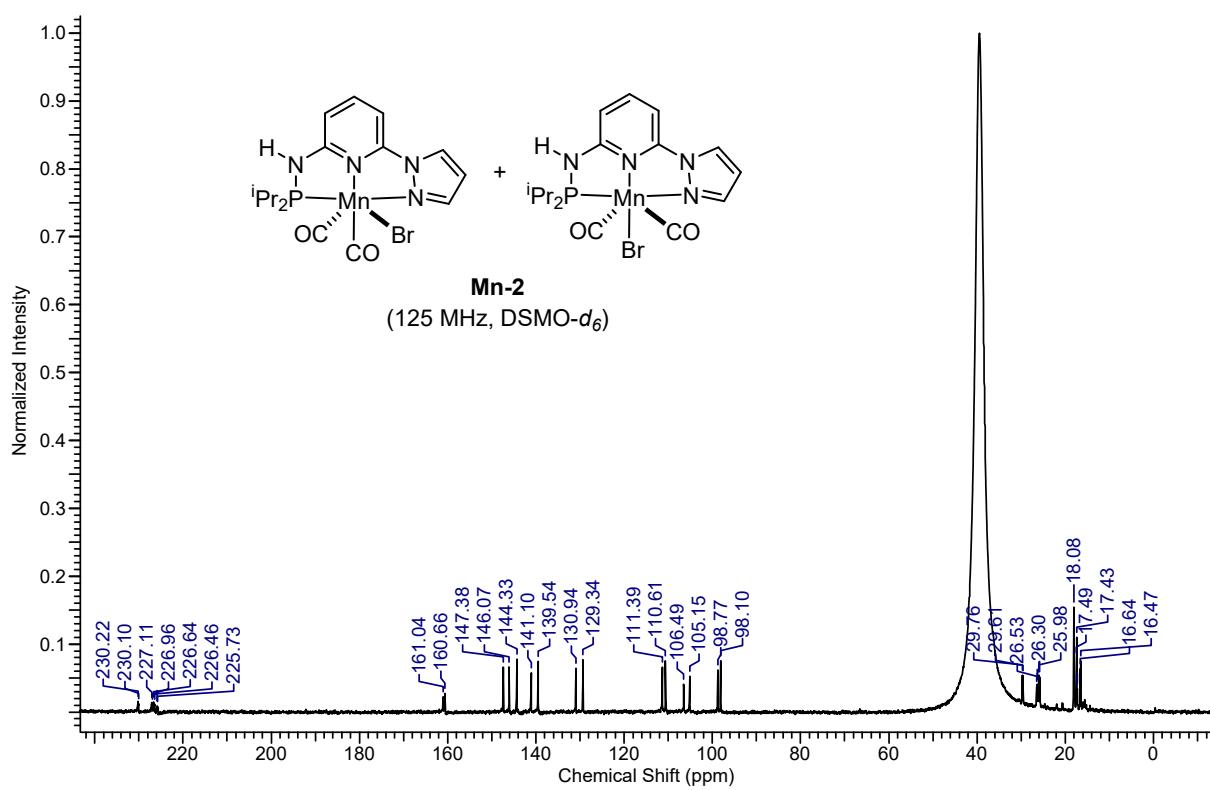
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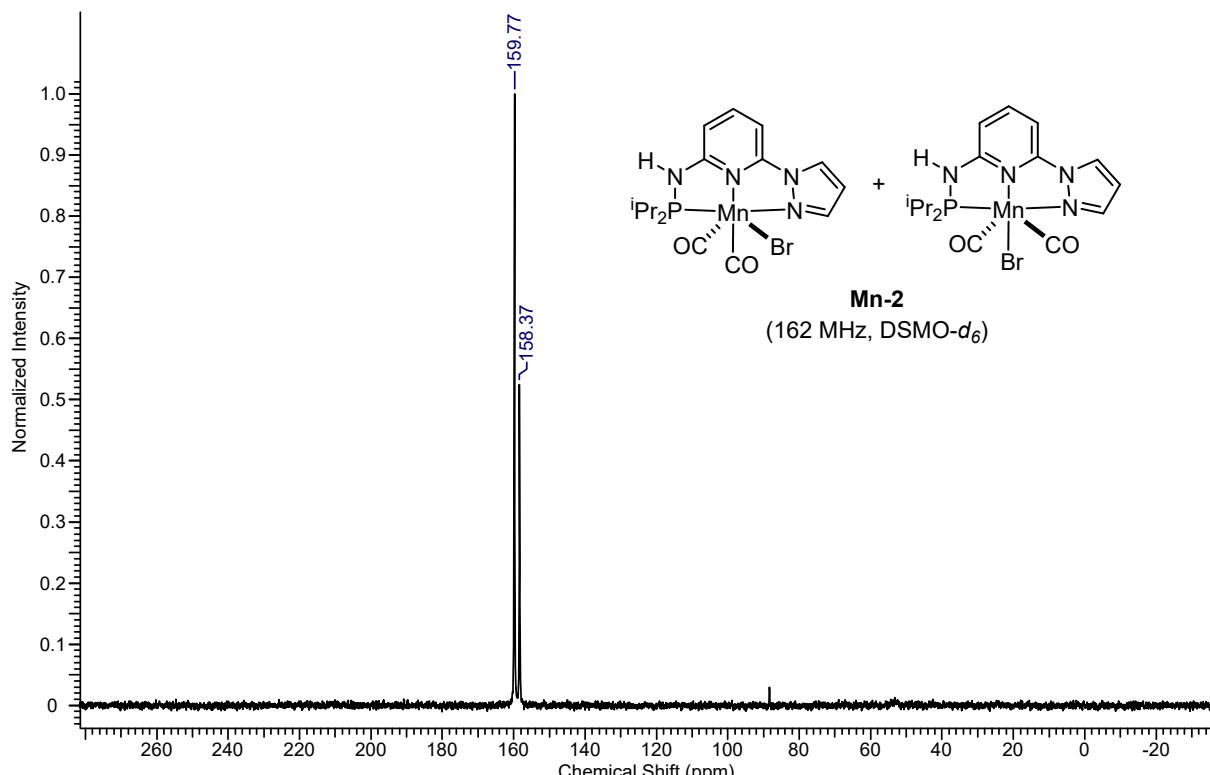
ESI-MS (-ve mode) of **Mn-1** complex



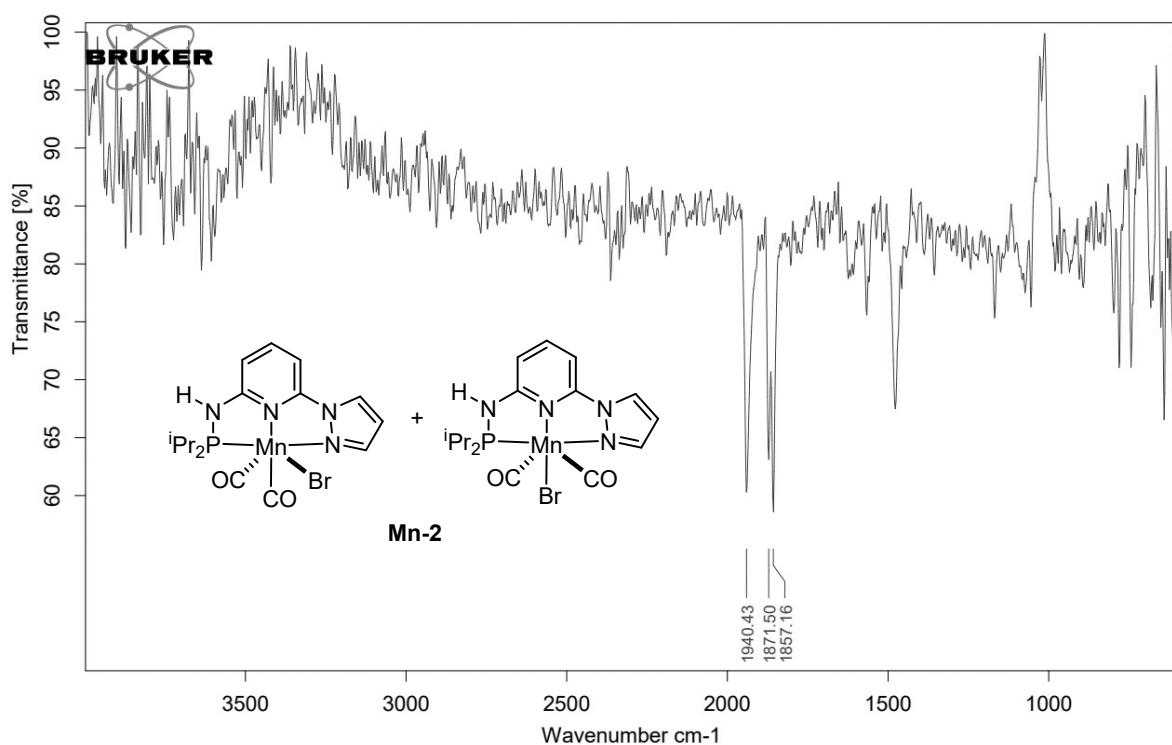
¹H-NMR spectrum of **Mn-2** complex (mixture of two isomers)



¹³C{¹H}-NMR spectrum of **Mn-2** complex (mixture of two isomers)

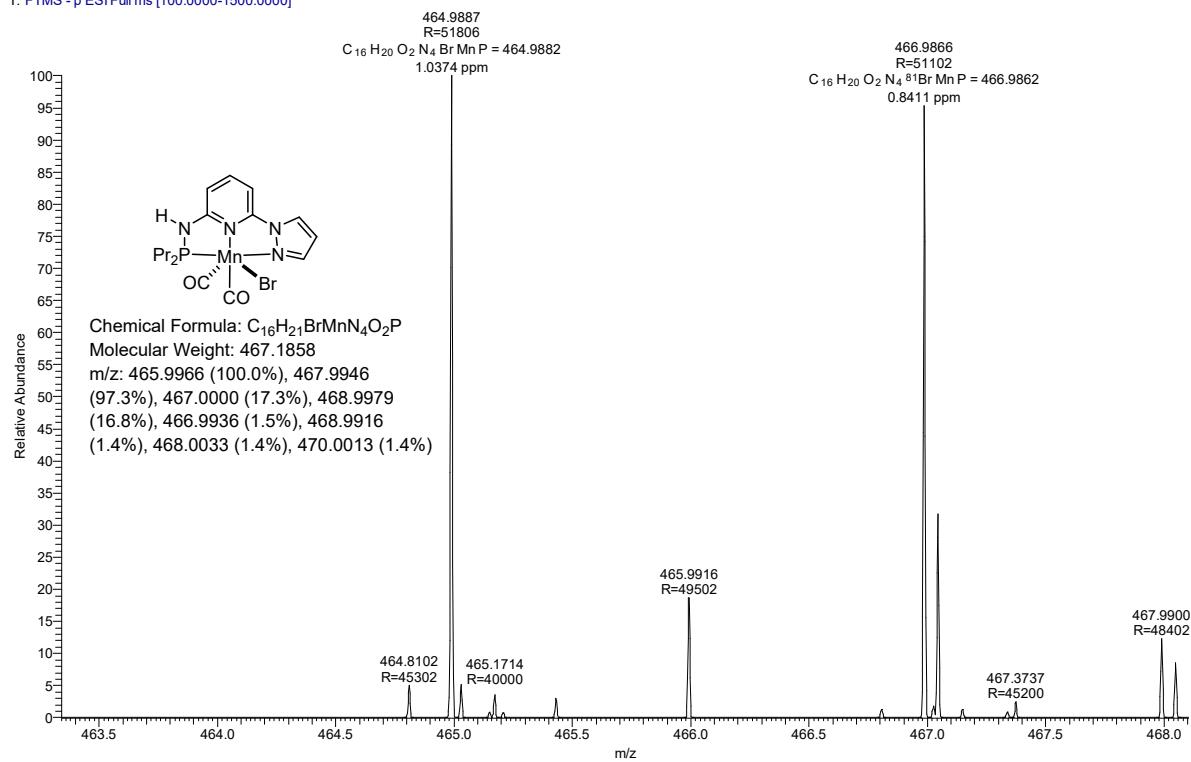


$^{31}\text{P}\{\text{H}\}$ -NMR spectrum of **Mn-2** complex (mixture of two isomers)

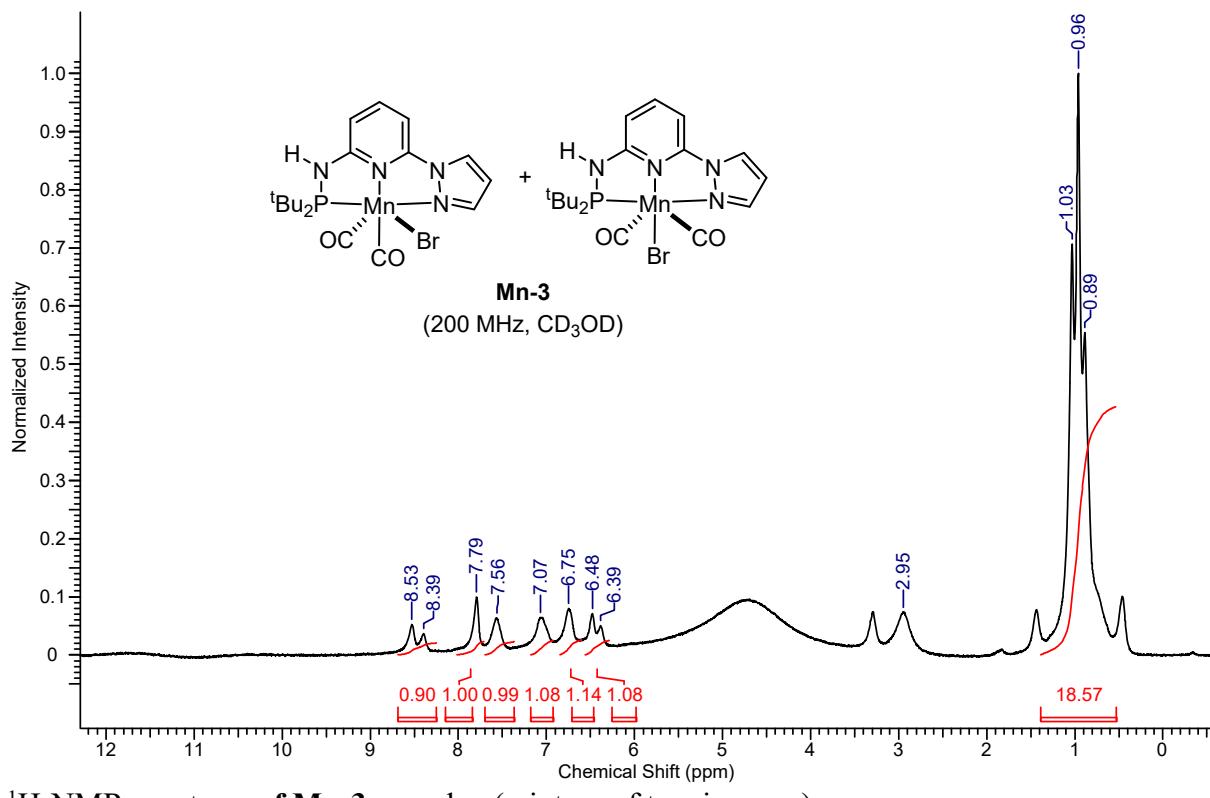


IR spectrum of **Mn-2** complex

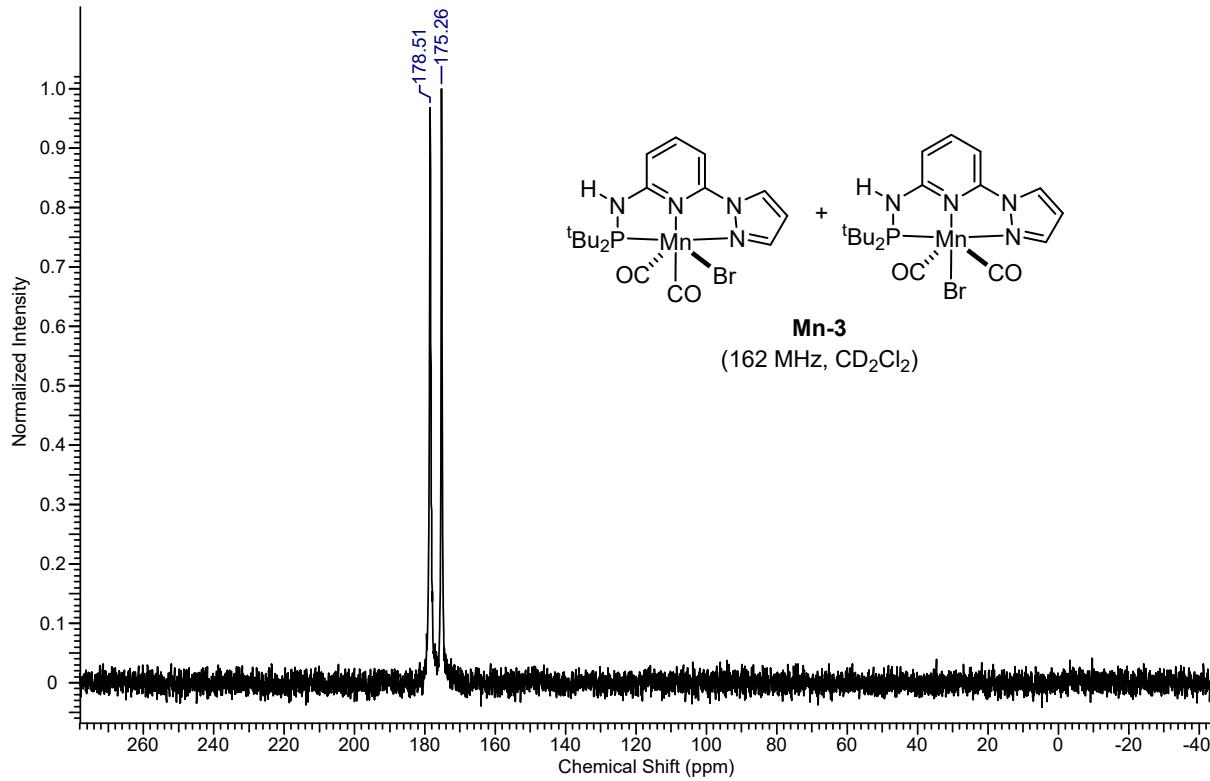
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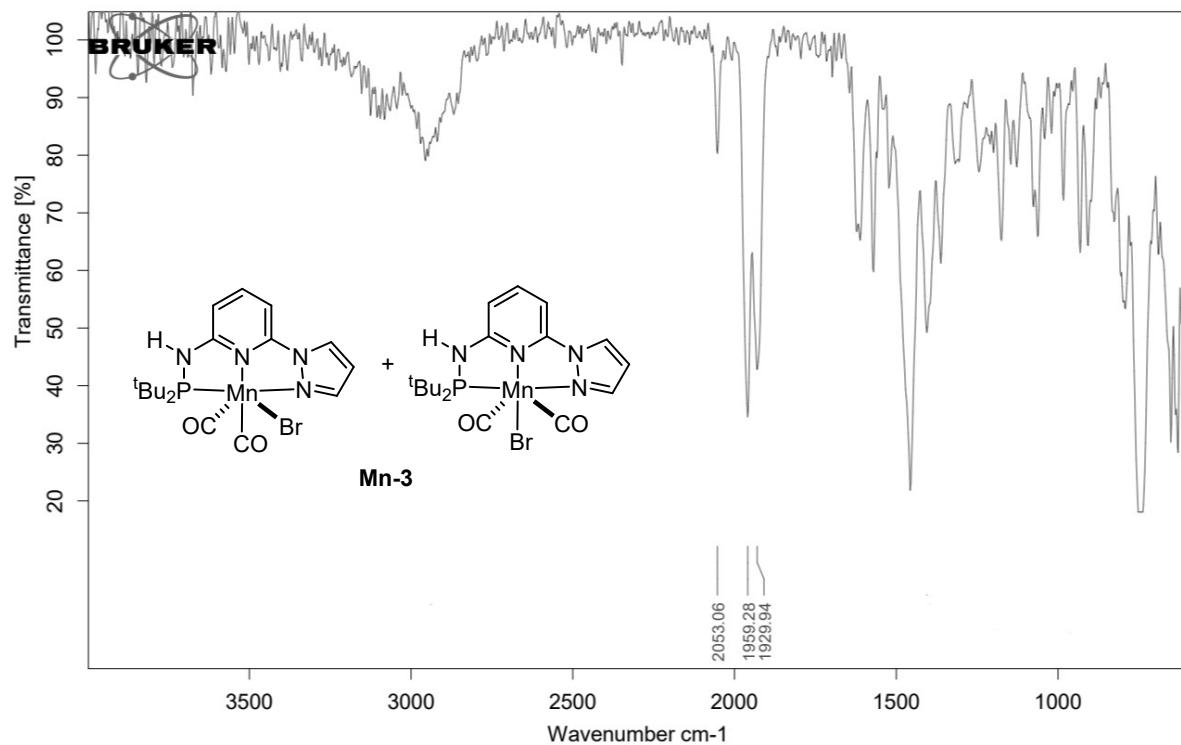
ESI-MS (-ve mode) of Mn-2 complex



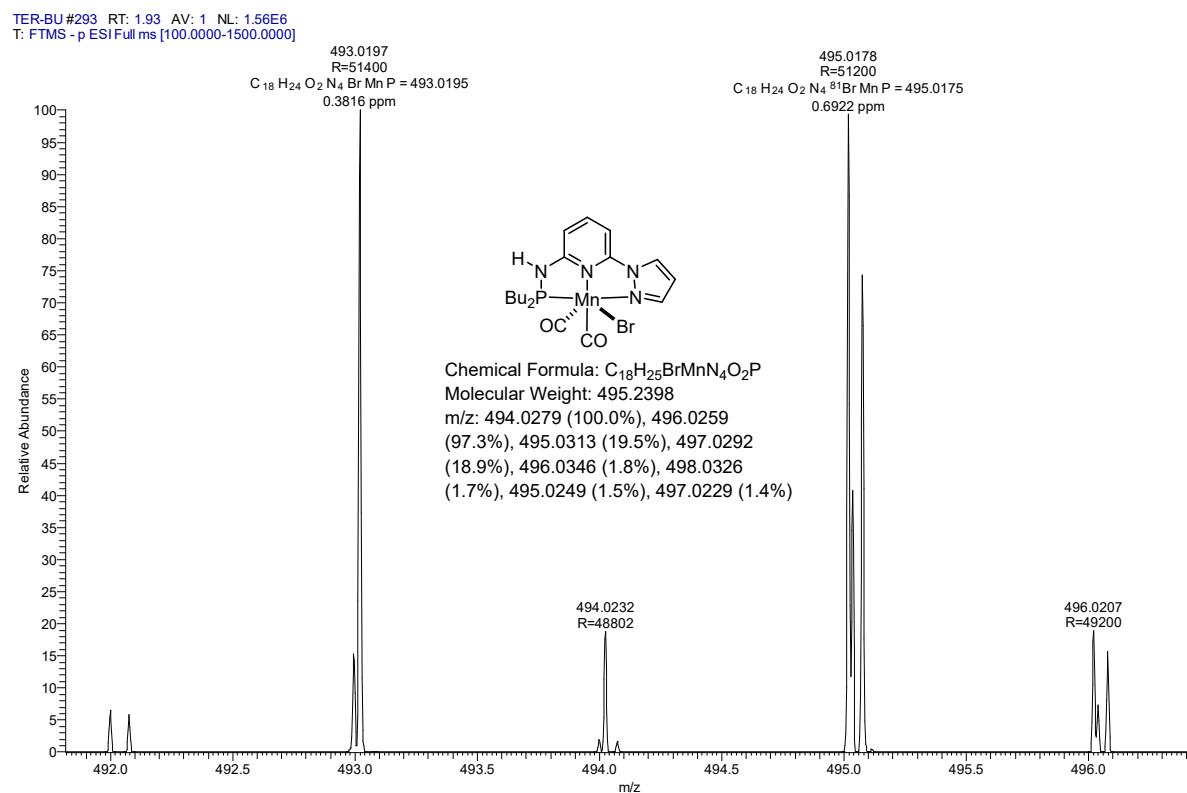
¹H-NMR spectrum of Mn-3 complex (mixture of two isomers)



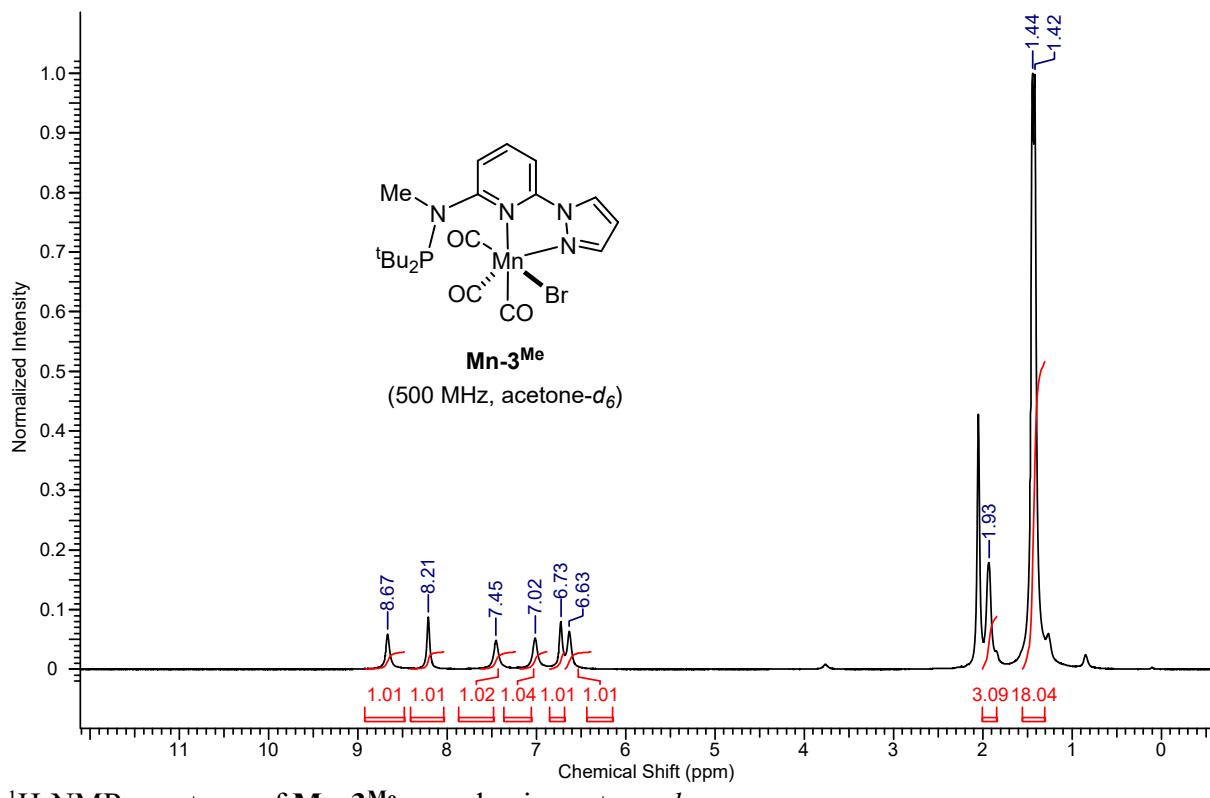
³¹P{¹H}-NMR spectrum of Mn-3 complex (mixture of two isomers)



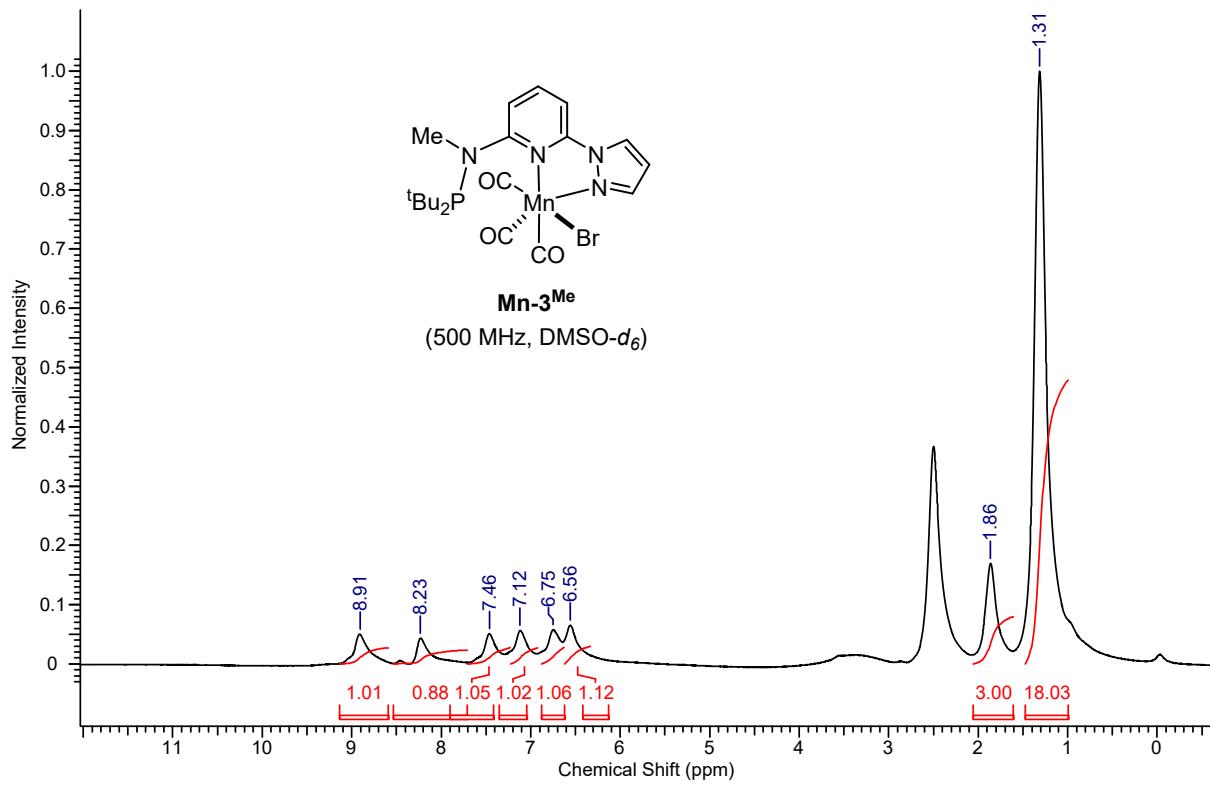
IR spectrum of **Mn-3** complex



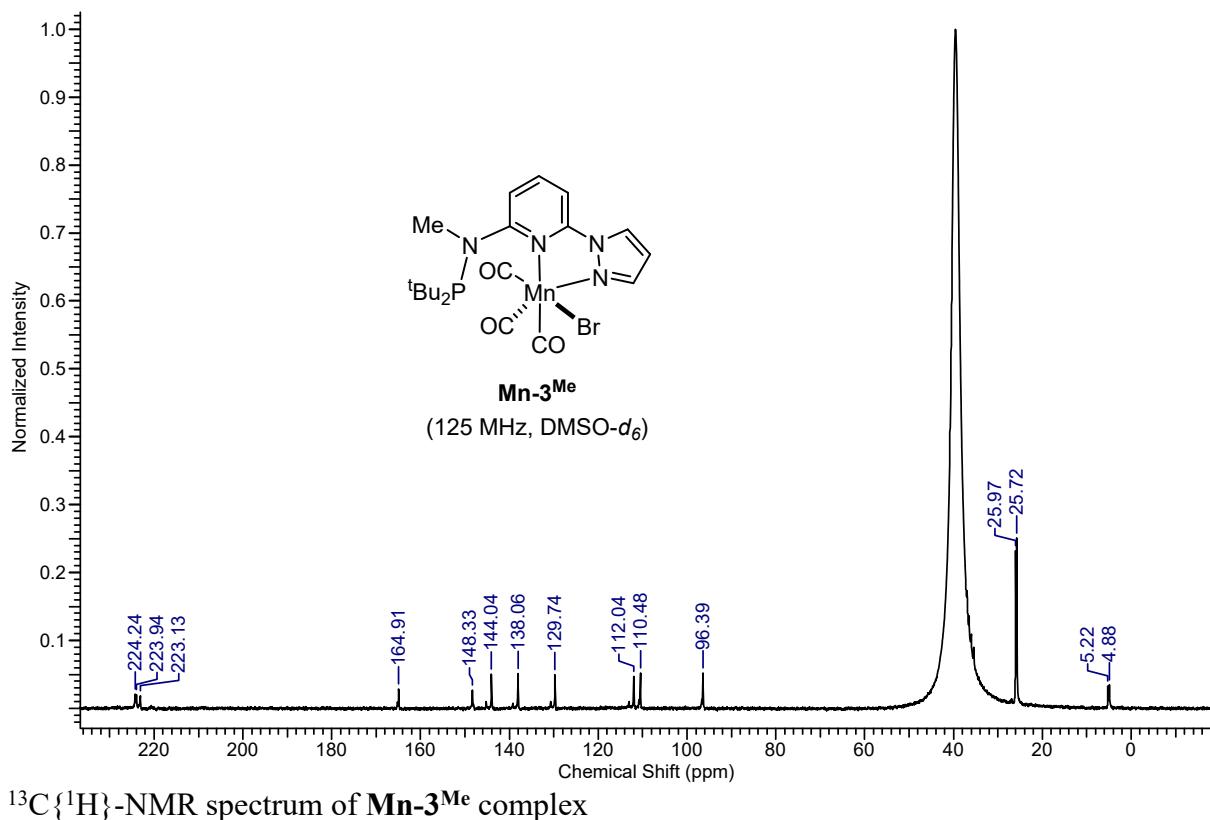
ESI-MS (-ve mode) of **Mn-3** complex



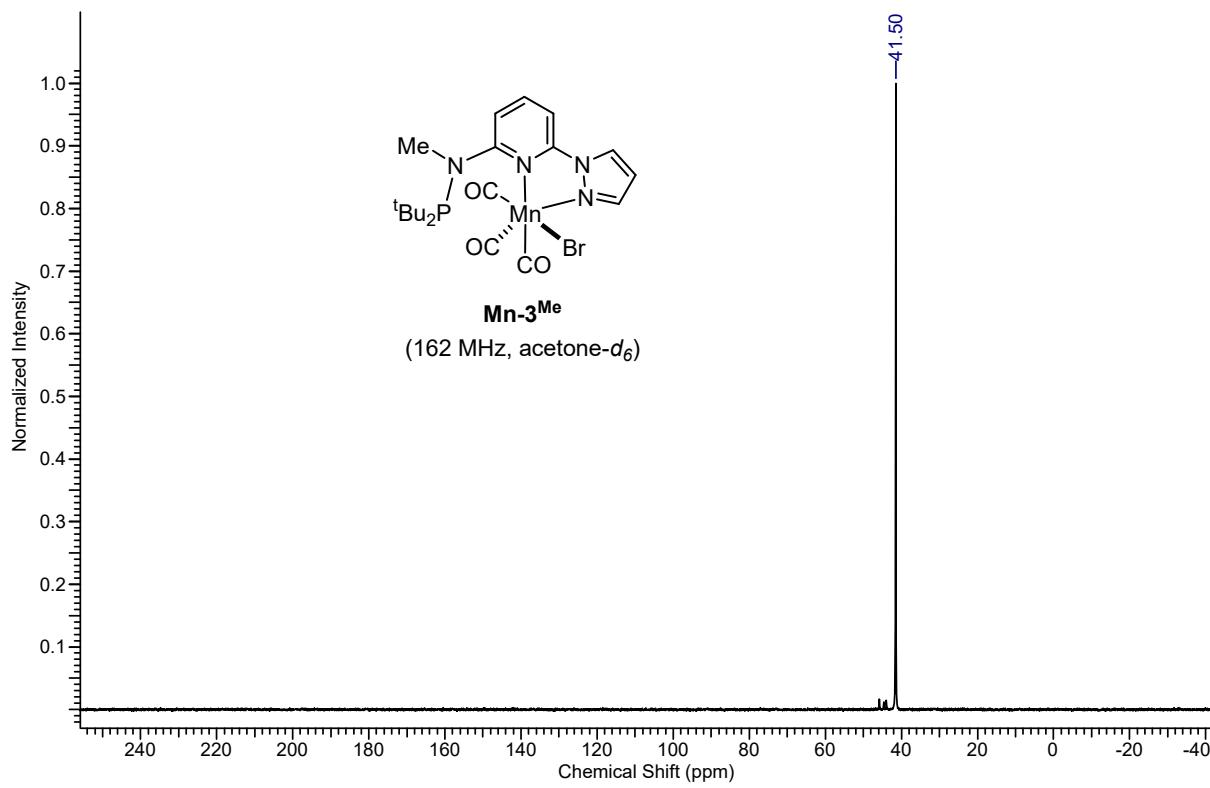
¹H-NMR spectrum of Mn-3^{Me} complex in acetone-*d*₆



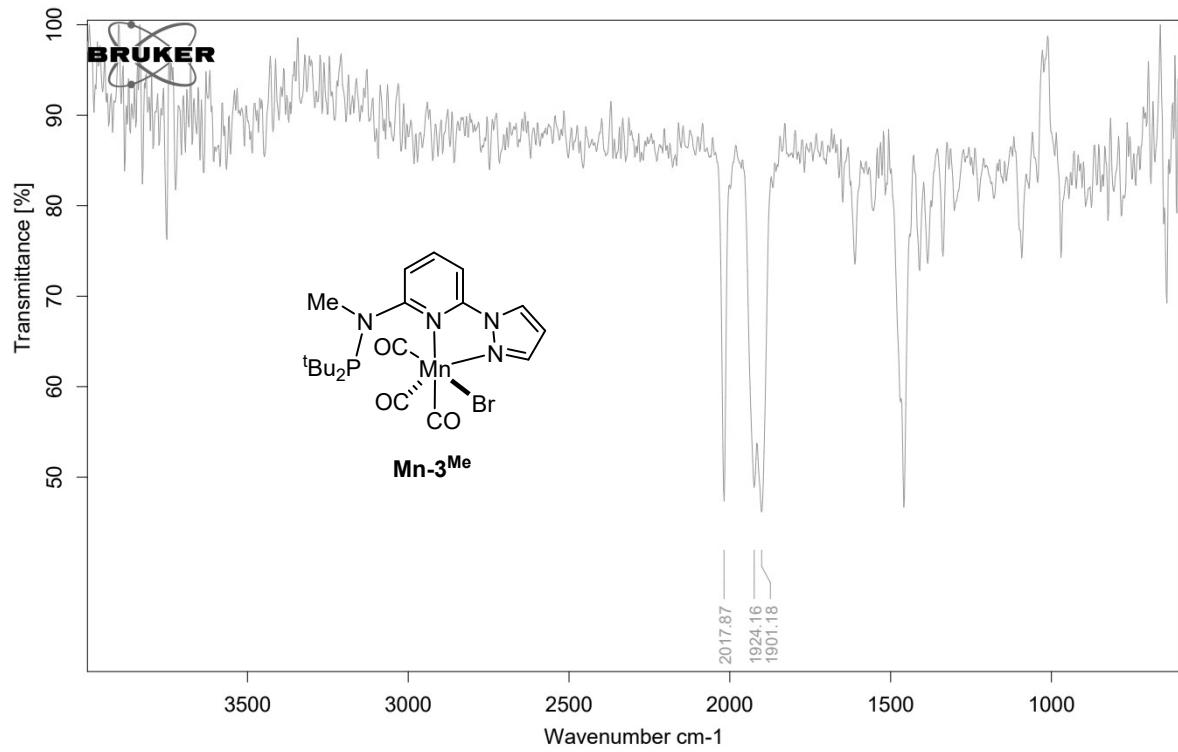
¹H-NMR spectrum of Mn-3^{Me} complex in DMSO-*d*₆



¹³C{¹H}-NMR spectrum of Mn-3^{Me} complex

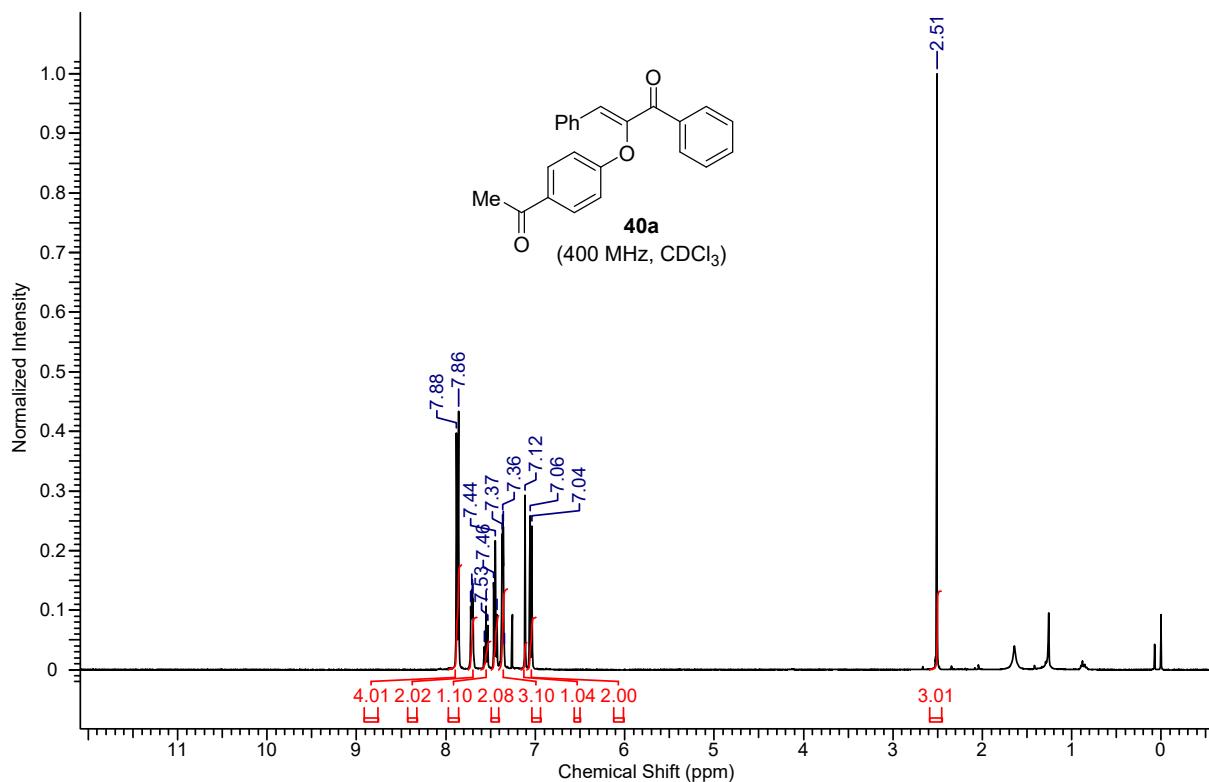


³¹P{¹H}-NMR spectrum of Mn-3^{Me} complex

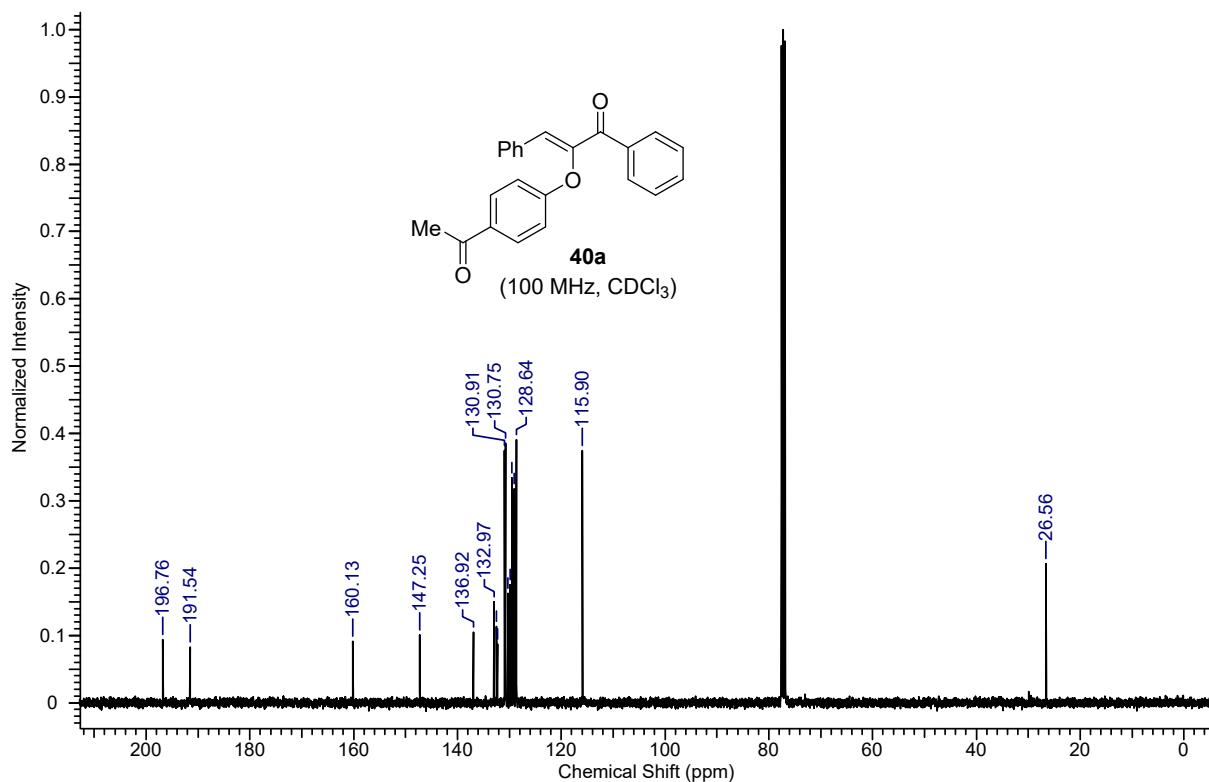


IR spectrum of **Mn-3^{Me}** complex

12. ^1H and $^{13}\text{C}\{^1\text{H}\}$ -NMR Spectra of Starting Compound

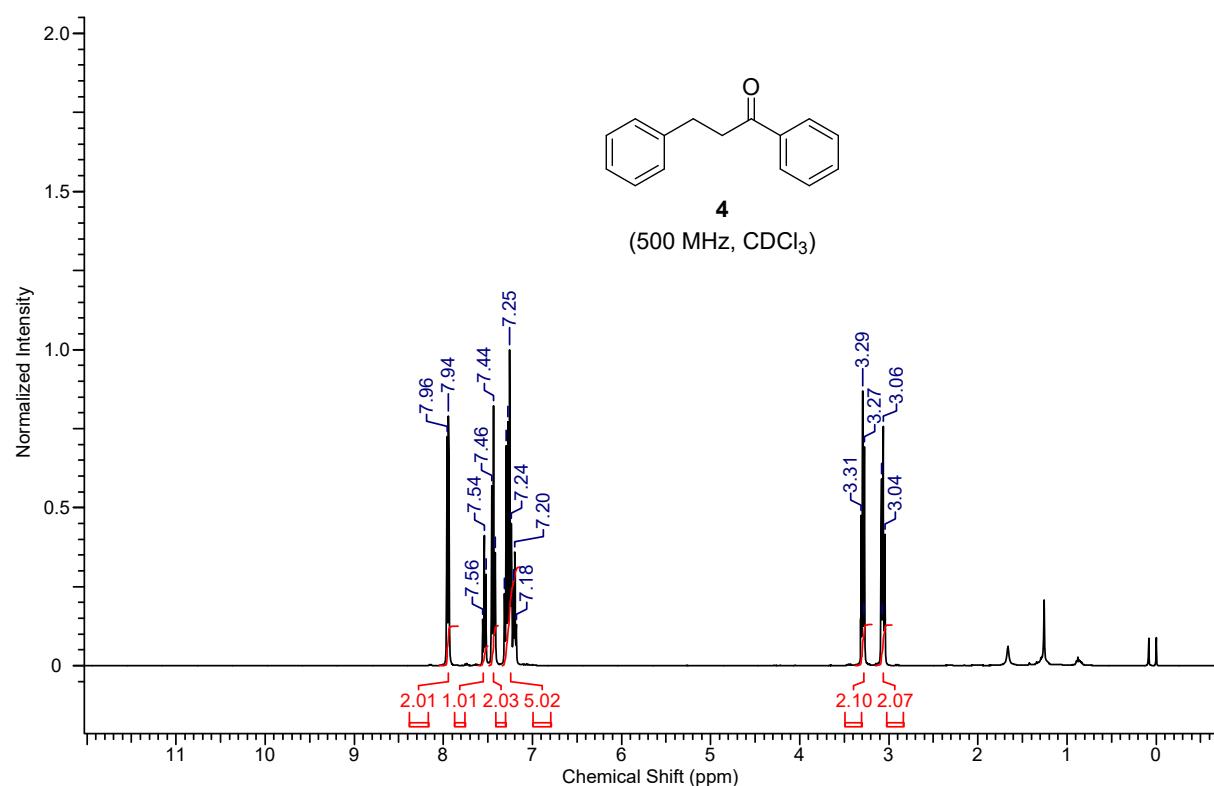


^1H -NMR spectrum of (Z) -2-(4-acetylphenoxy)-1,3-diphenylprop-2-en-1-one (**40a**)

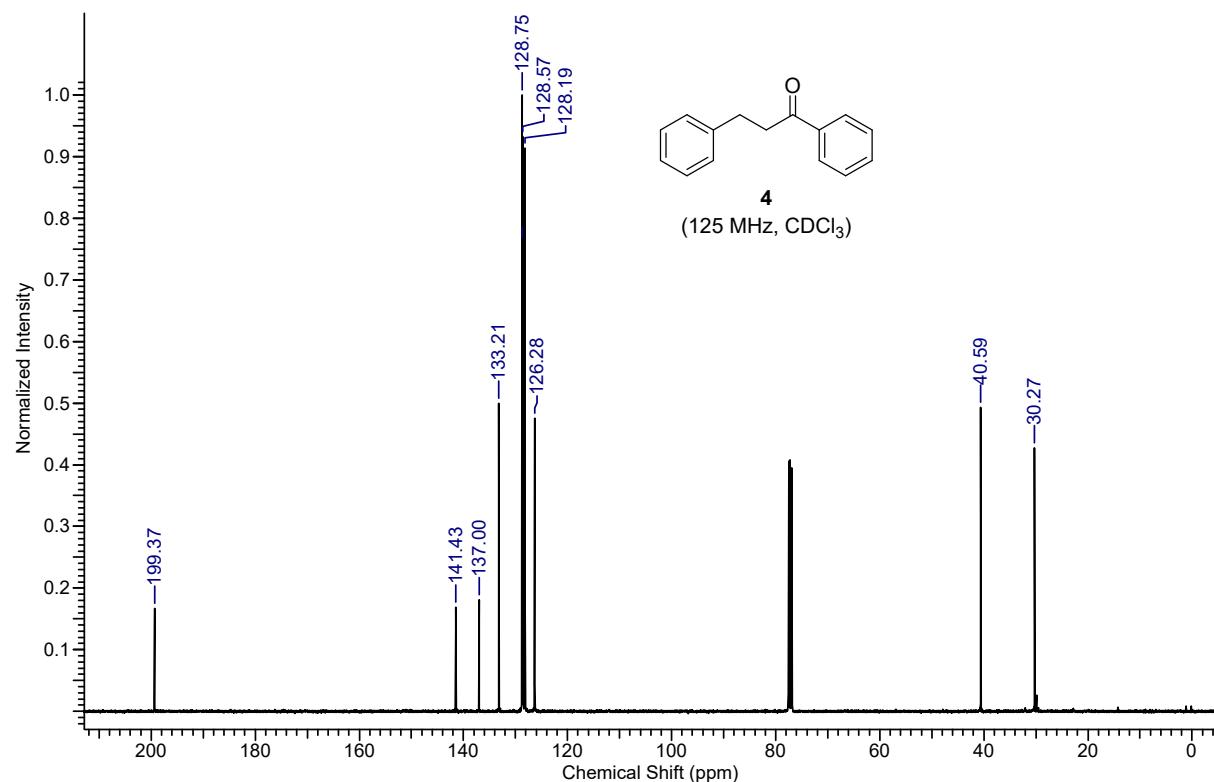


$^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum of (Z) -2-(4-acetylphenoxy)-1,3-diphenylprop-2-en-1-one (**40a**)

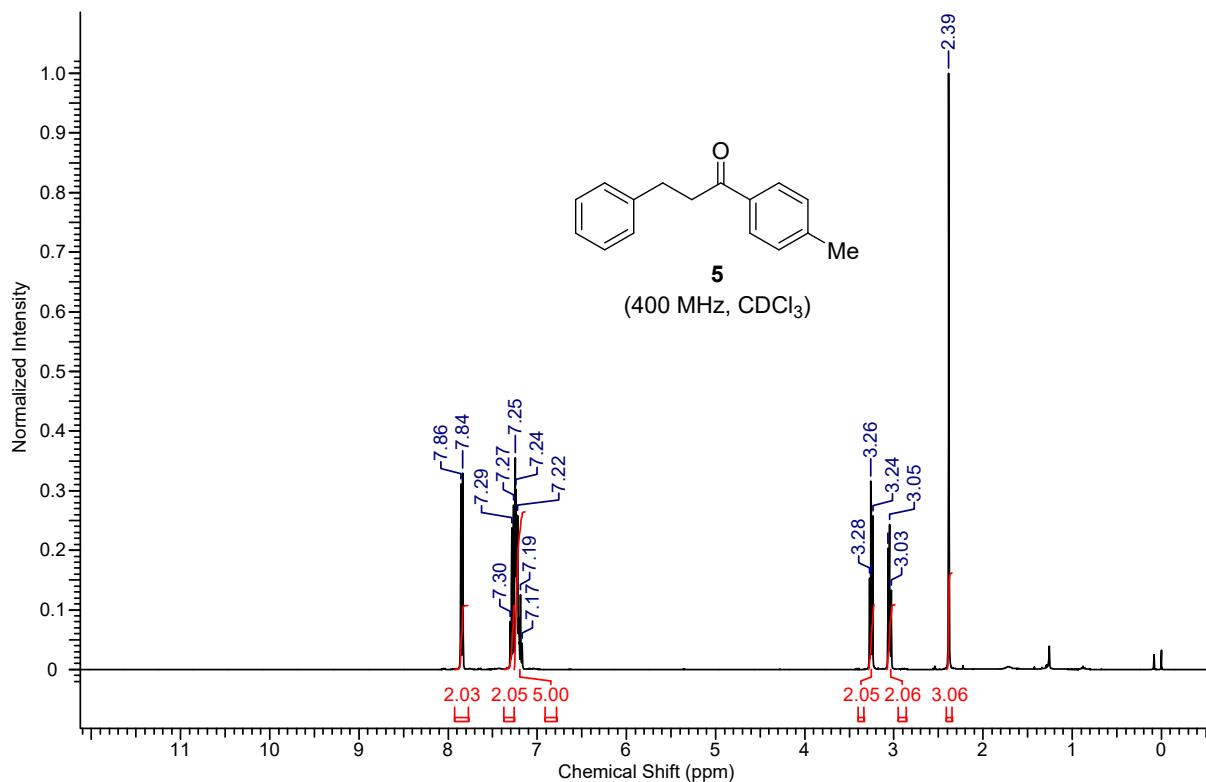
13. ^1H and $^{13}\text{C}\{^1\text{H}\}$ -NMR Spectra of Hydrogenated Compounds



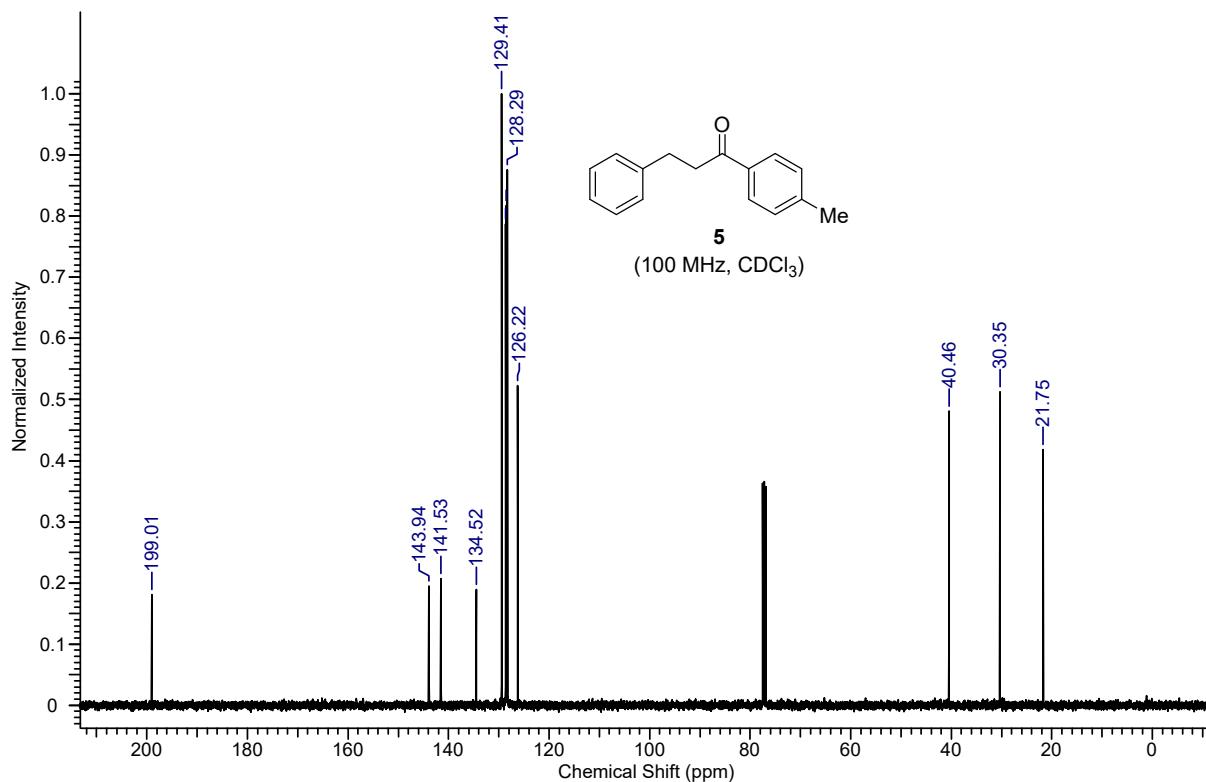
^1H -NMR spectrum of 1,3-diphenylpropan-1-one (**4**)



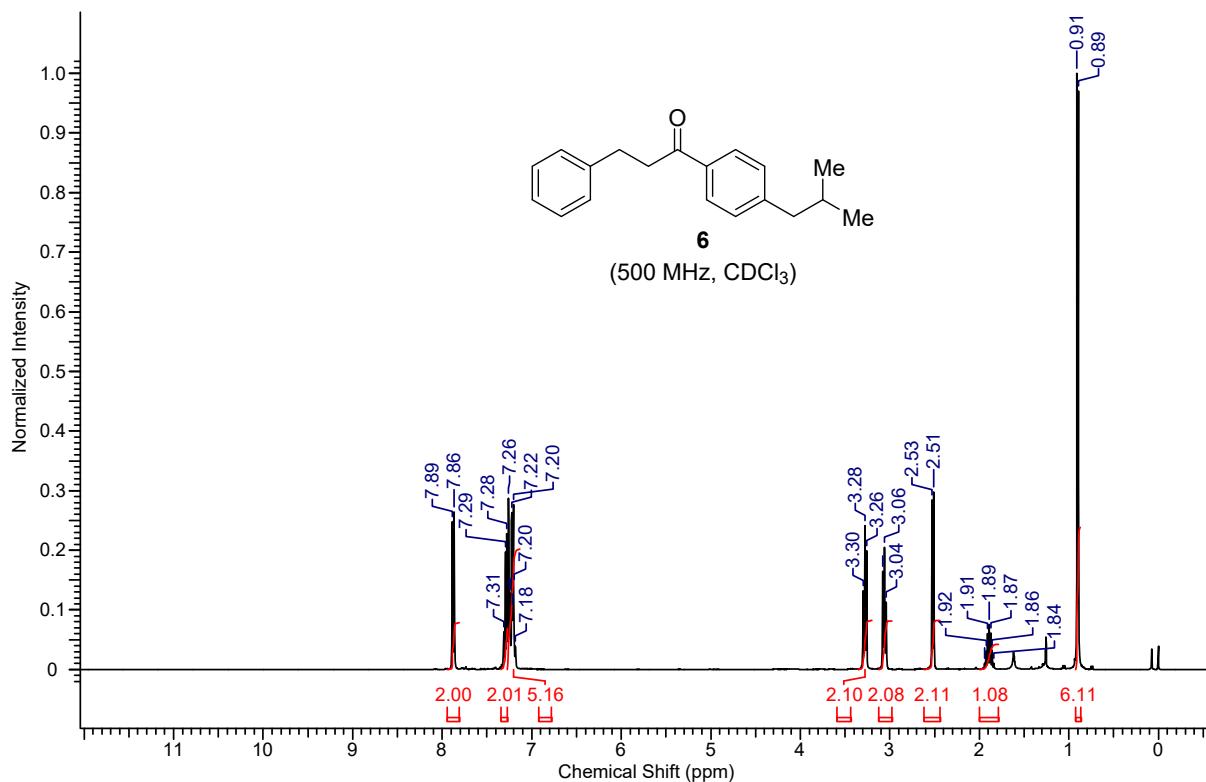
$^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum of 1,3-diphenylpropan-1-one (**4**)



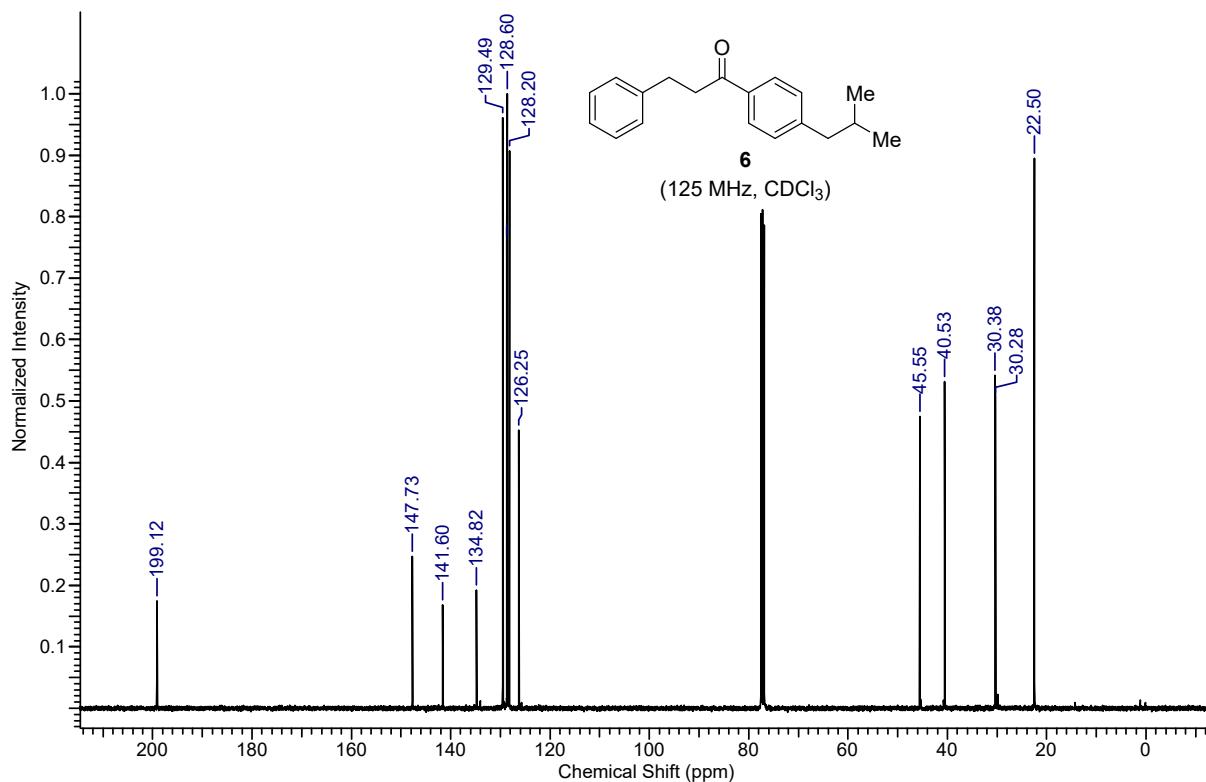
¹H-NMR spectrum of 3-phenyl-1-(p-tolyl)propan-1-one (**5**)



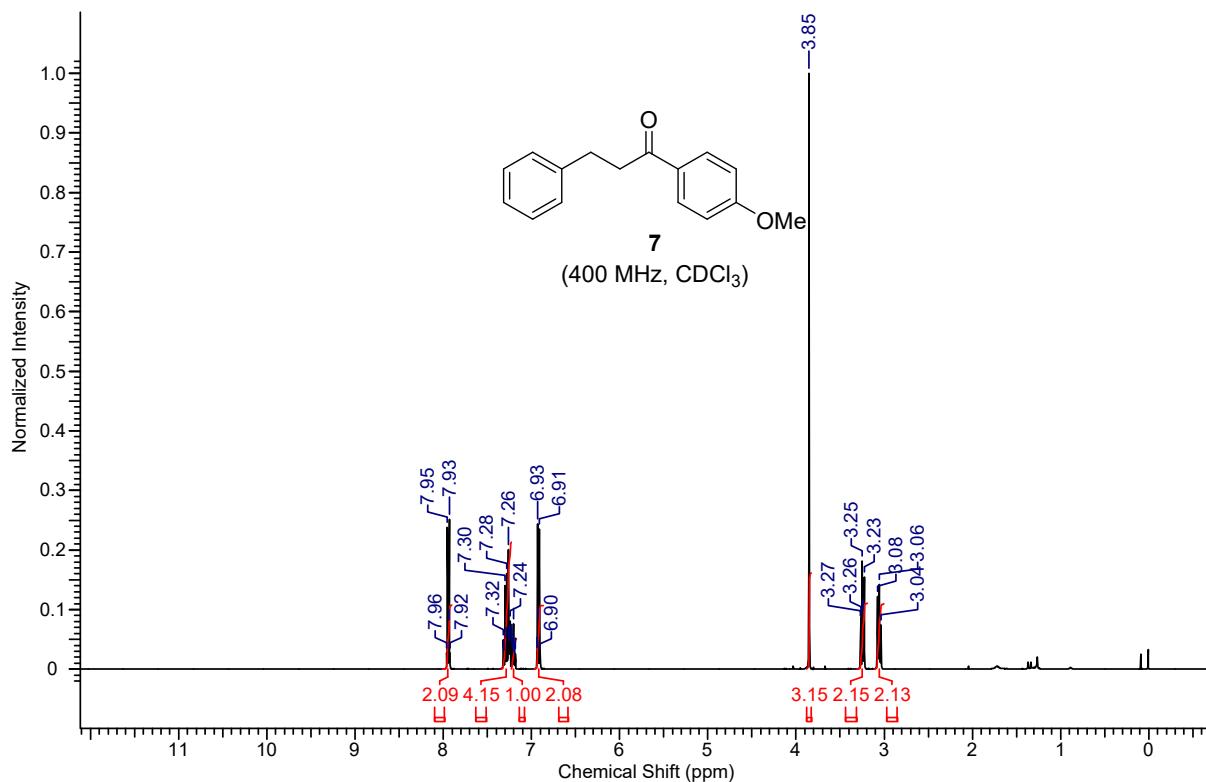
¹³C{¹H}-NMR spectrum of 3-phenyl-1-(p-tolyl)propan-1-one (**5**)



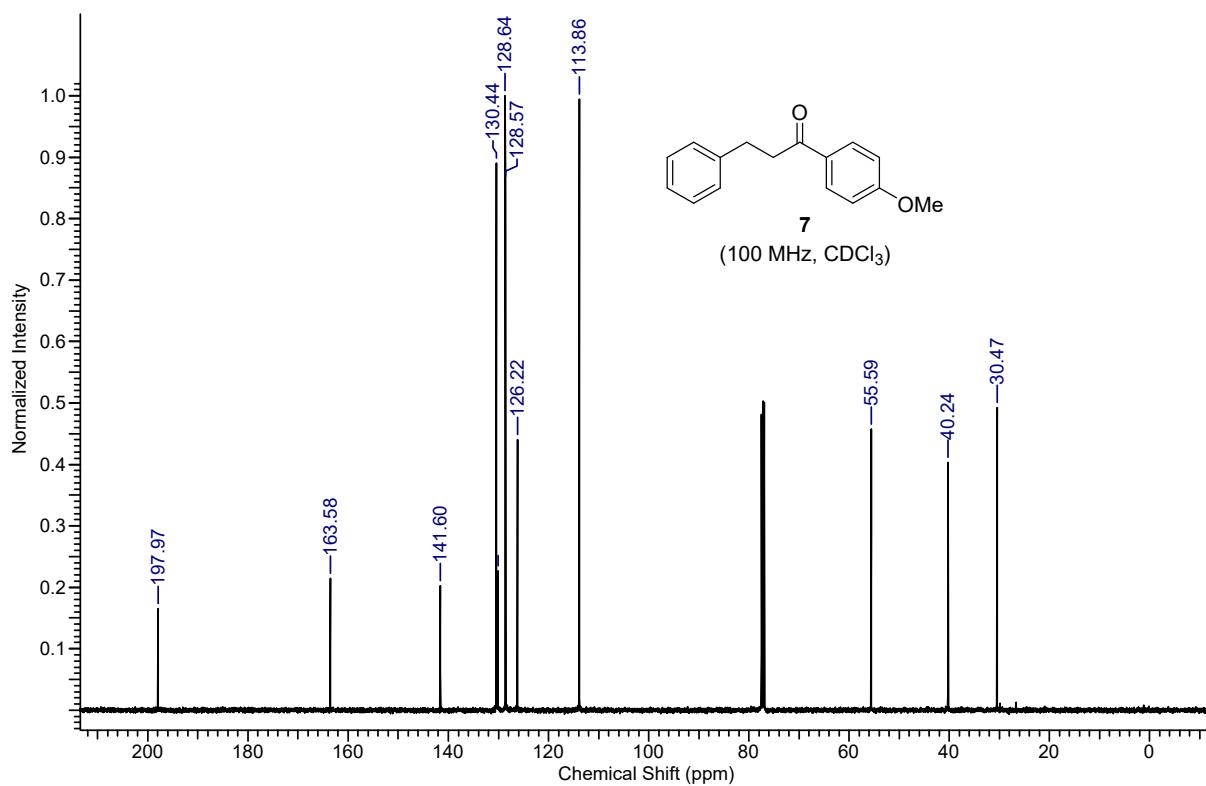
¹H-NMR spectrum of 1-(4-isobutylphenyl)-3-phenylpropan-1-one (**6**)



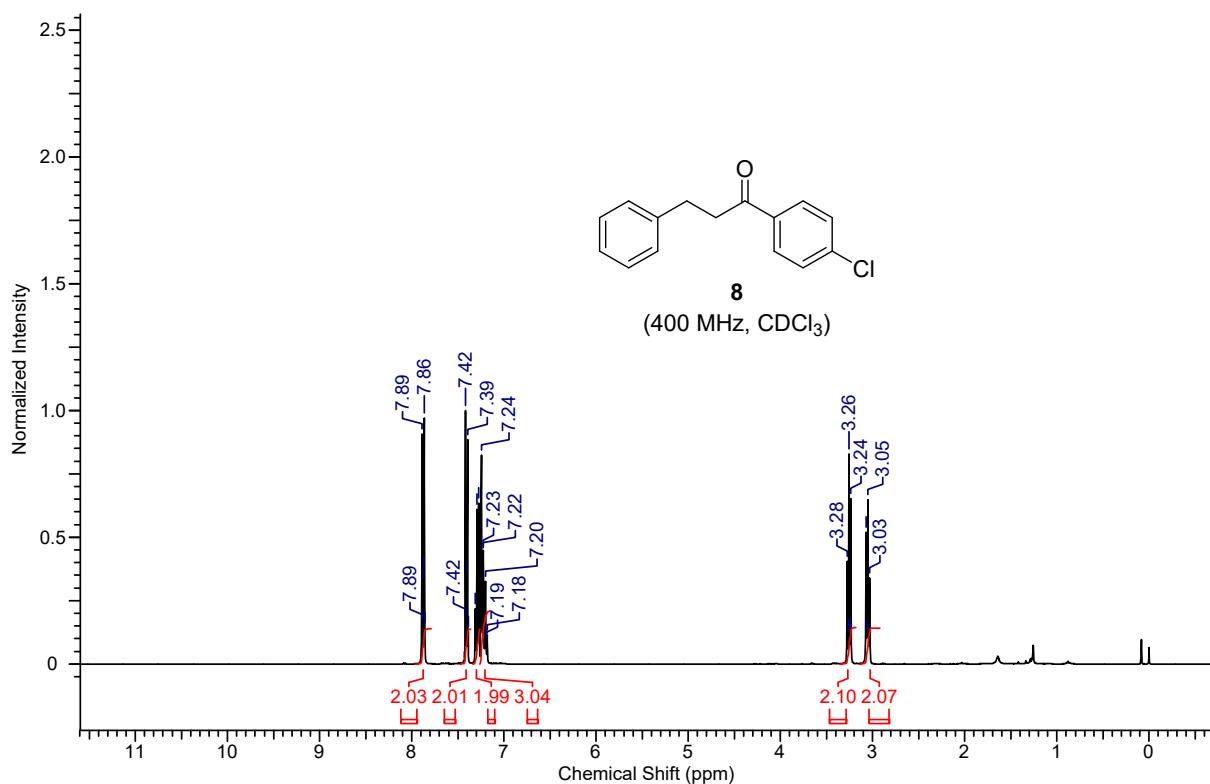
¹³C{¹H}-NMR spectrum of 1-(4-isobutylphenyl)-3-phenylpropan-1-one (**6**)



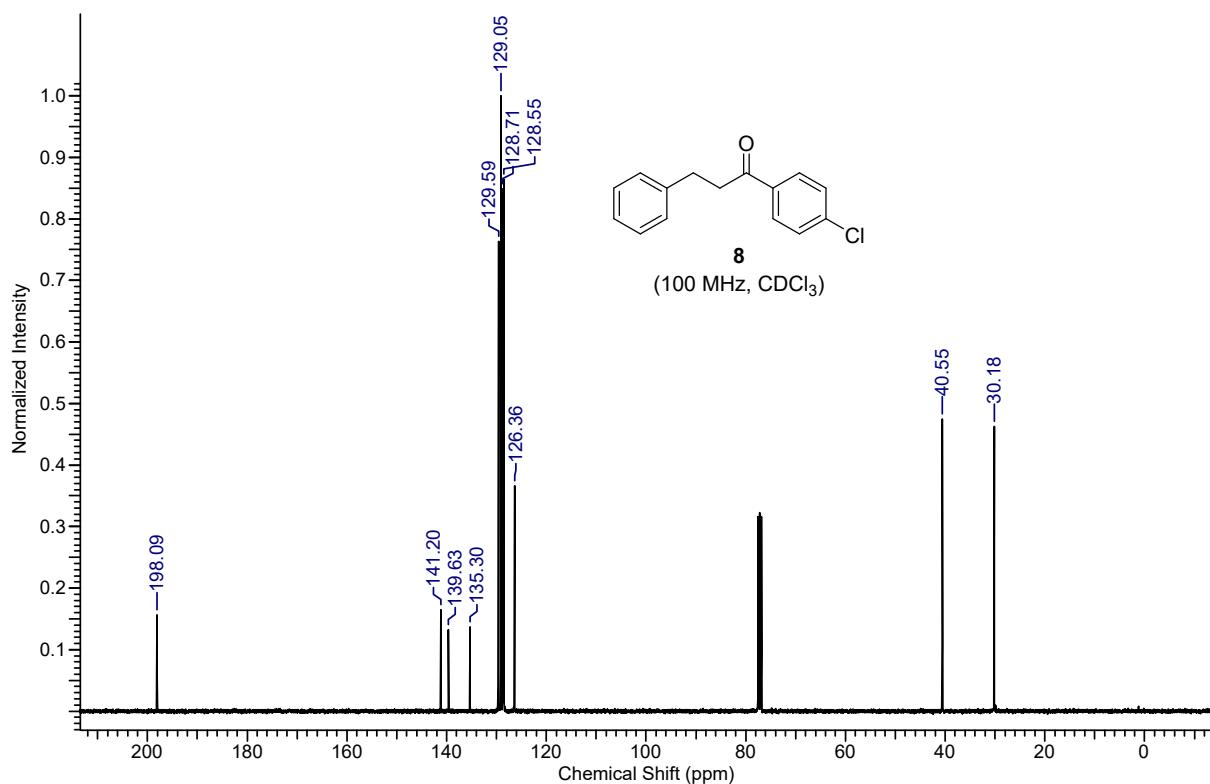
¹H-NMR spectrum of 1-(4-methoxyphenyl)-3-phenylpropan-1-one (**7**)



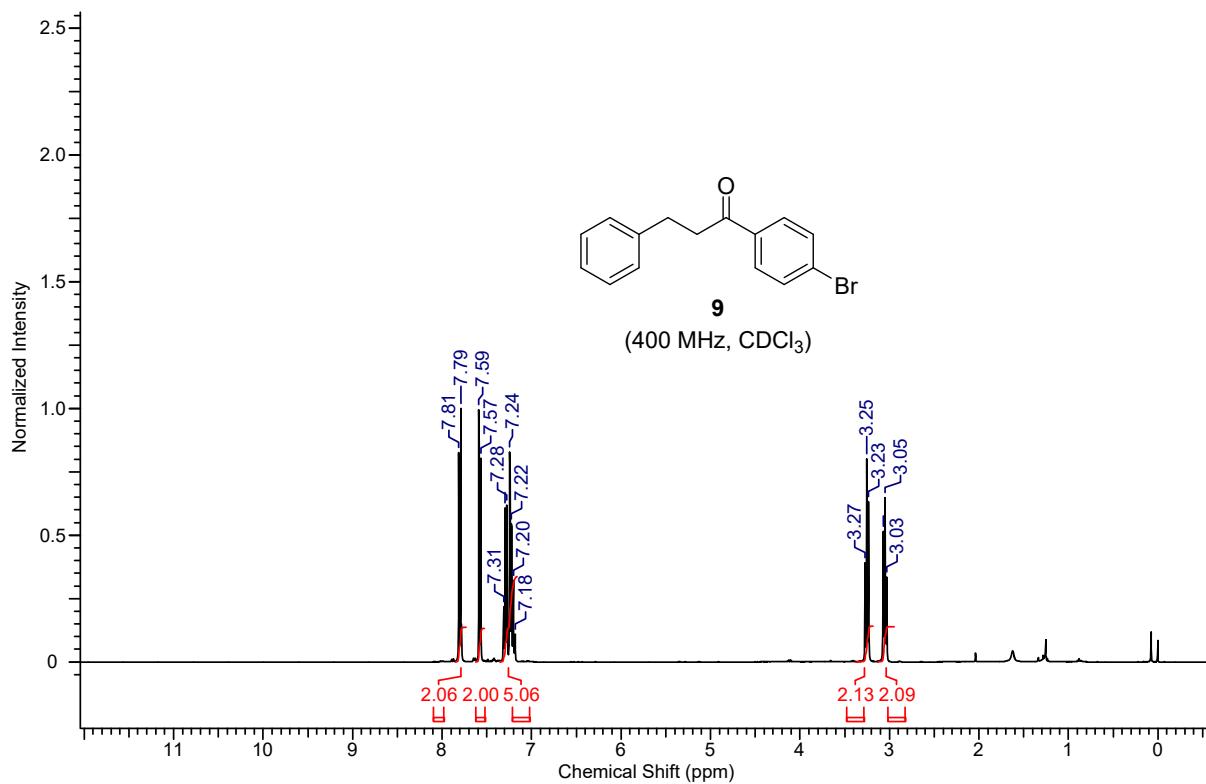
¹³C{¹H}-NMR spectrum of 1-(4-methoxyphenyl)-3-phenylpropan-1-one (**7**)



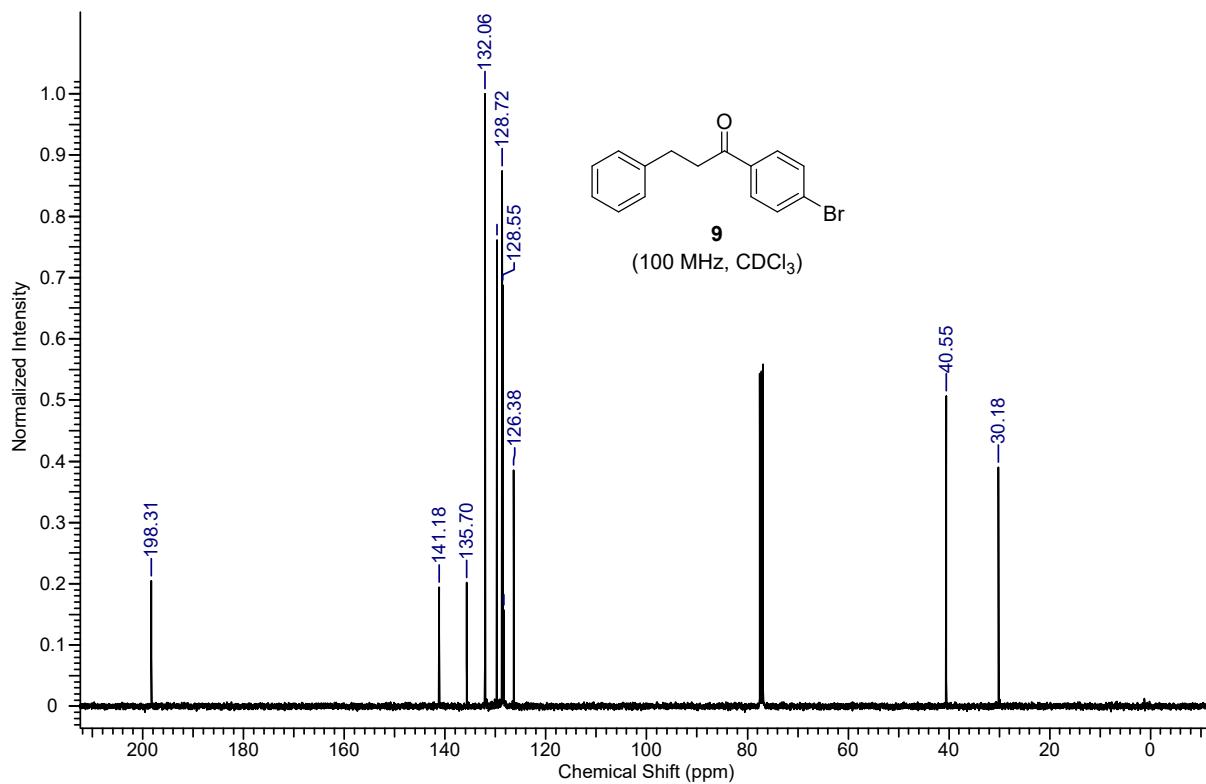
¹H-NMR spectrum of 1-(4-chlorophenyl)-3-phenylpropan-1-one (**8**)



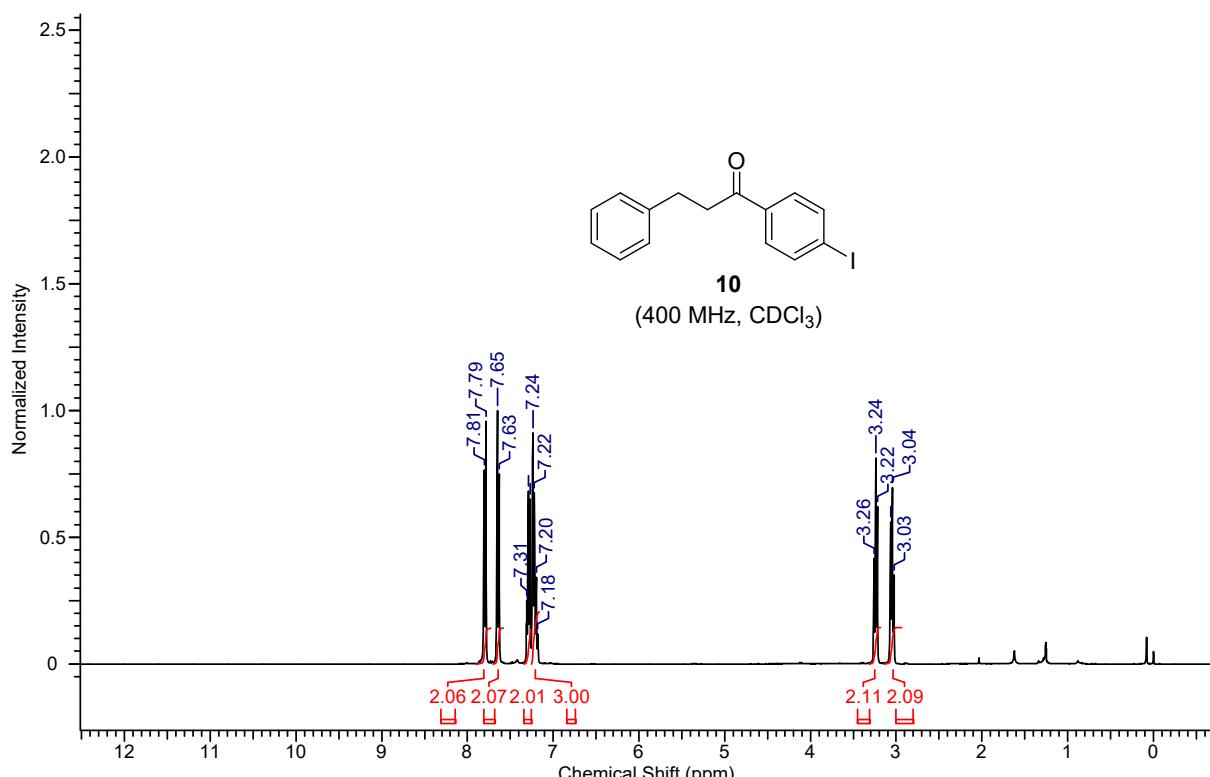
¹³C{¹H}-NMR spectrum of 1-(4-chlorophenyl)-3-phenylpropan-1-one (**8**)



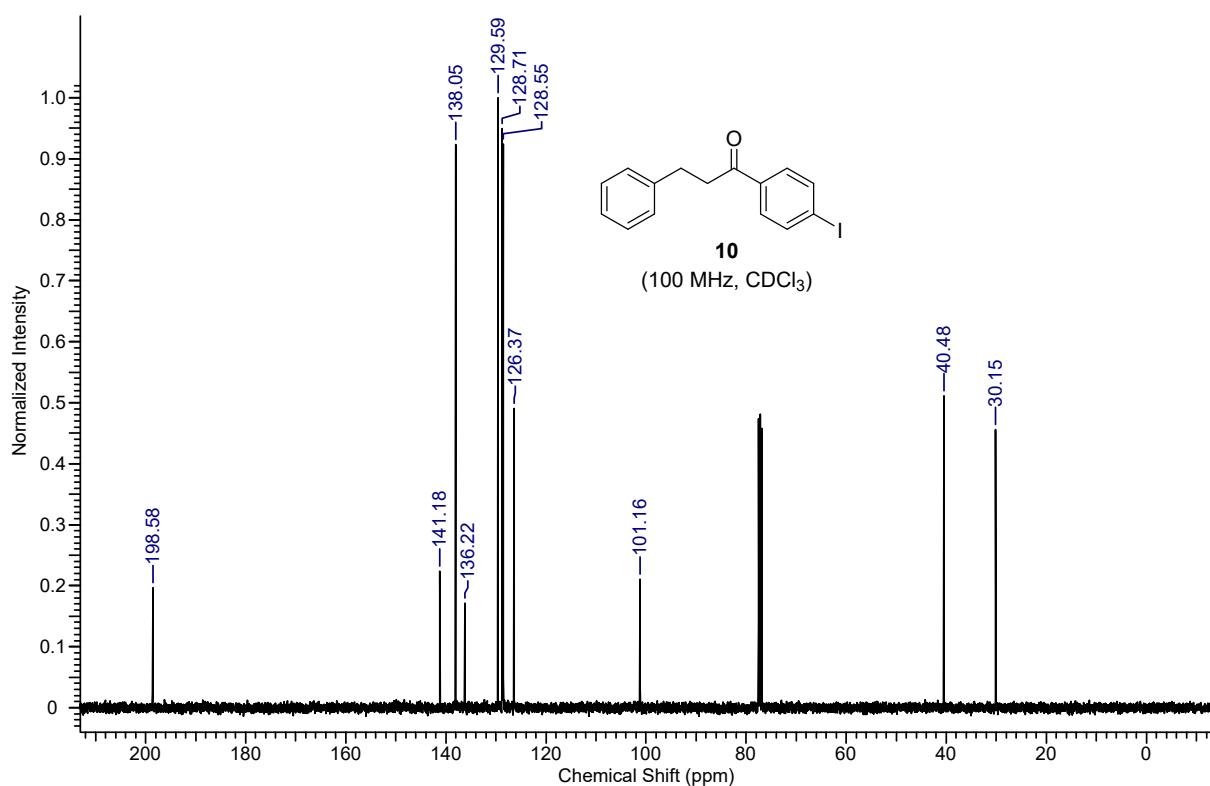
¹H-NMR spectrum of 1-(4-bromophenyl)-3-phenylpropan-1-one (**9**)



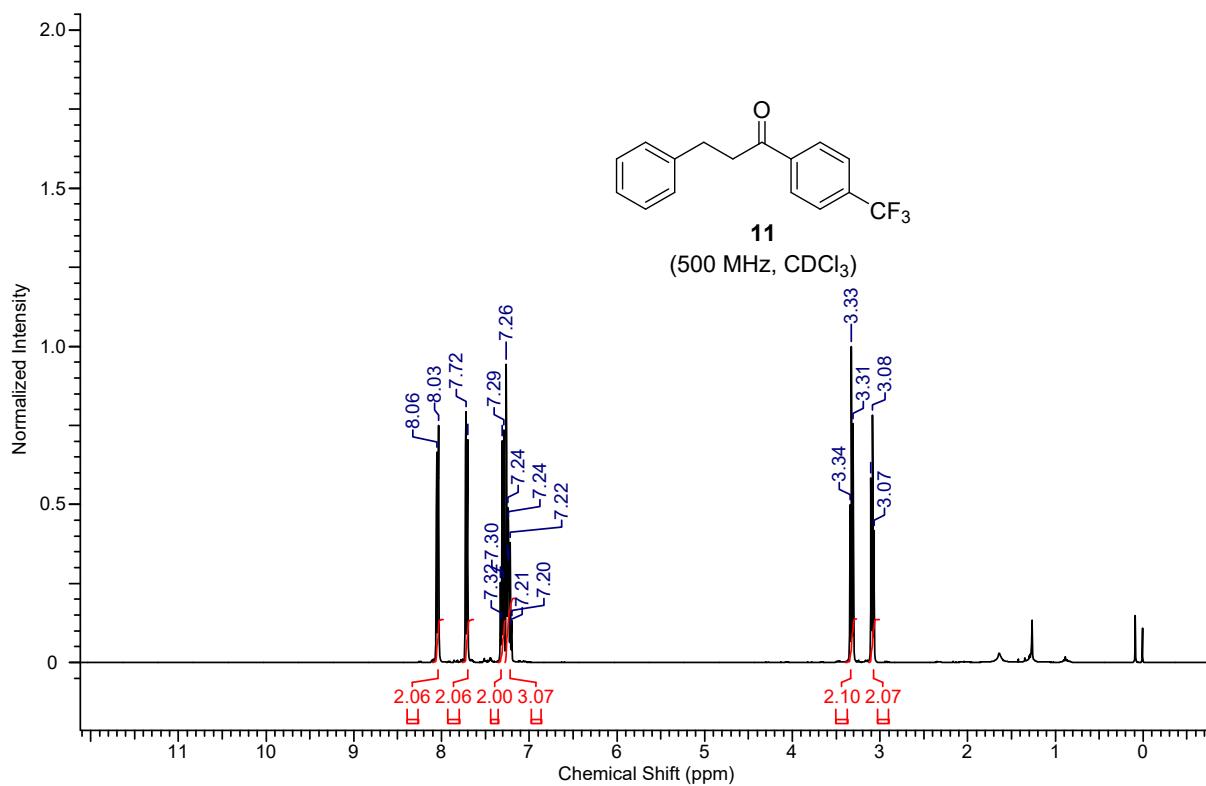
¹³C{¹H}-NMR spectrum of 1-(4-bromophenyl)-3-phenylpropan-1-one (**9**)



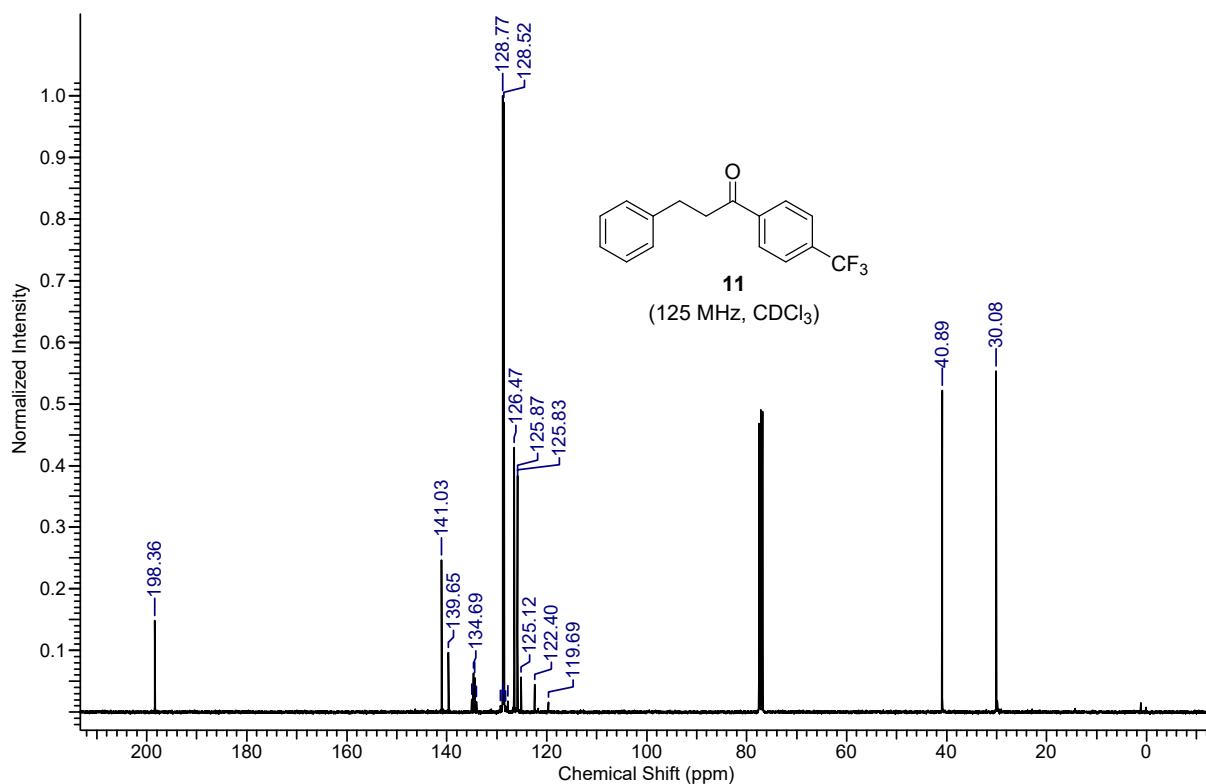
¹H-NMR spectrum of 1-(4-iodophenyl)-3-phenylpropan-1-one (**10**)



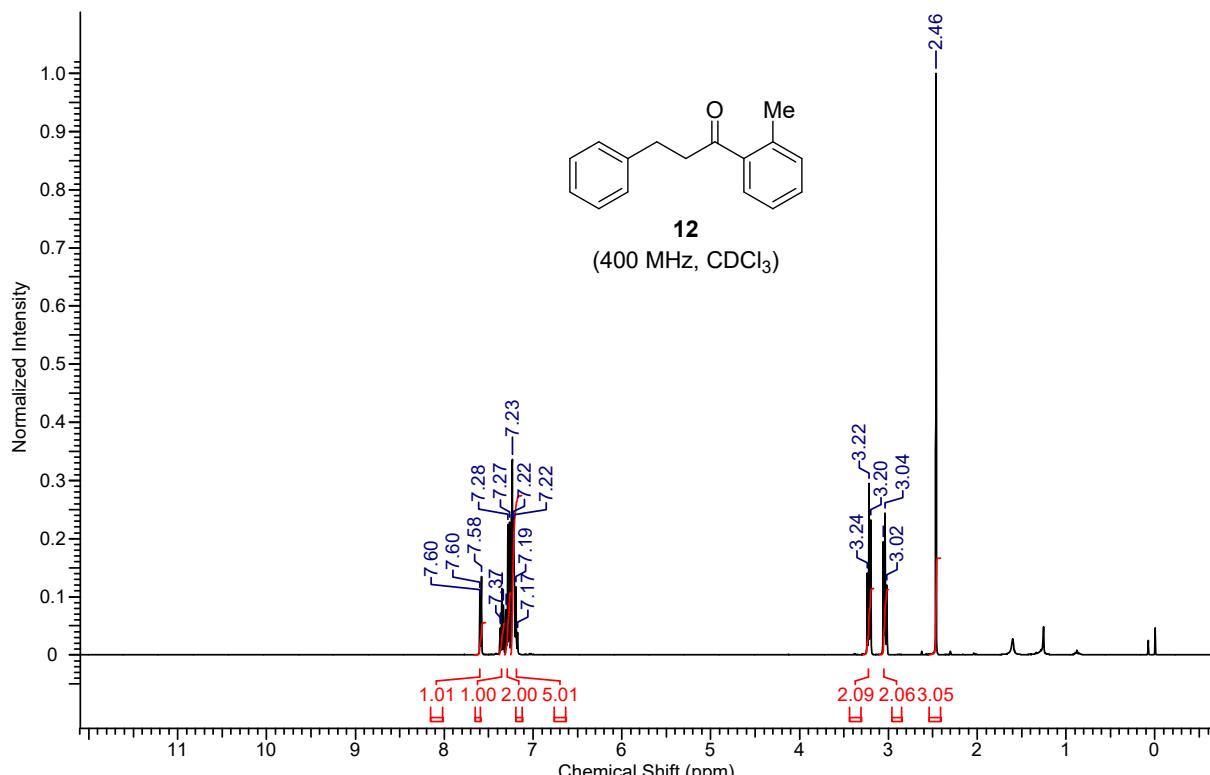
¹³C{¹H}-NMR spectrum of 1-(4-iodophenyl)-3-phenylpropan-1-one (**10**)



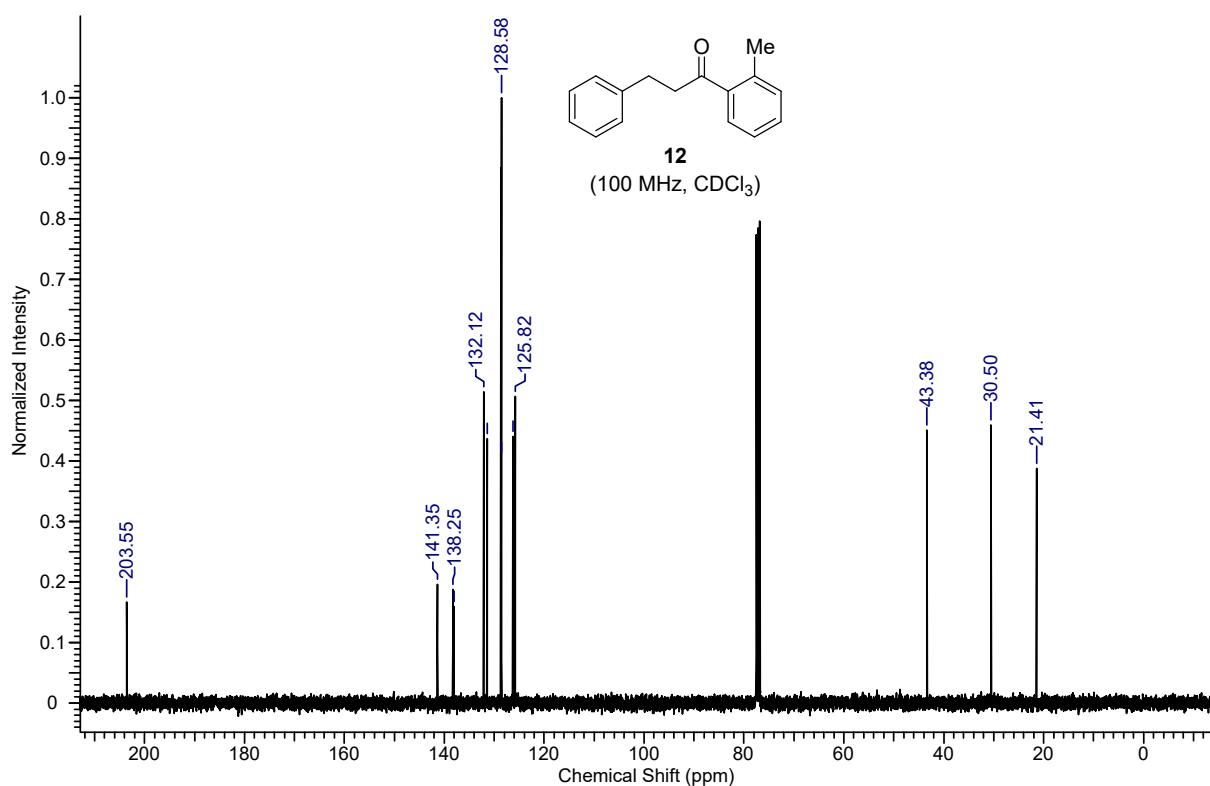
^1H -NMR spectrum of 3-phenyl-1-(4-(trifluoromethyl)phenyl)propan-1-one (**11**)



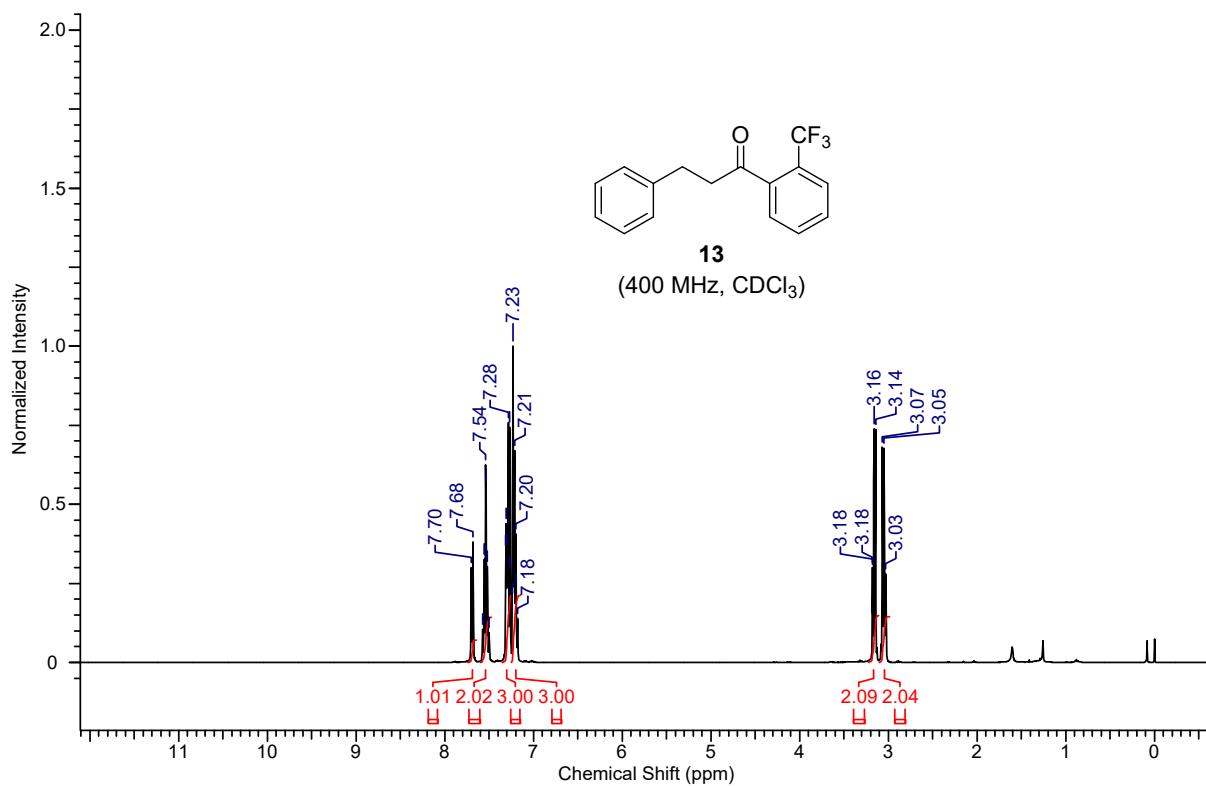
$^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum of 3-phenyl-1-(4-(trifluoromethyl)phenyl)propan-1-one (**11**)



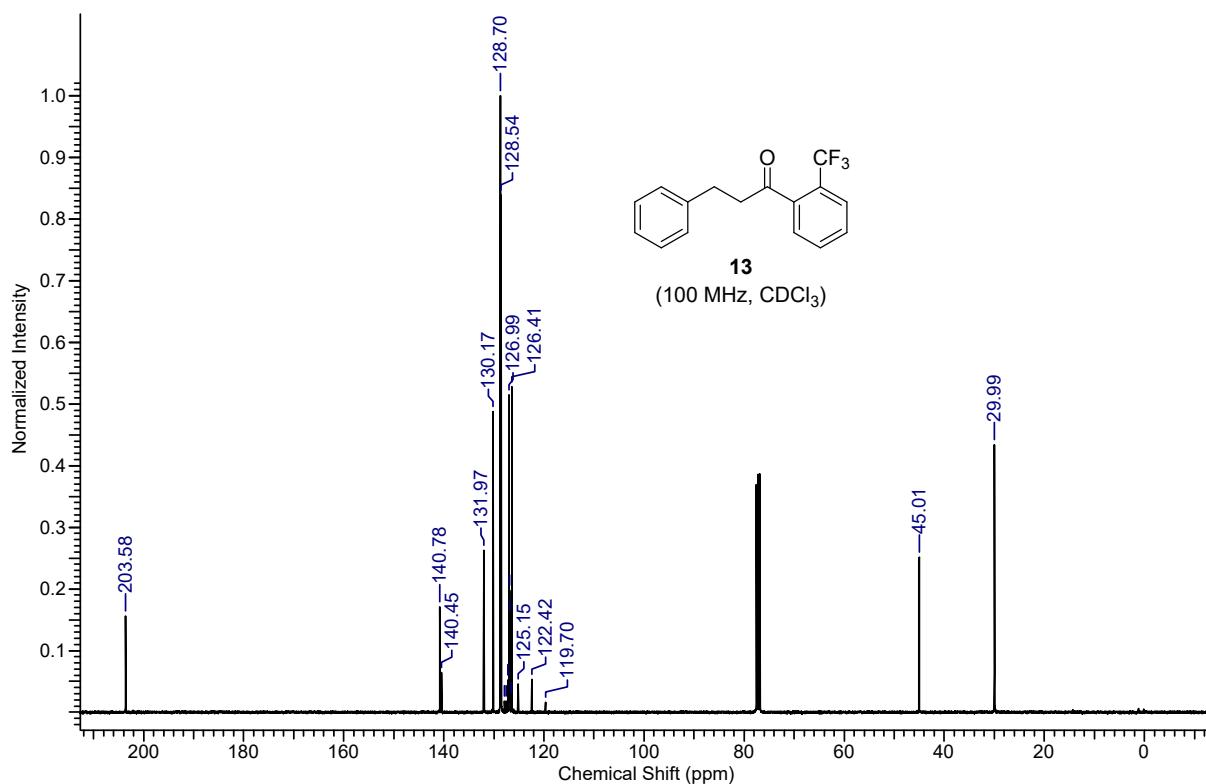
¹H-NMR spectrum of 3-phenyl-1-(*o*-tolyl)propan-1-one (**12**)



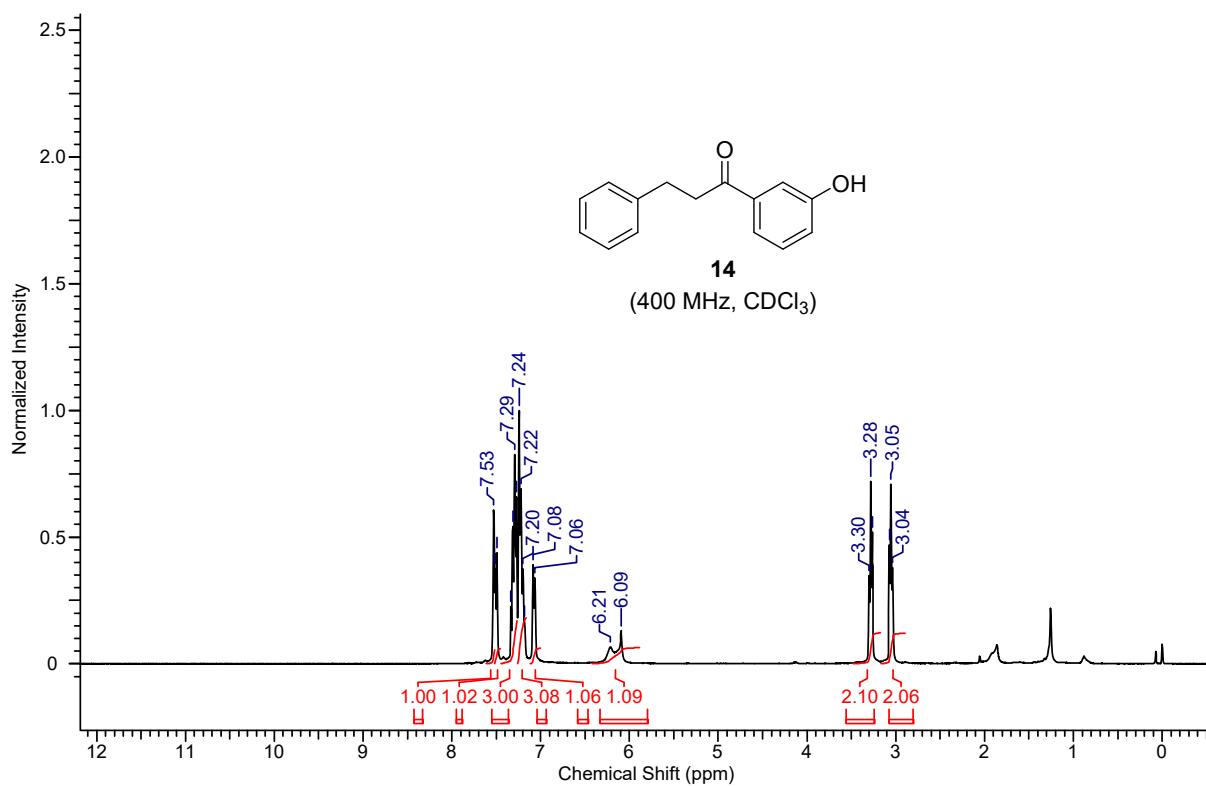
¹³C{¹H}-NMR spectrum of 3-phenyl-1-(*o*-tolyl)propan-1-one (**12**)



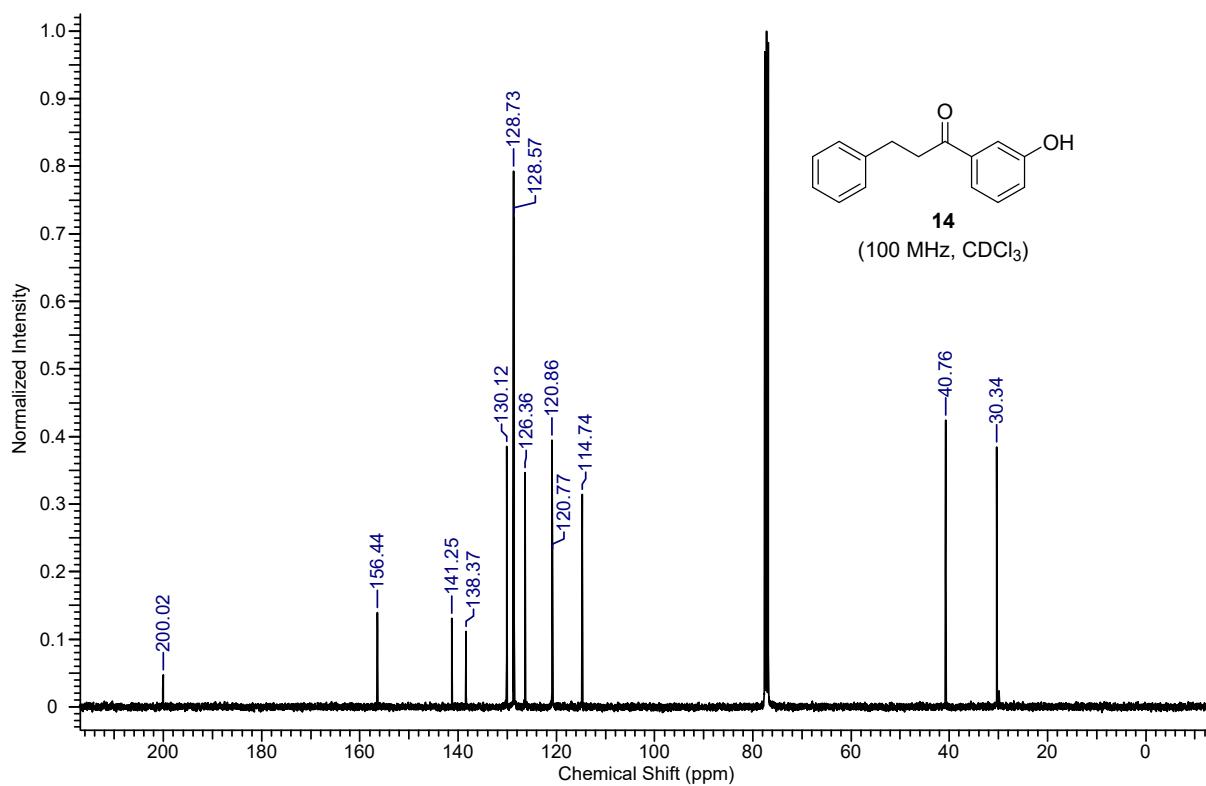
¹H-NMR spectrum of 3-phenyl-1-(2-(trifluoromethyl)phenyl)propan-1-one (**13**)



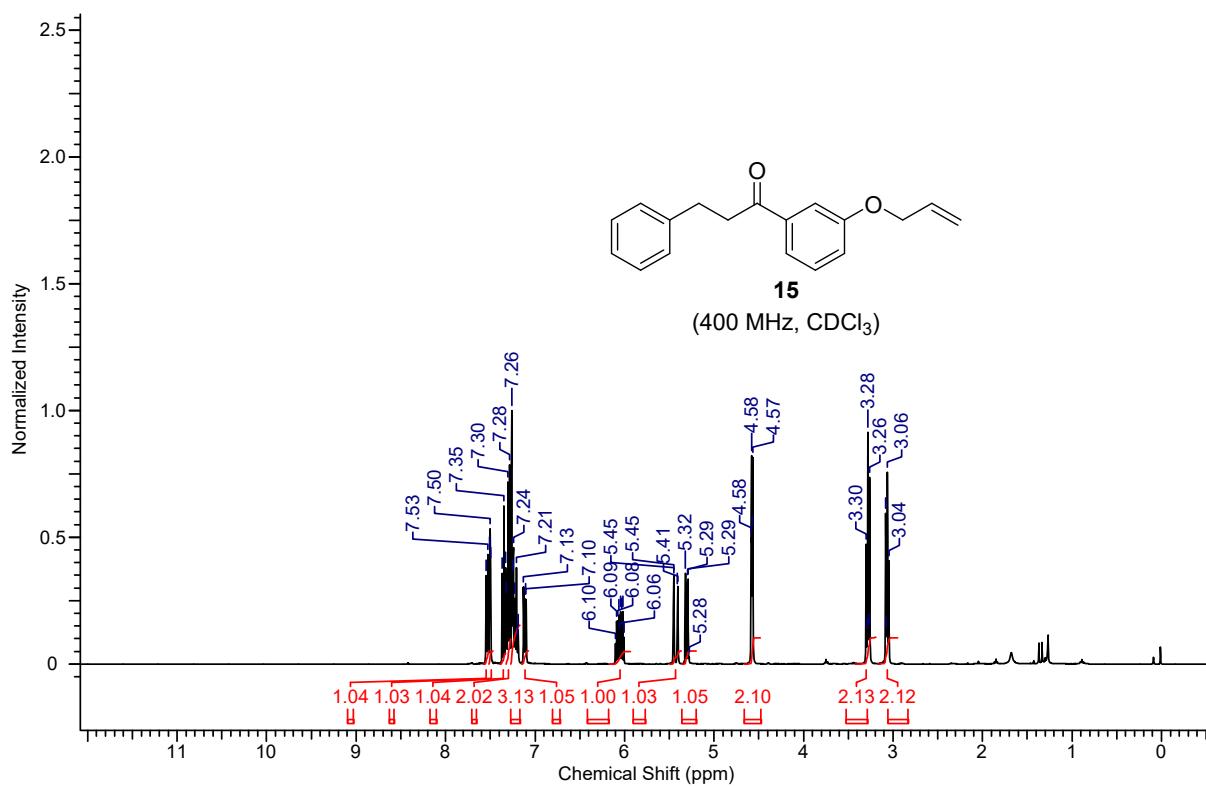
¹³C{¹H}-NMR spectrum of 3-phenyl-1-(2-(trifluoromethyl)phenyl)propan-1-one (**13**)



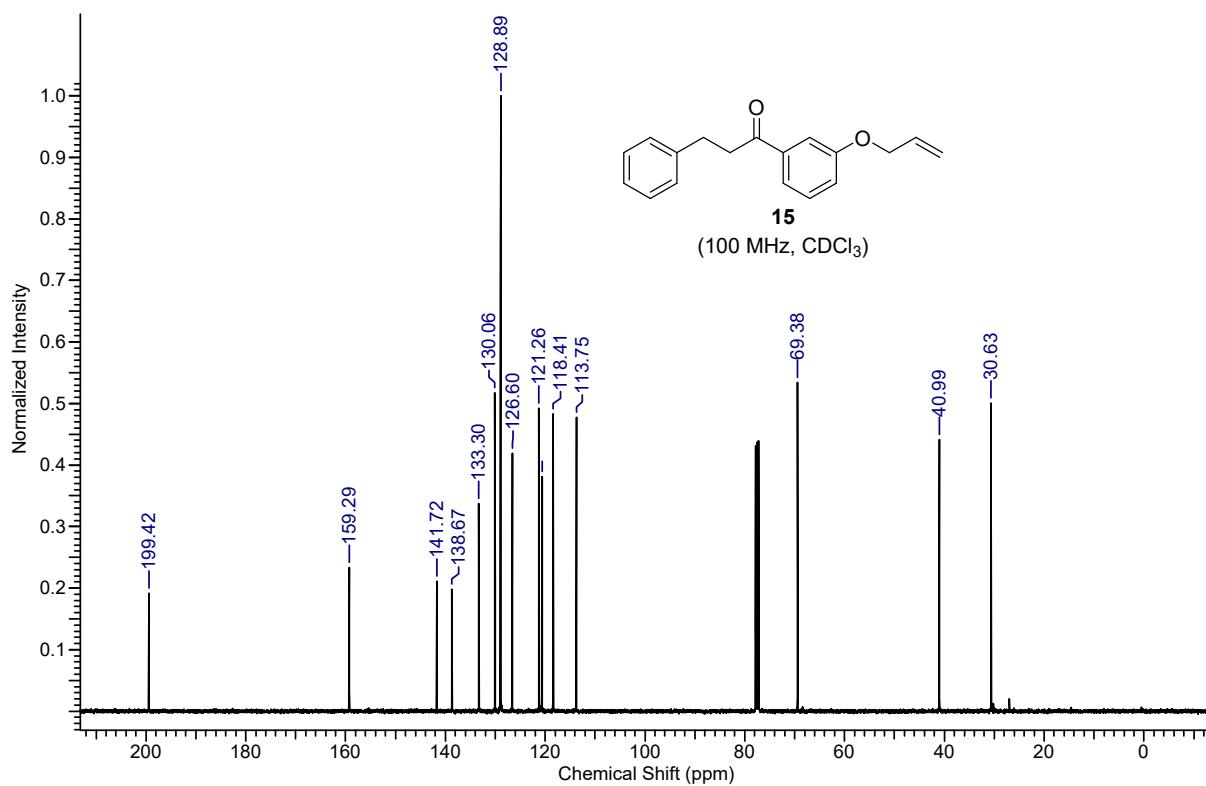
¹H-NMR spectrum of 1-(3-hydroxyphenyl)-3-phenylpropan-1-one (**14**)



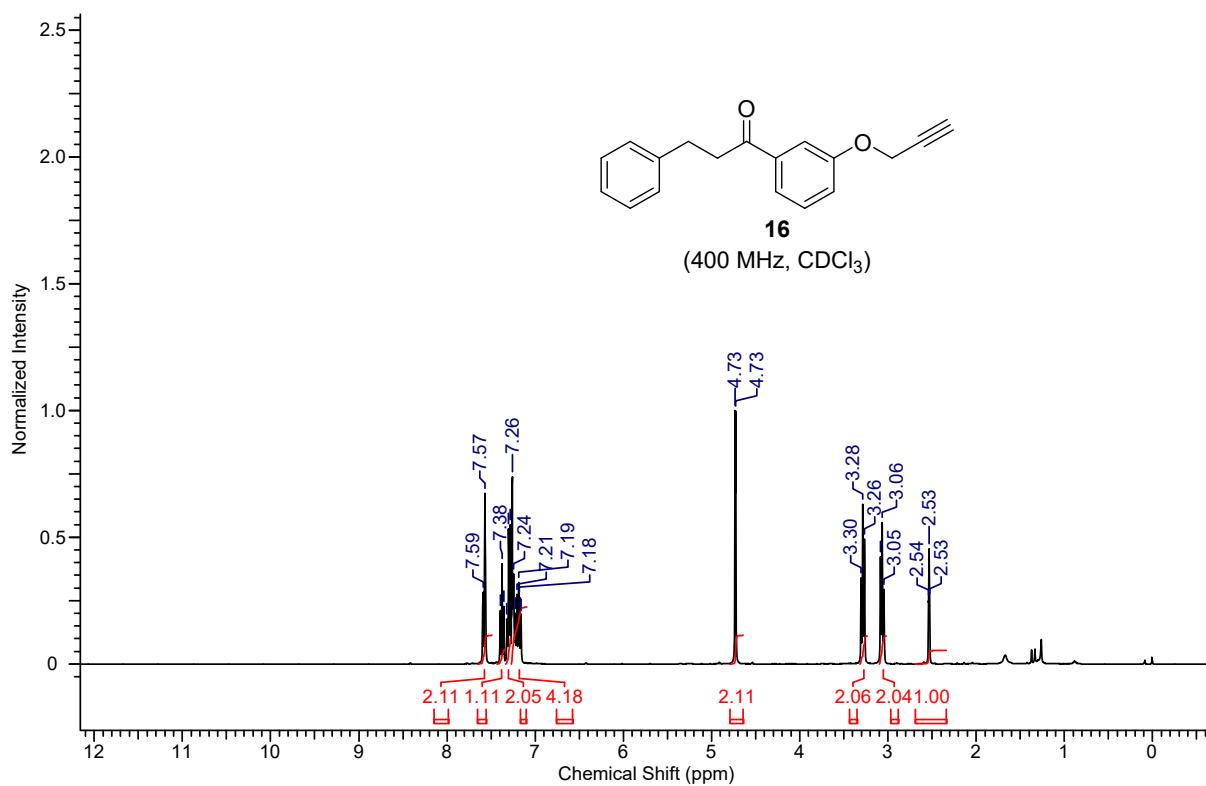
¹³C{¹H}-NMR spectrum of 1-(3-hydroxyphenyl)-3-phenylpropan-1-one (**14**)



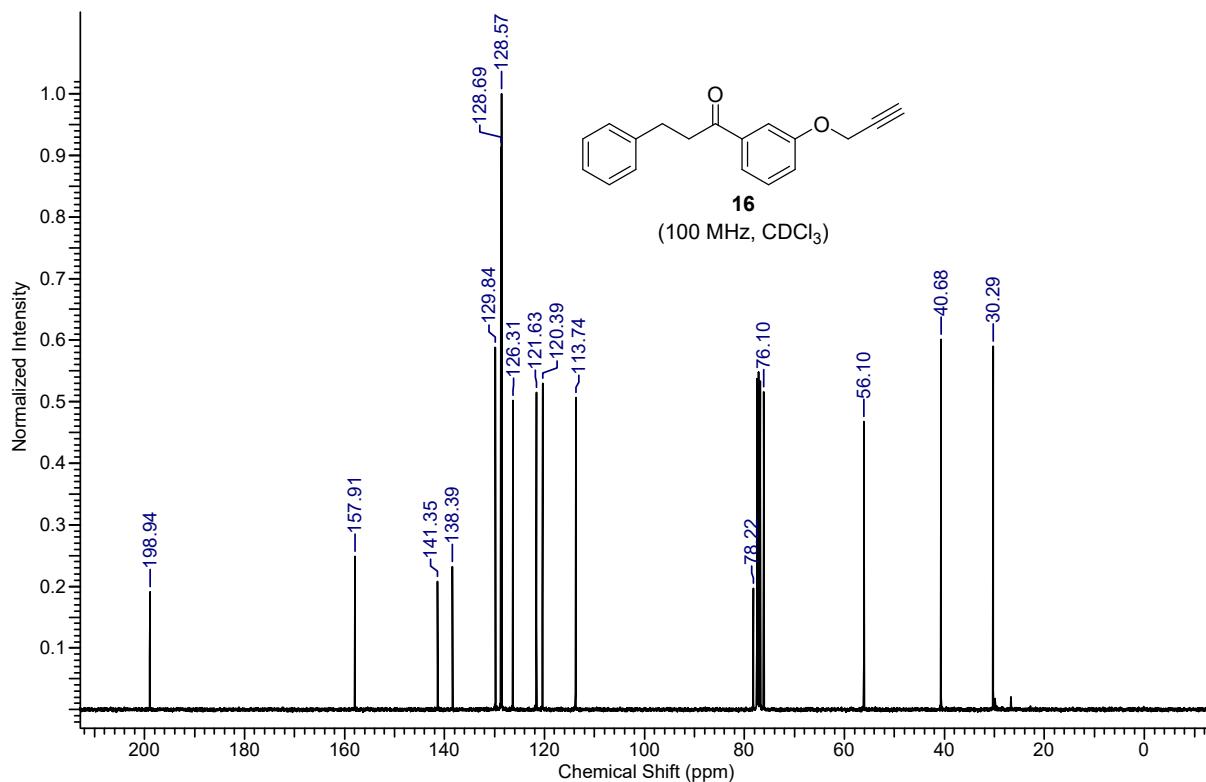
¹H-NMR spectrum of 1-(3-(allyloxy)phenyl)-3-phenylpropan-1-one (**15**)



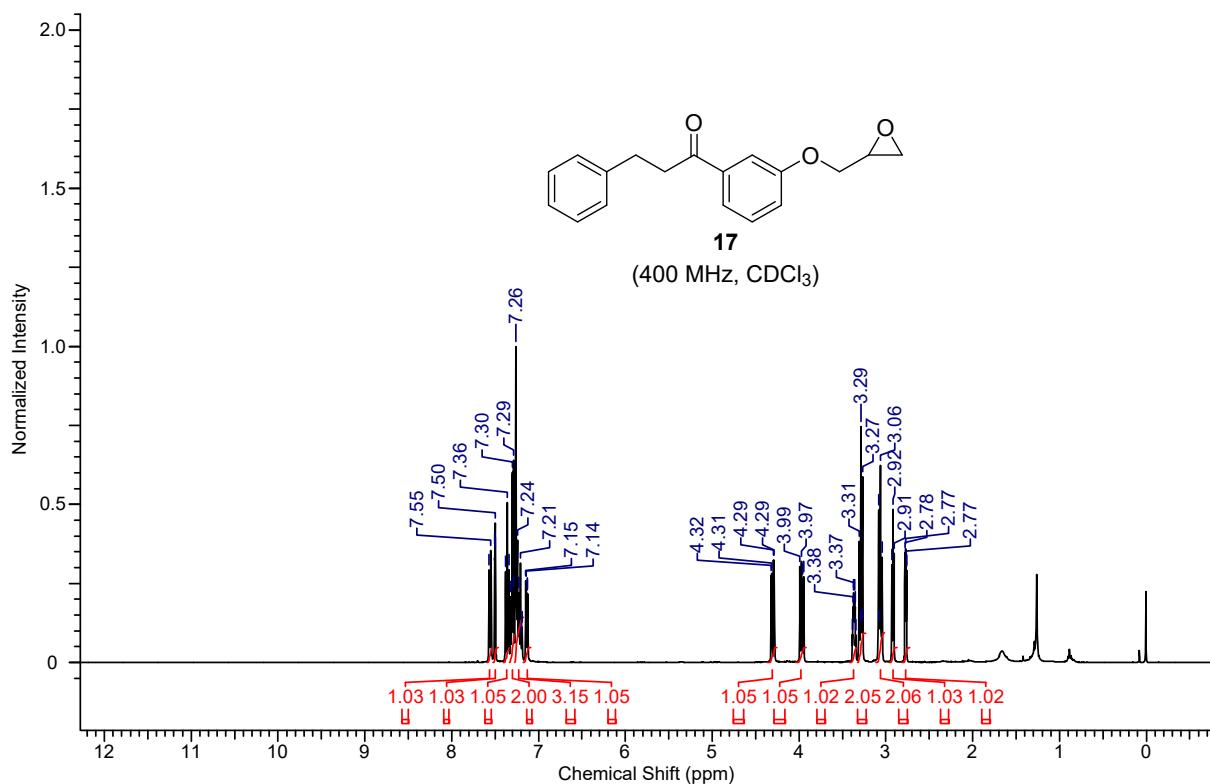
¹³C{¹H}-NMR spectrum of 1-(3-(allyloxy)phenyl)-3-phenylpropan-1-one (**15**)



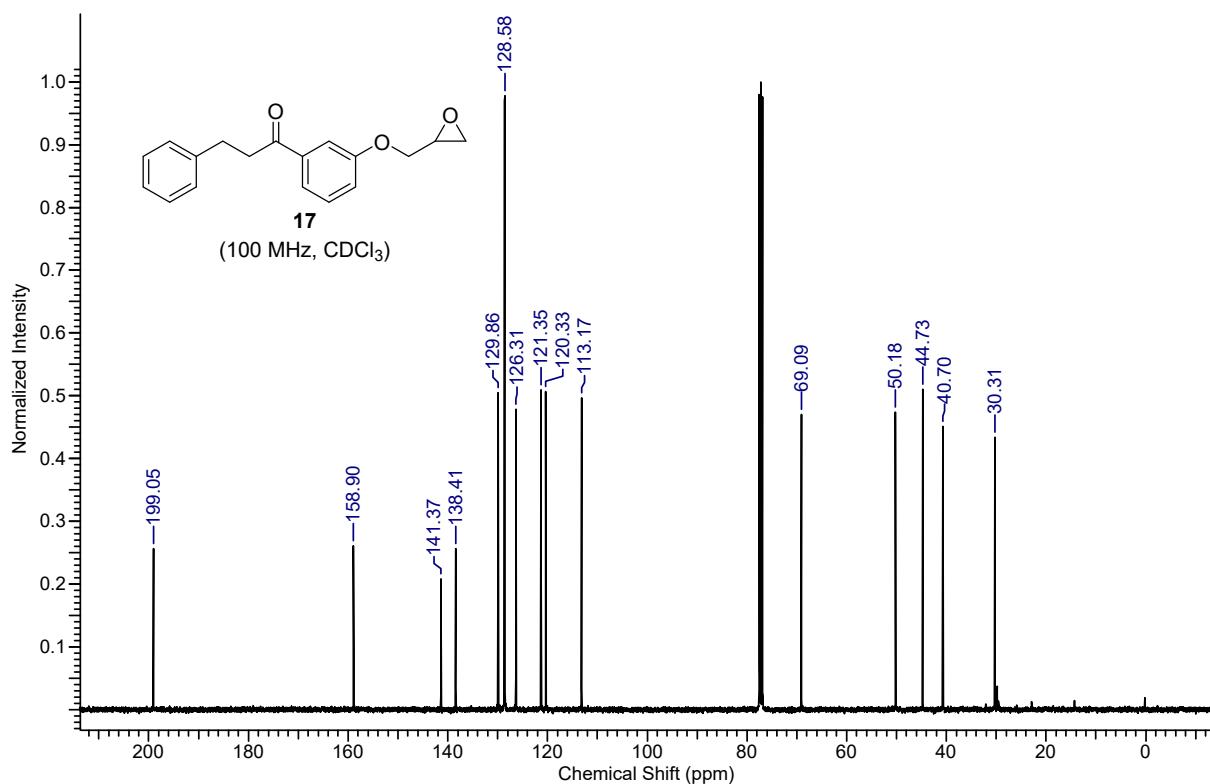
¹H-NMR spectrum of 3-phenyl-1-(3-(prop-2-yn-1-yloxy)phenyl)propan-1-one (**16**)



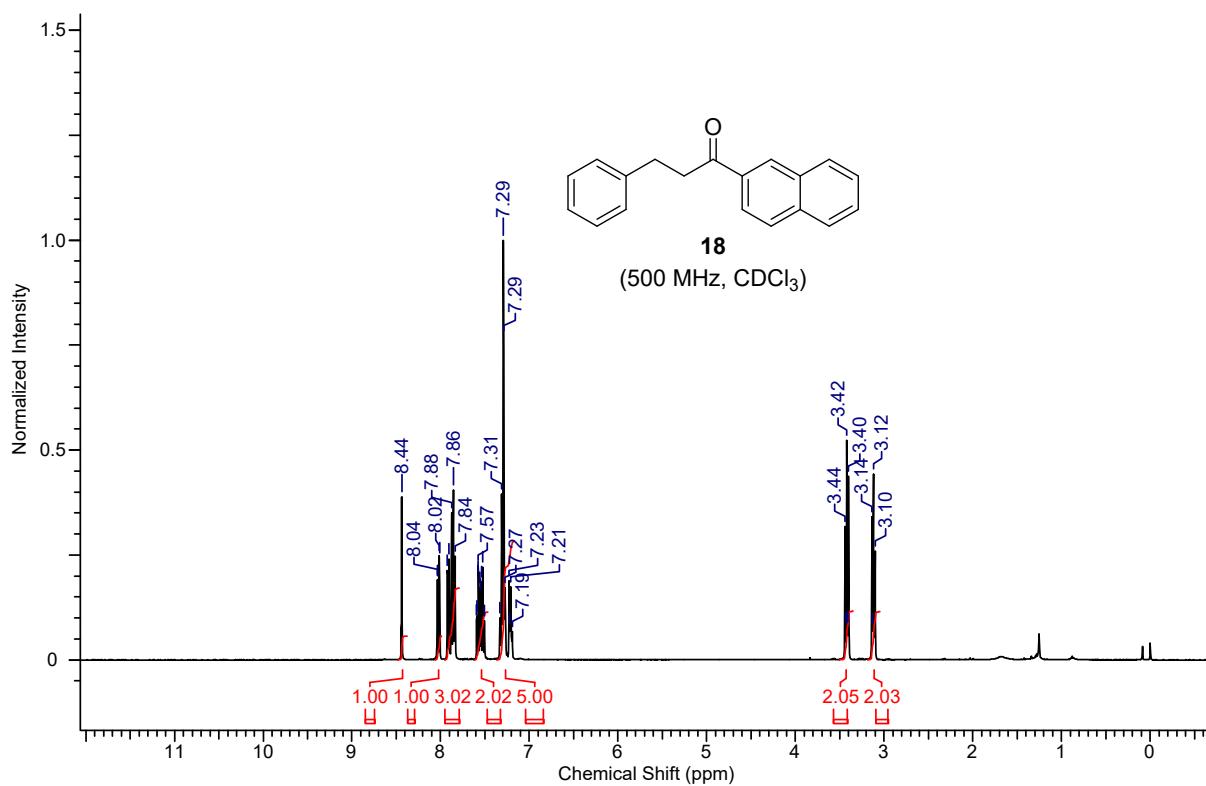
¹³C{¹H}-NMR spectrum of 3-phenyl-1-(3-(prop-2-yn-1-yloxy)phenyl)propan-1-one (**16**)



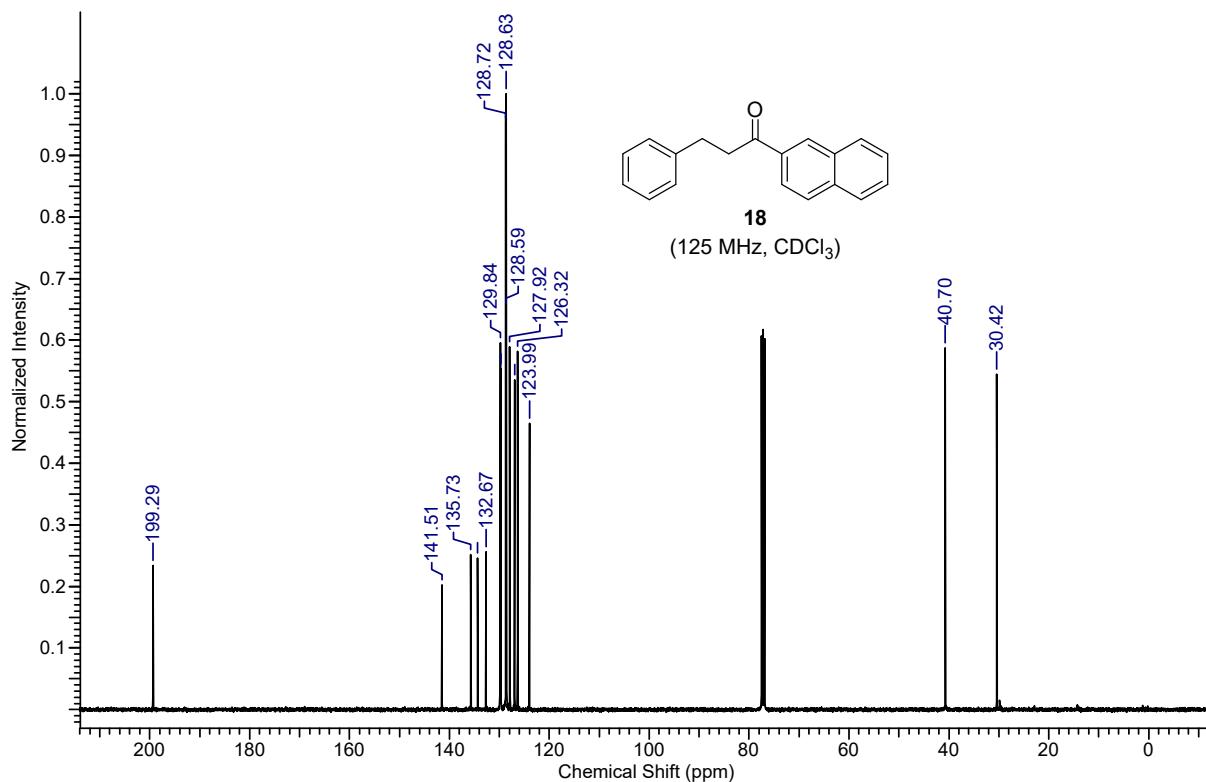
¹H-NMR spectrum of 1-(3-(oxiran-2-ylmethoxy)phenyl)-3-phenylpropan-1-one (**17**)



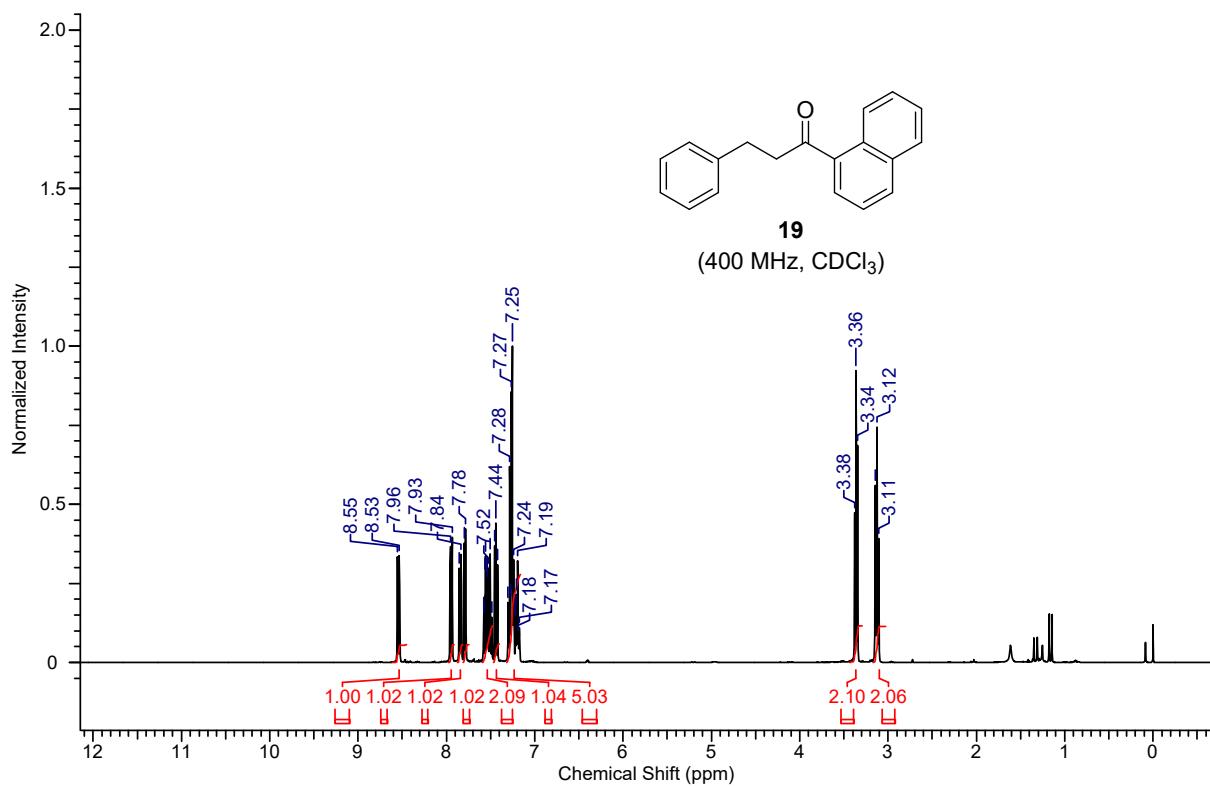
¹³C{¹H}-NMR spectrum of 1-(3-(oxiran-2-ylmethoxy)phenyl)-3-phenylpropan-1-one (**17**)



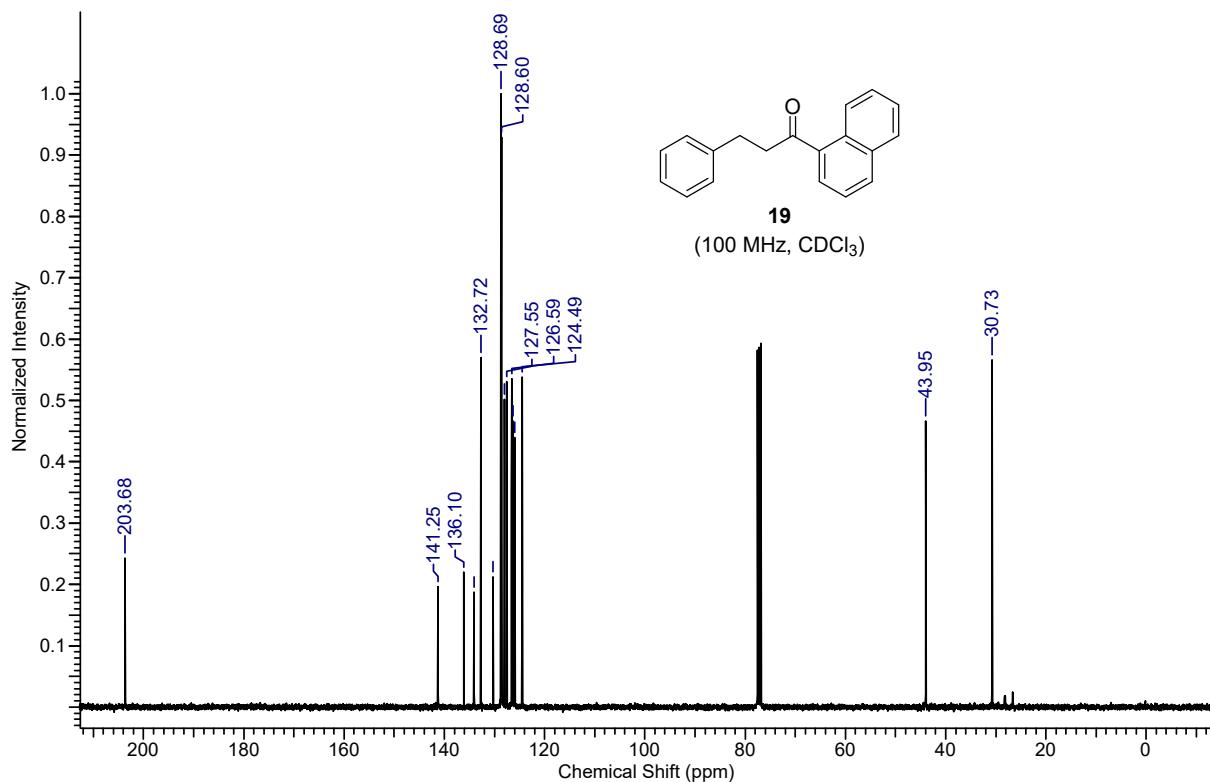
¹H-NMR spectrum of 1-(naphthalen-2-yl)-3-phenylpropan-1-one (**18**)



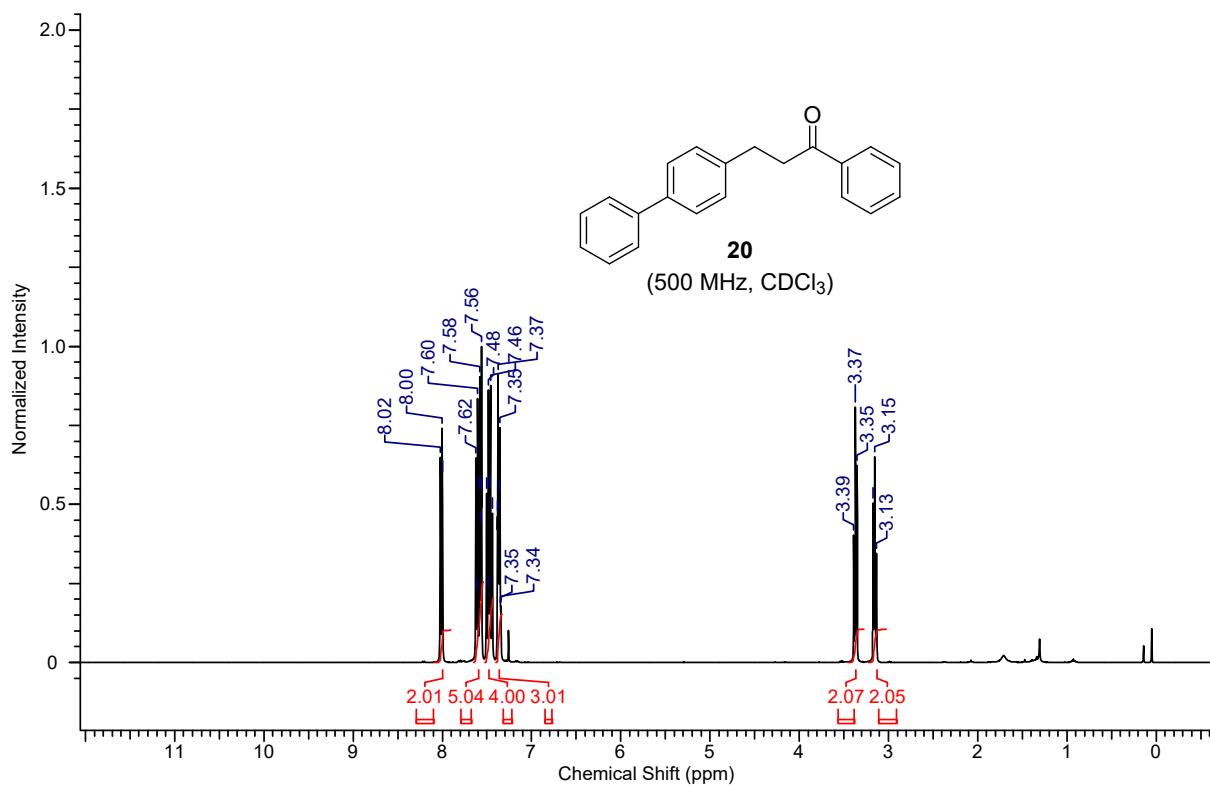
¹³C{¹H}-NMR spectrum of 1-(naphthalen-2-yl)-3-phenylpropan-1-one (**18**)



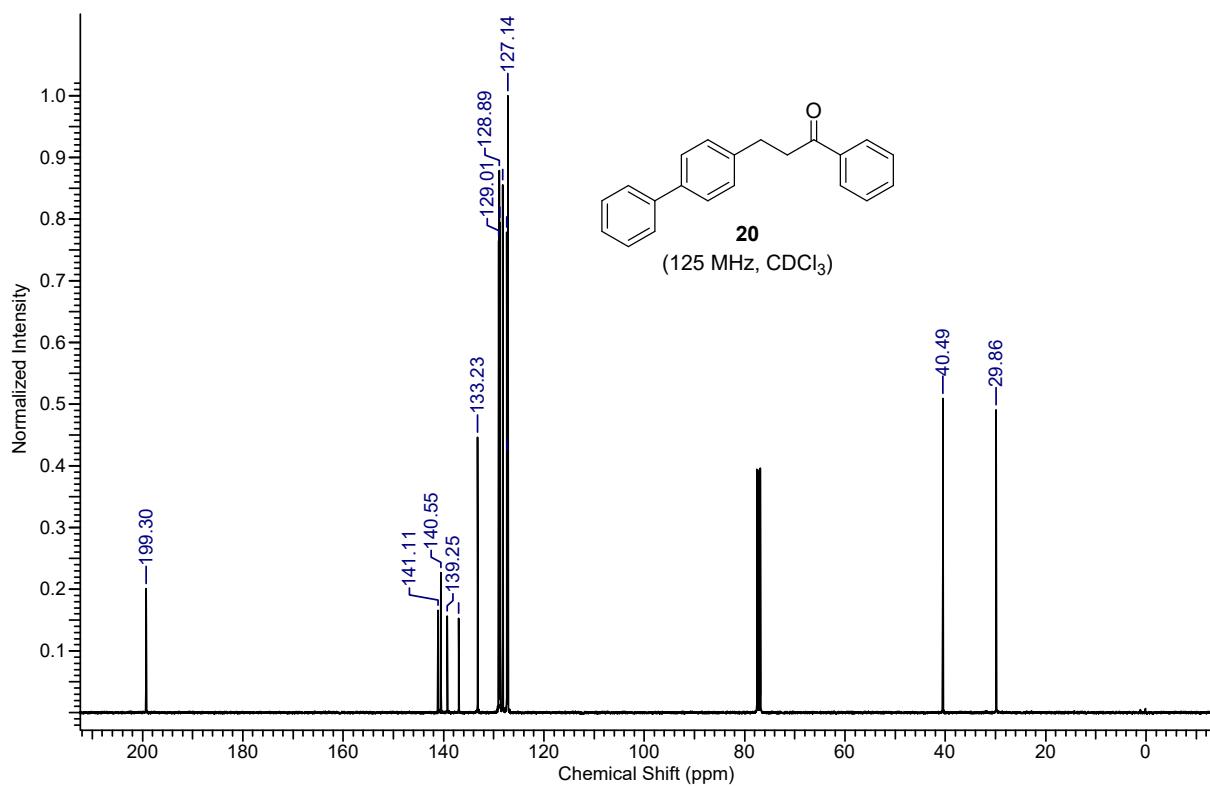
¹H-NMR spectrum of 1-(naphthalen-1-yl)-3-phenylpropan-1-one (**19**)



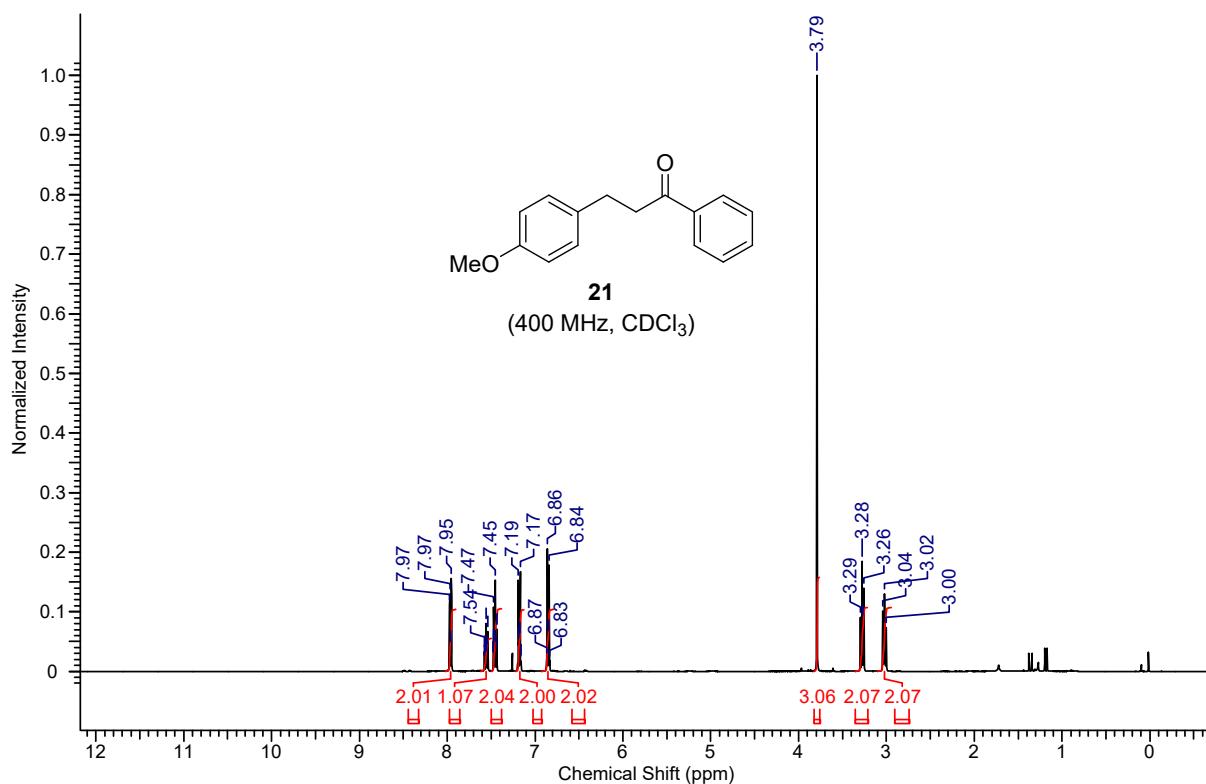
¹³C{¹H}-NMR spectrum of 1-(naphthalen-1-yl)-3-phenylpropan-1-one (**19**)



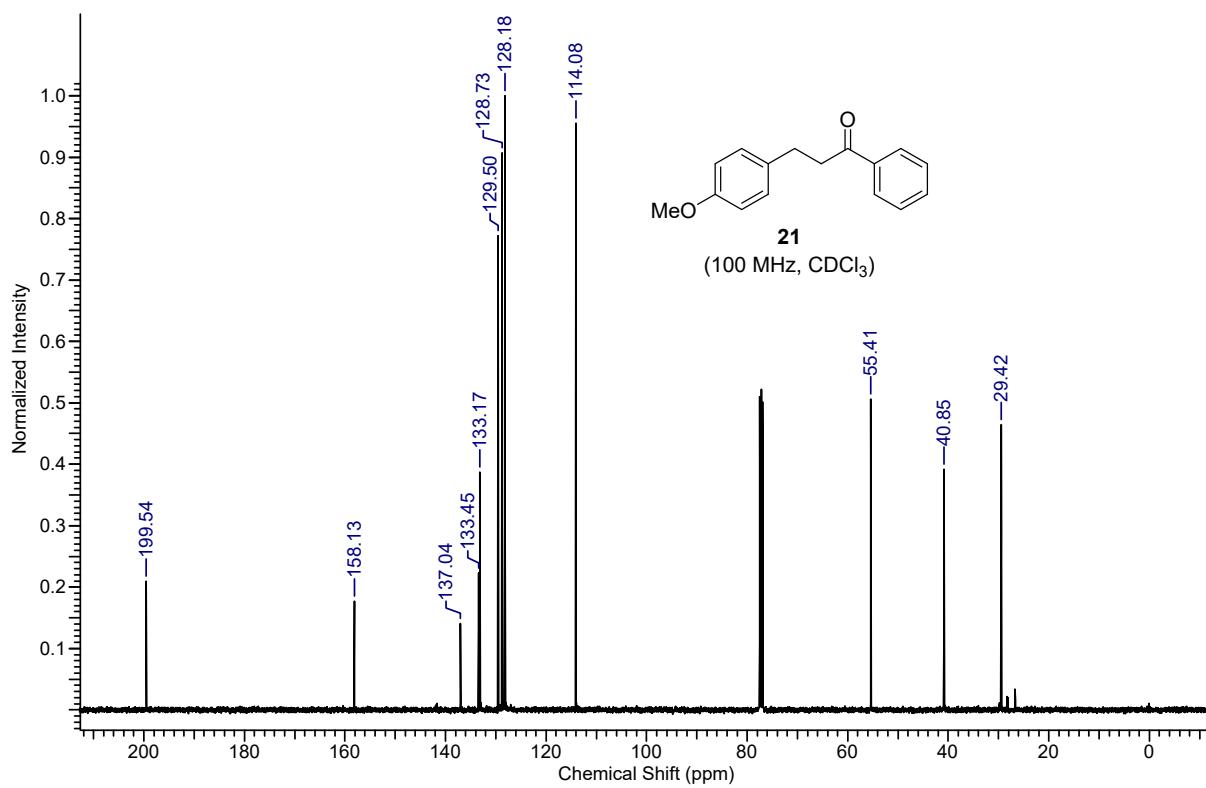
¹H-NMR spectrum of 3-([1,1'-biphenyl]-4-yl)-1-phenylpropan-1-one (**20**)



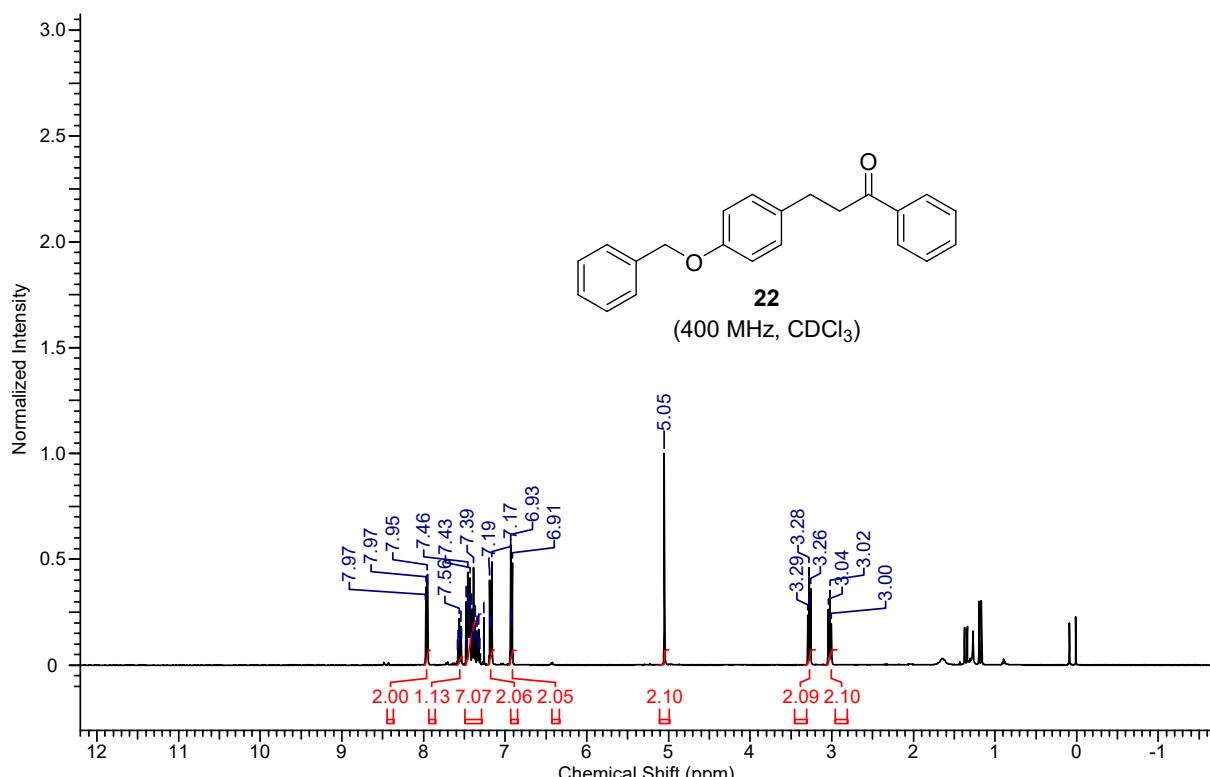
¹³C{¹H}-NMR spectrum of 3-([1,1'-biphenyl]-4-yl)-1-phenylpropan-1-one (**20**)



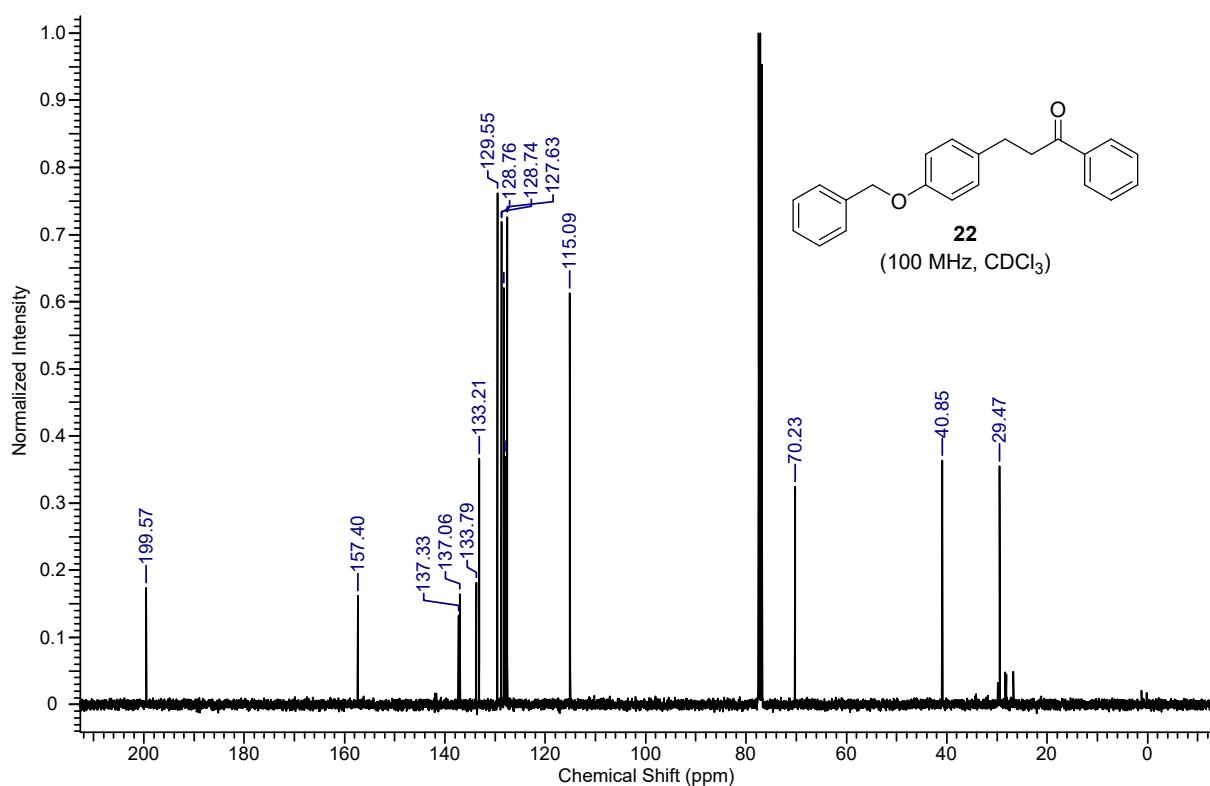
¹H-NMR spectrum of 3-(4-methoxyphenyl)-1-phenylpropan-1-one (**21**)



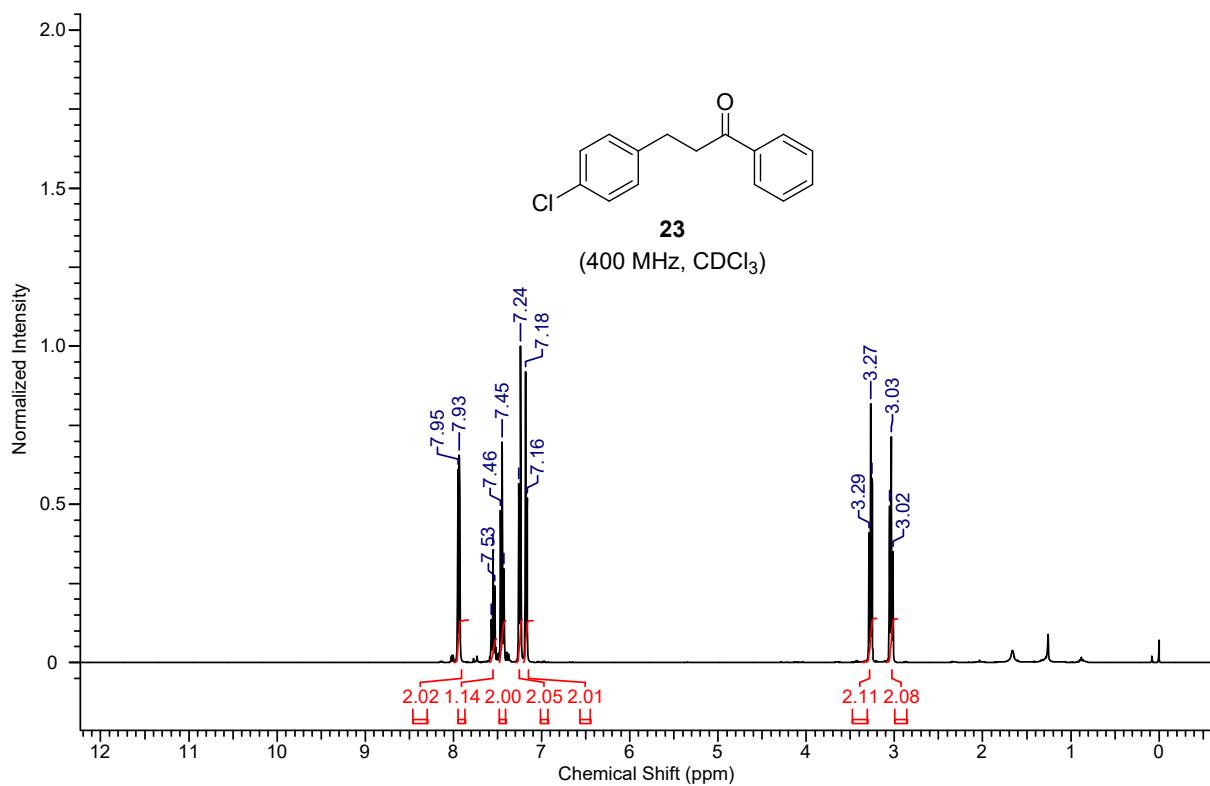
¹³C{¹H}-NMR spectrum of 3-(4-methoxyphenyl)-1-phenylpropan-1-one (**21**)



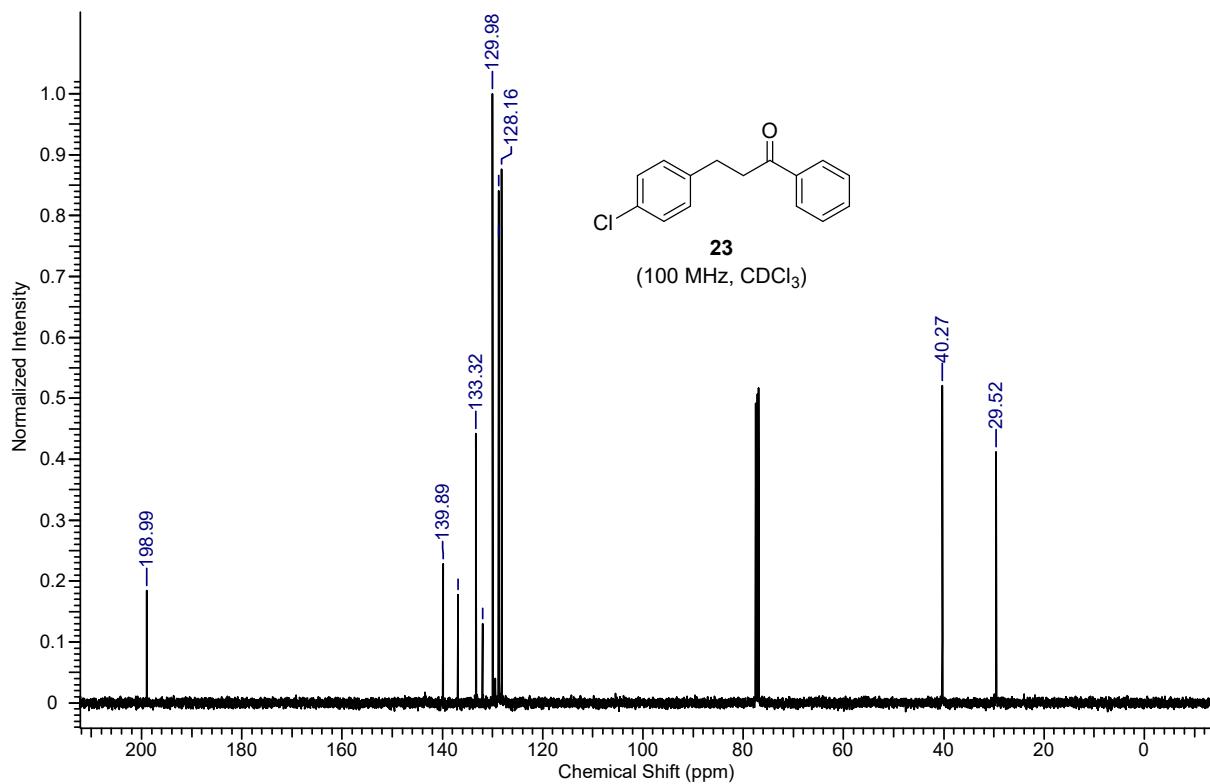
¹H-NMR spectrum of 3-(4-(benzyloxy)phenyl)-1-phenylpropan-1-one (**22**)



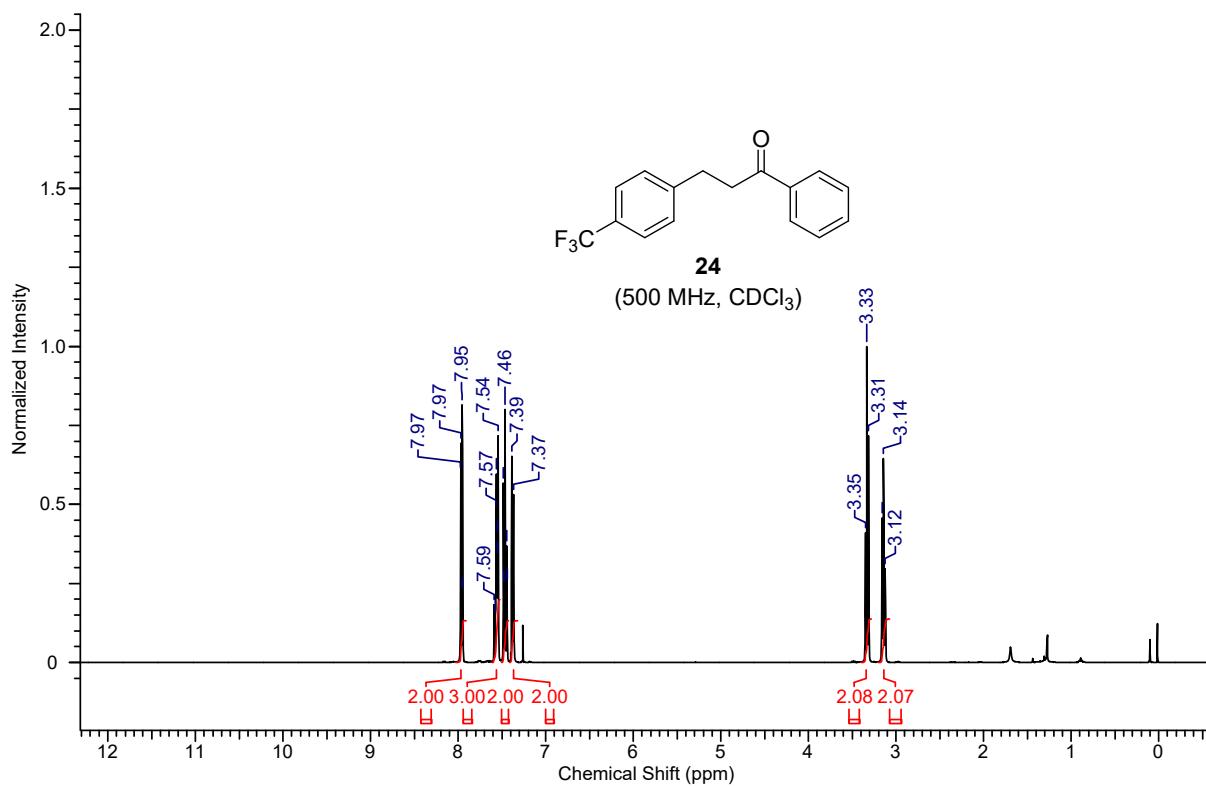
¹³C{¹H}-NMR spectrum of 3-(4-(benzyloxy)phenyl)-1-phenylpropan-1-one (**22**)



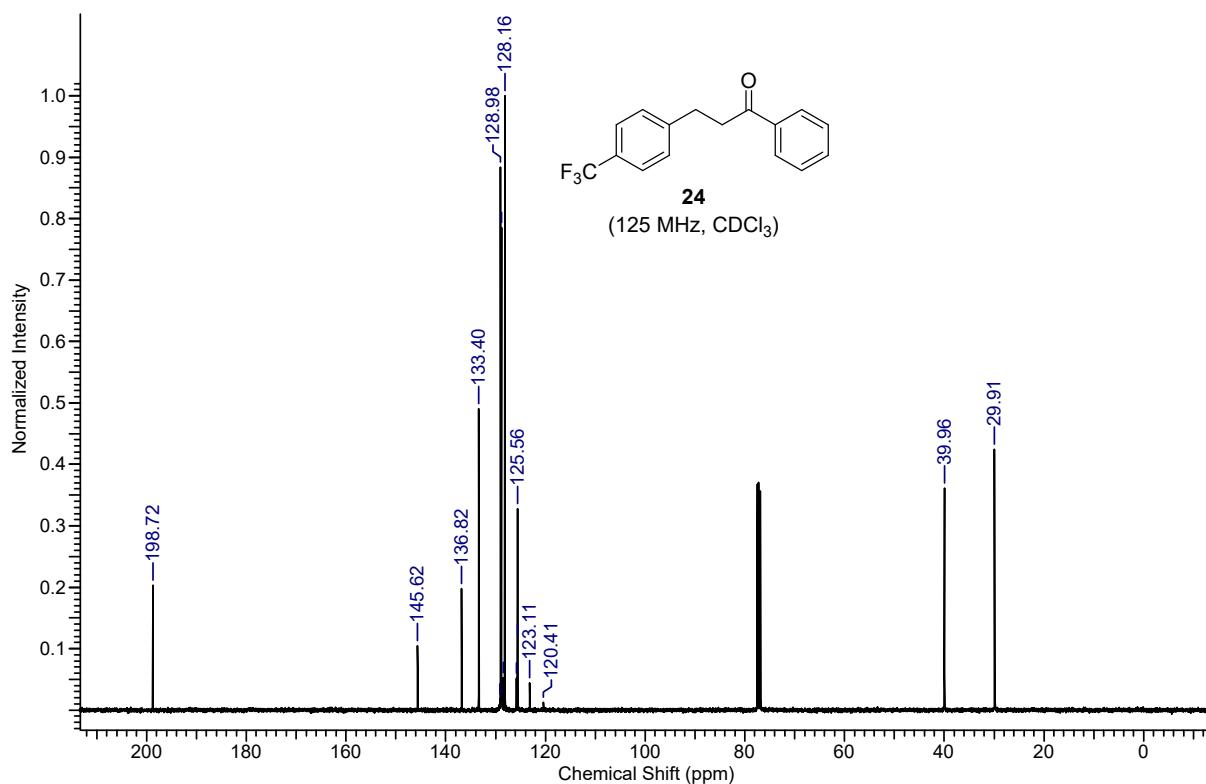
¹H-NMR spectrum of 3-(4-chlorophenyl)-1-phenylpropan-1-one (**23**)



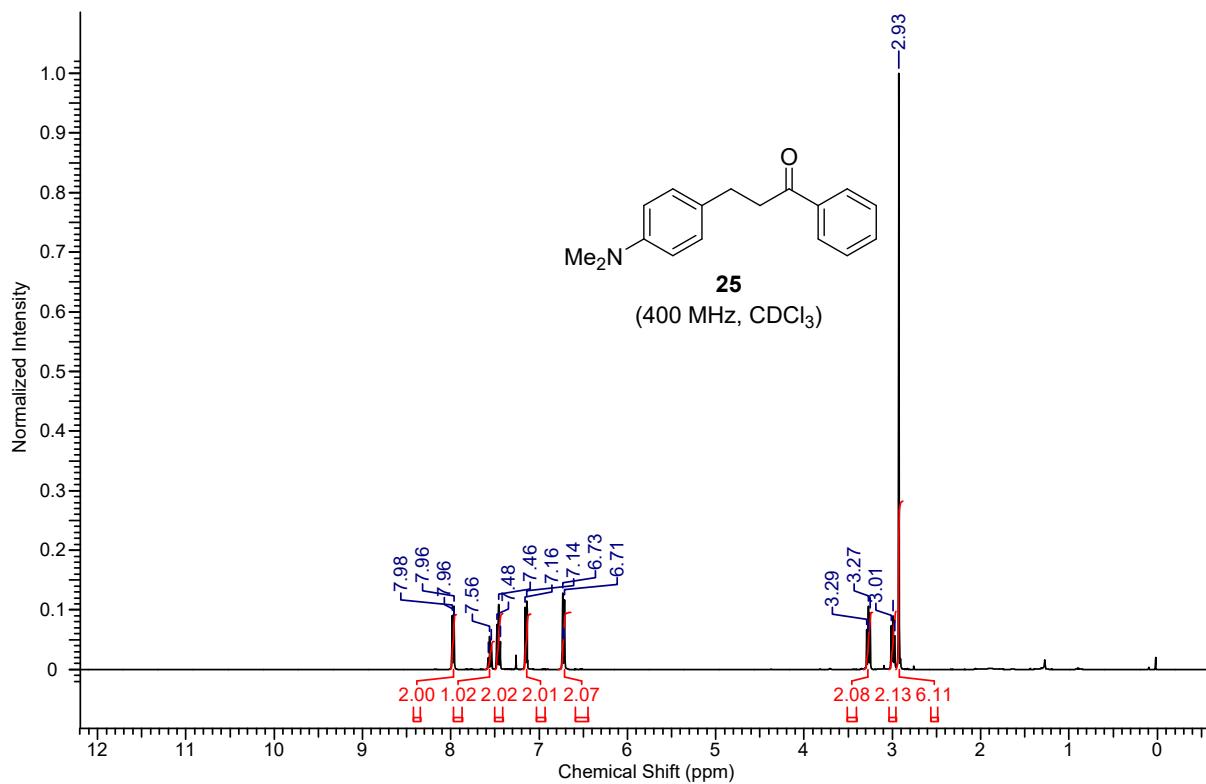
¹³C{¹H}-NMR spectrum of 3-(4-chlorophenyl)-1-phenylpropan-1-one (**23**)



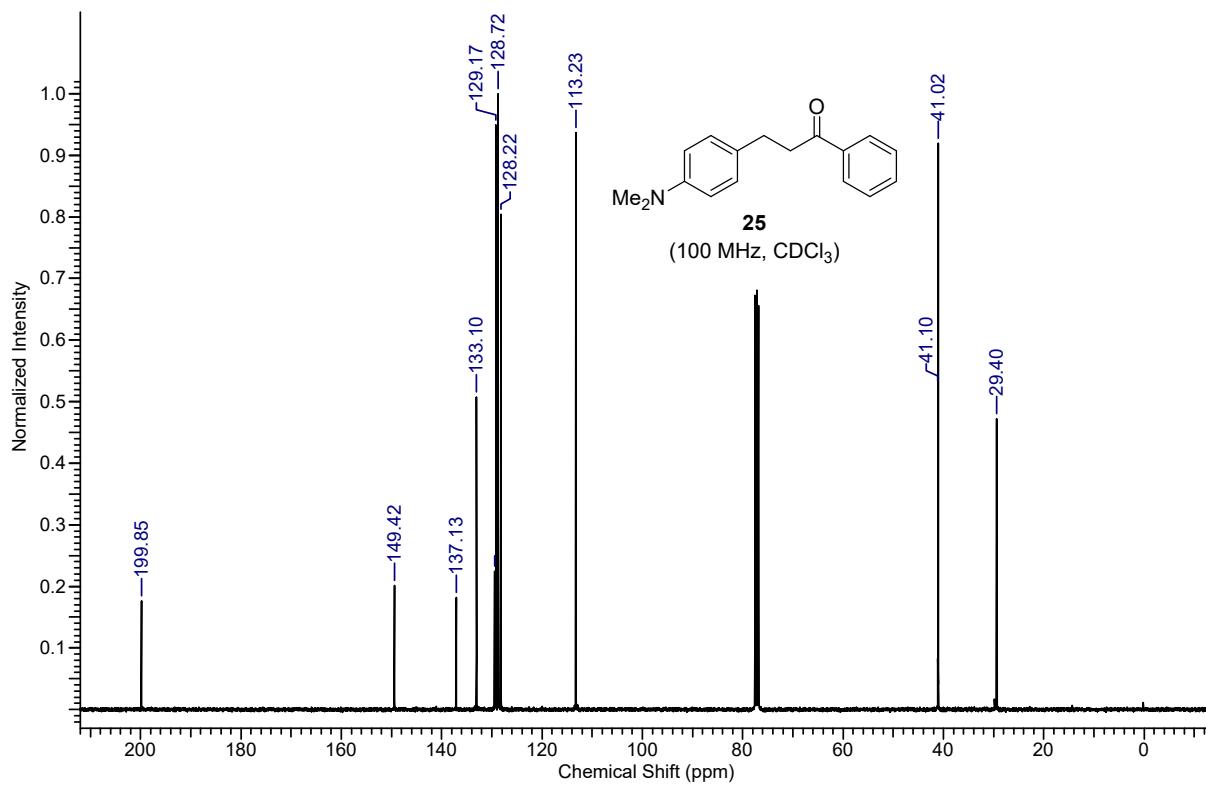
¹H-NMR spectrum of 1-phenyl-3-(4-(trifluoromethyl)phenyl)propan-1-one (**24**)



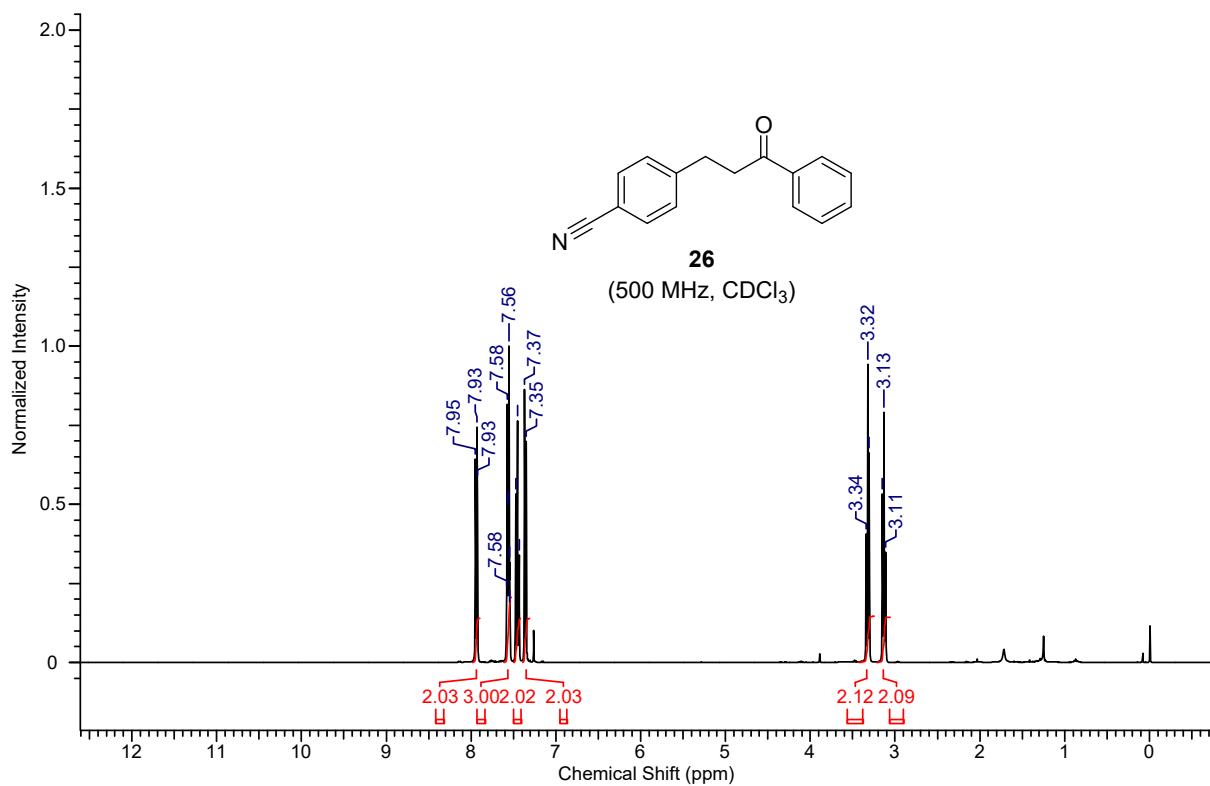
¹³C{¹H}-NMR spectrum of 1-phenyl-3-(4-(trifluoromethyl)phenyl)propan-1-one (**24**)



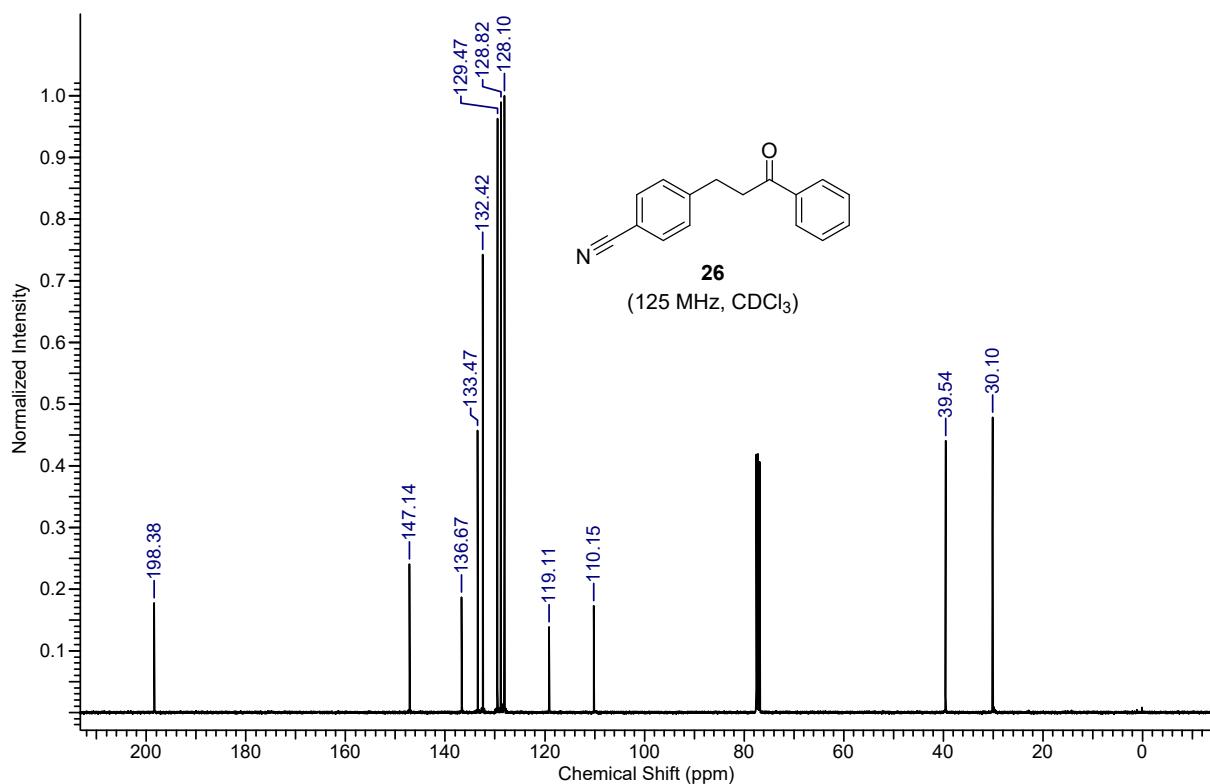
¹H-NMR spectrum of 3-(4-(dimethylamino)phenyl)-1-phenylpropan-1-one (**25**)



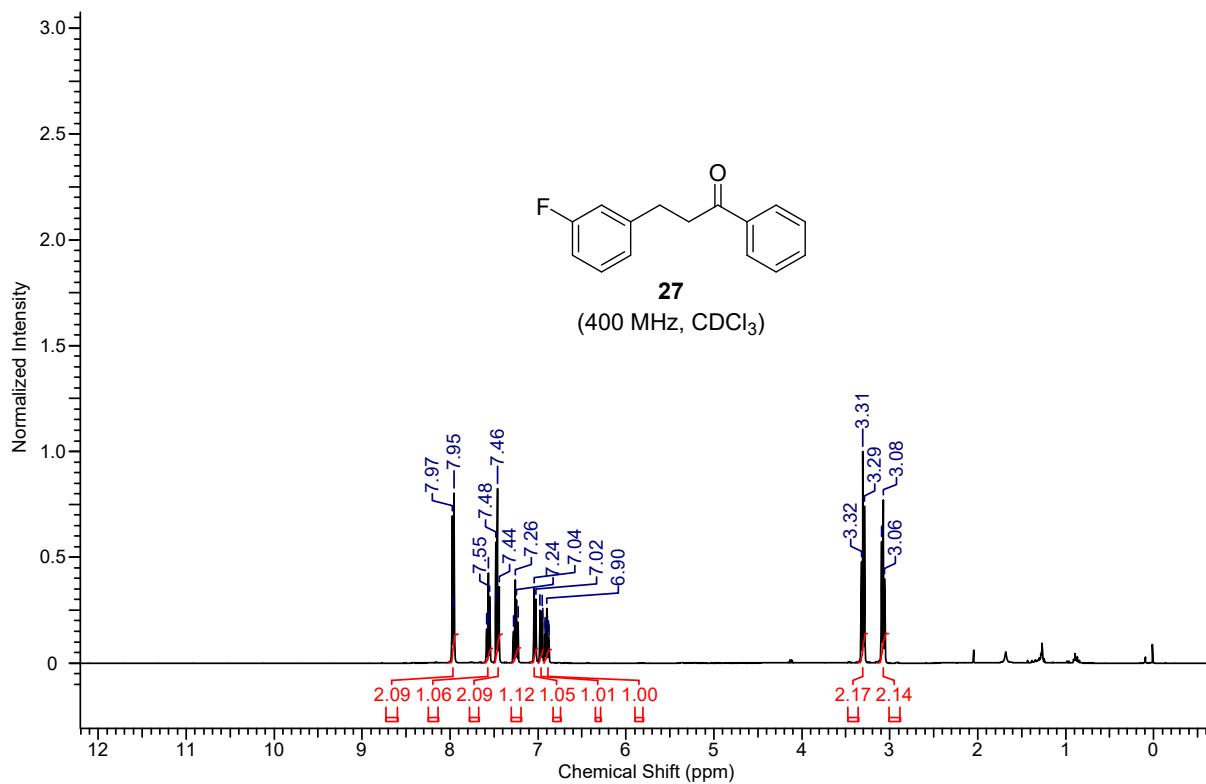
¹³C{¹H}-NMR spectrum of 3-(4-(dimethylamino)phenyl)-1-phenylpropan-1-one (**25**)



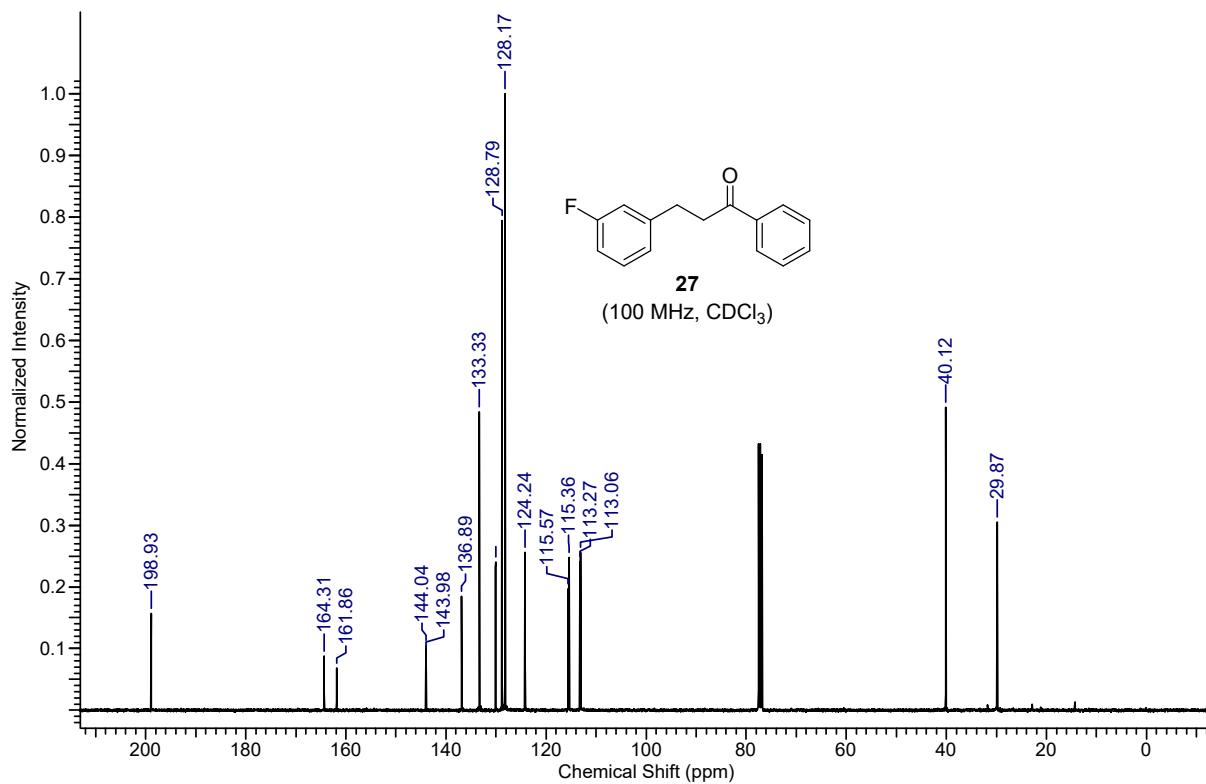
^1H -NMR spectrum of 4-(3-oxo-3-phenylpropyl)benzonitrile (**26**)



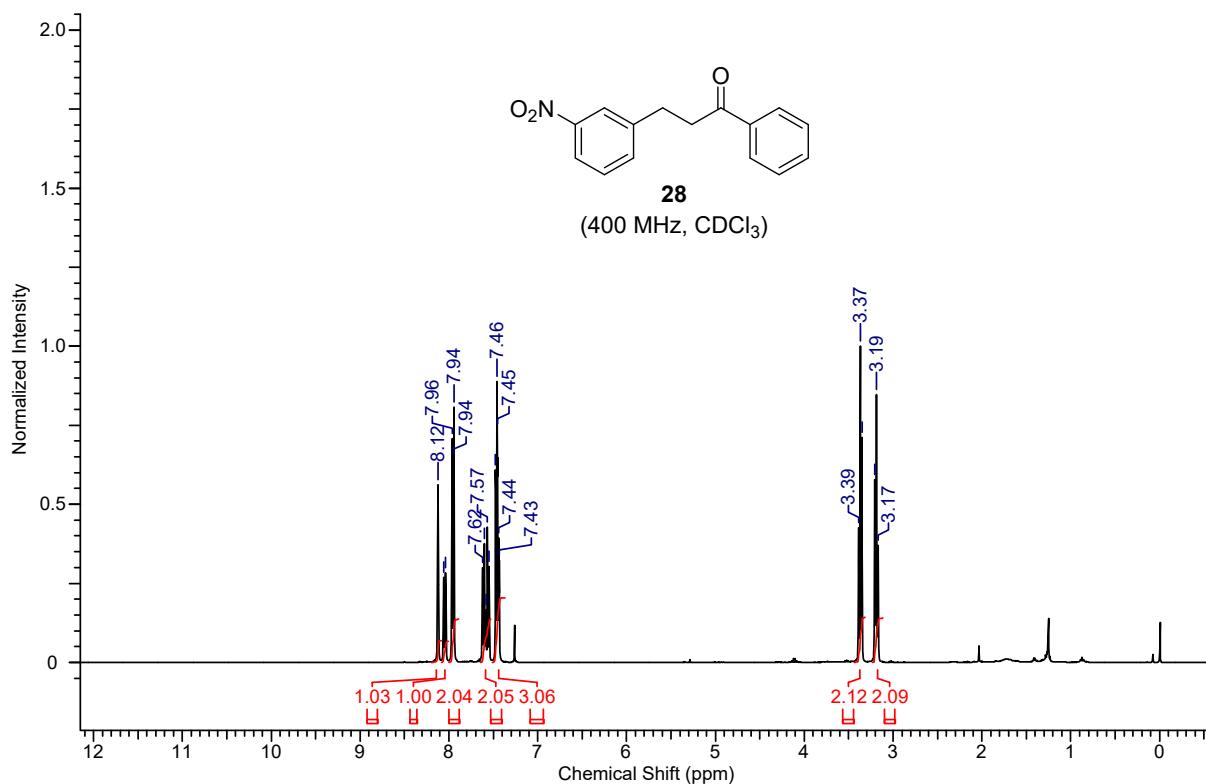
$^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum of 4-(3-oxo-3-phenylpropyl)benzonitrile (**26**)



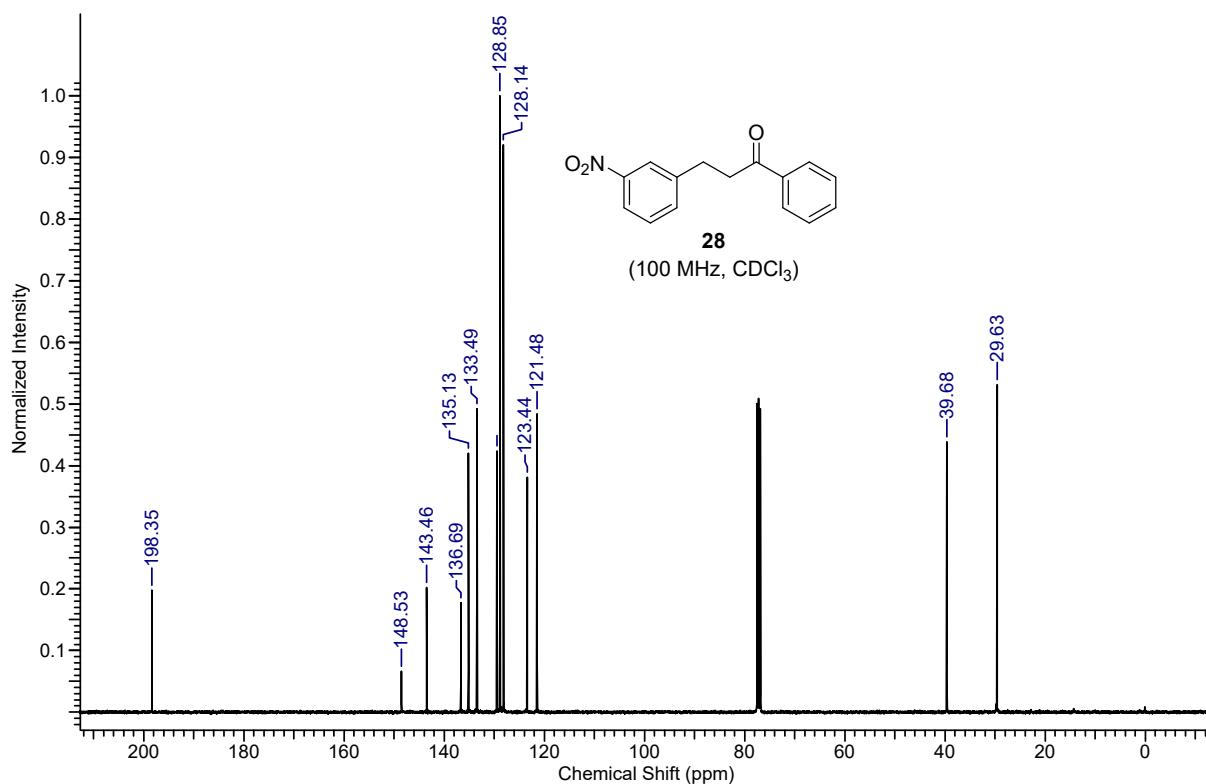
¹H-NMR spectrum of 3-(3-fluorophenyl)-1-phenylpropan-1-one (**27**)



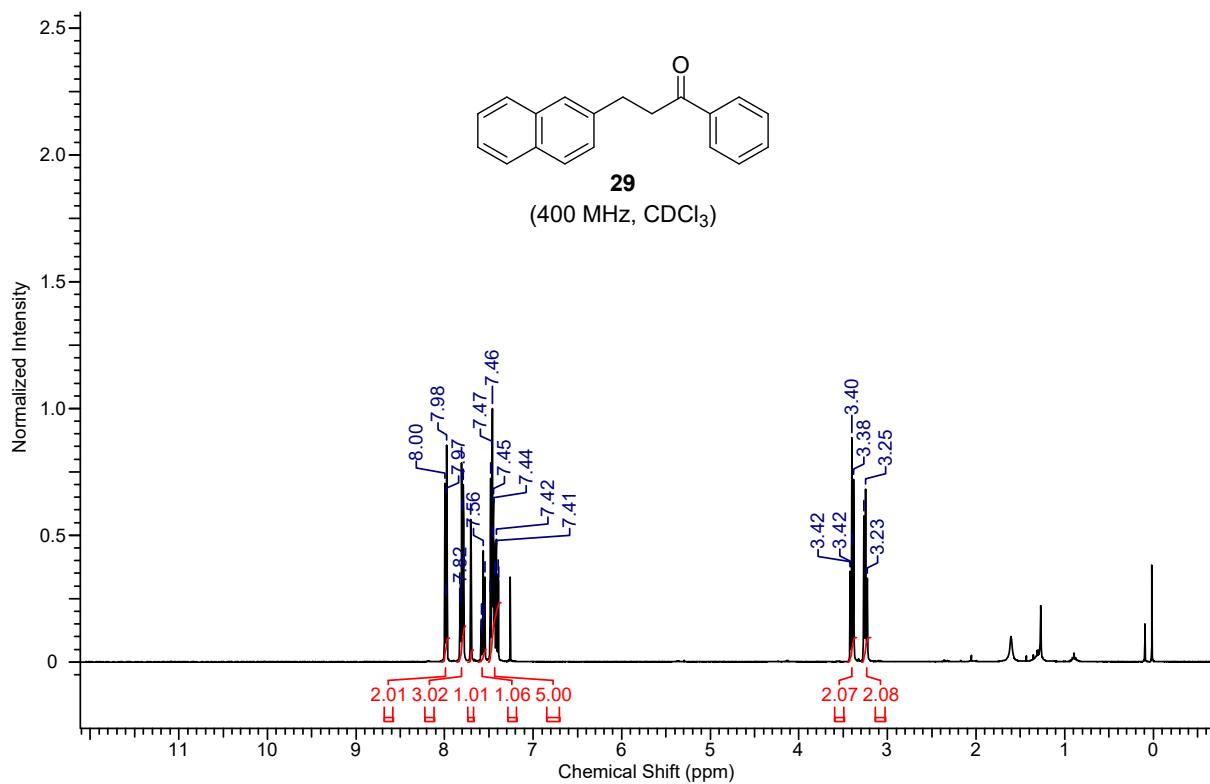
¹³C{¹H}-NMR spectrum of 3-(3-fluorophenyl)-1-phenylpropan-1-one (**27**)



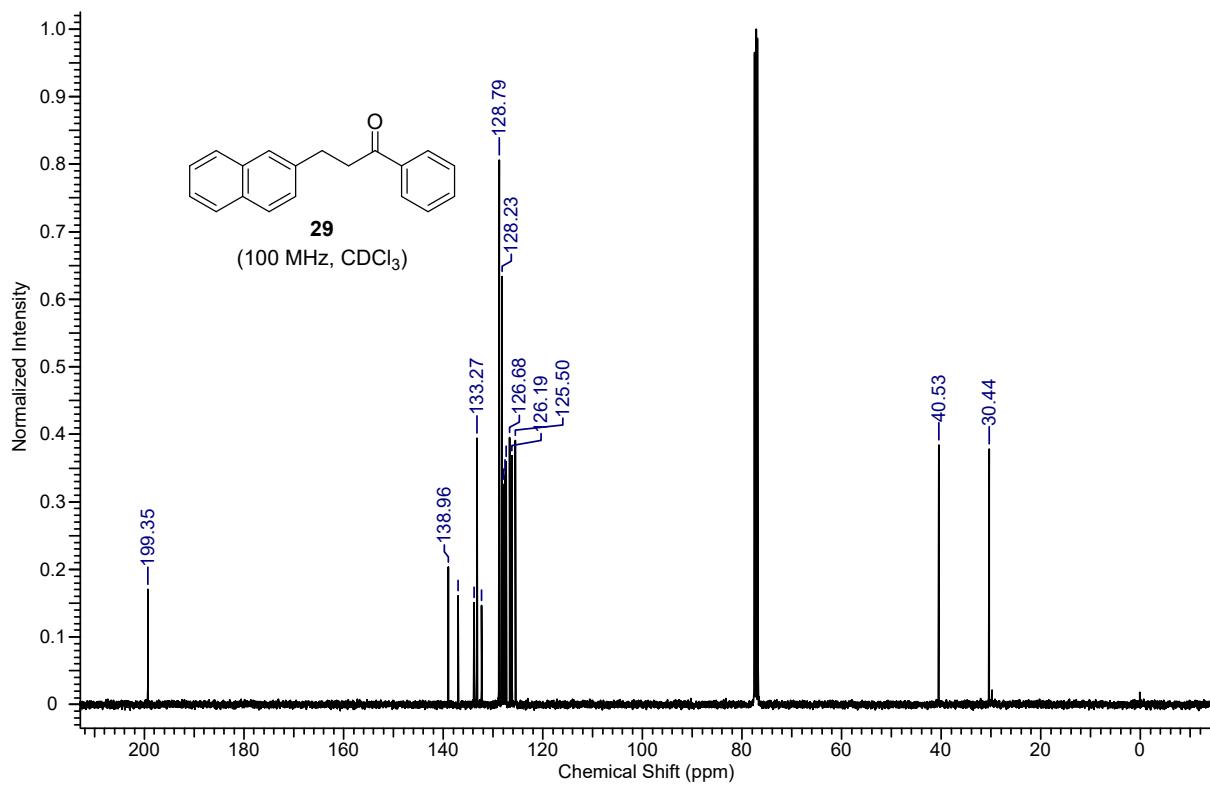
¹H-NMR spectrum of 3-(3-nitrophenyl)-1-phenylpropan-1-one (**28**)



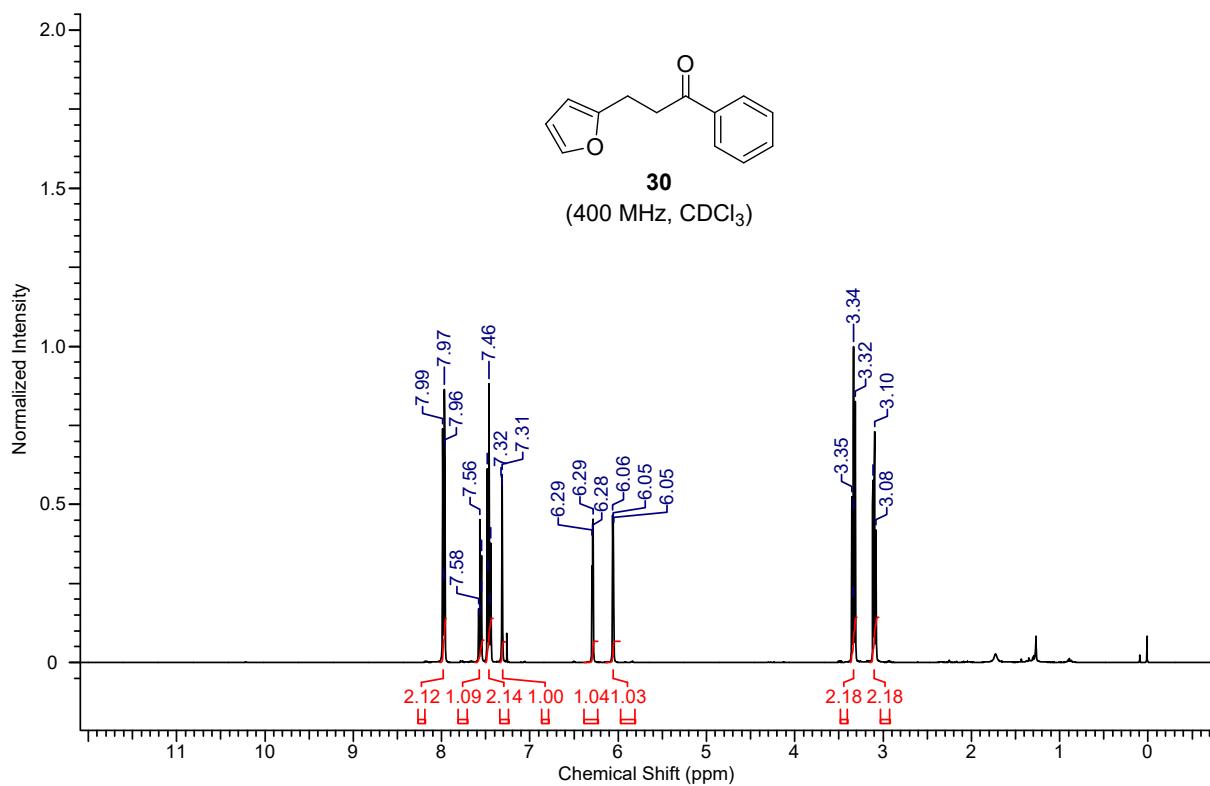
¹³C{¹H}-NMR spectrum of 3-(3-nitrophenyl)-1-phenylpropan-1-one (**28**)



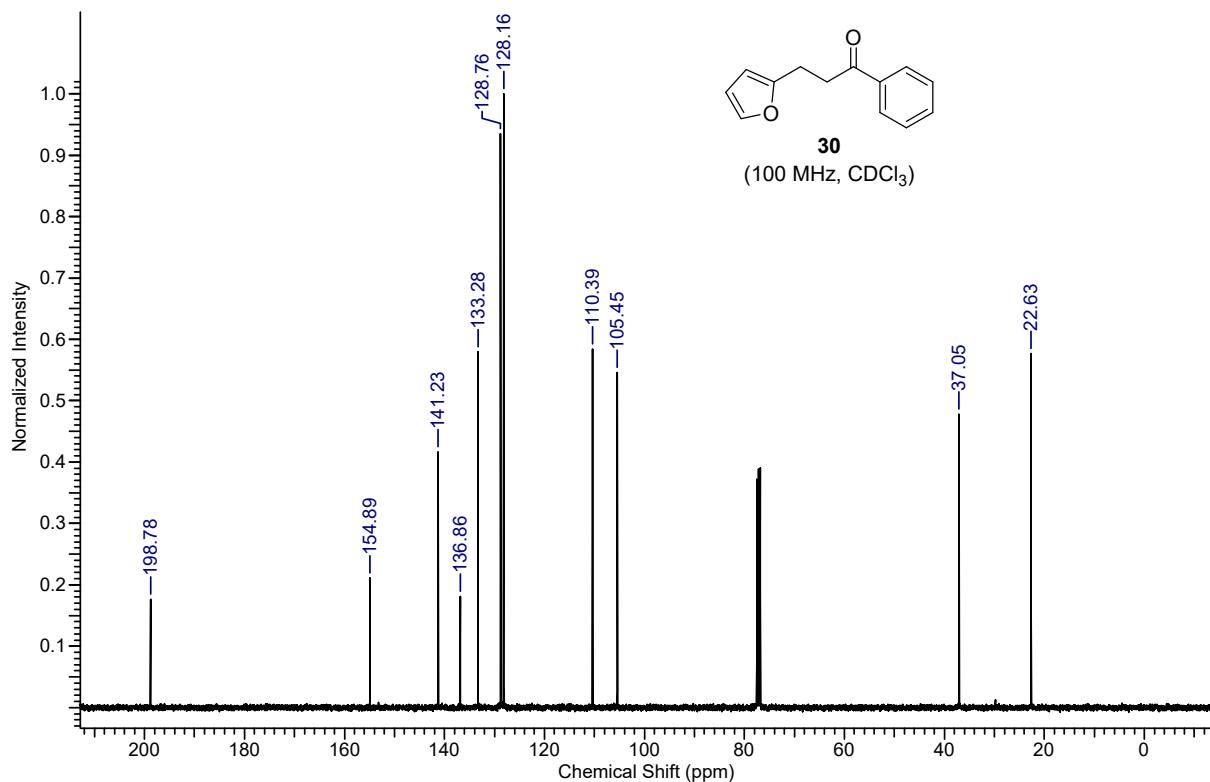
¹H-NMR spectrum of 3-(naphthalen-2-yl)-1-phenylpropan-1-one (**29**)



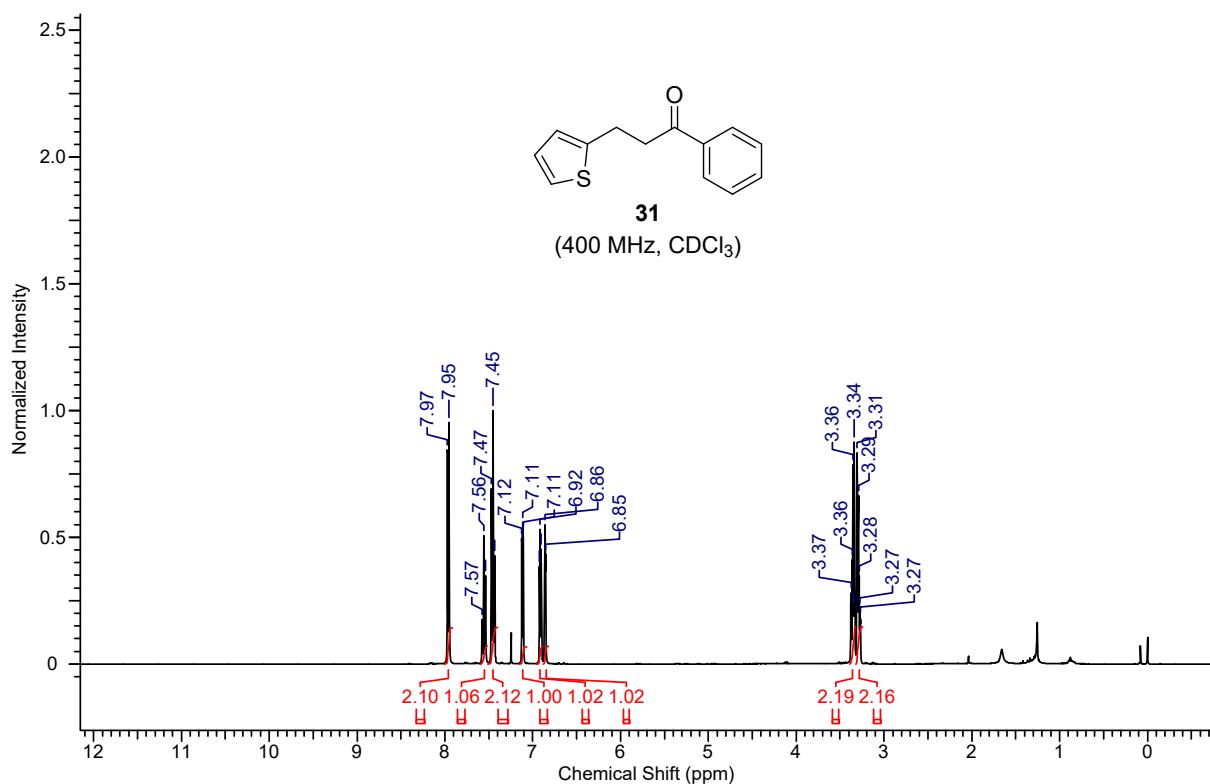
¹³C{¹H}-NMR spectrum of 3-(naphthalen-2-yl)-1-phenylpropan-1-one (**29**)



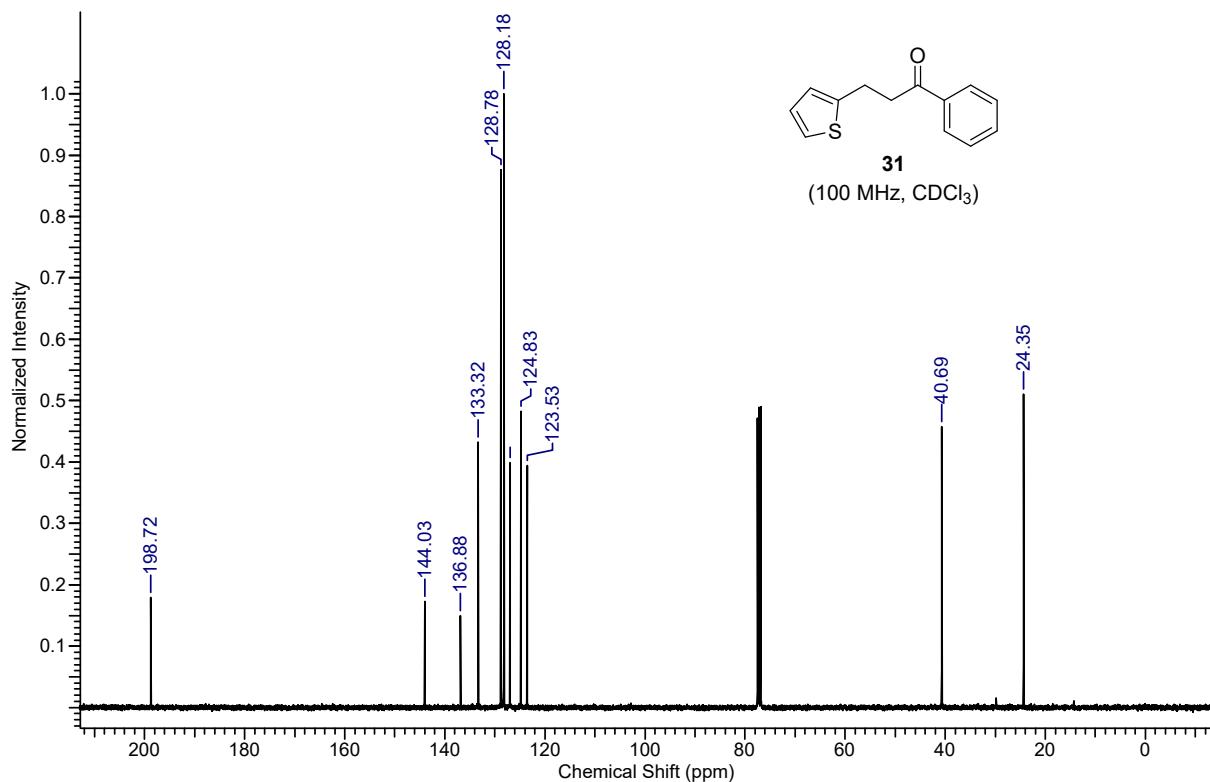
¹H-NMR spectrum of 3-(furan-2-yl)-1-phenylpropan-1-one (**30**)



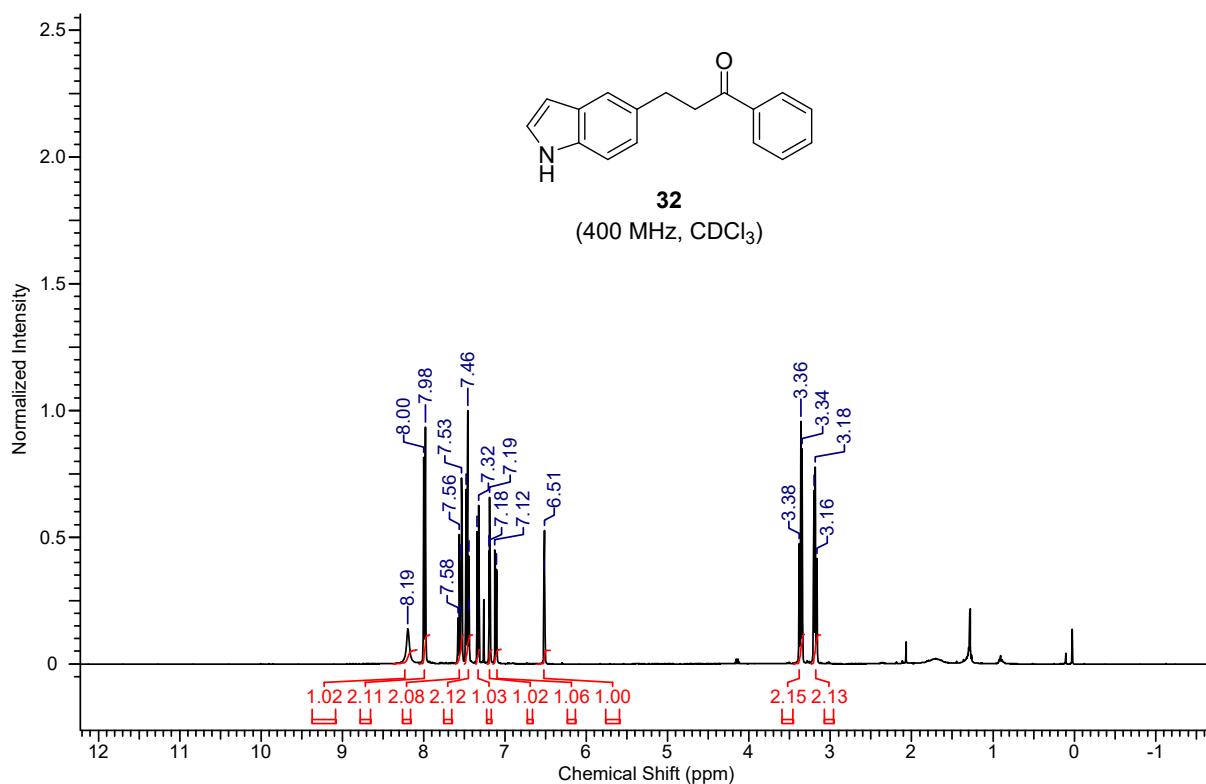
¹³C{¹H}-NMR spectrum of 3-(furan-2-yl)-1-phenylpropan-1-one (**30**)



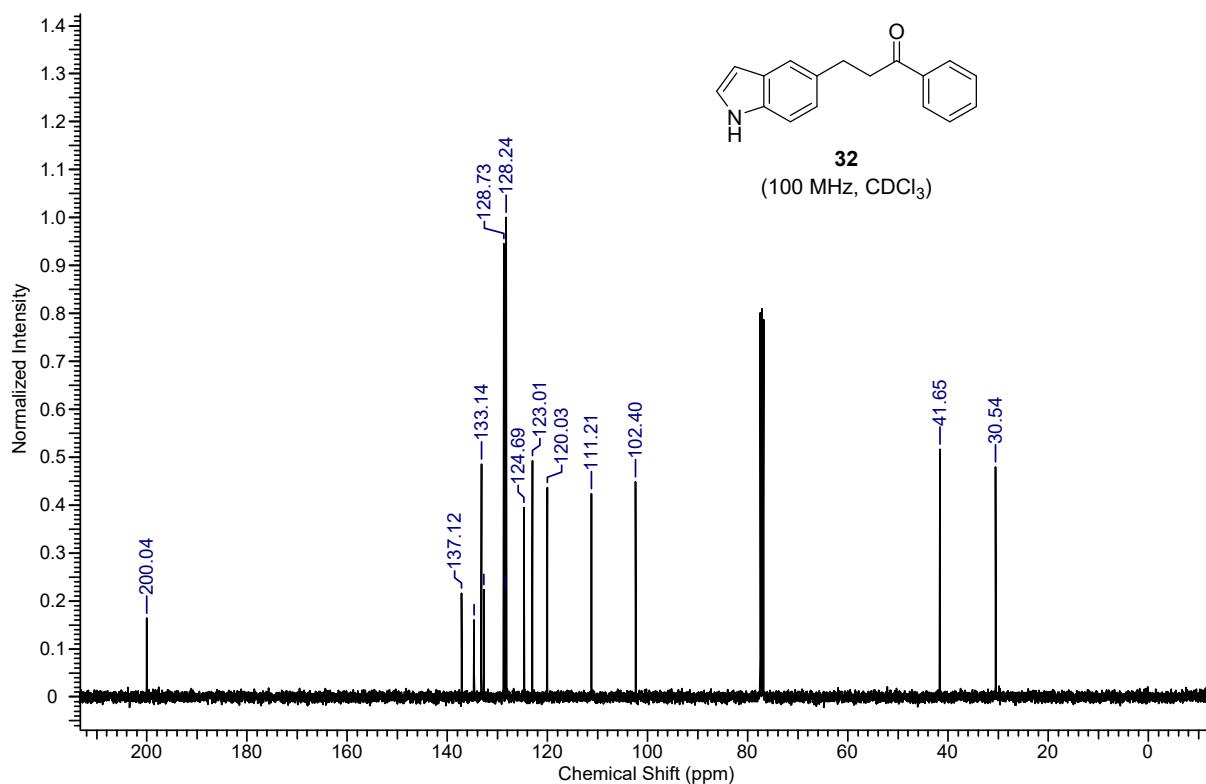
¹H-NMR spectrum of 1-phenyl-3-(thiophen-2-yl)propan-1-one (**31**)



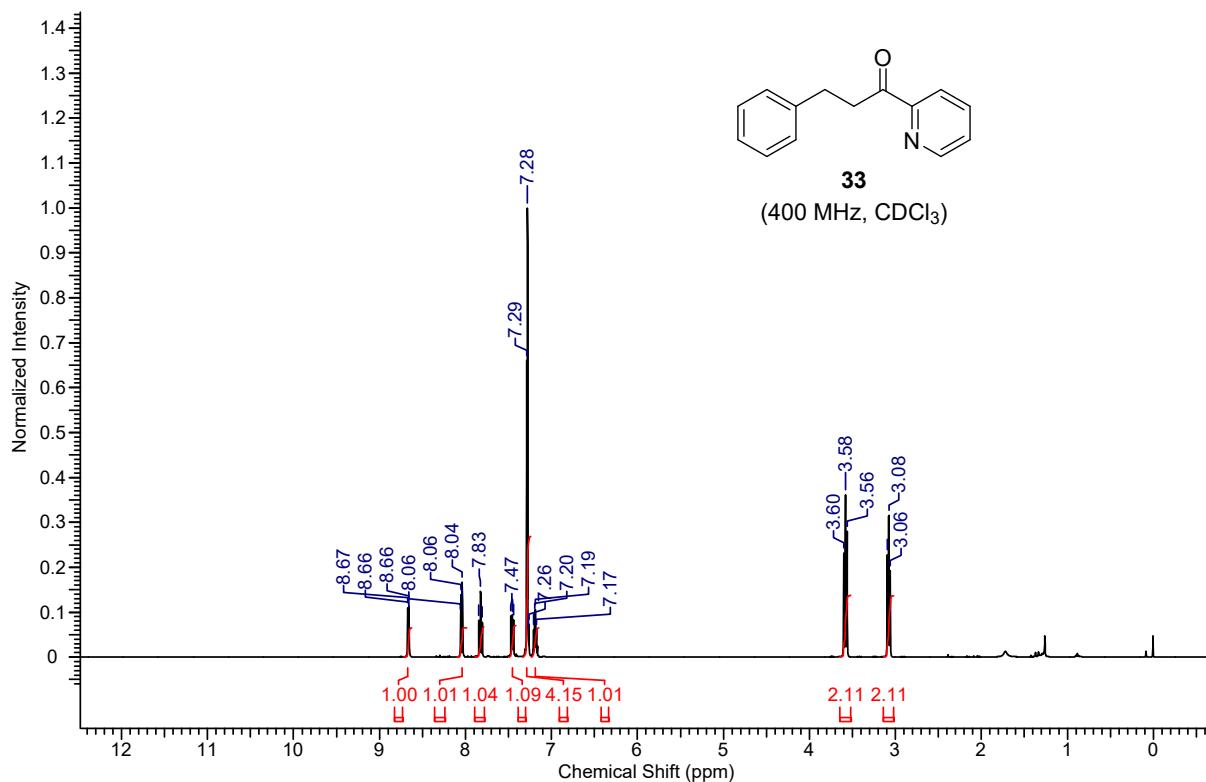
¹³C{¹H}-NMR spectrum of 1-phenyl-3-(thiophen-2-yl)propan-1-one (**31**)



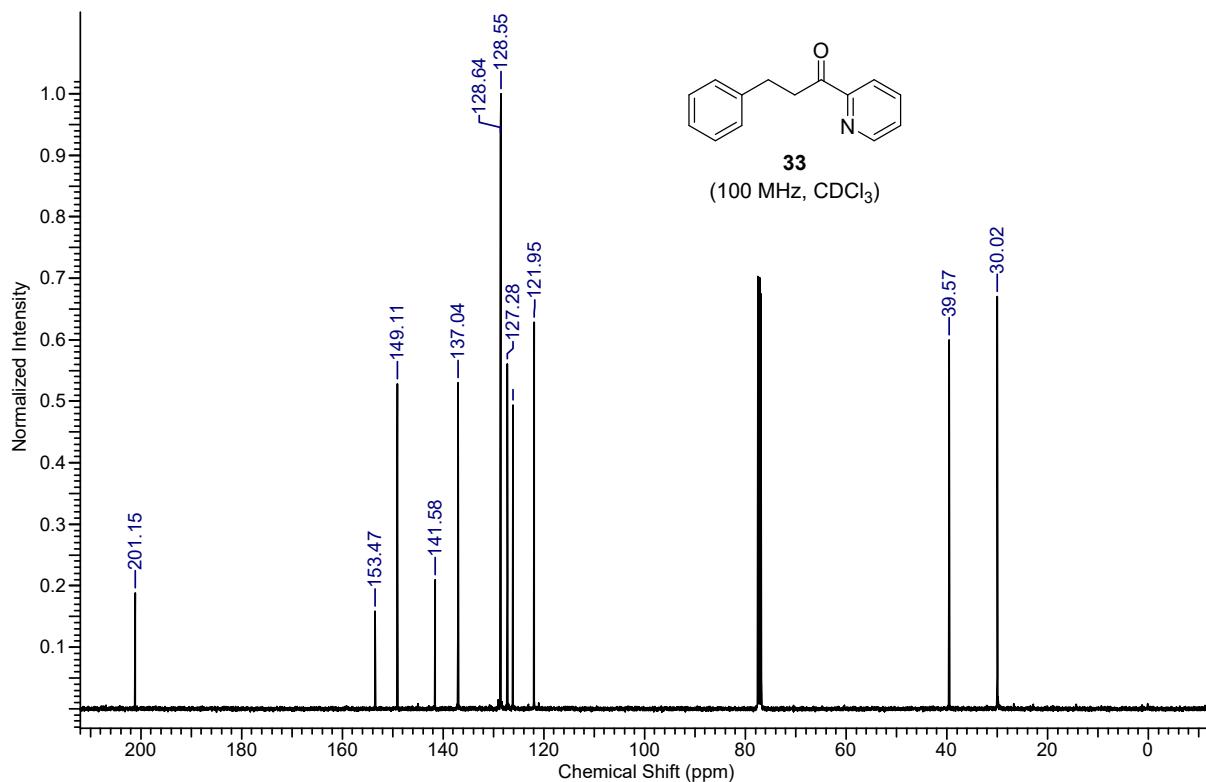
¹H-NMR spectrum of 3-(1*H*-indol-5-yl)-1-phenylpropan-1-one (**32**)



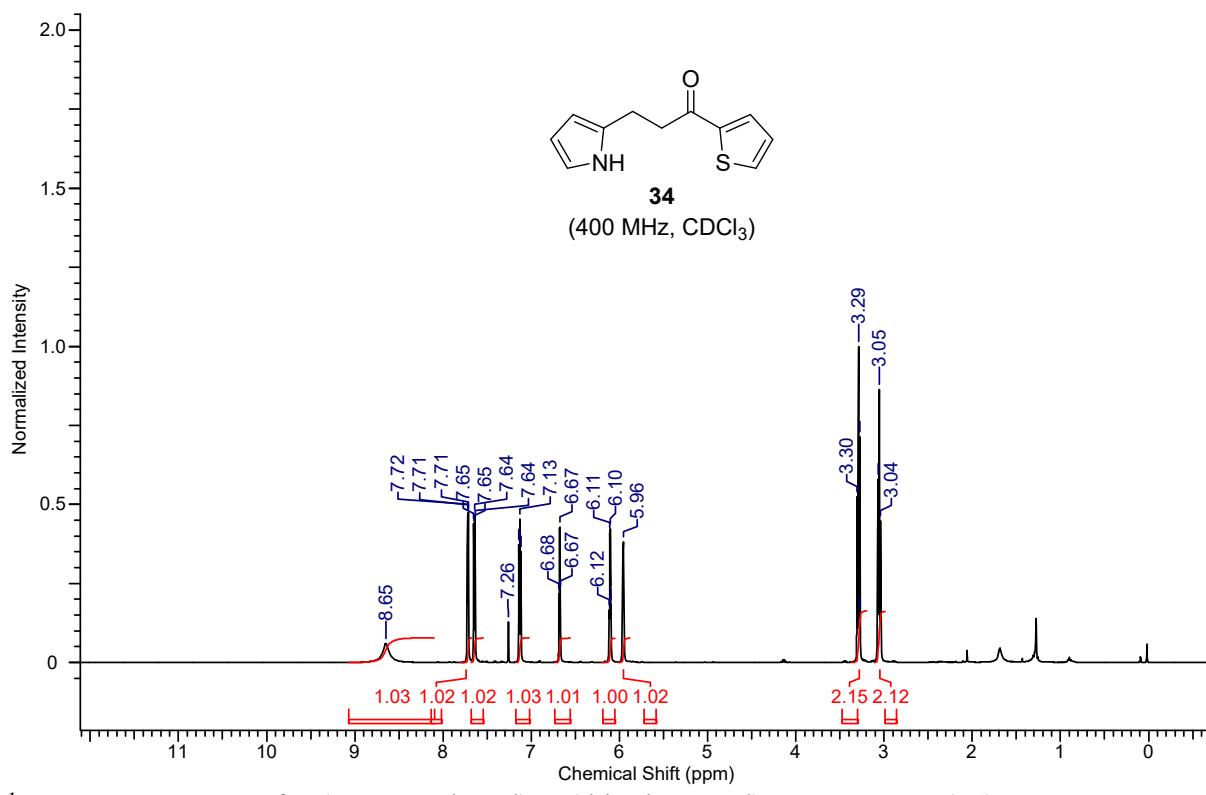
¹³C{¹H}-NMR spectrum of 3-(1*H*-indol-5-yl)-1-phenylpropan-1-one (**32**)



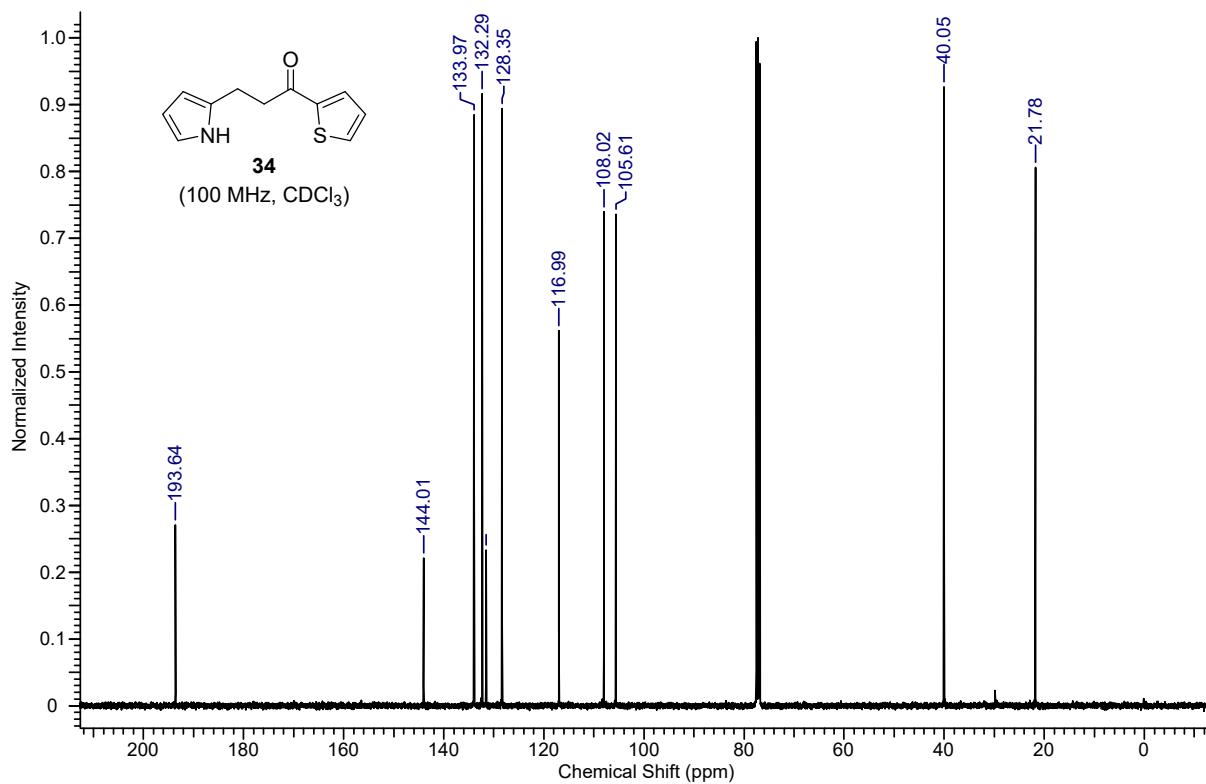
¹H-NMR spectrum of 3-phenyl-1-(pyridin-2-yl)propan-1-one (**33**)



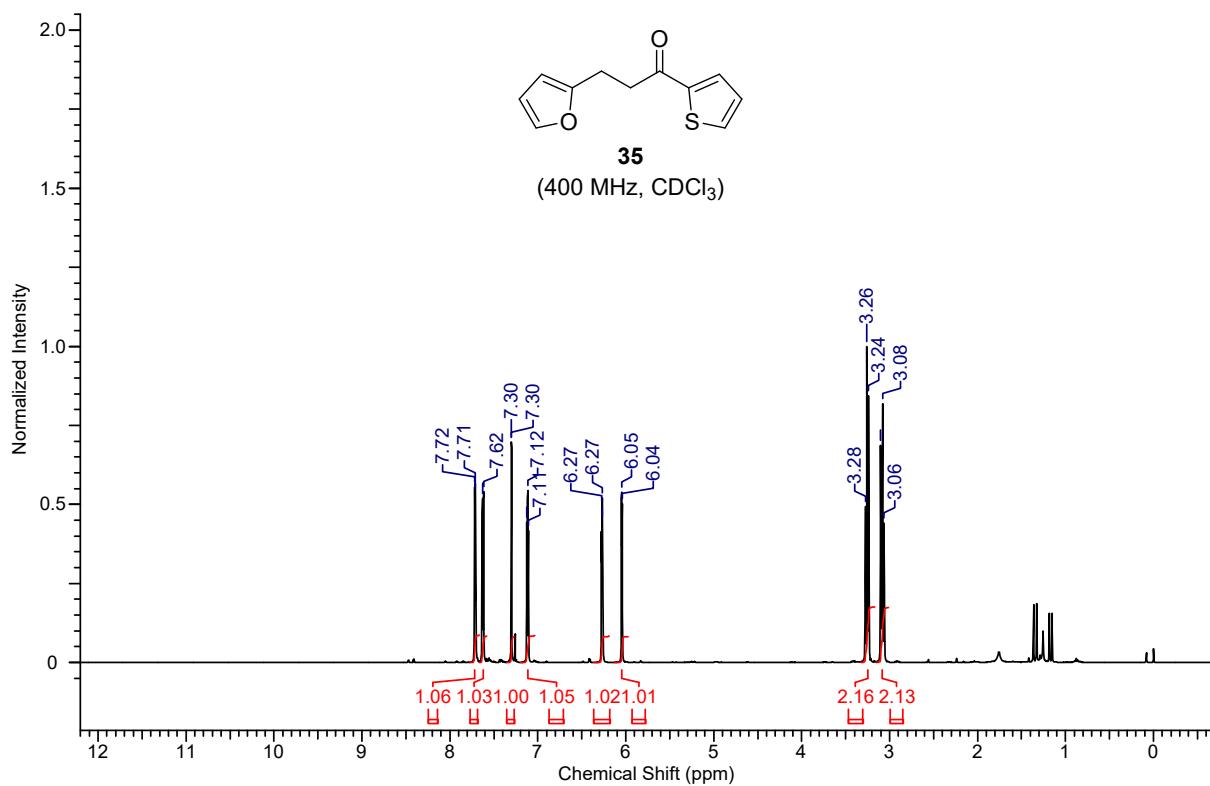
¹³C{¹H}-NMR spectrum of 3-phenyl-1-(pyridin-2-yl)propan-1-one (**33**)



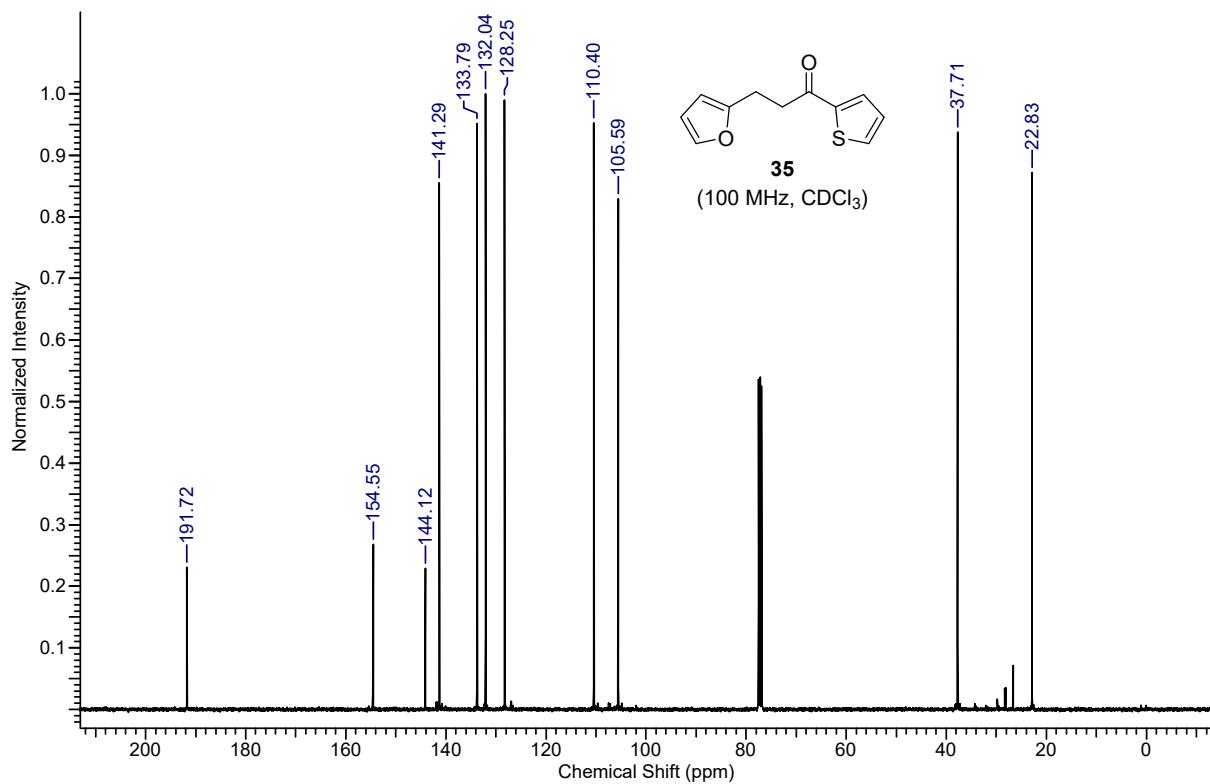
¹H-NMR spectrum of 3-(1*H*-pyrrol-2-yl)-1-(thiophen-2-yl)propan-1-one (**34**)



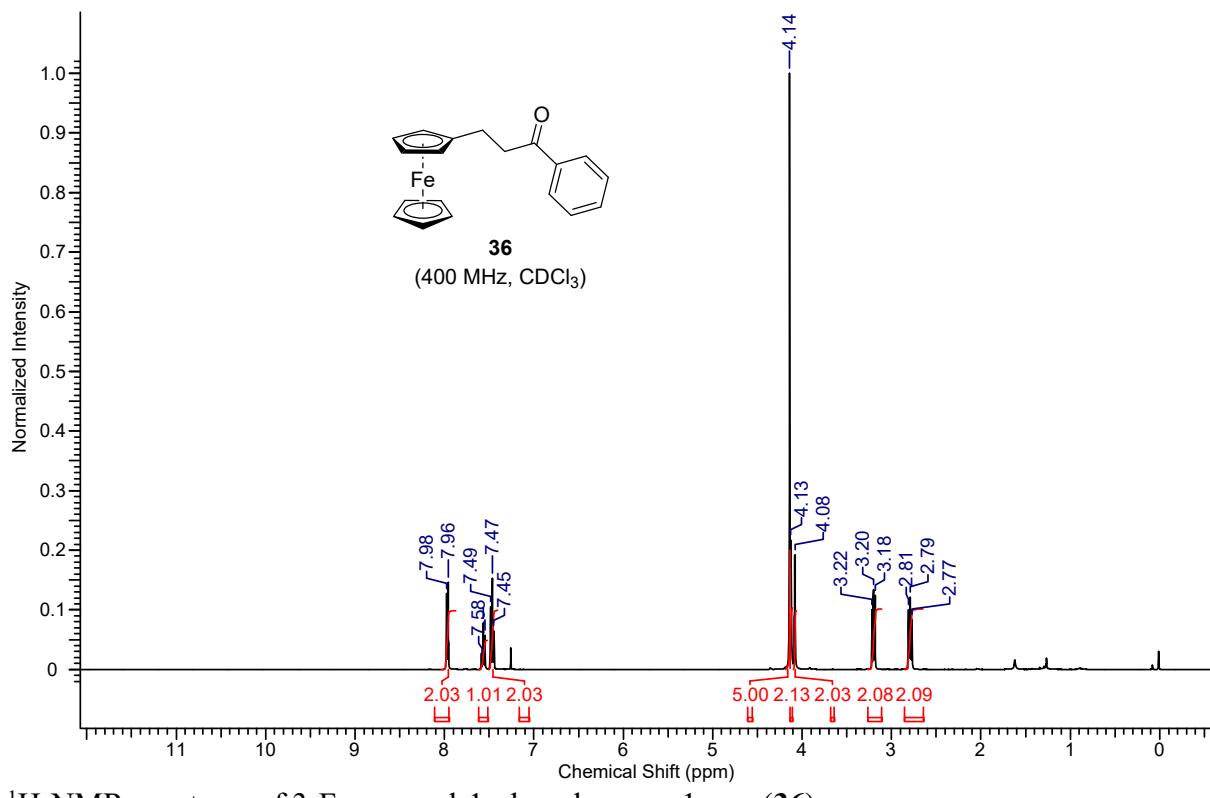
¹³C{¹H}-NMR spectrum of 3-(1*H*-pyrrol-2-yl)-1-(thiophen-2-yl)propan-1-one (**34**)



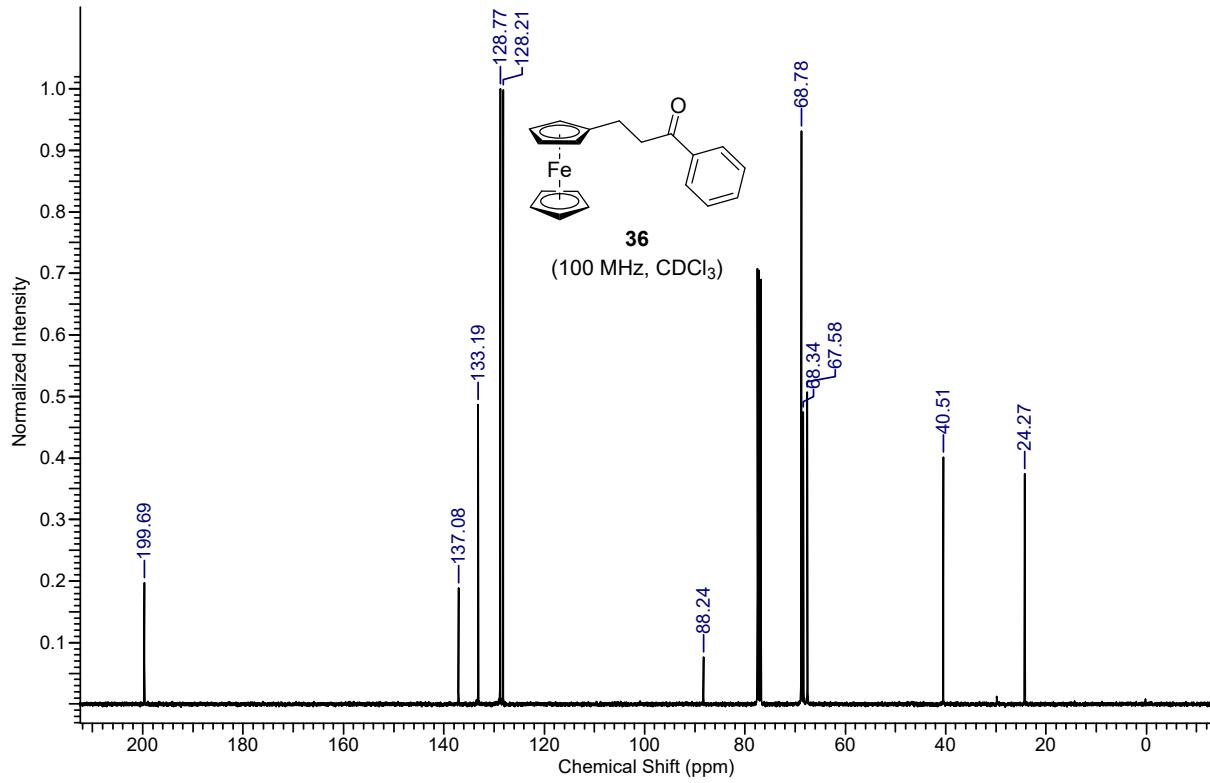
¹H-NMR spectrum of 3-(furan-2-yl)-1-(thiophen-2-yl)propan-1-one (**35**)



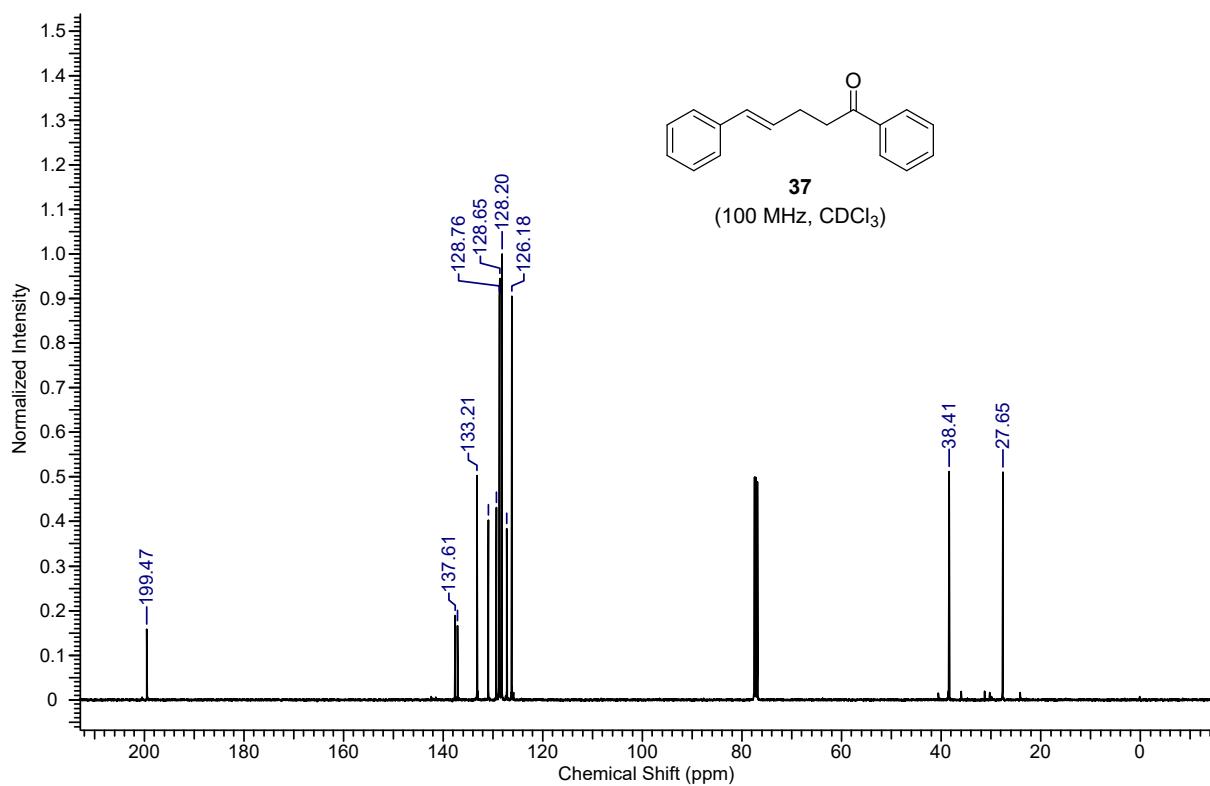
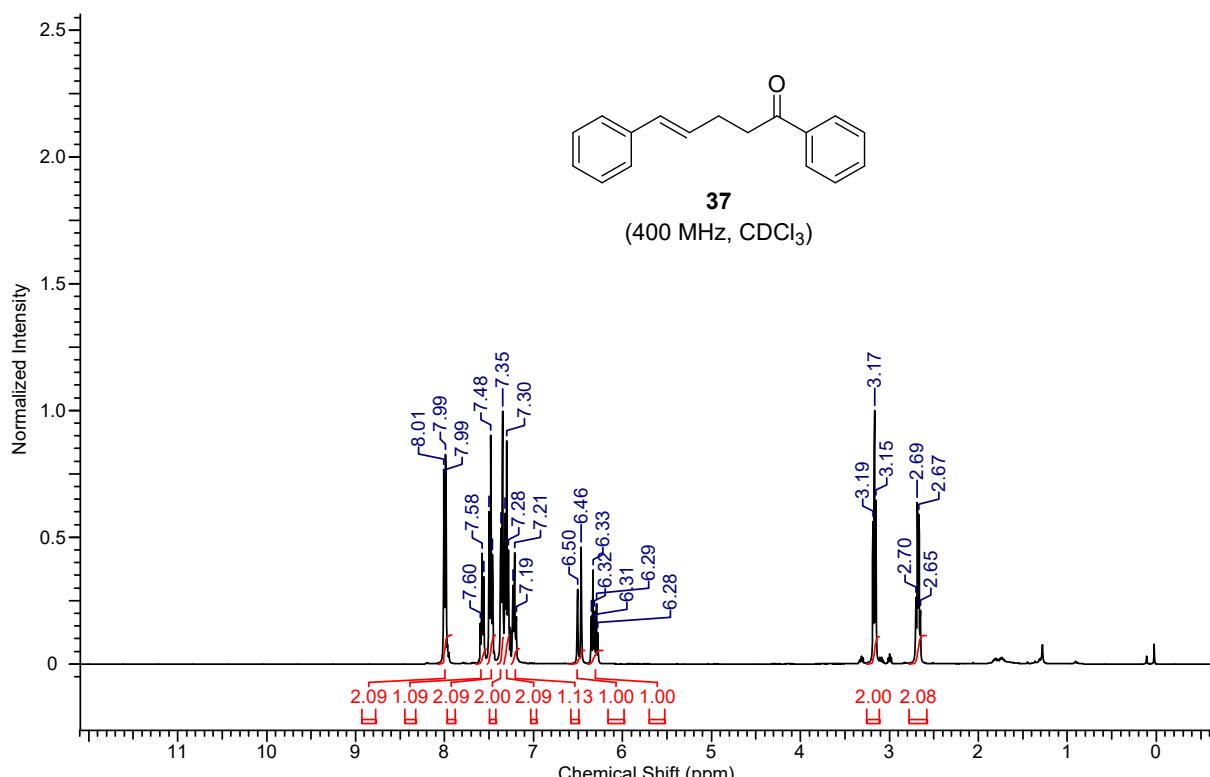
¹³C{¹H}-NMR spectrum of 3-(furan-2-yl)-1-(thiophen-2-yl)propan-1-one (**35**)

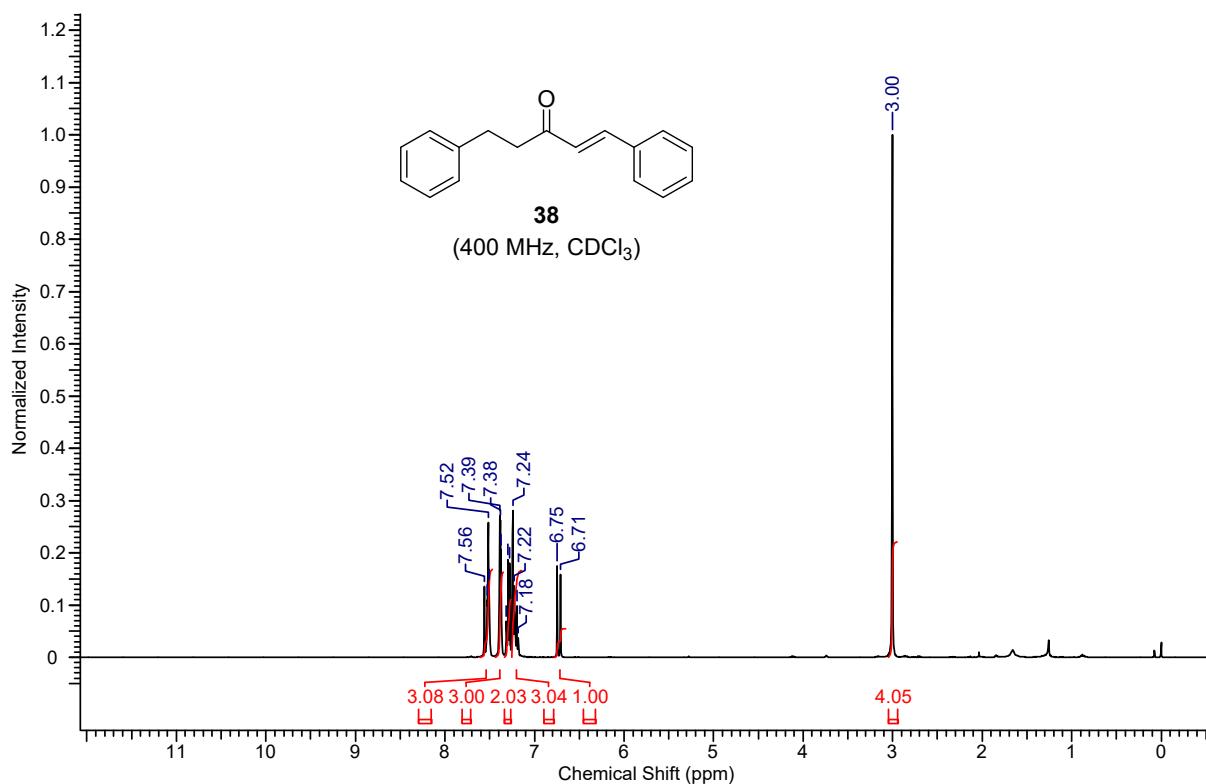


¹H-NMR spectrum of 3-Ferrocenyl-1-phenylpropan-1-one (**36**)

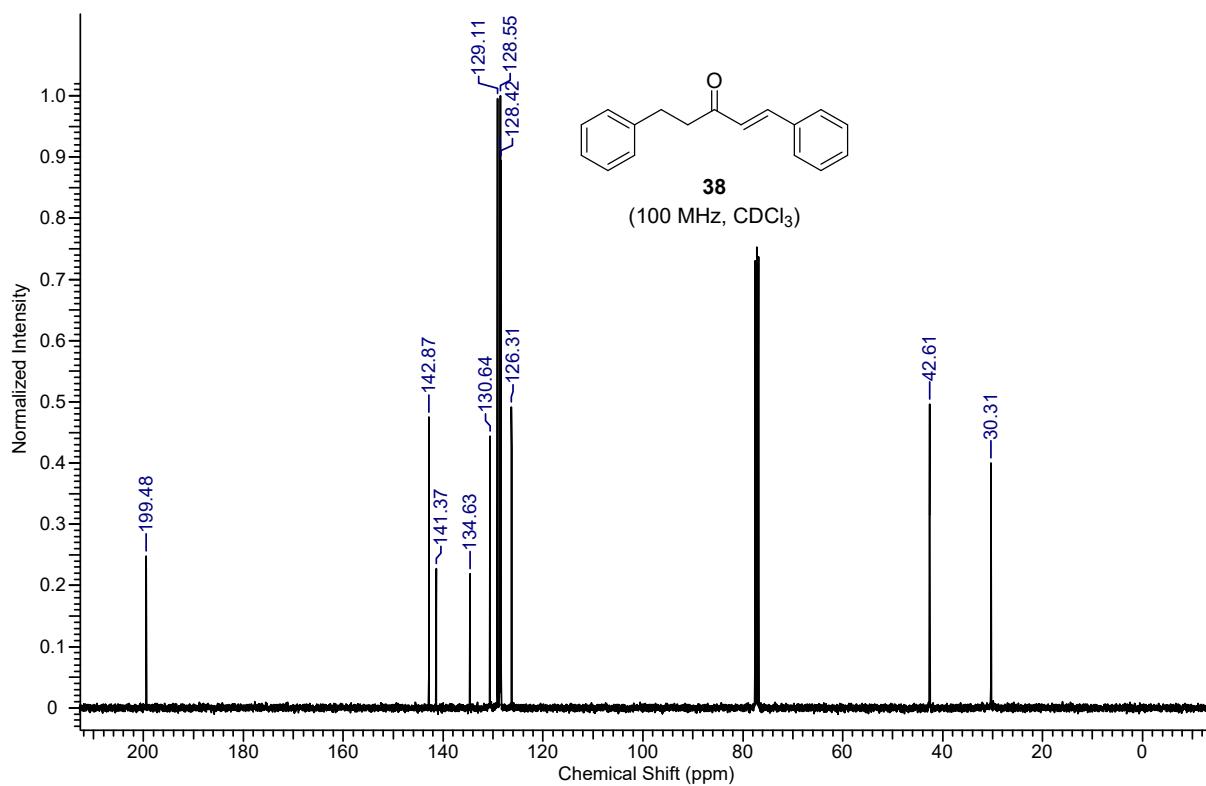


¹³C{¹H}-NMR spectrum of 3-Ferrocenyl-1-phenylpropan-1-one (**36**)

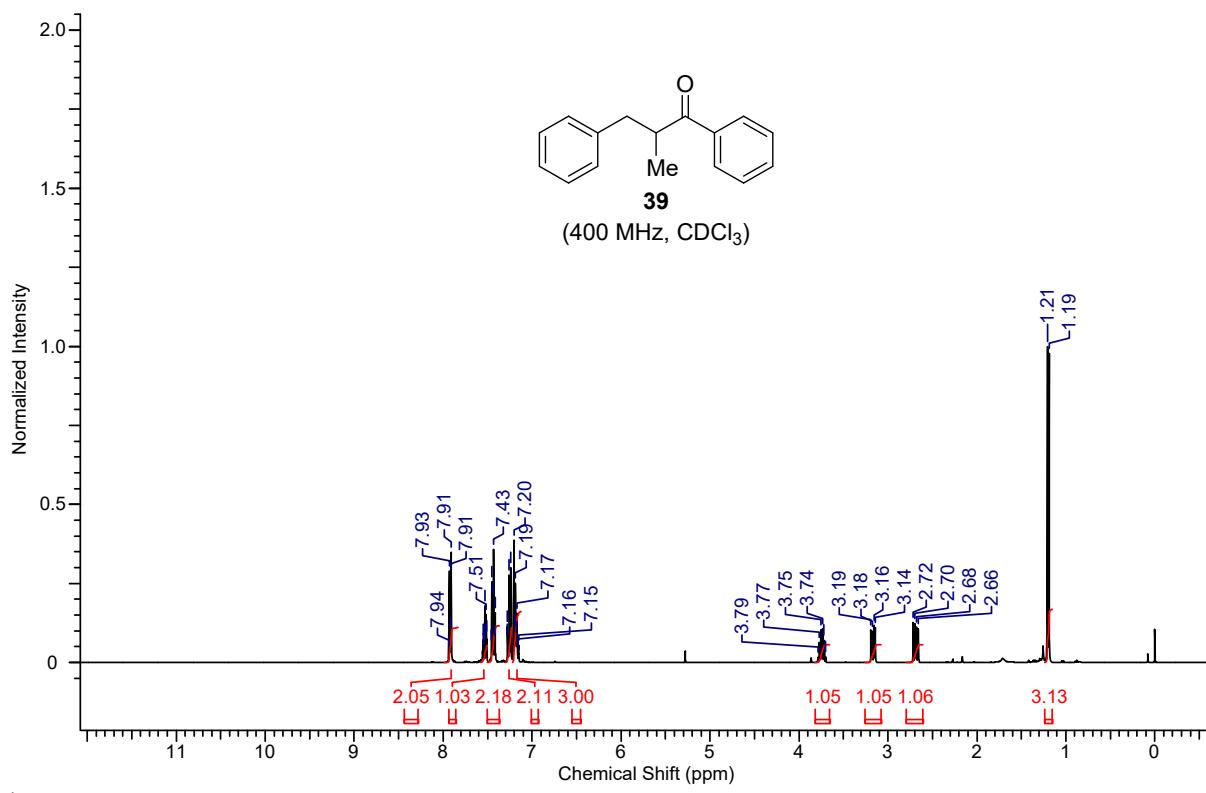




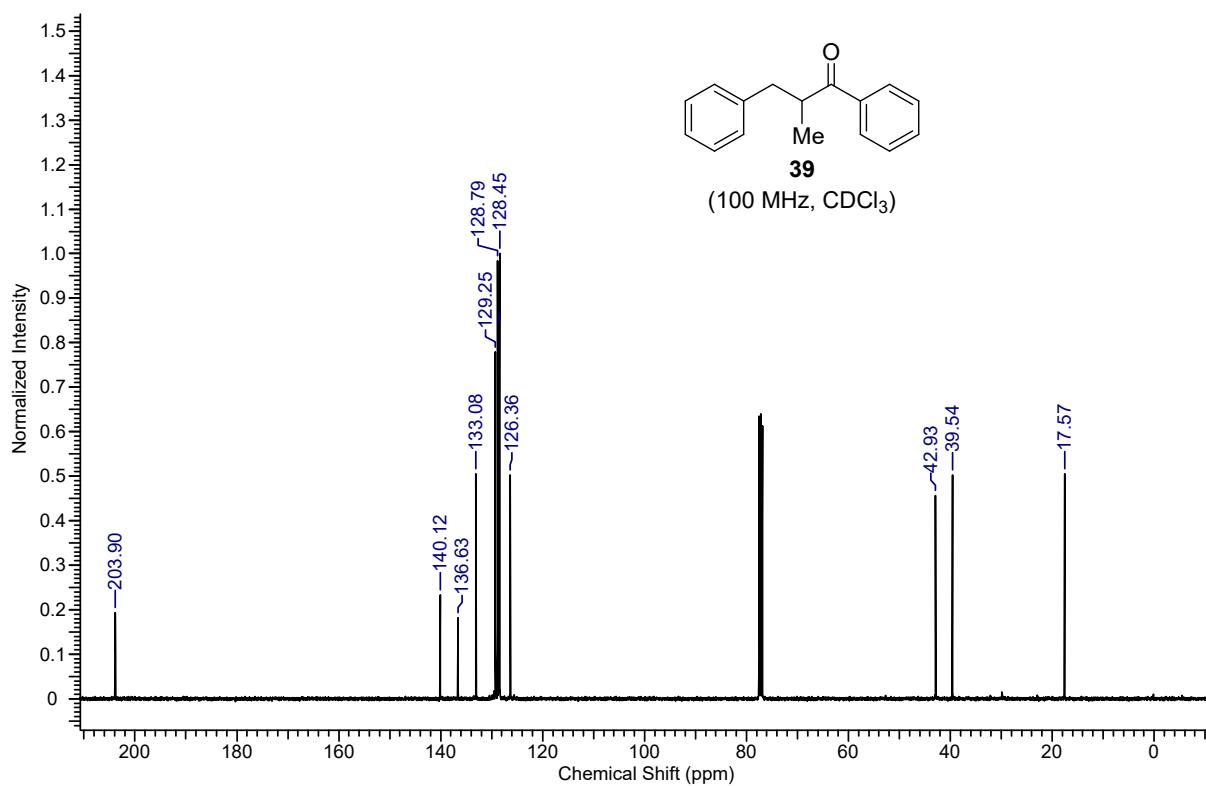
¹H-NMR spectrum of (*E*)-1,5-diphenylpent-1-en-3-one (**38**)



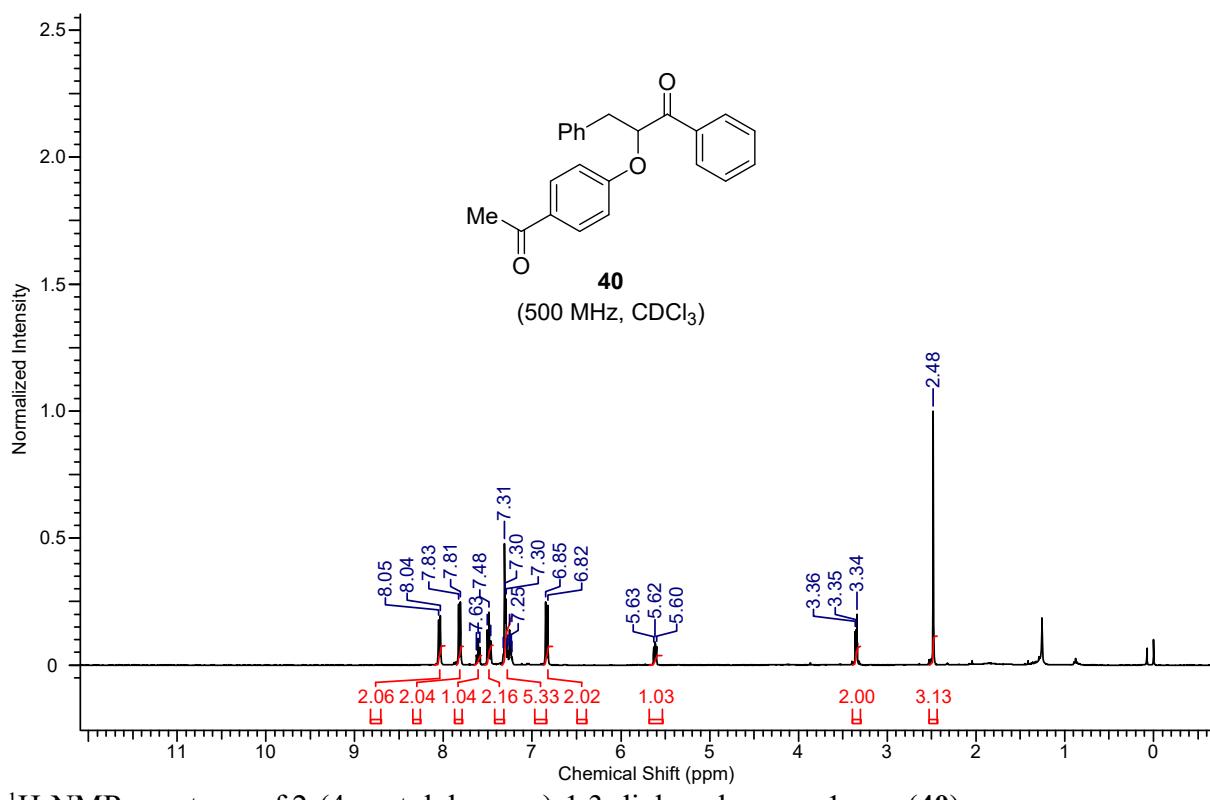
¹³C{¹H}-NMR spectrum of (*E*)-1,5-diphenylpent-1-en-3-one (**38**)



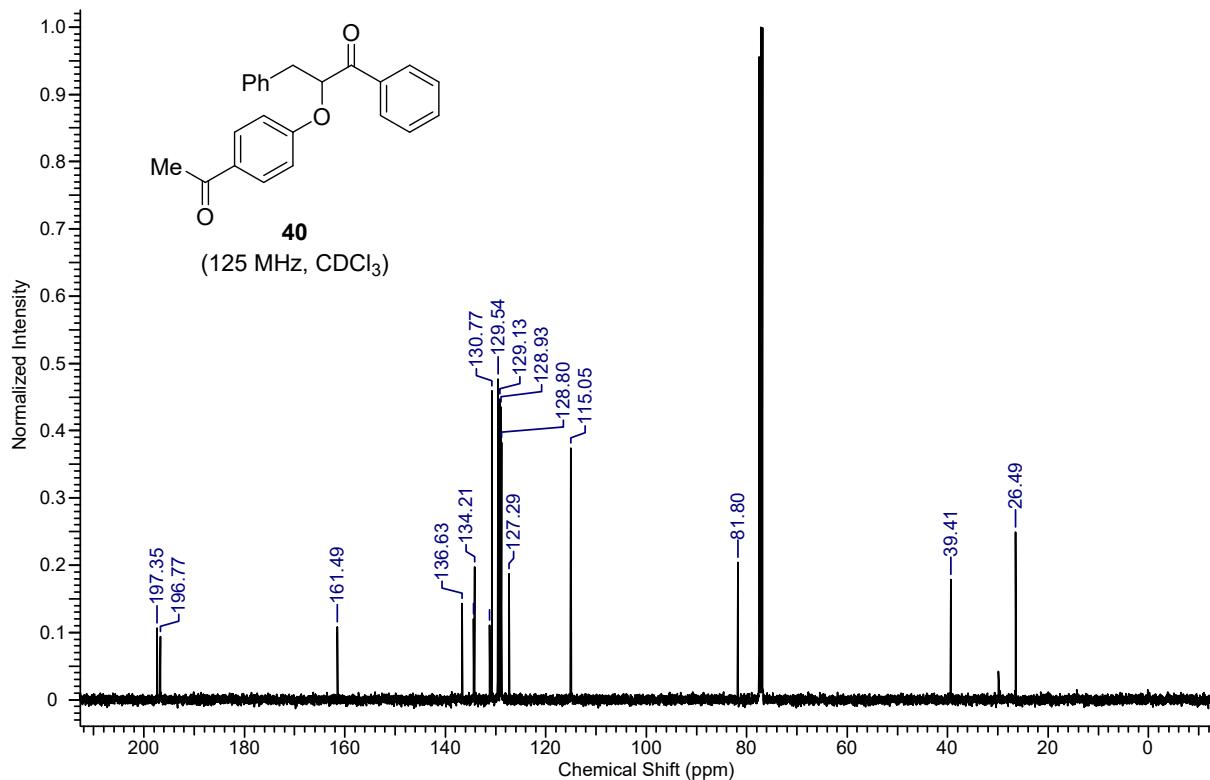
¹H-NMR spectrum of 2-methyl-1,3-diphenylpropan-1-one (**39**)



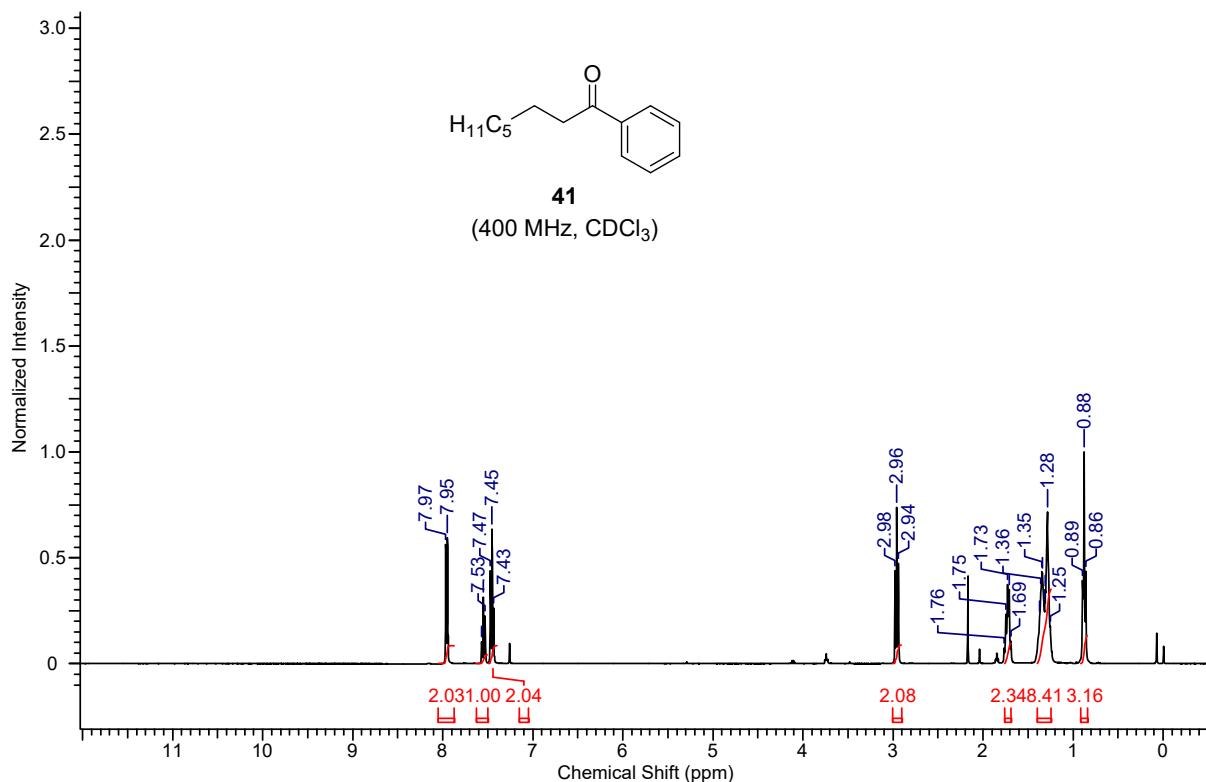
¹³C{¹H}-NMR spectrum of 2-methyl-1,3-diphenylpropan-1-one (**39**)



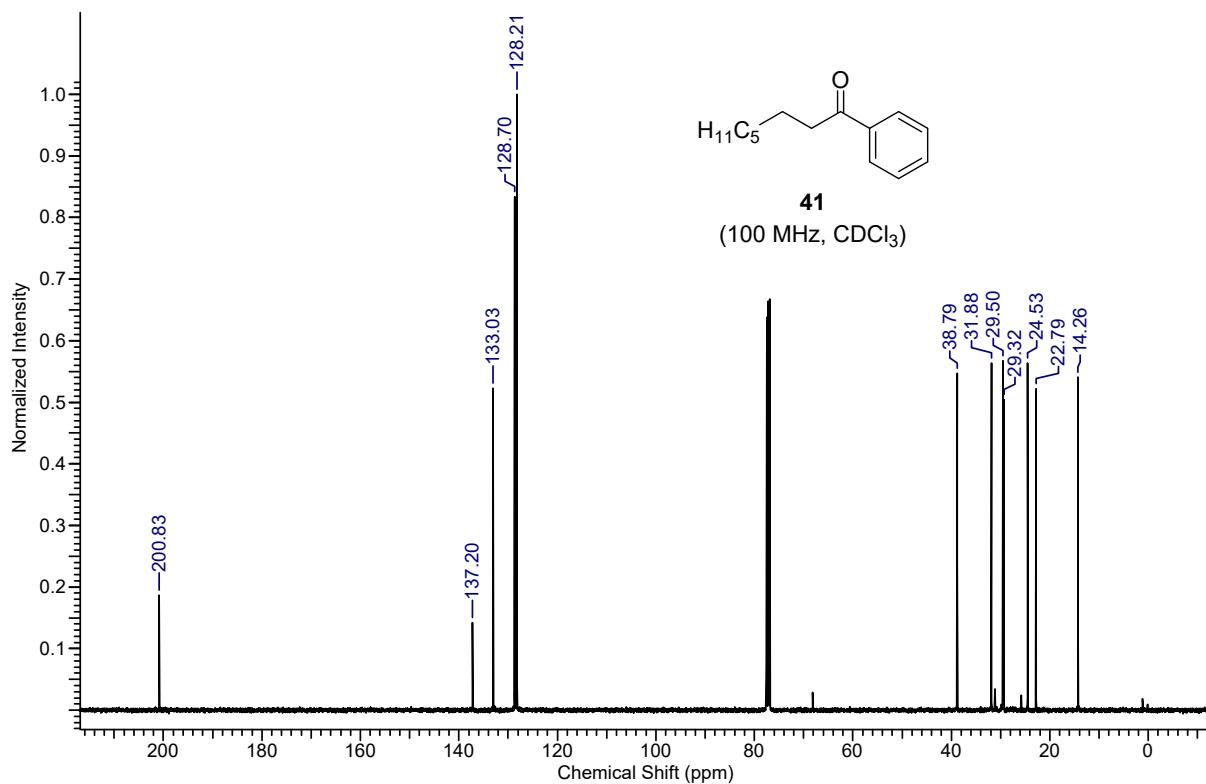
¹H-NMR spectrum of 2-(4-acetylphenoxy)-1,3-diphenylpropan-1-one (**40**)



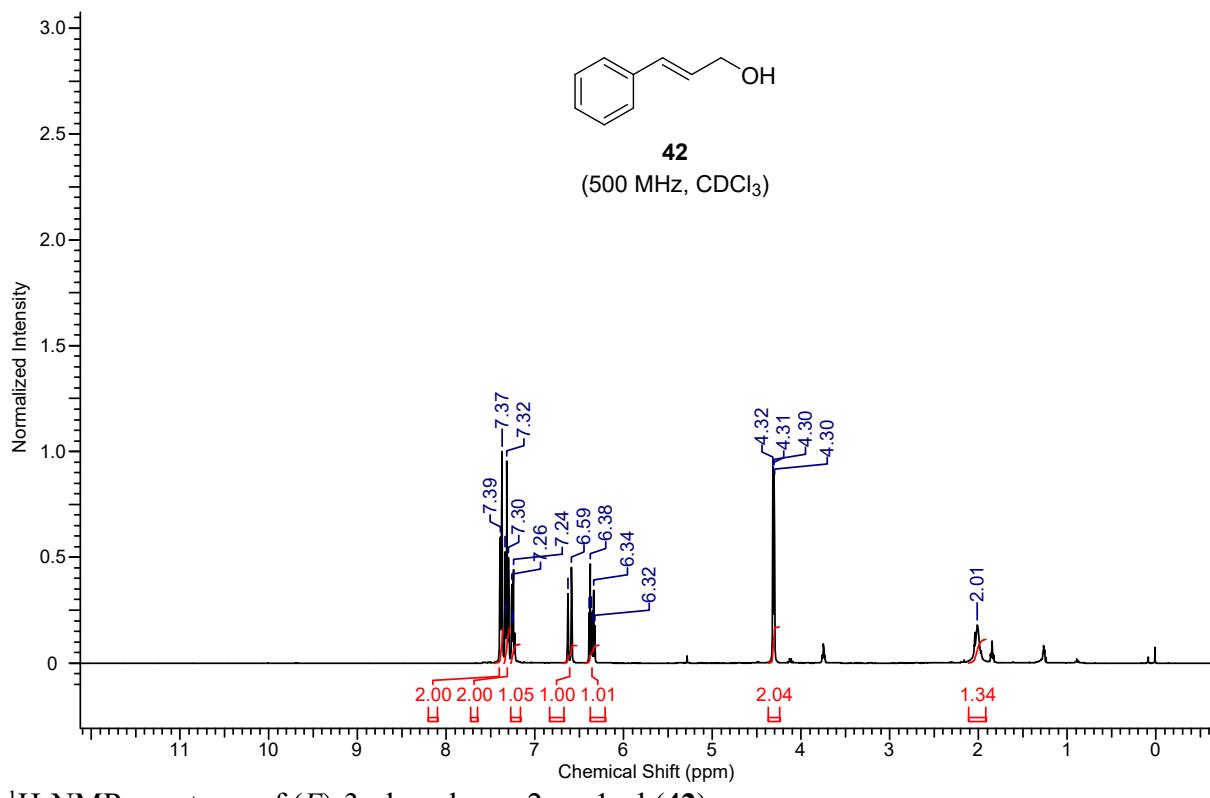
¹³C{¹H}-NMR spectrum of 2-(4-acetylphenoxy)-1,3-diphenylpropan-1-one (**40**)



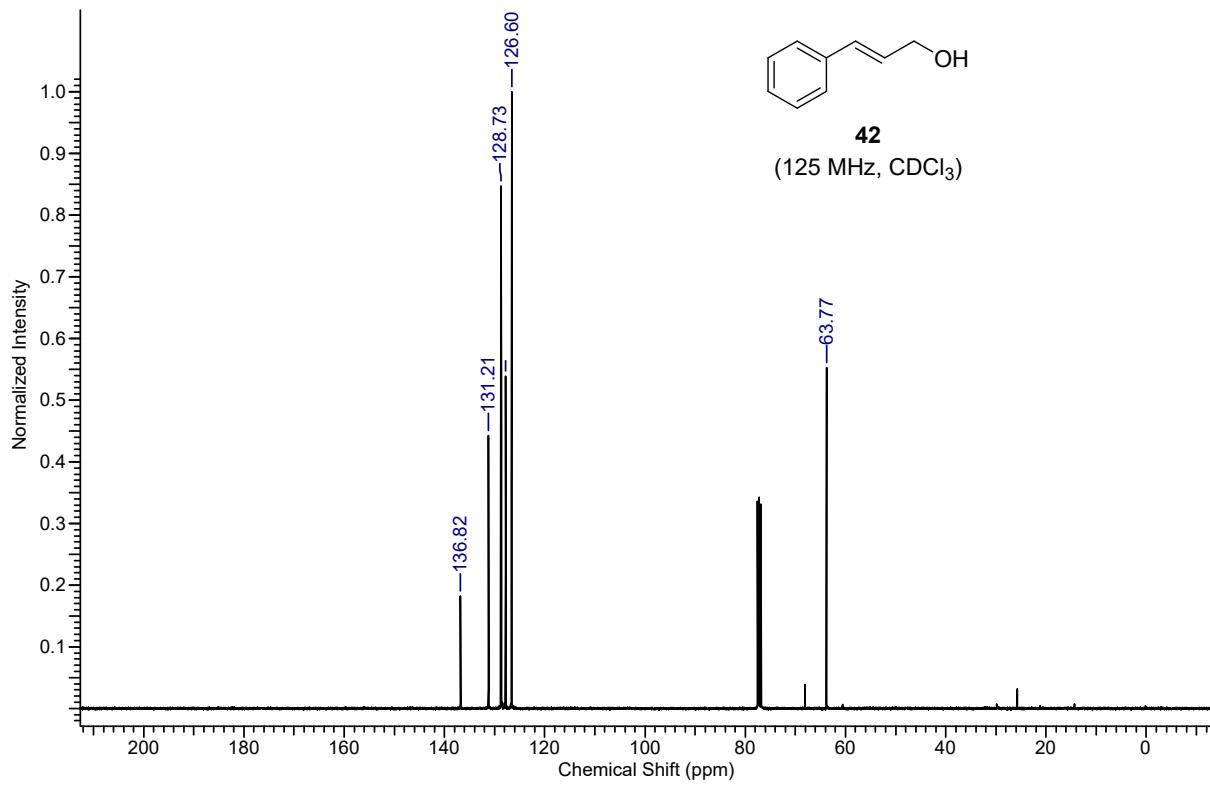
¹H-NMR spectrum of 1-phenyloctan-1-one (**41**)



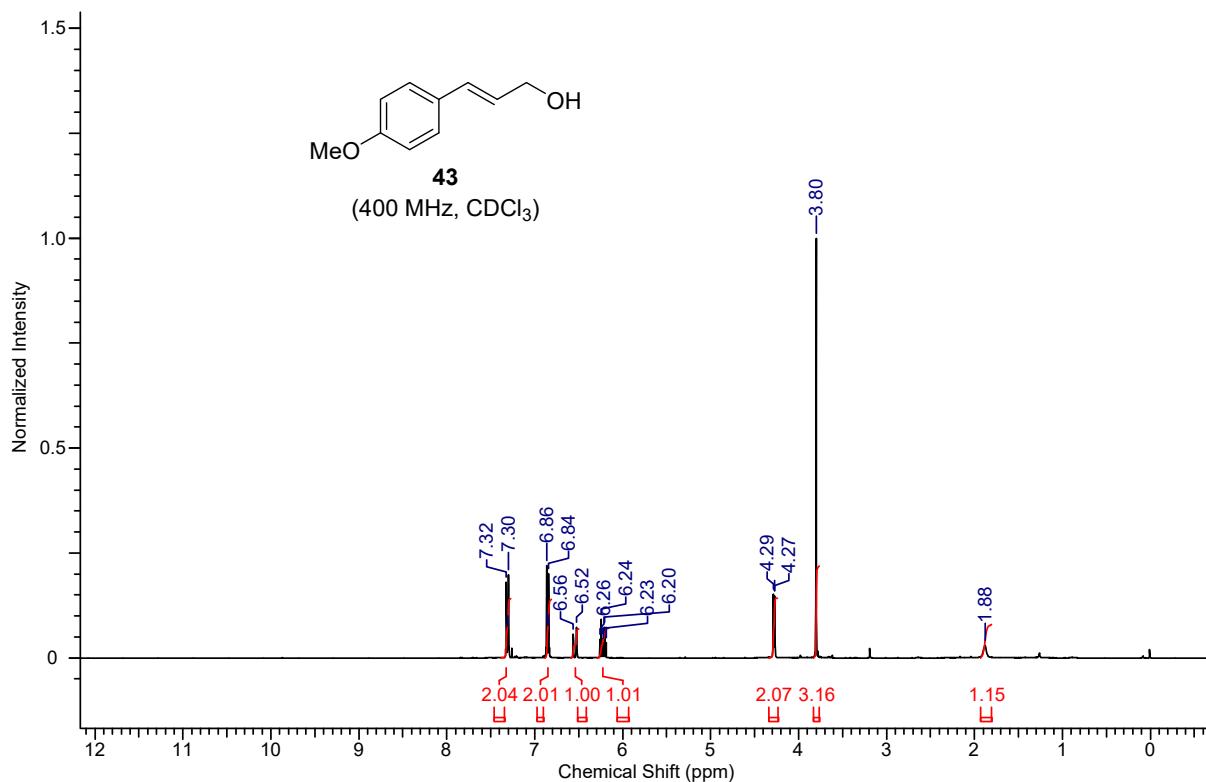
¹³C{¹H}-NMR spectrum of 1-phenyloctan-1-one (**41**)



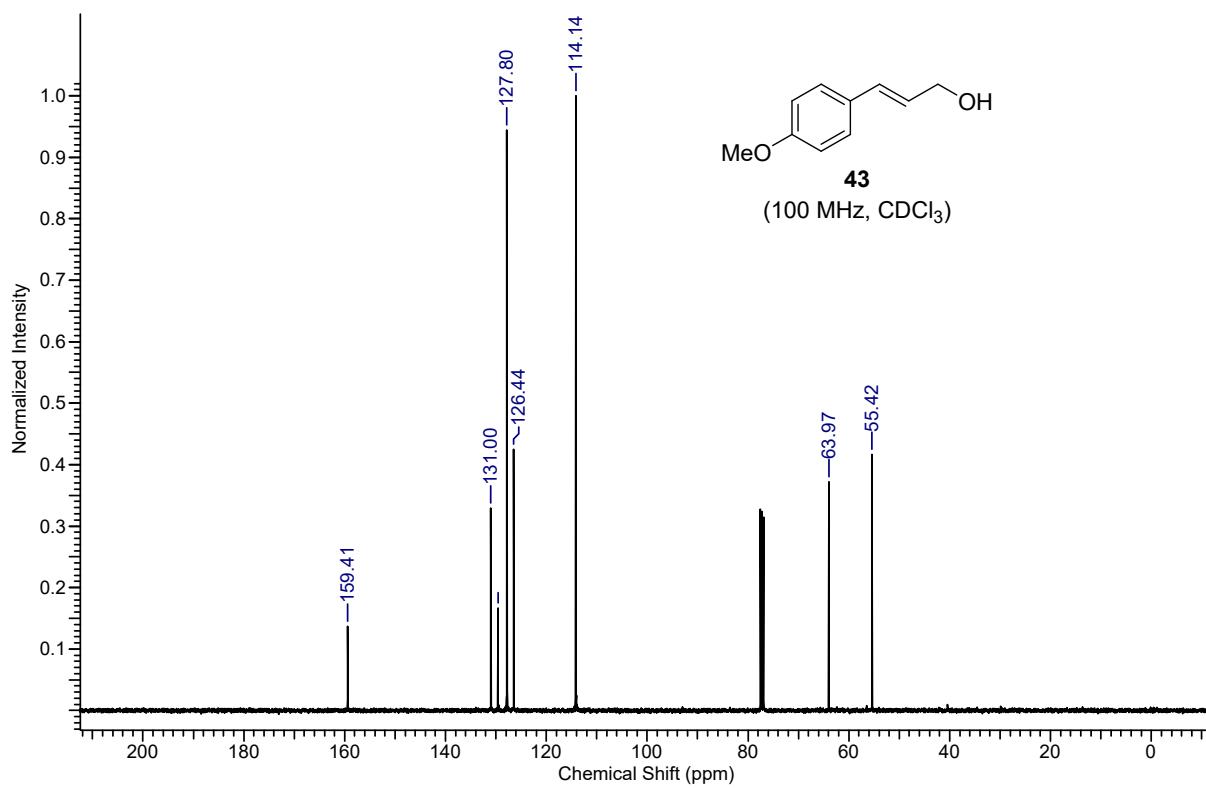
¹H-NMR spectrum of (*E*)-3-phenylprop-2-en-1-ol (**42**)



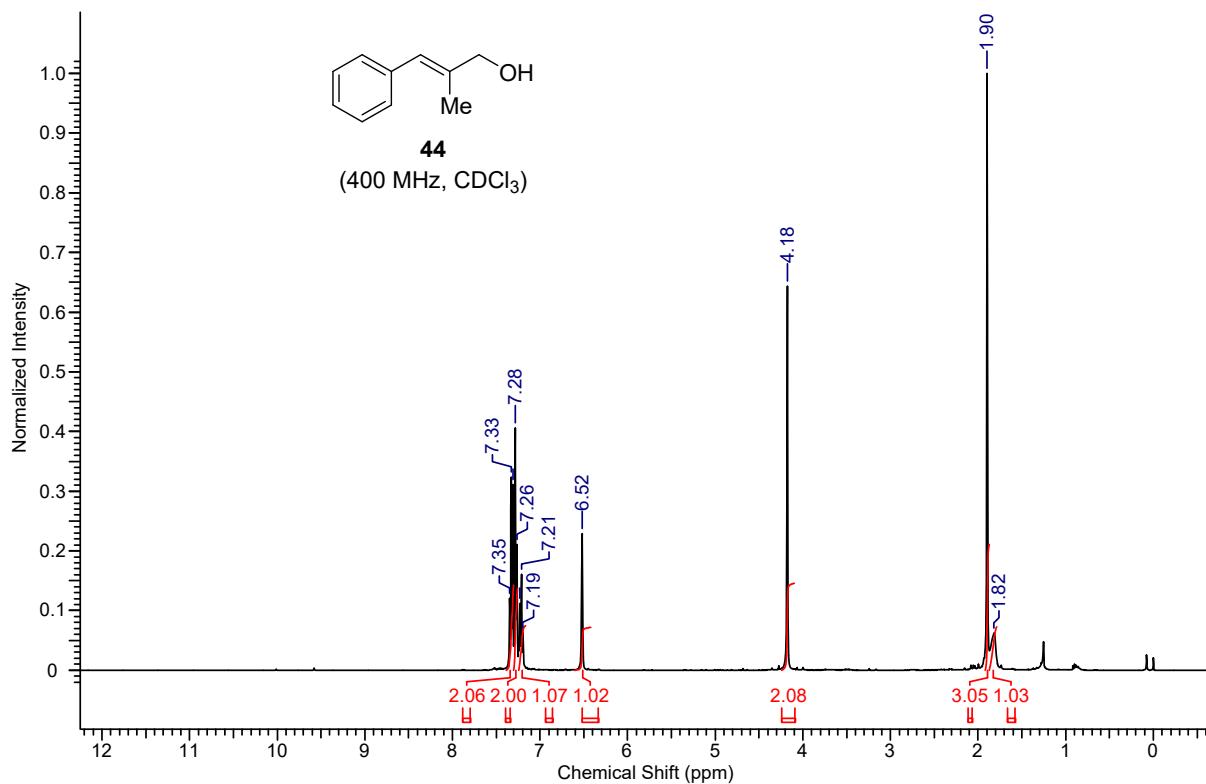
¹³C{¹H}-NMR spectrum of (*E*)-3-phenylprop-2-en-1-ol (**42**)



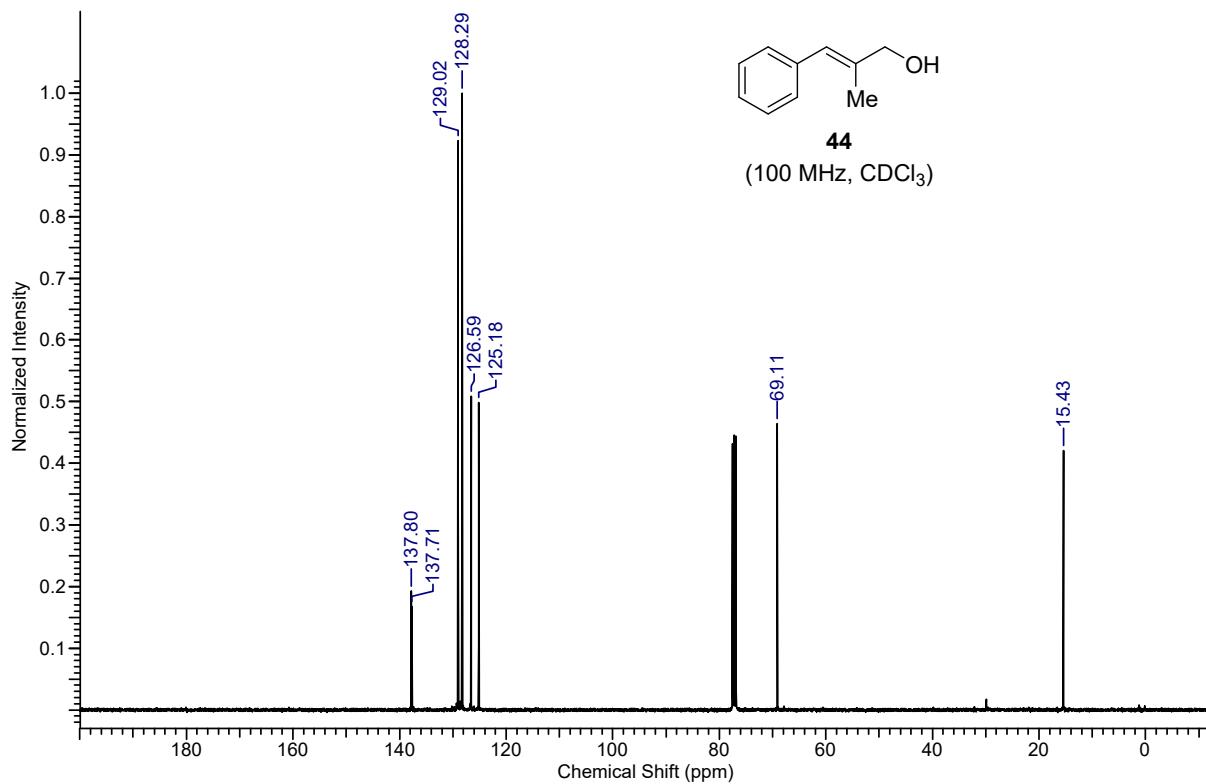
¹H-NMR spectrum of (*E*)-3-(4-methoxyphenyl)prop-2-en-1-ol (**43**)



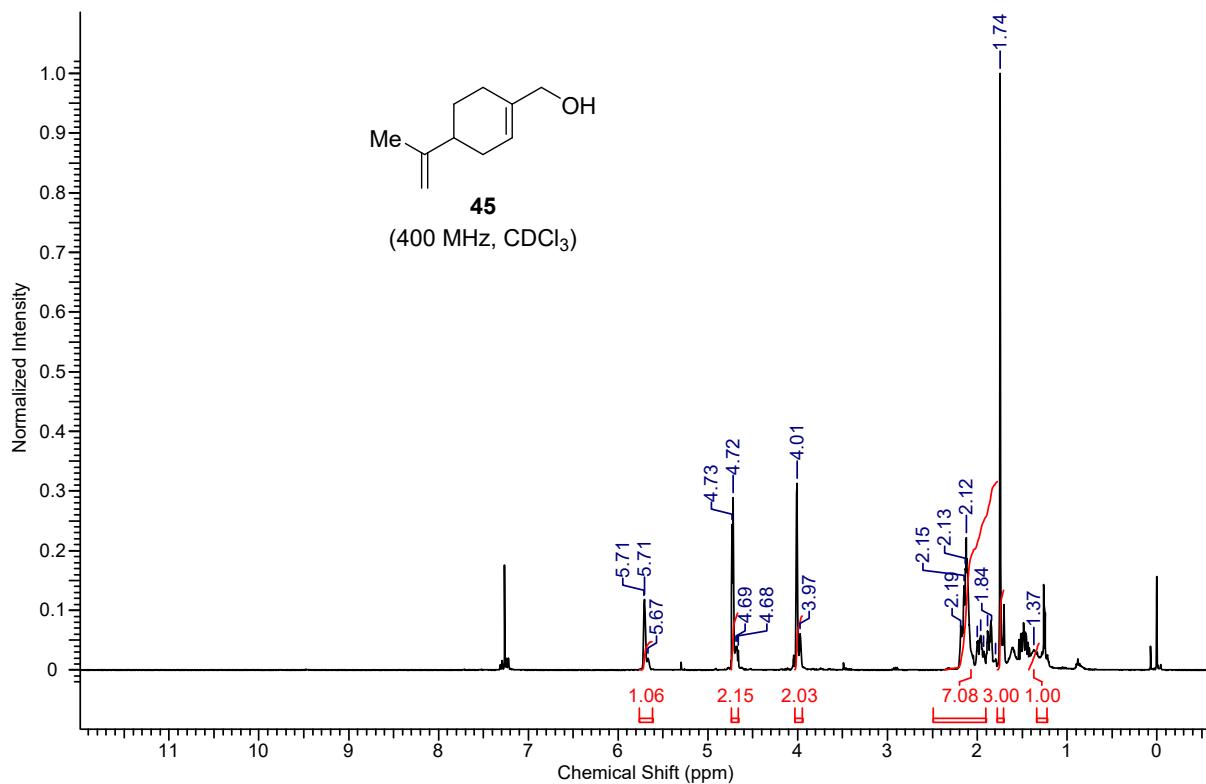
¹³C{¹H}-NMR spectrum of (*E*-3-(4-methoxyphenyl)prop-2-en-1-ol (**43**)



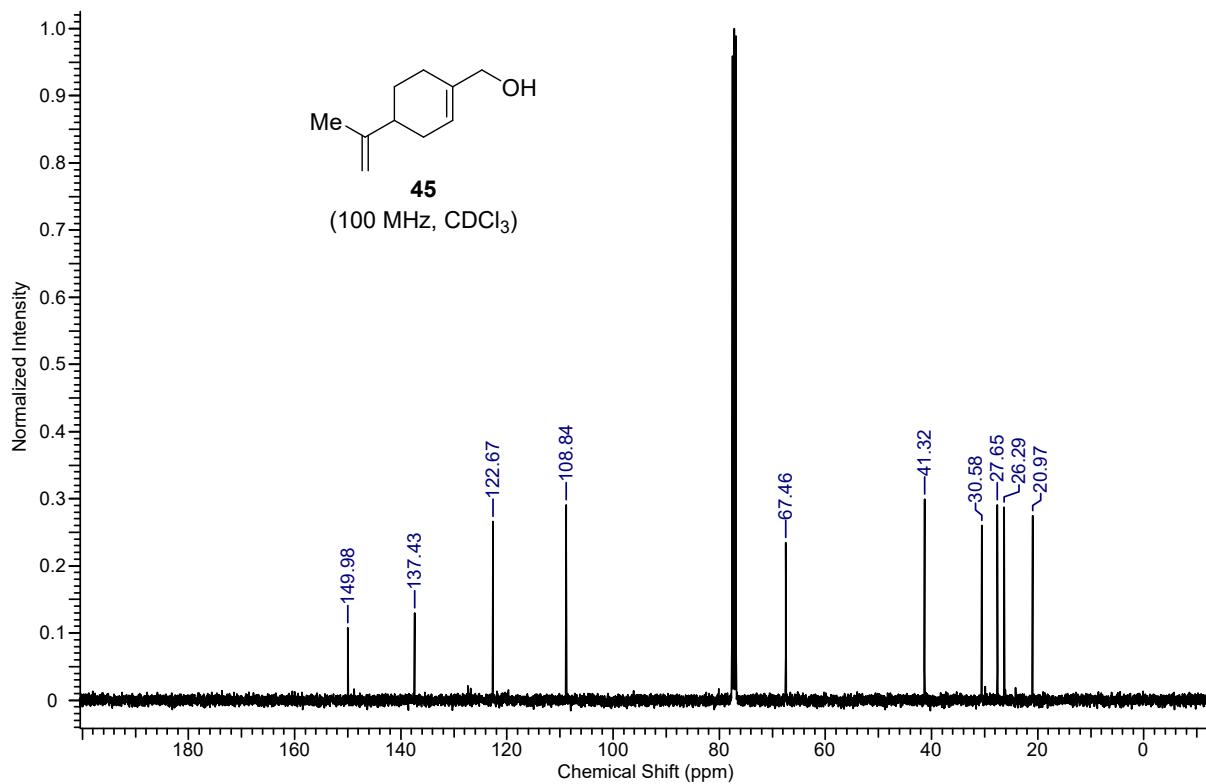
¹H-NMR spectrum of (*E*)-2-methyl-3-phenylprop-2-en-1-ol (**44**)



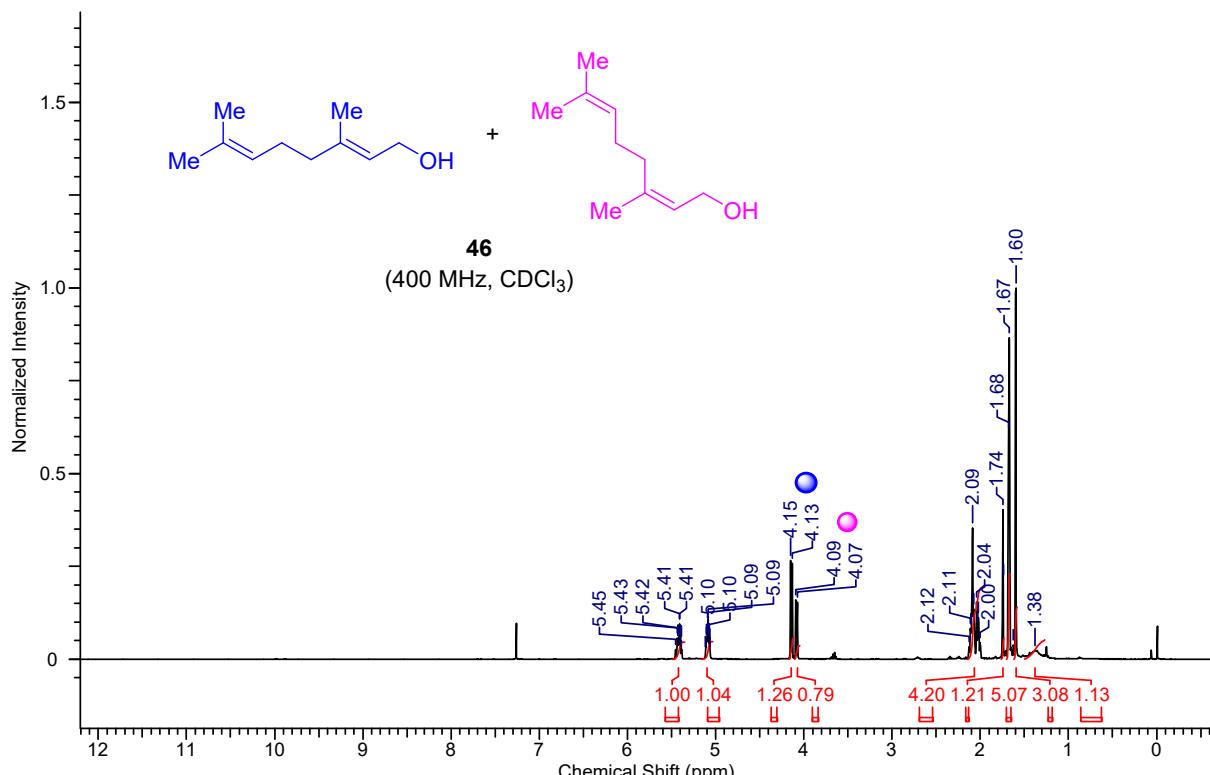
¹³C{¹H}-NMR spectrum of (*E*)-2-methyl-3-phenylprop-2-en-1-ol (**44**)



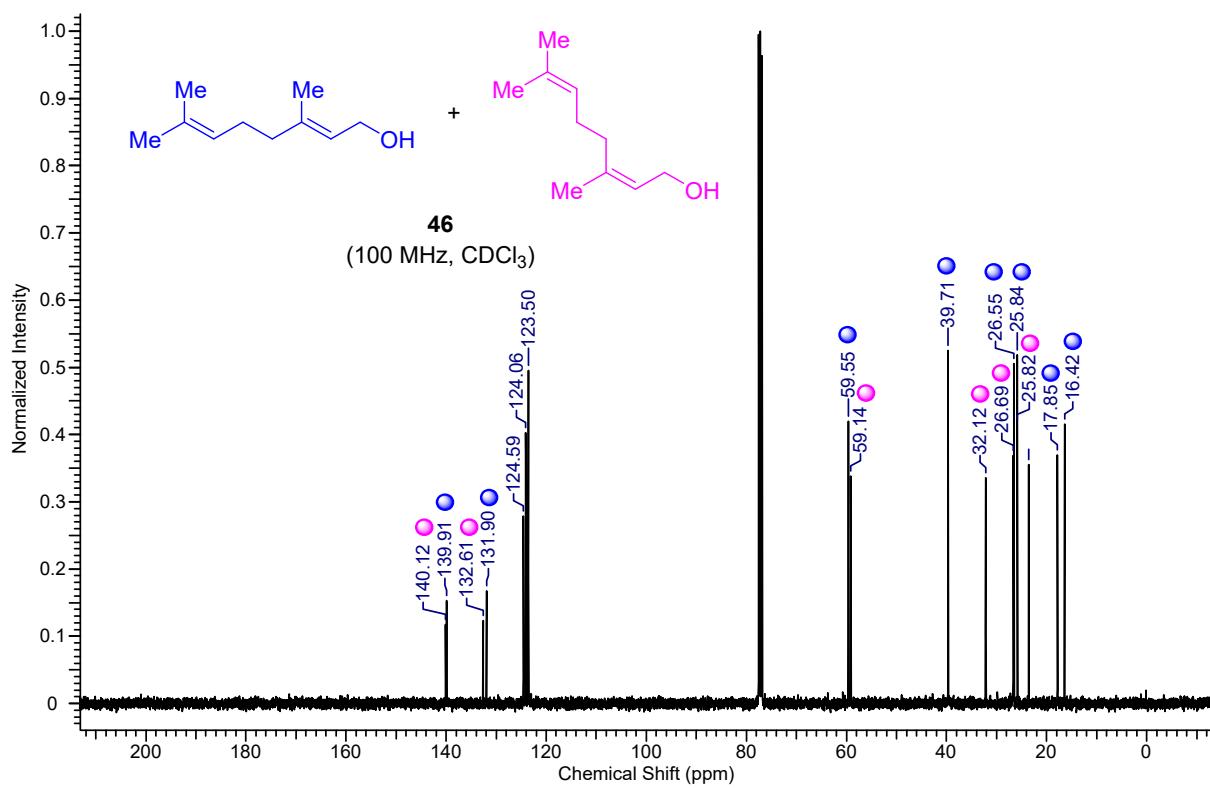
¹H-NMR spectrum of (4-(prop-1-en-2-yl)cyclohex-1-en-1-yl)methanol (**45**)



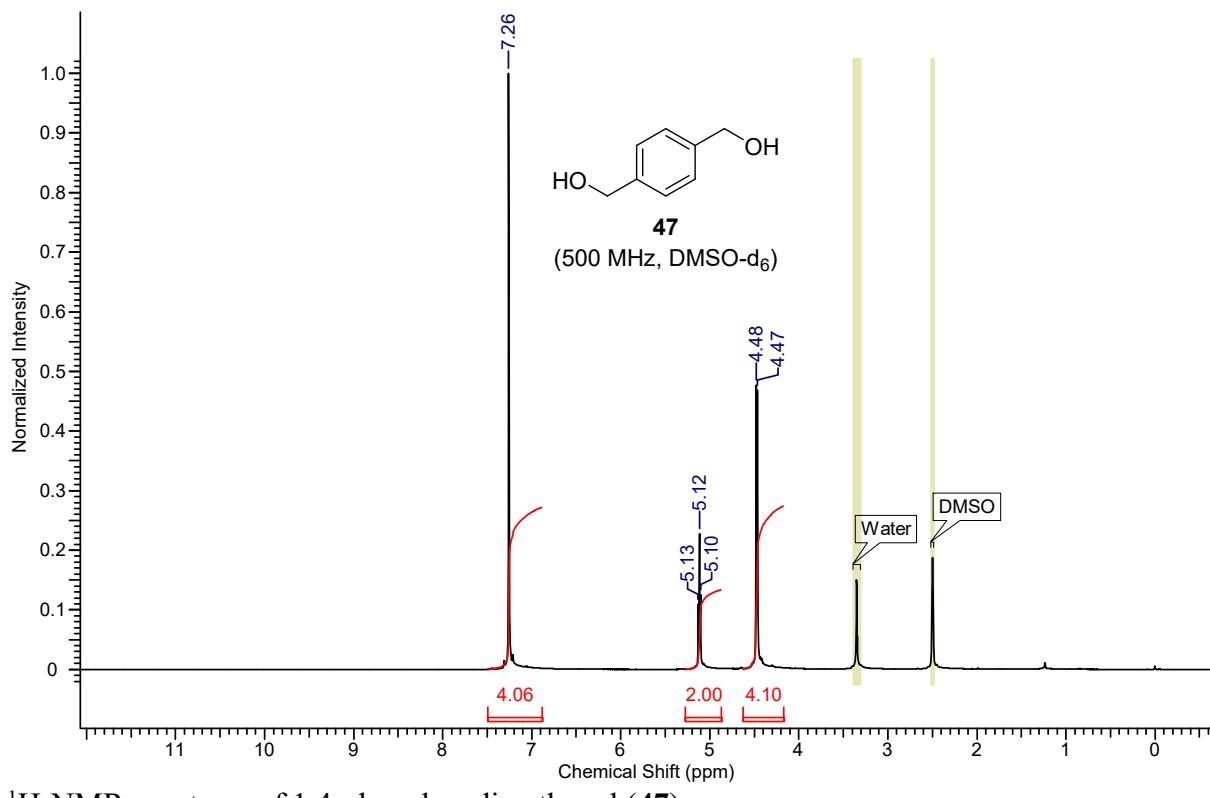
¹³C{¹H}-NMR spectrum of (4-(prop-1-en-2-yl)cyclohex-1-en-1-yl)methanol (**45**)



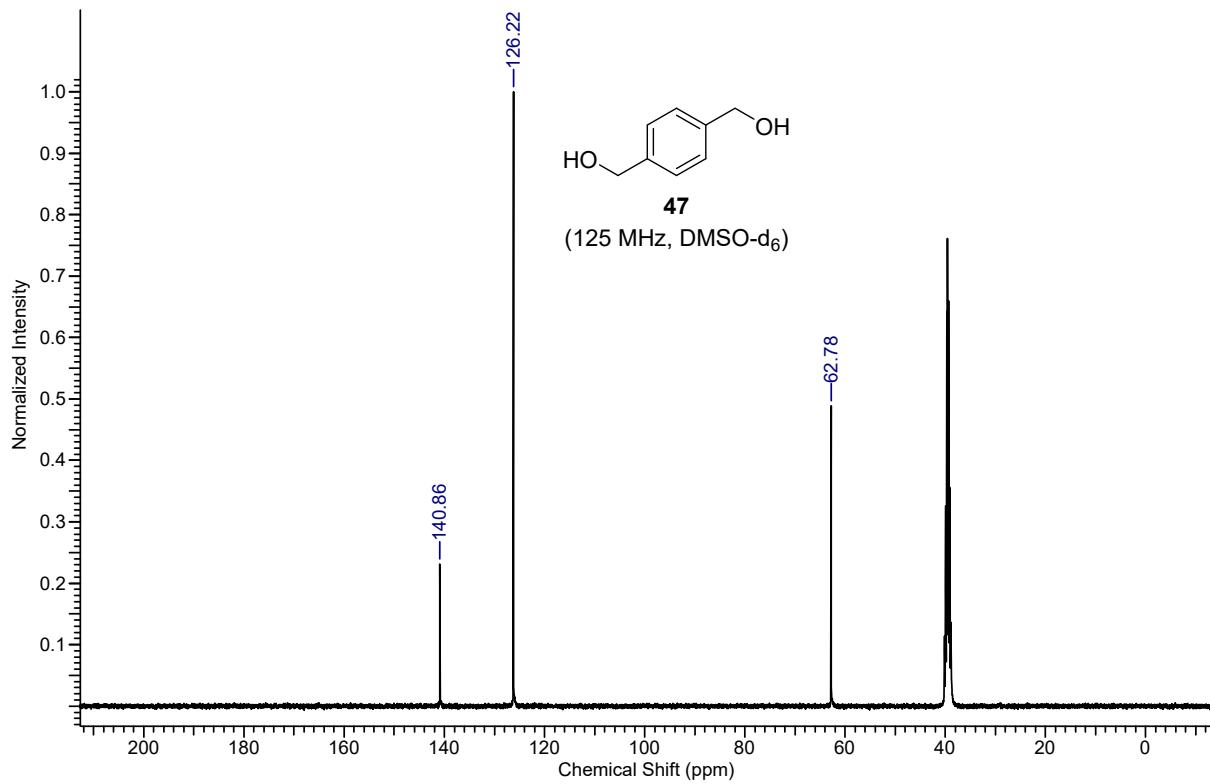
^1H -NMR spectrum of (*E/Z*)-3,7-dimethylocta-2,6-dien-1-ol (**46**)



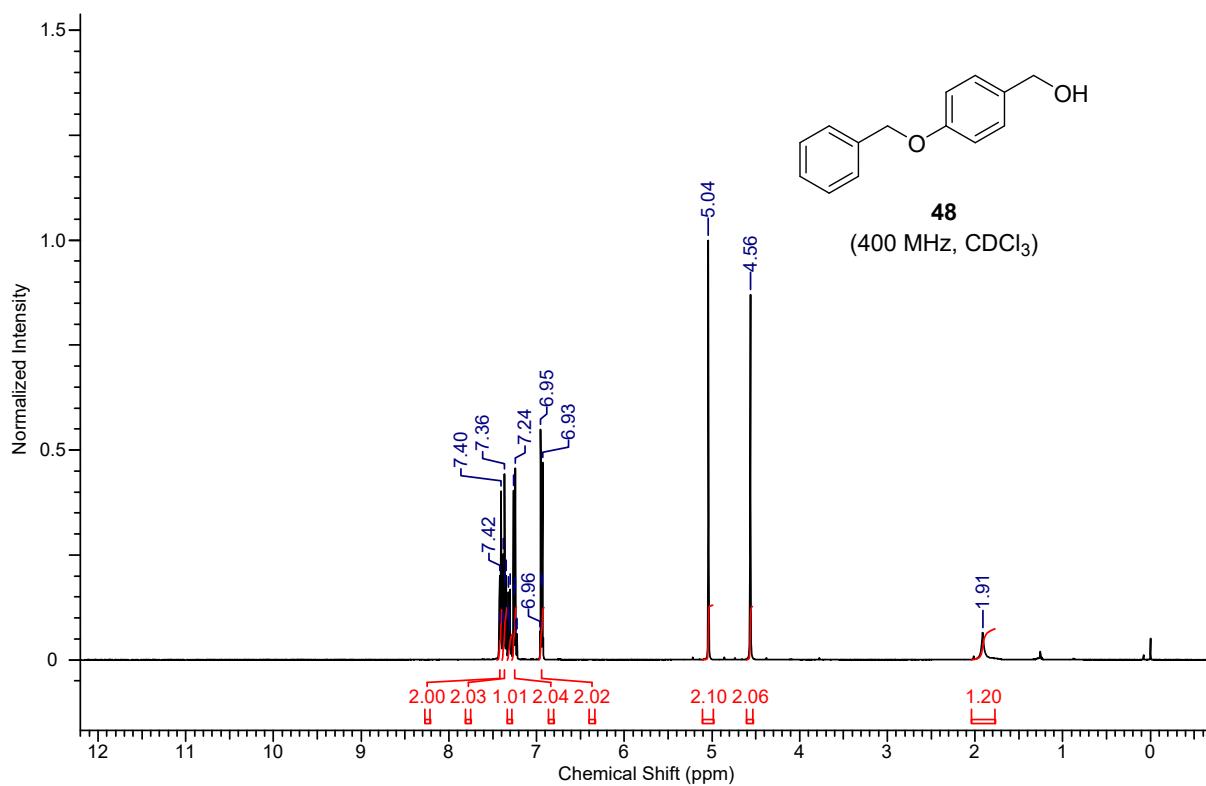
$^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum of (*E/Z*)-3,7-dimethylocta-2,6-dien-1-ol (**46**)



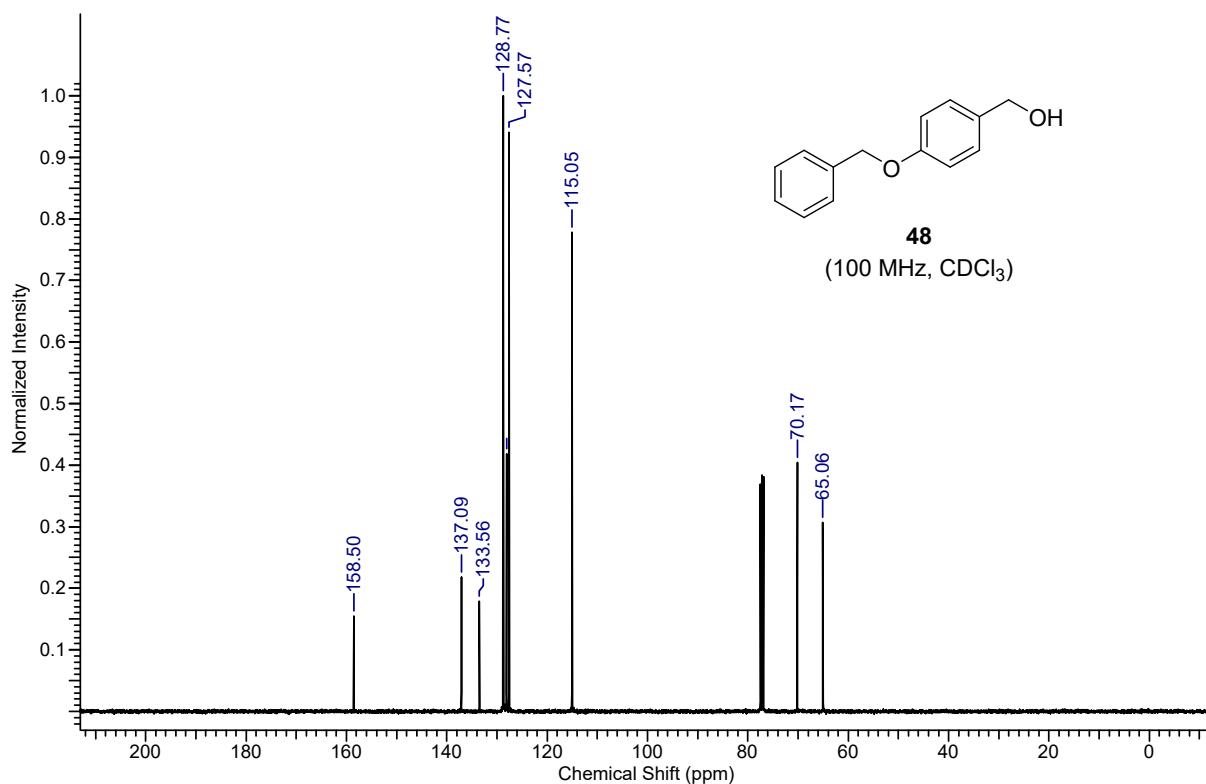
¹H-NMR spectrum of 1,4-phenylenedimethanol (**47**)



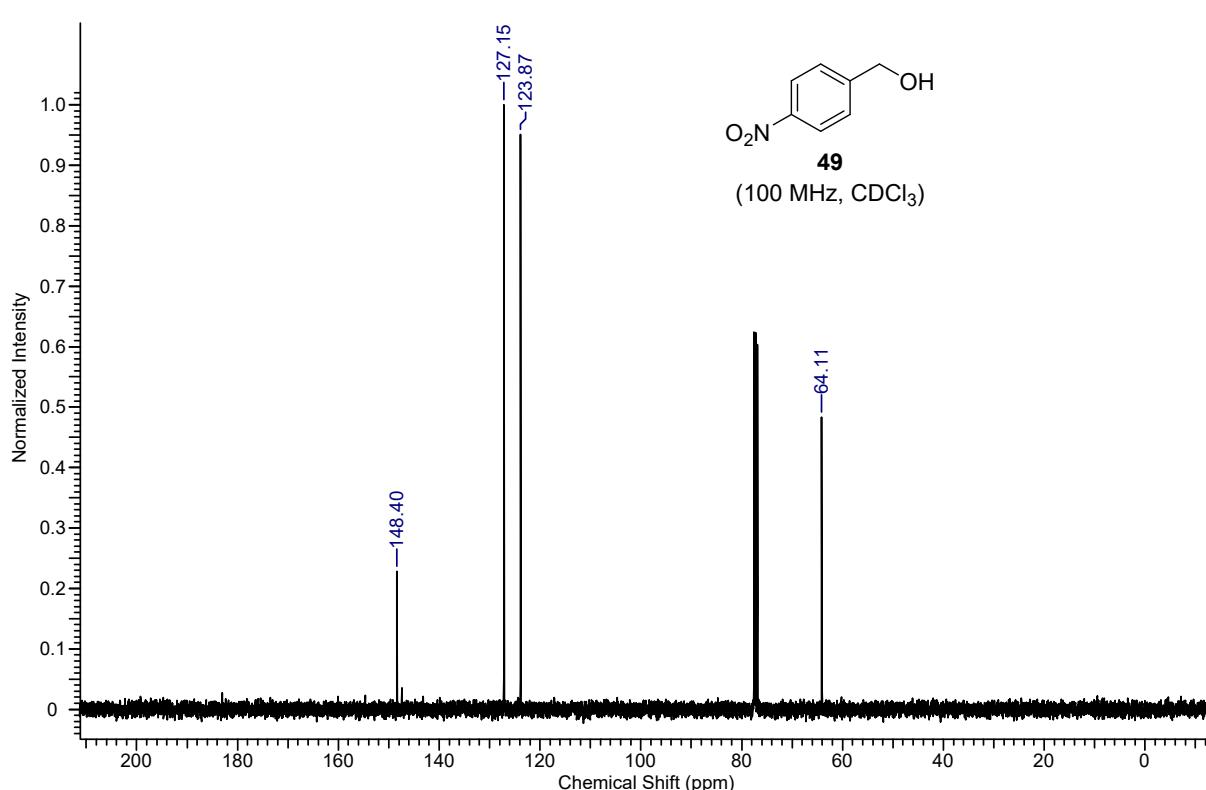
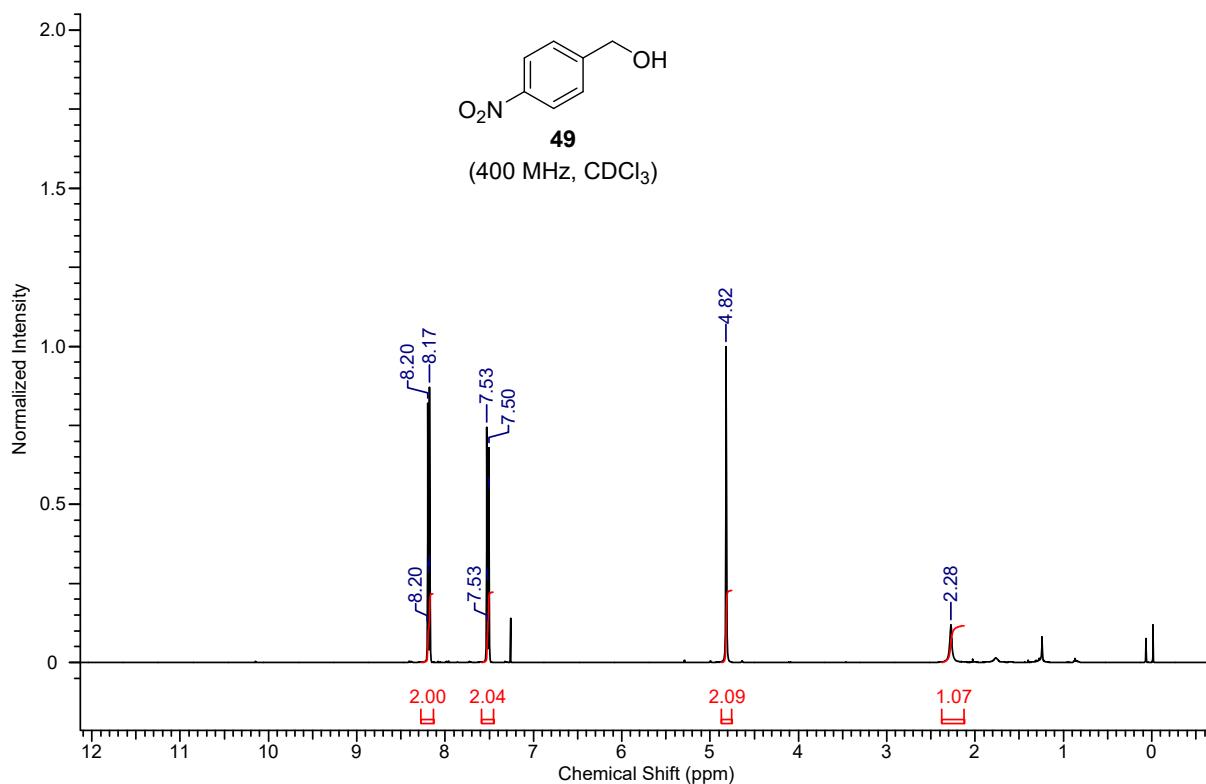
¹³C{¹H}-NMR spectrum of 1,4-phenylenedimethanol (**47**)

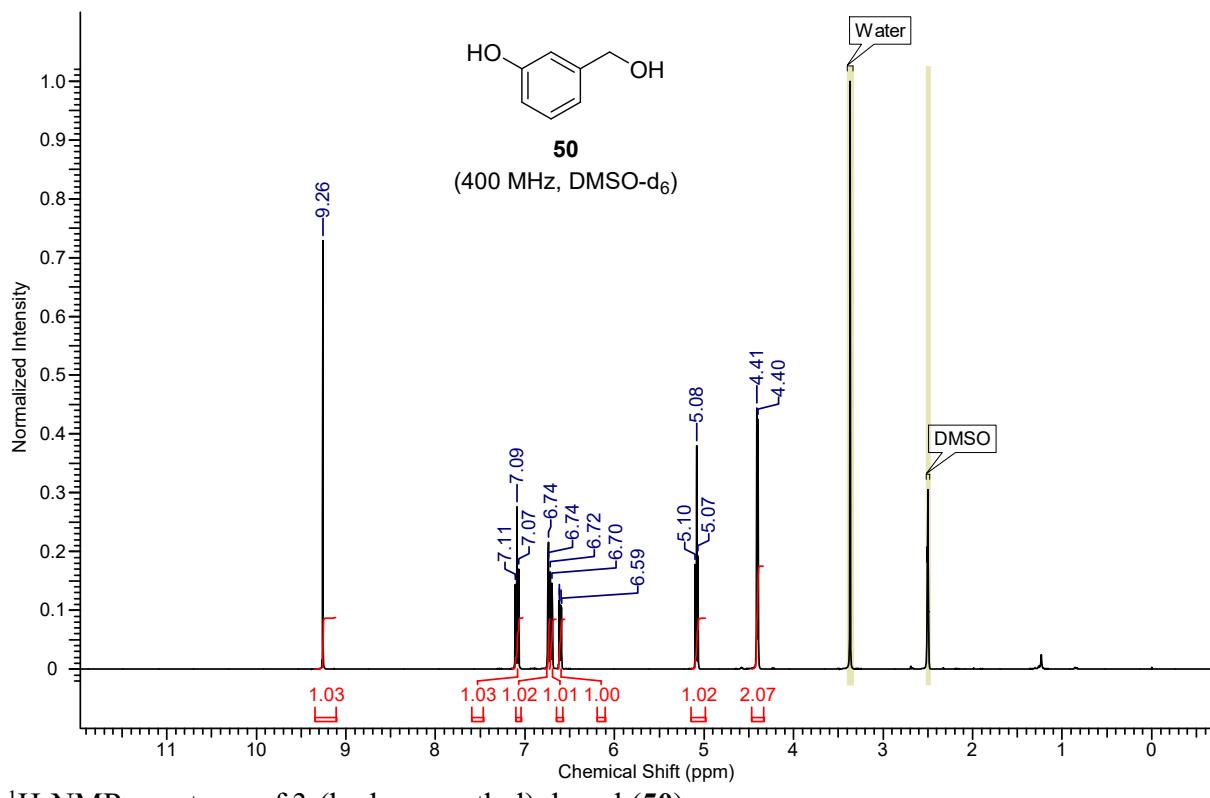


¹H-NMR spectrum of (4-(benzyloxy)phenyl)methanol (**48**)

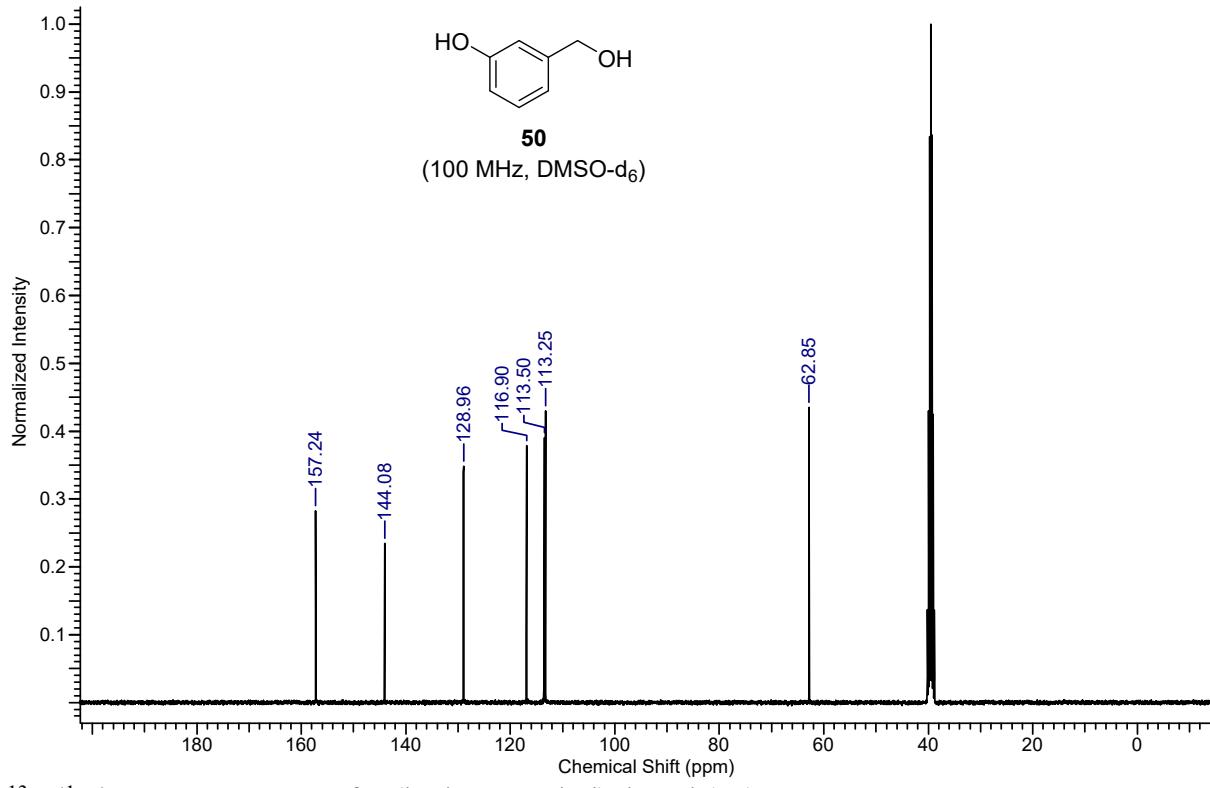


¹³C{¹H}-NMR spectrum of (4-(benzyloxy)phenyl)methanol (**48**)

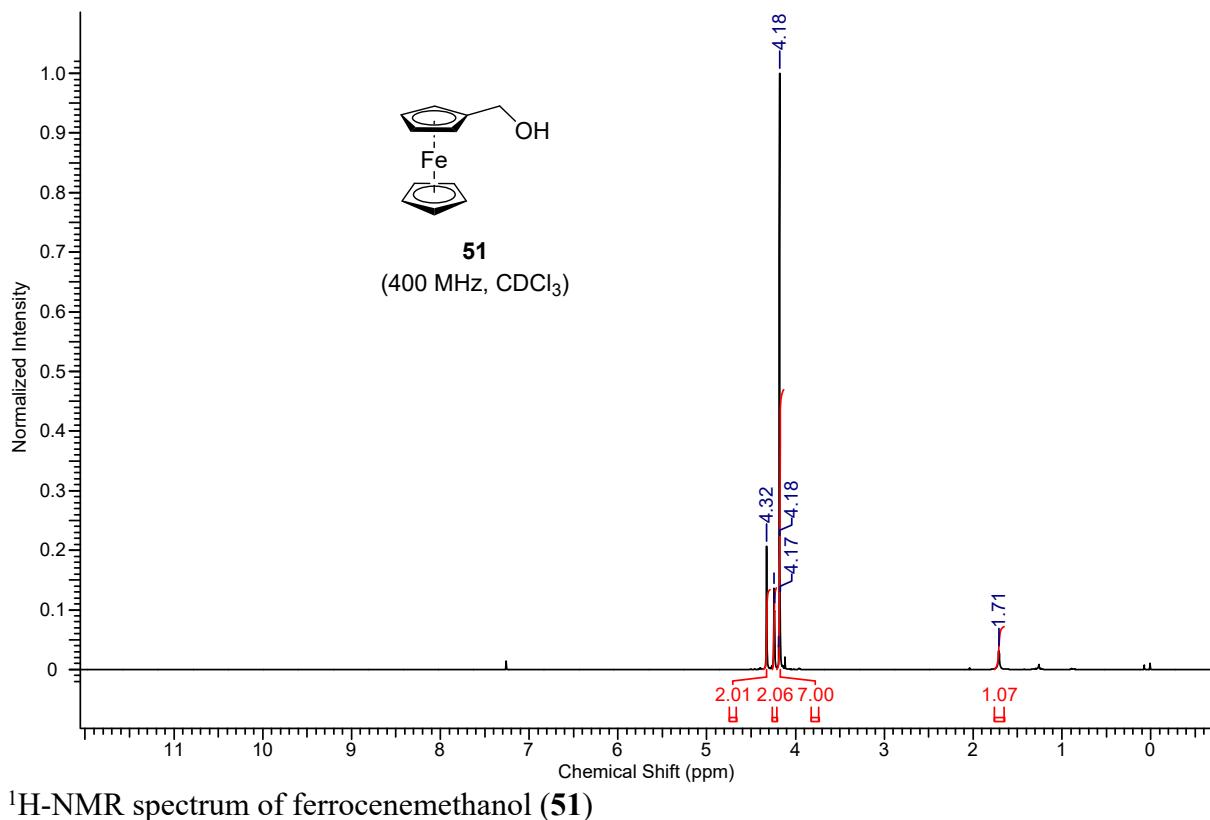




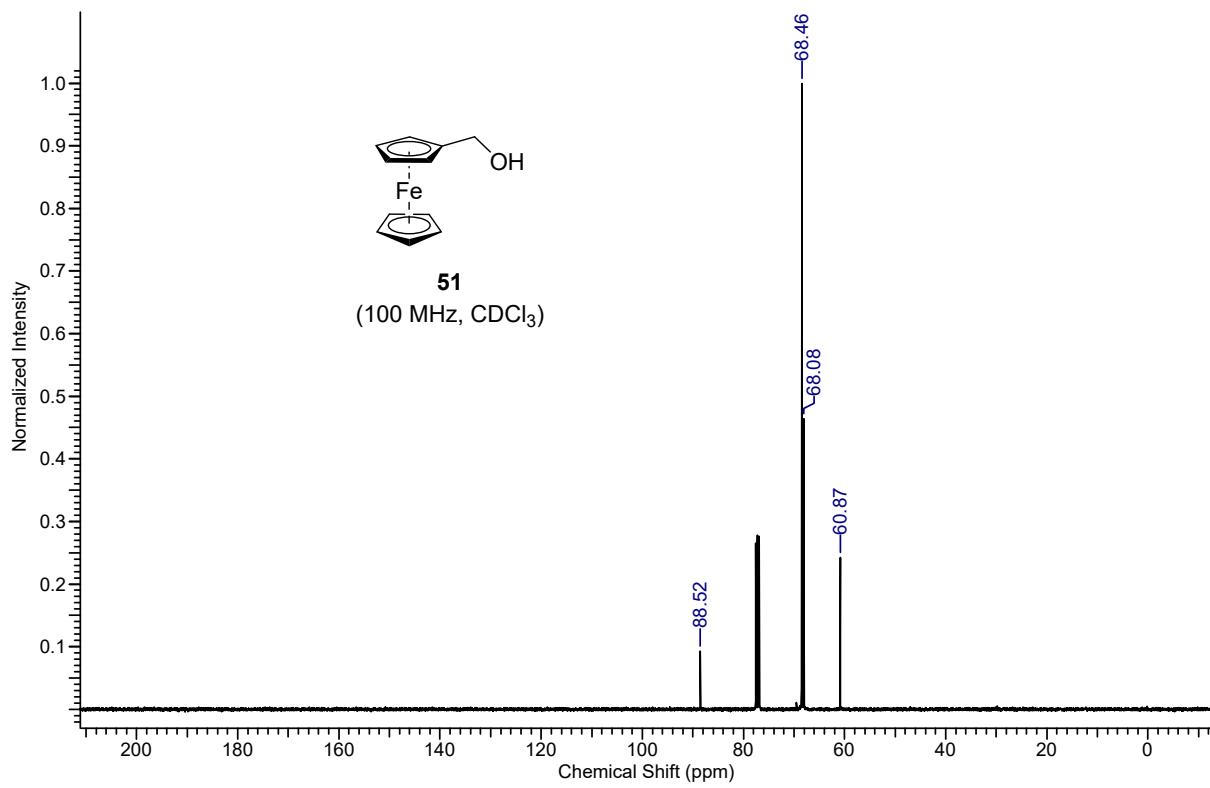
¹H-NMR spectrum of 3-(hydroxymethyl)phenol (**50**)



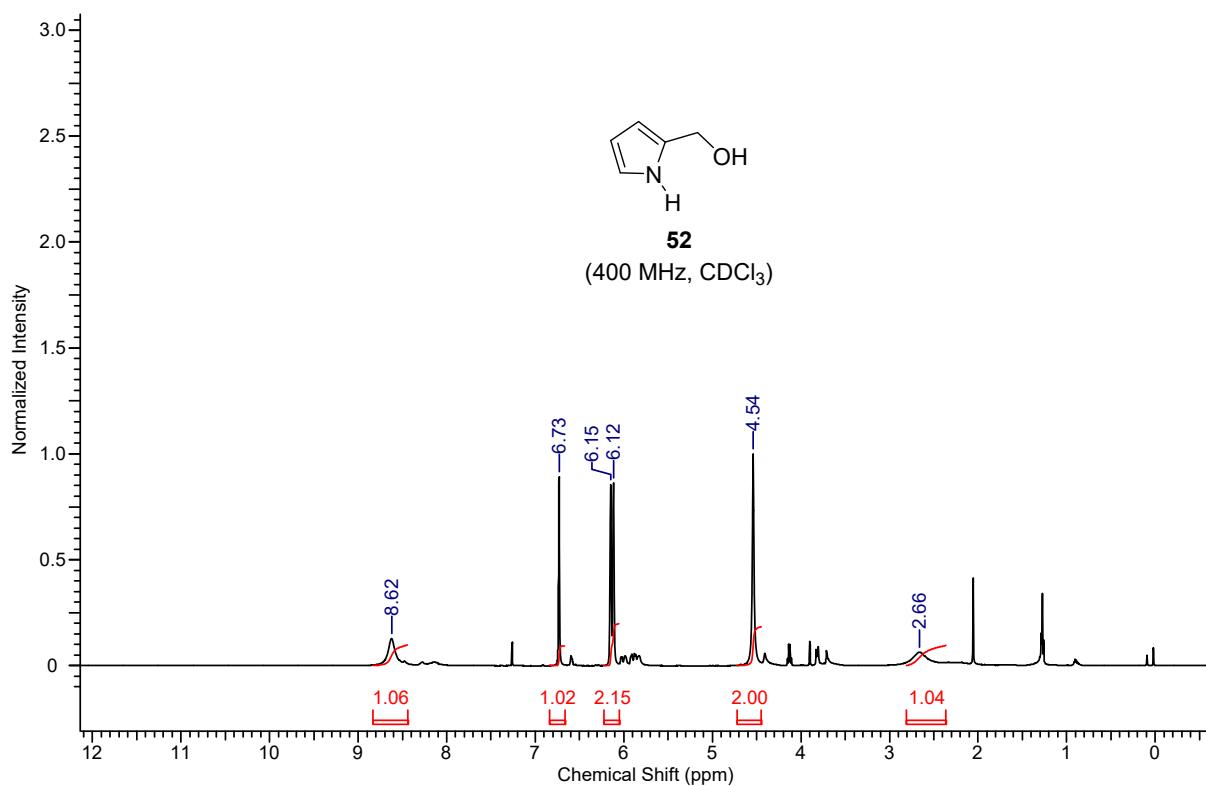
¹³C{¹H}-NMR spectrum of 3-(hydroxymethyl)phenol (**50**)



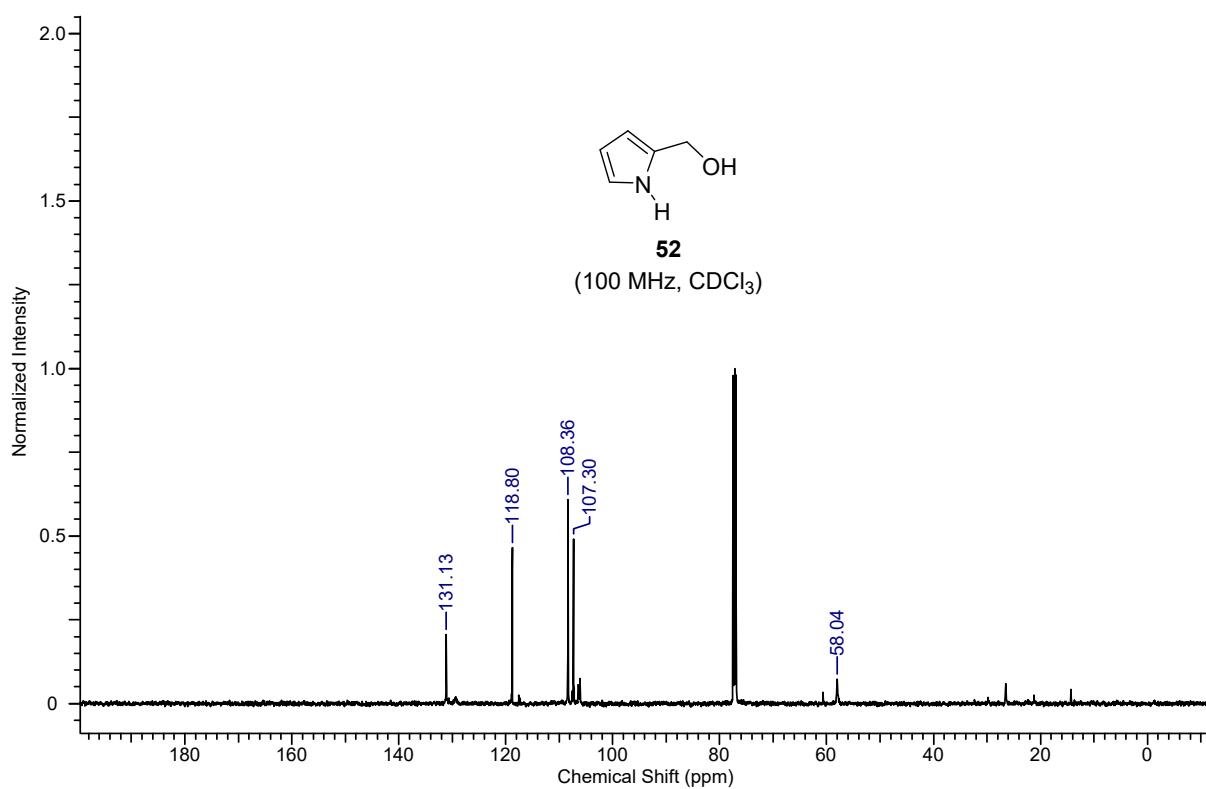
¹H-NMR spectrum of ferrocenemethanol (**51**)



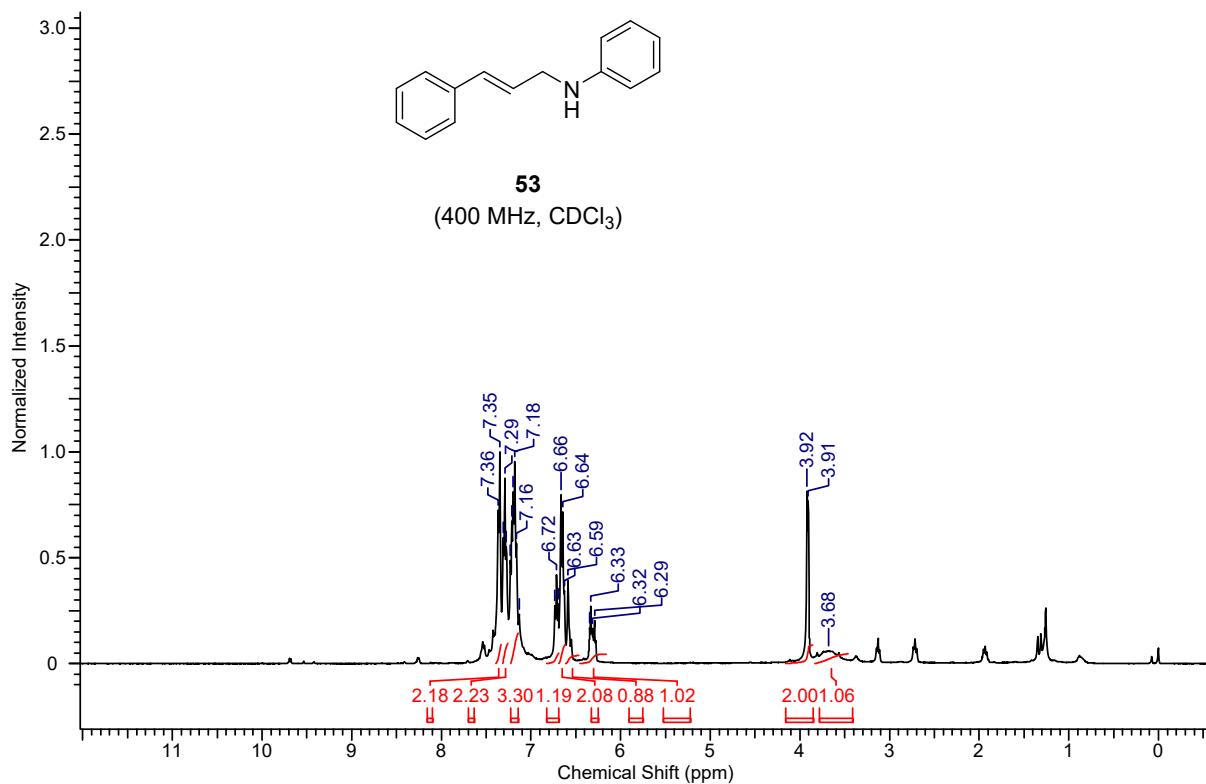
¹³C{¹H}-NMR spectrum of ferrocenemethanol (**51**)



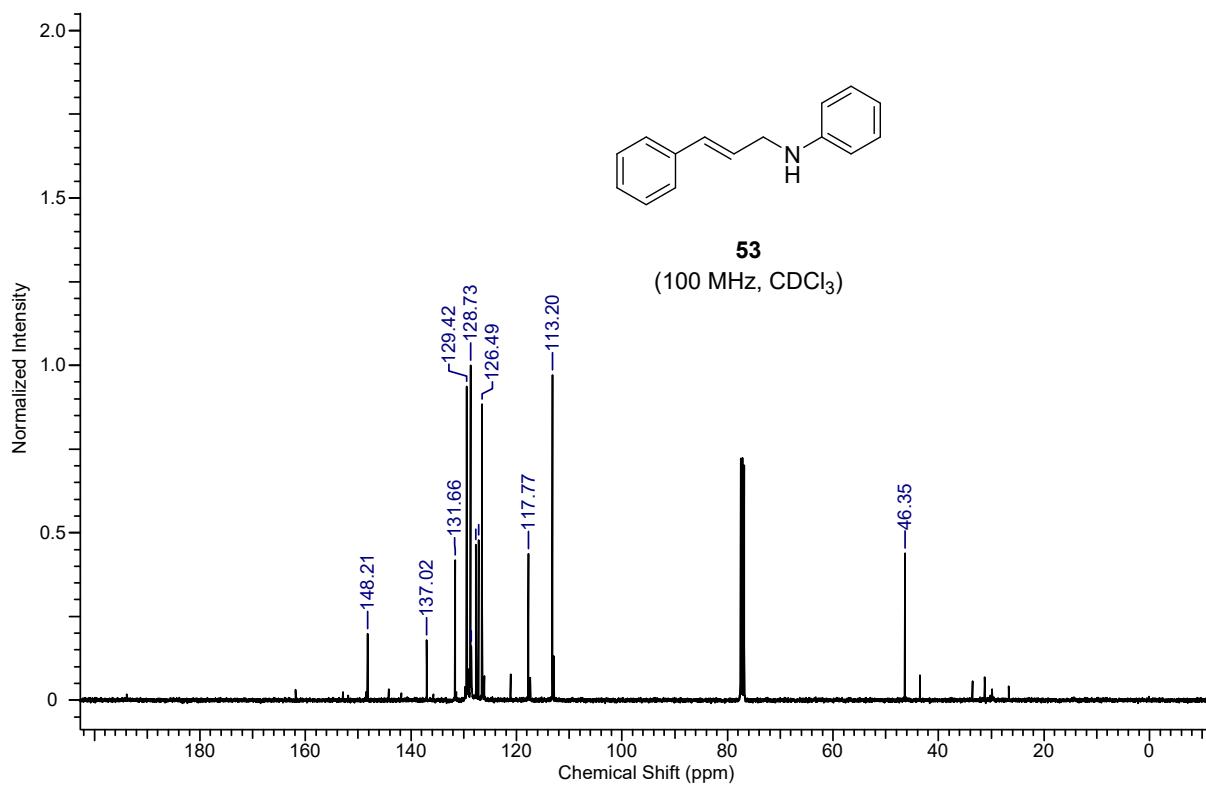
¹H-NMR spectrum of (1*H*-pyrrol-2-yl)methanol (**52**)



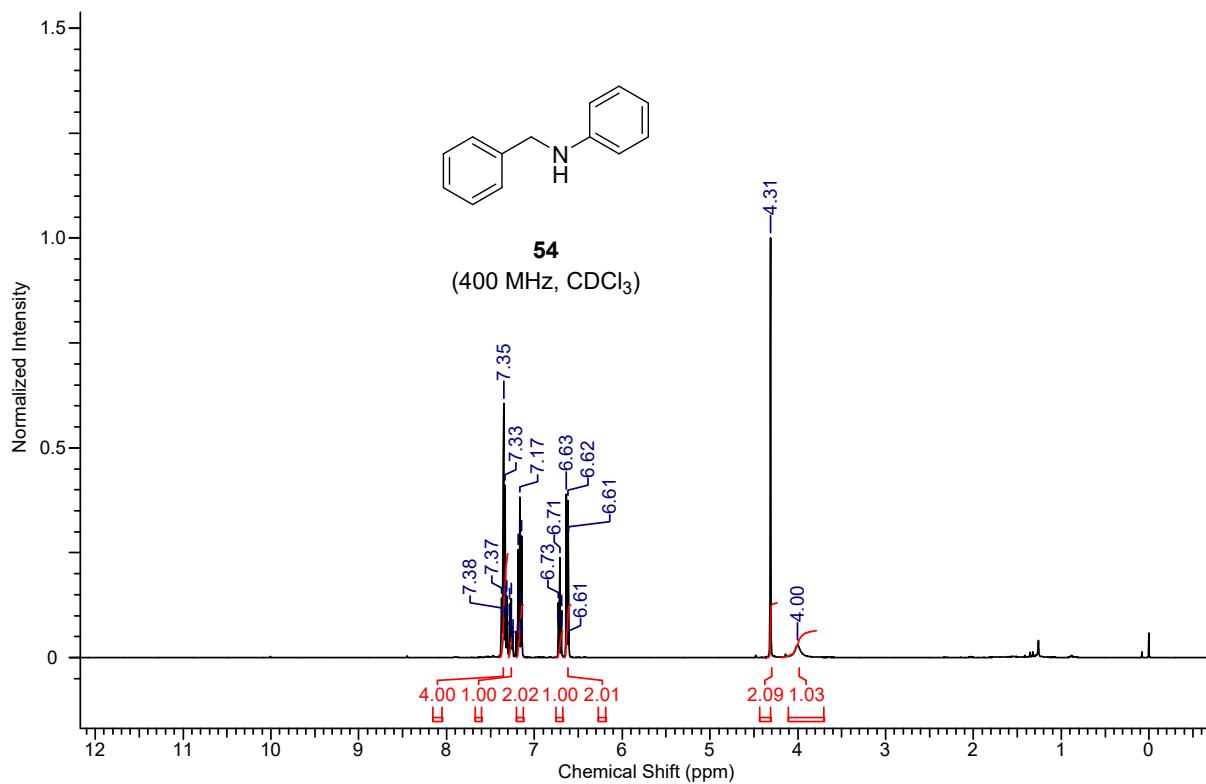
¹³C{¹H}-NMR spectrum of (1*H*-pyrrol-2-yl)methanol (**52**)



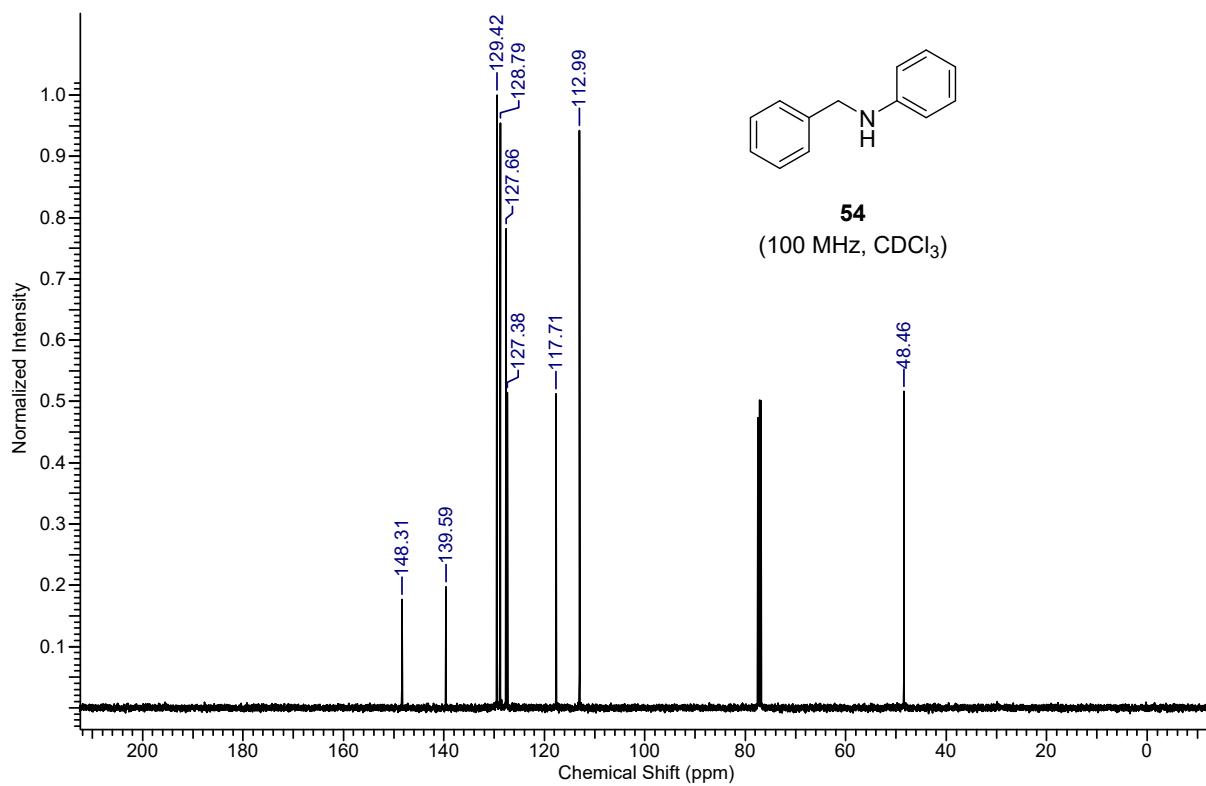
¹H-NMR spectrum of *N*-cinnamylaniline (**53**)



¹³C{¹H}-NMR spectrum of *N*-cinnamylaniline (**53**)



¹H-NMR spectrum of *N*-benzyylaniline (**54**)



¹³C{¹H}-NMR spectrum of *N*-benzyylaniline (**54**)