Supporting information

Transition Metal Complexes of a Bis(carbene) Ligand Featuring 1,2,4-Triazolin-5-ylidene Donors: Structural Diversity and Catalytic Applications

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Table of contents

1. Characterization data of the ligands and metal complexes

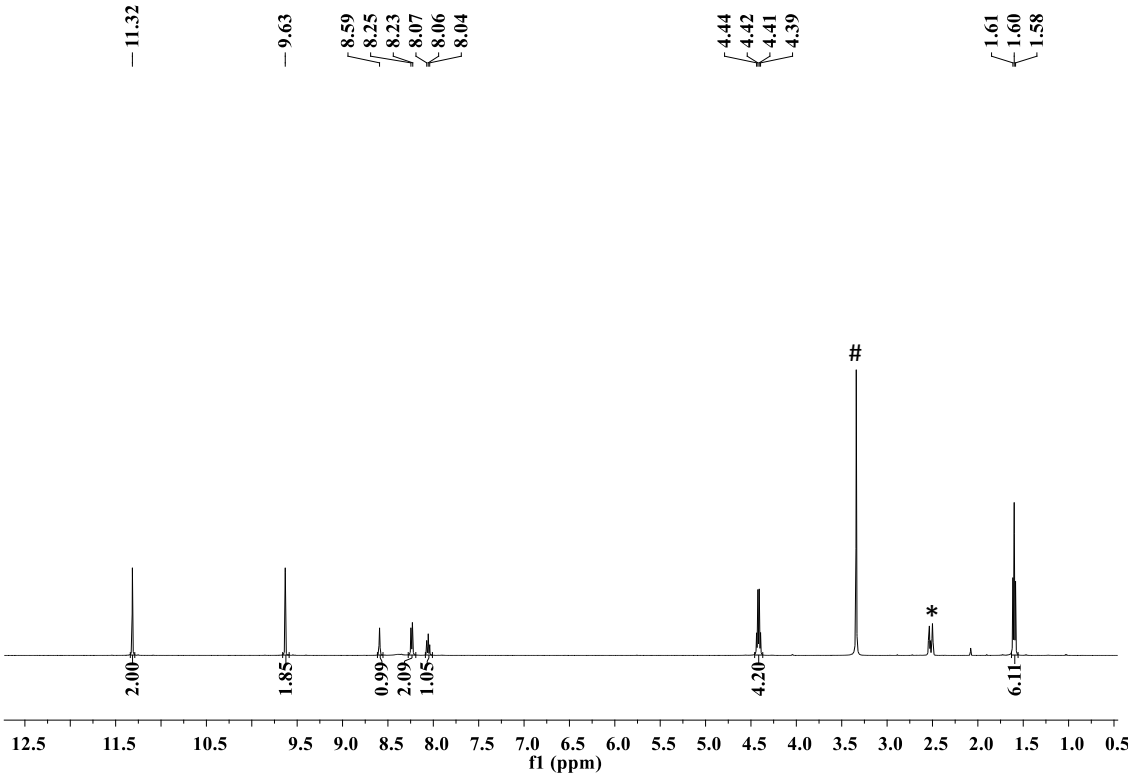


Figure S1. ^{1}H NMR spectrum of **1** in DMSO-d_6 (*). # indicates solvent impurity of H_2O in DMSO-d_6.

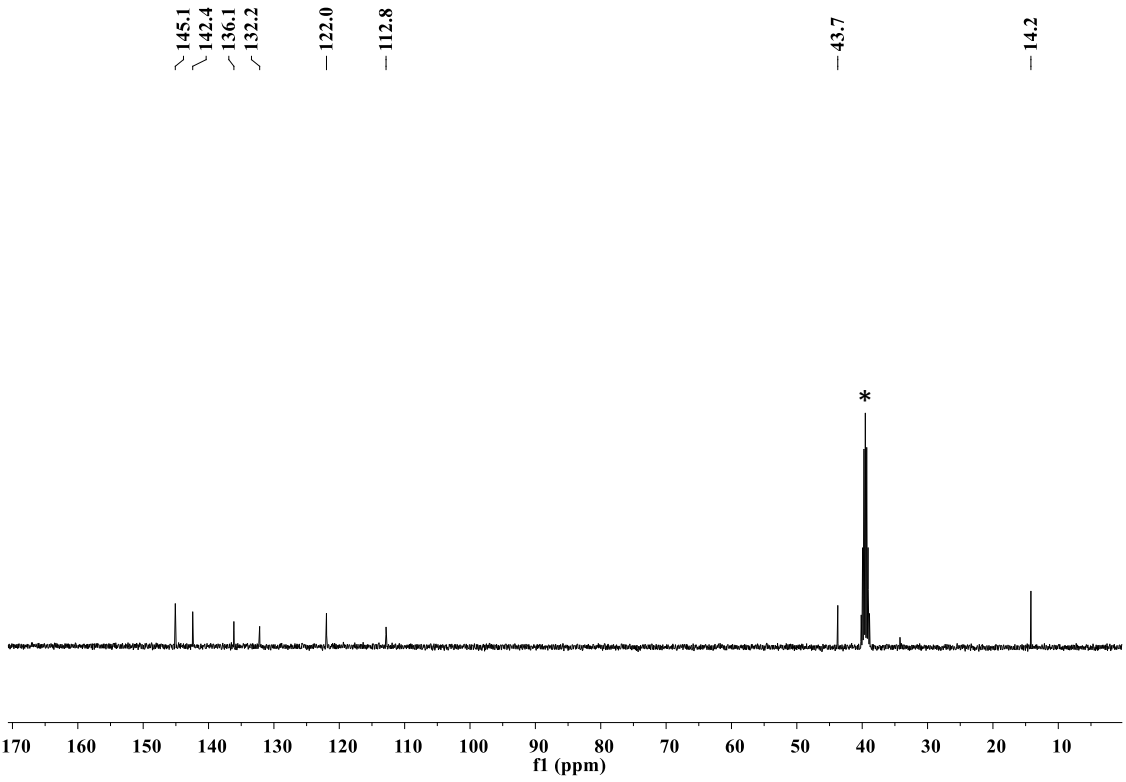


Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of **1** in DMSO-d_6 (*).

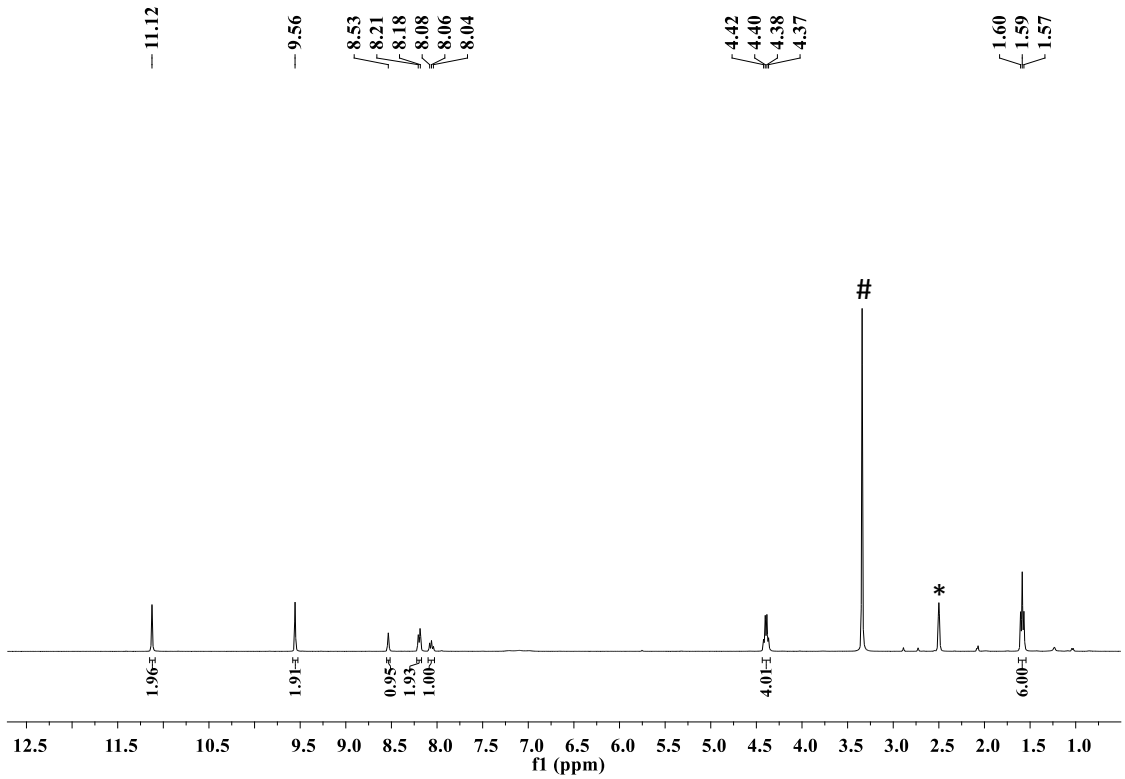


Figure S3. ^{1}H NMR spectrum of **2** in DMSO-d_6 (*). # indicates solvent impurity of H_2O in DMSO-d_6.

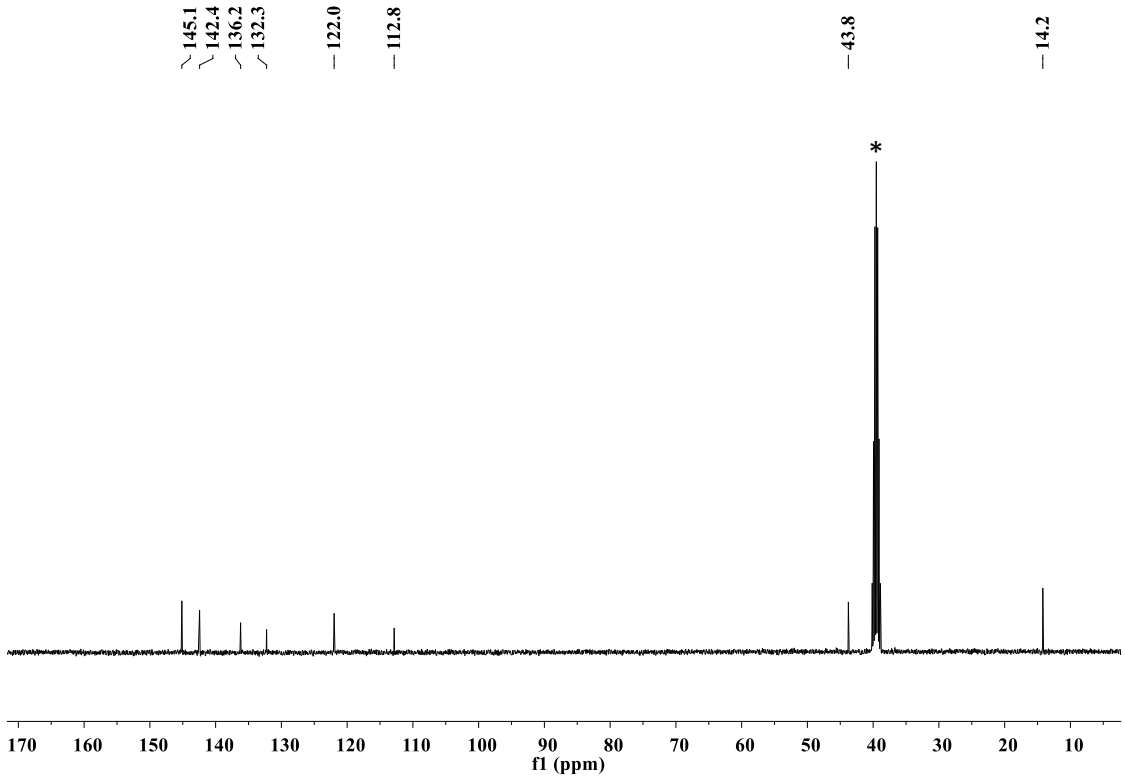


Figure S4. $^{13}C\{^{1}H\}$ NMR spectrum of **2** in DMSO-d_6 (*).

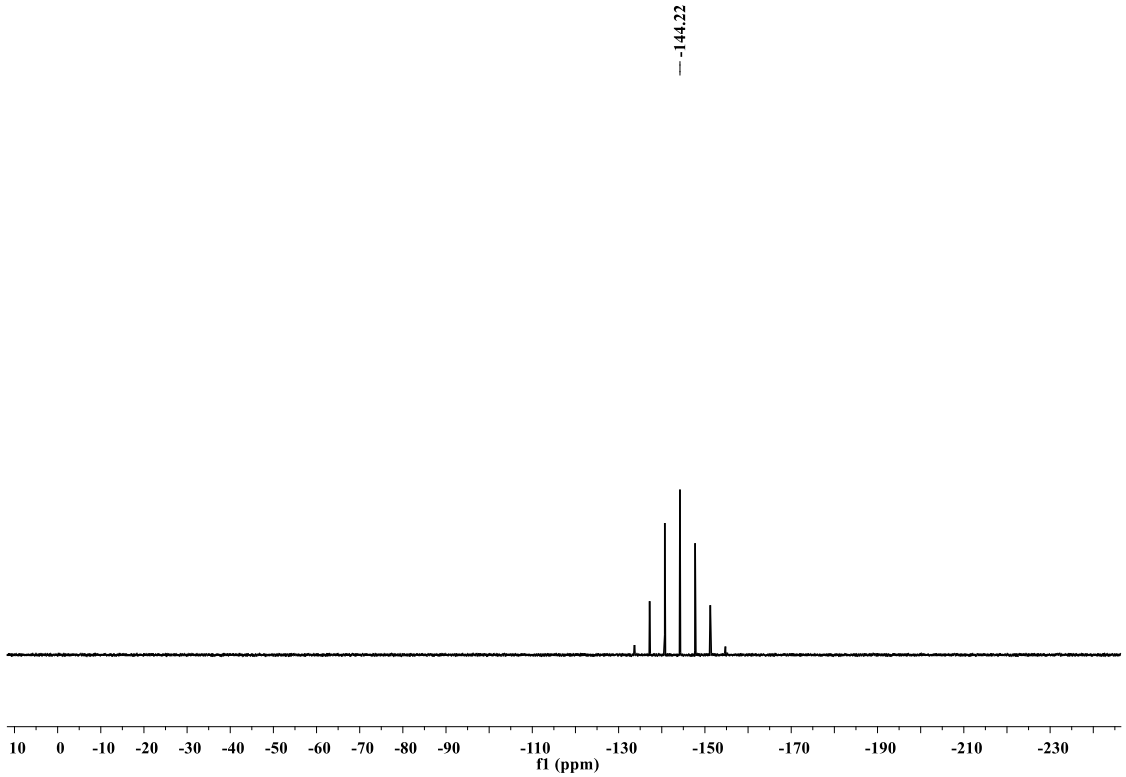


Figure S5. $^{31}P\{^{1}H\}$ NMR spectrum of **2** in DMSO-d_6.

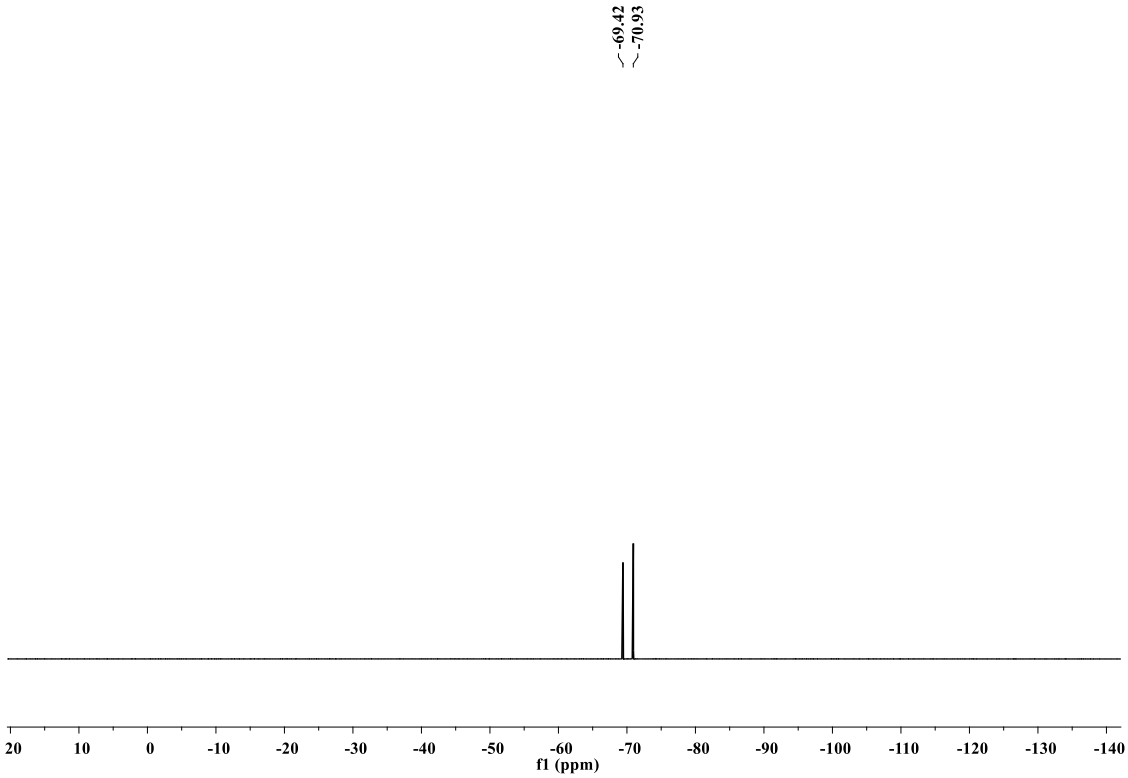


Figure S6. $^{19}F\{^{1}H\}$ NMR spectrum of **2** in DMSO-d_6.

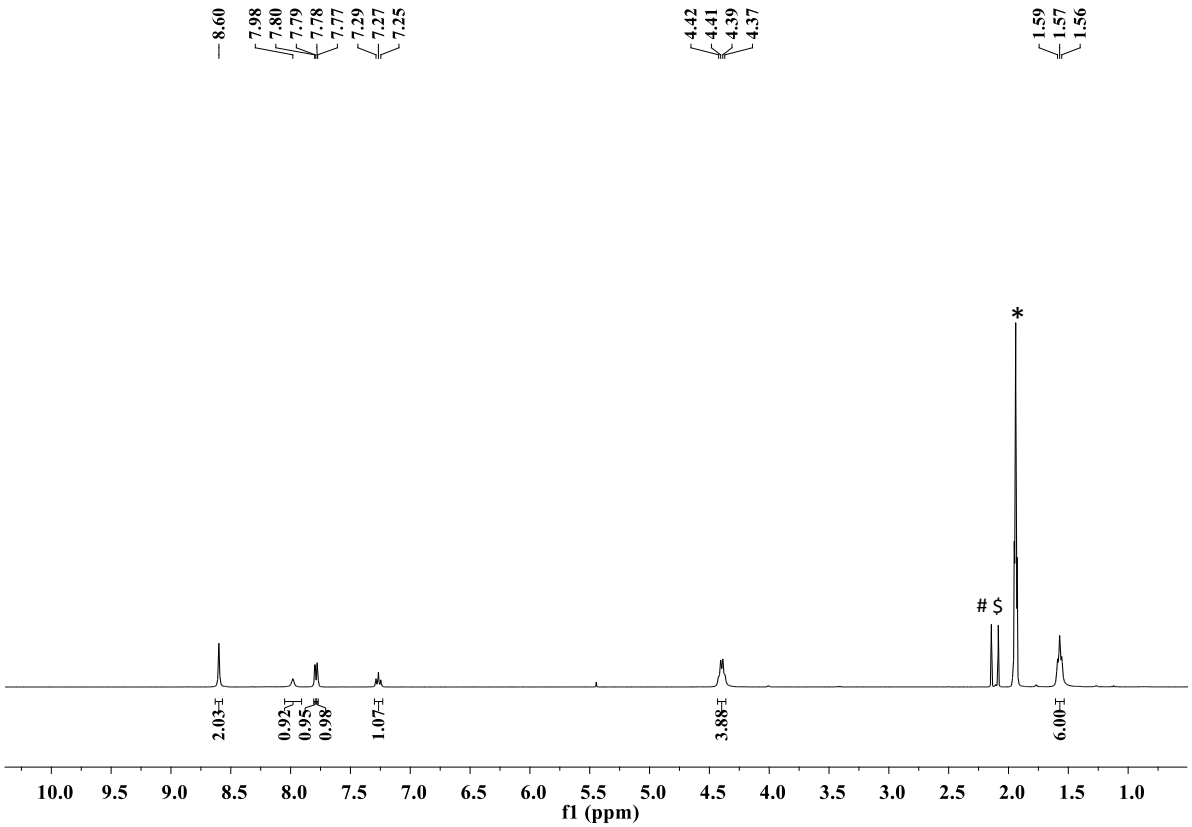


Figure S7. ^{1}H NMR spectrum of **3** in CD_3CN (*). # and $ indicate the solvent impurities of H_2O and acetone, respectively.

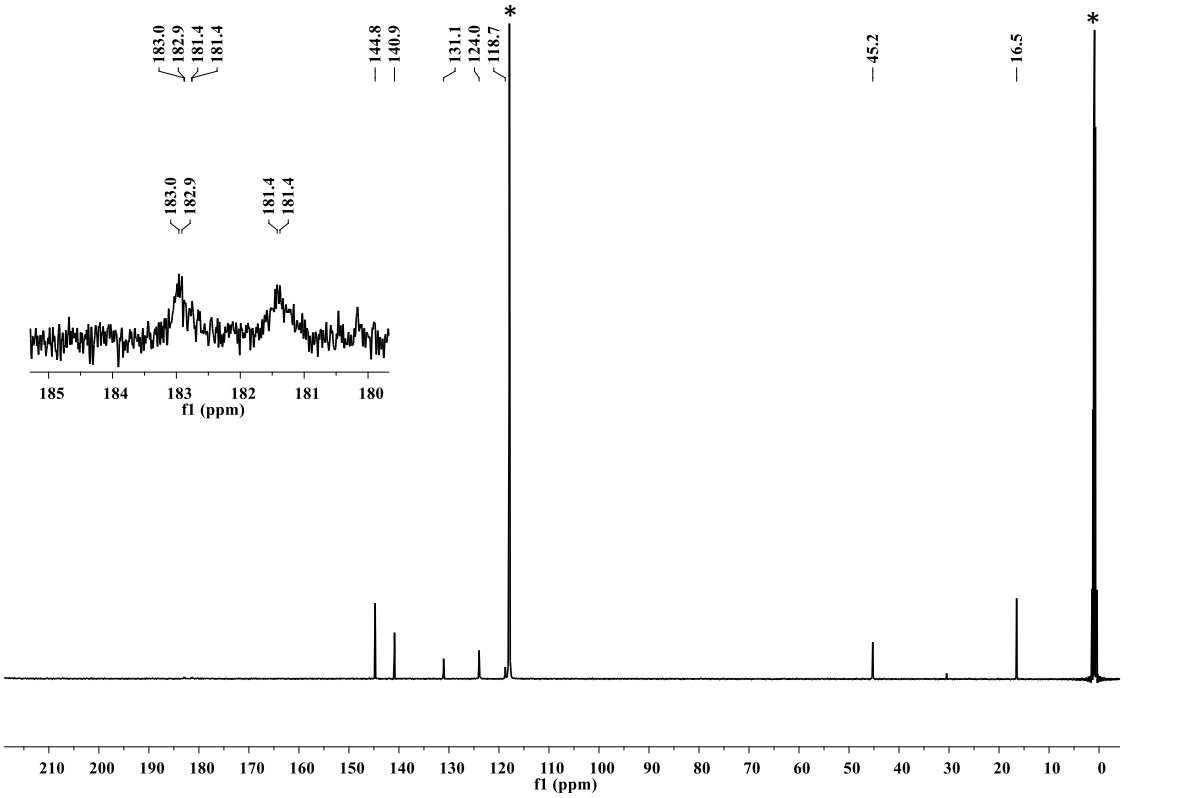


Figure S8. $^{13}C\{^{1}H\}$ NMR spectrum of **3** in CD_3CN (*).

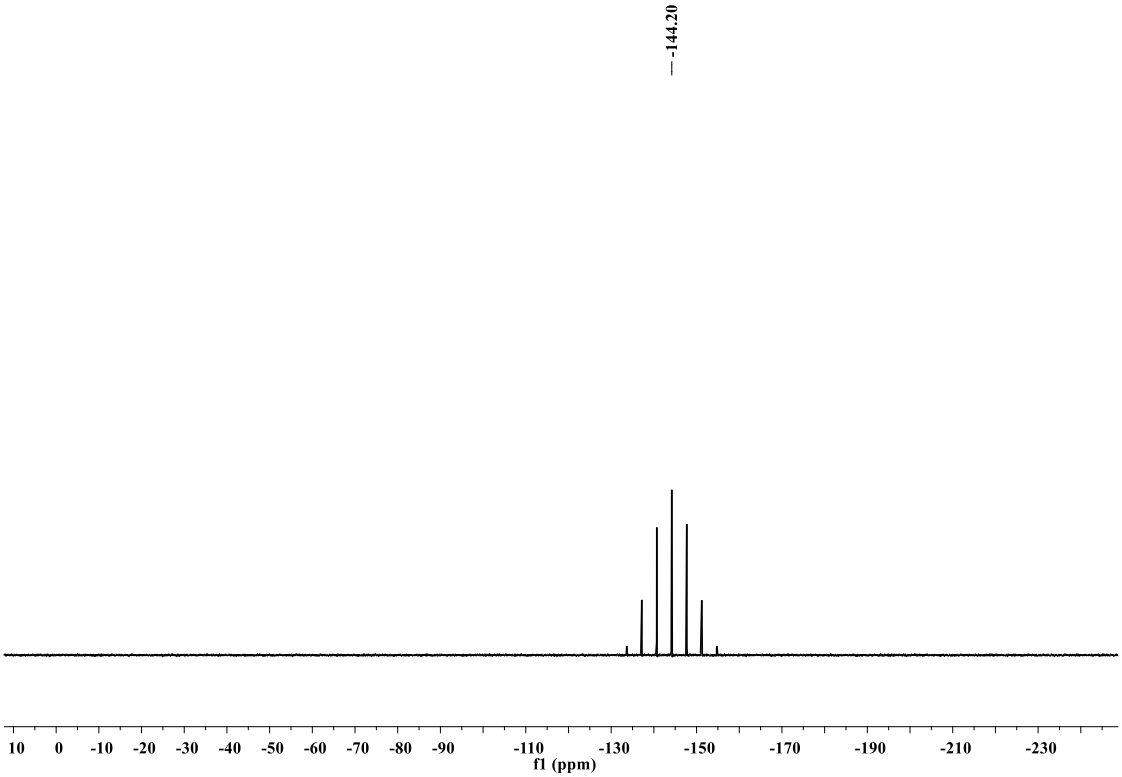


Figure S9. $^{31}P\{^{1}H\}$ NMR spectrum of **3** in CD_3CN.

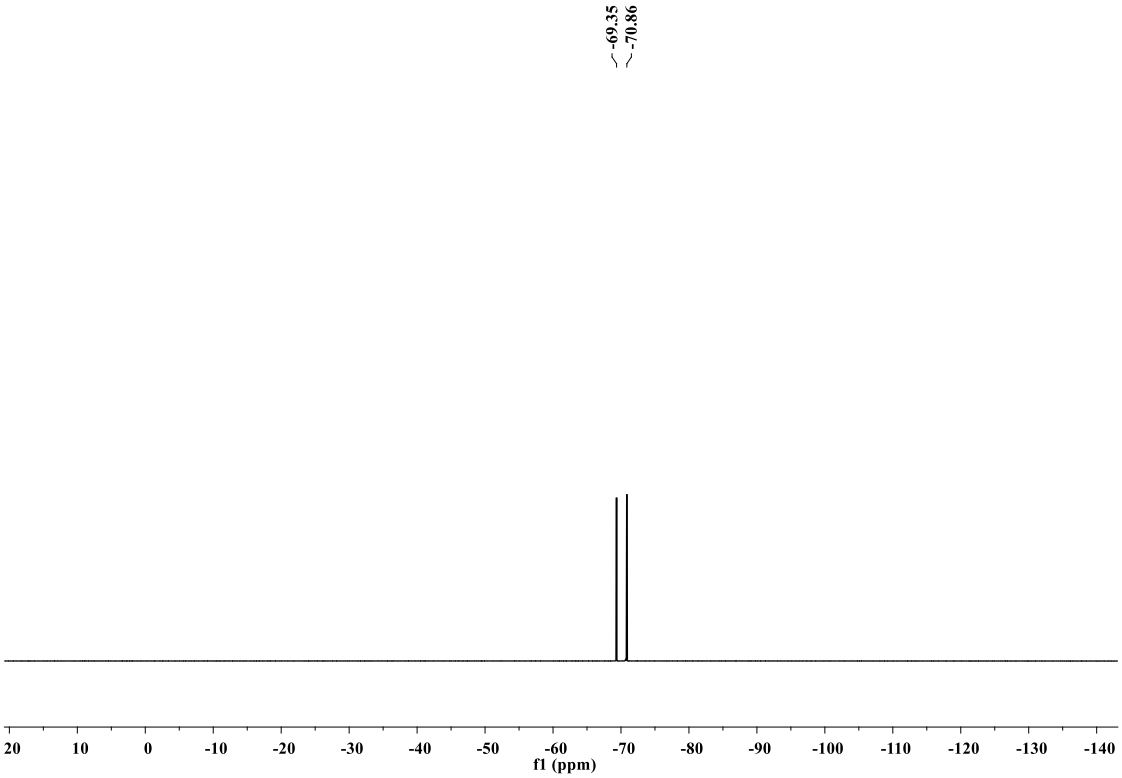


Figure S10. $^{19}F\{^{1}H\}$ NMR spectrum of **3** in CD_3CN.

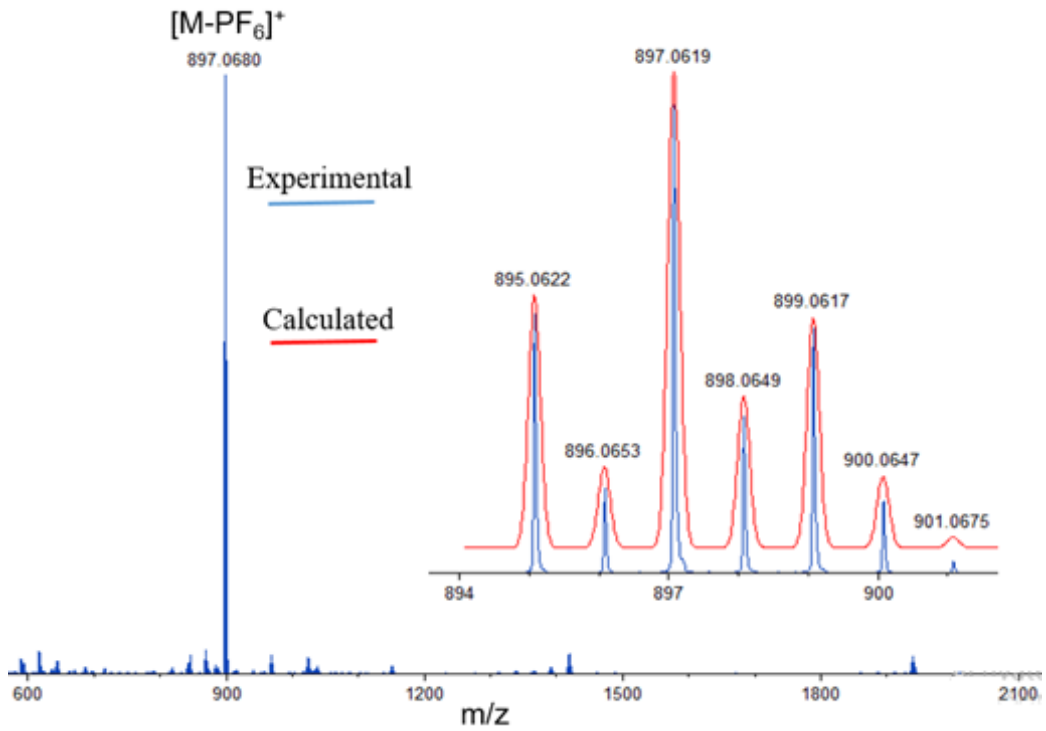


Figure S11. ESI mass spectrum of the dinuclear Ag(I)-NHC complex $[(\mathbf{L})_2Ag_2](PF_6)_2$, **3**.

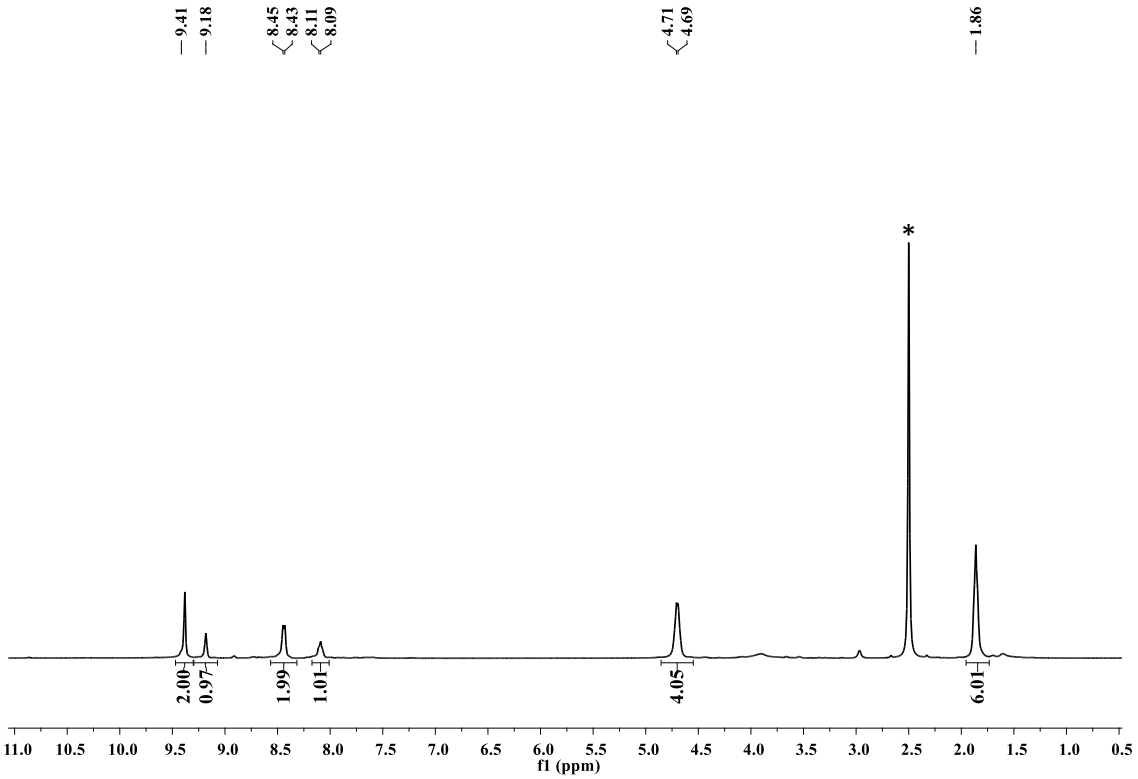


Figure S12. ^{1}H NMR spectrum of **4** in DMSO-d_6 (*).

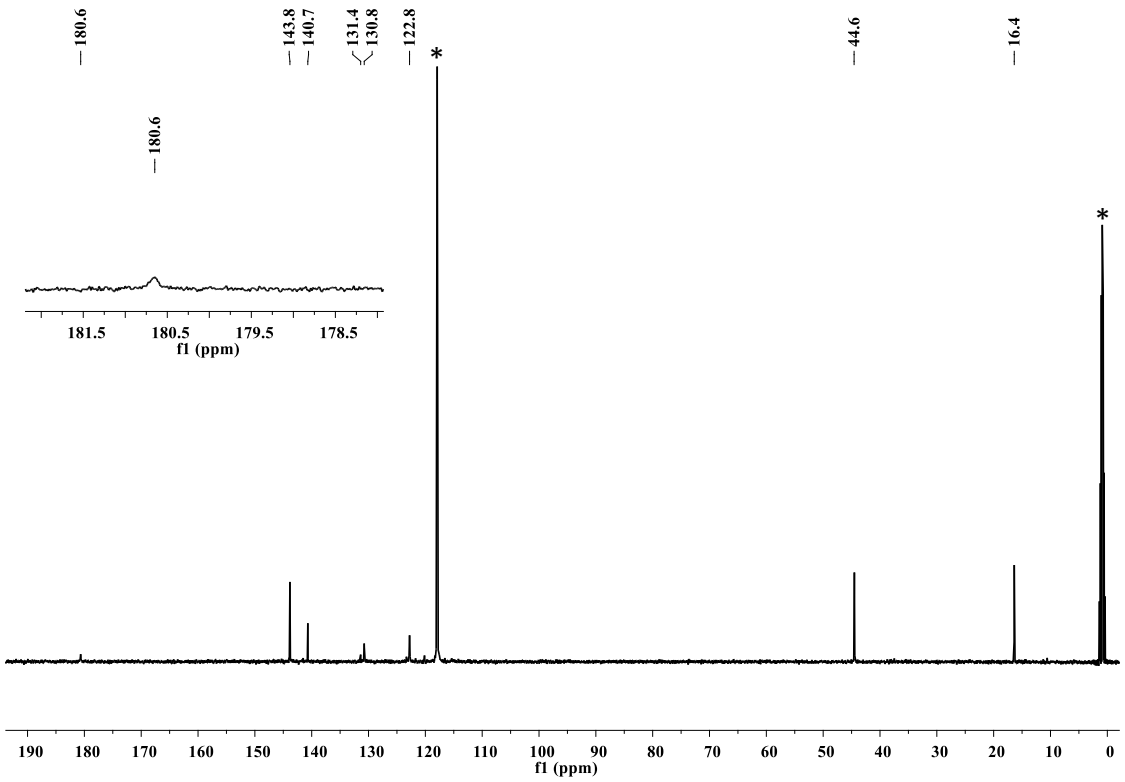


Figure S13. $^{13}C\{^{1}H\}$ NMR spectrum of **4** in CD_3CN (*).

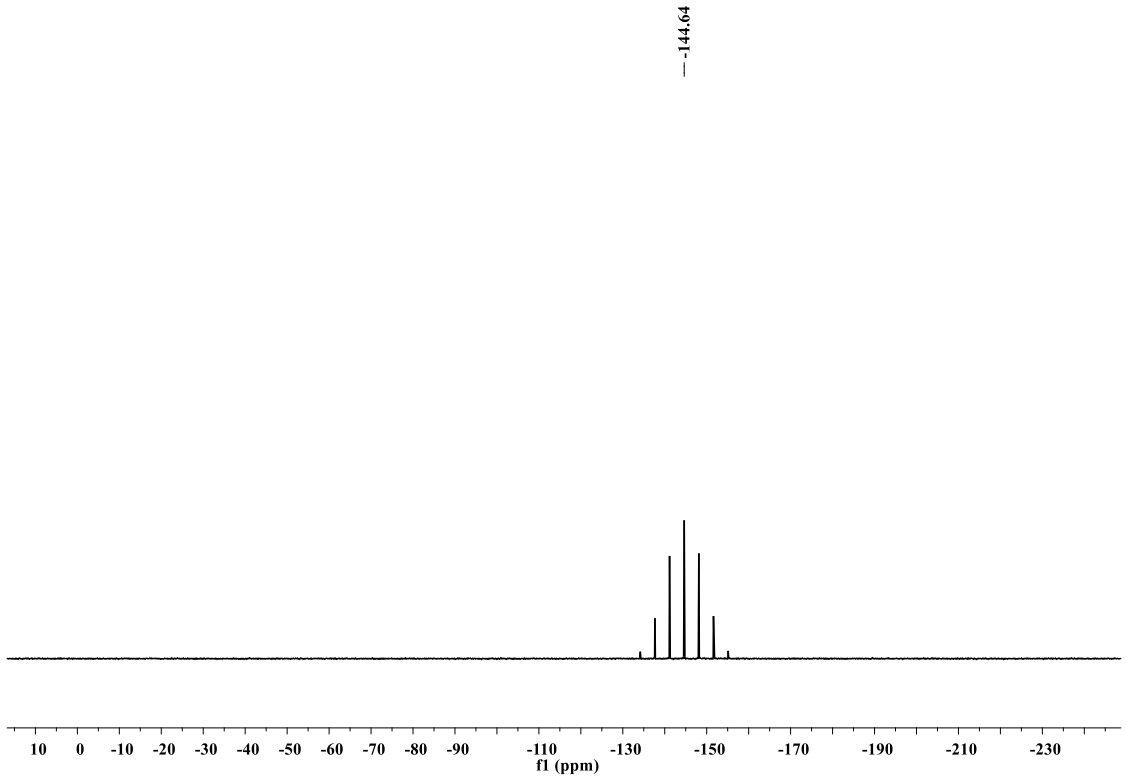


Figure S14. $^{31}P\{^{1}H\}$ NMR spectrum of **4** in CD_3CN.

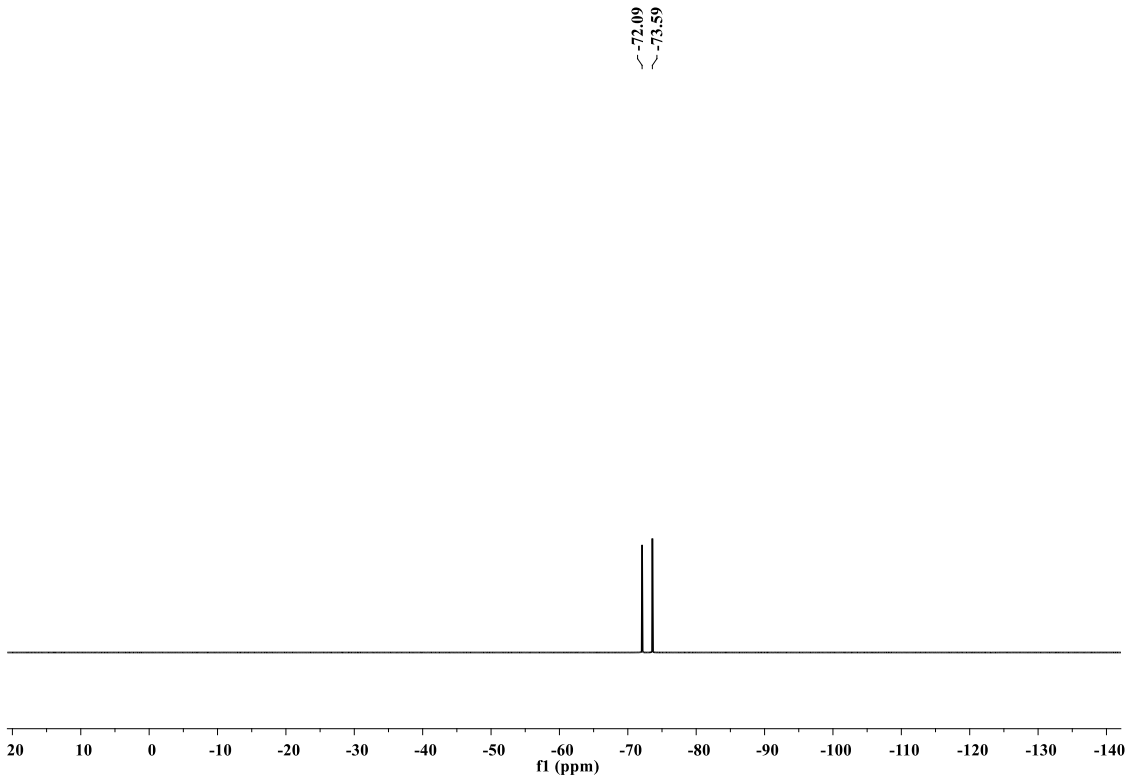


Figure S15. $^{19}F\{^{1}H\}$ NMR spectrum of **4** in CD_3CN.

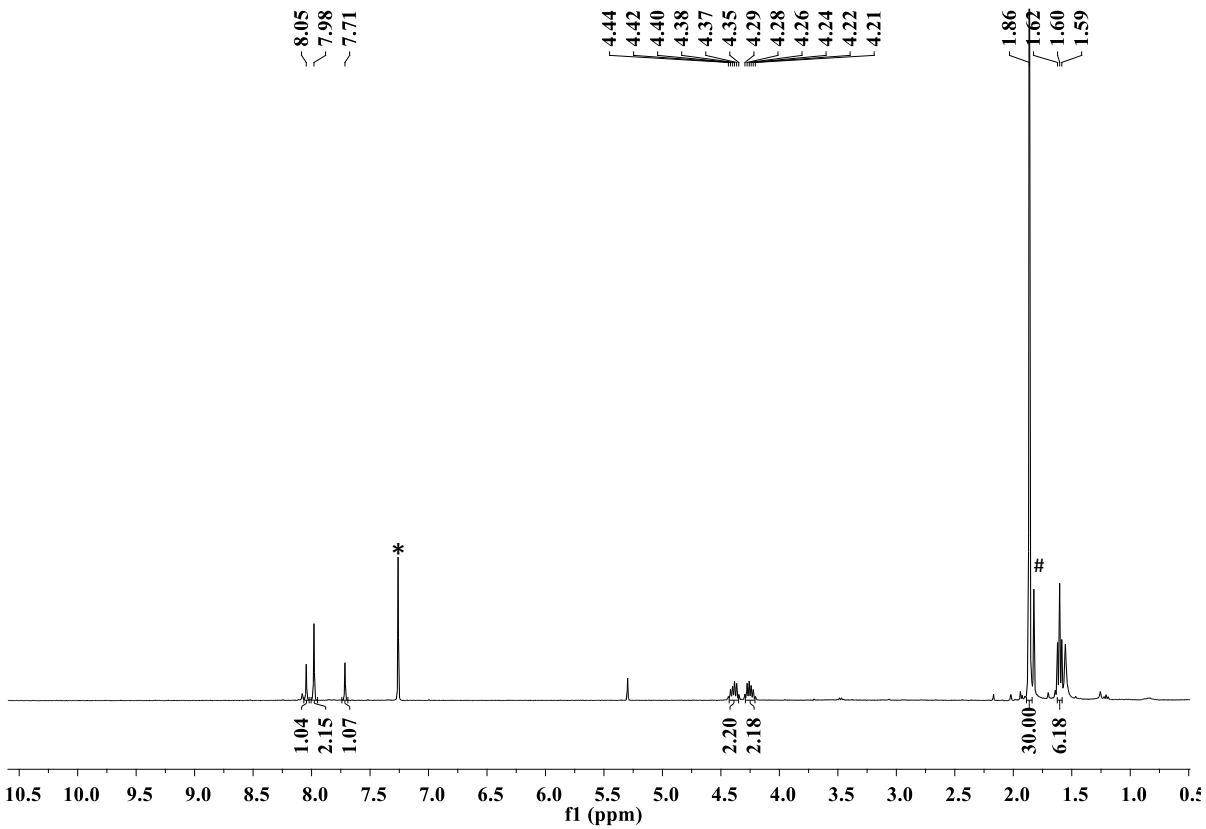


Figure S16. ^{1}H NMR spectrum of **5** in $CDCl_3$ (*). # indicates solvent impurity of H_2O in $CDCl_3$.

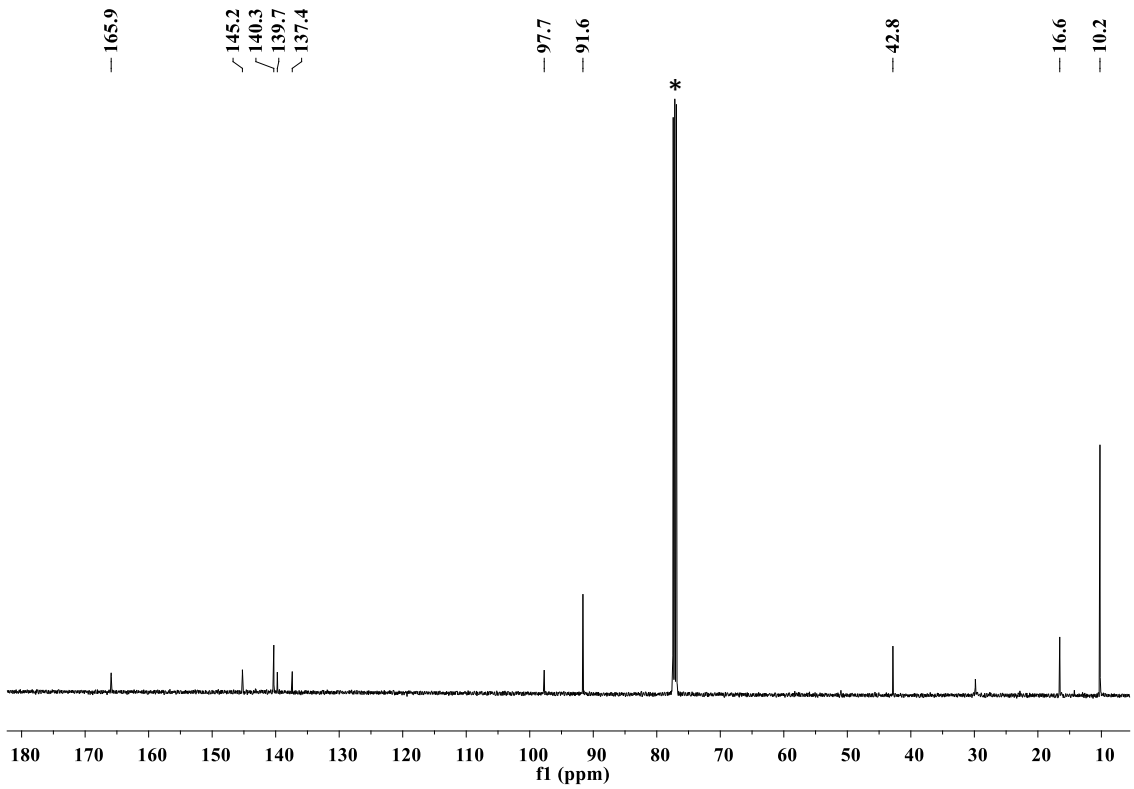


Figure S17. $^{13}C\{^{1}H\}$ NMR spectrum of **5** in $CDCl_3$ (*).

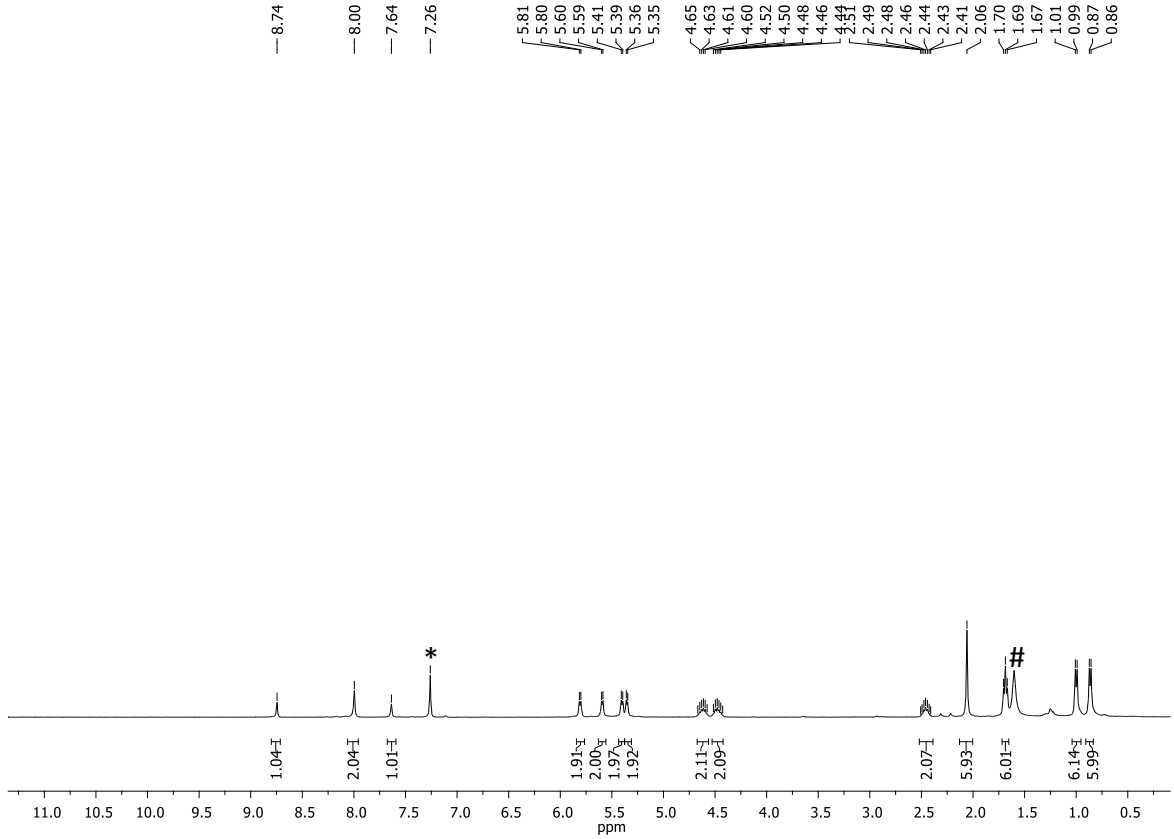


Figure S18. ^{1}H NMR spectrum of **6** in $CDCl_3$ (*). # indicates solvent impurity of H_2O in $CDCl_3$.

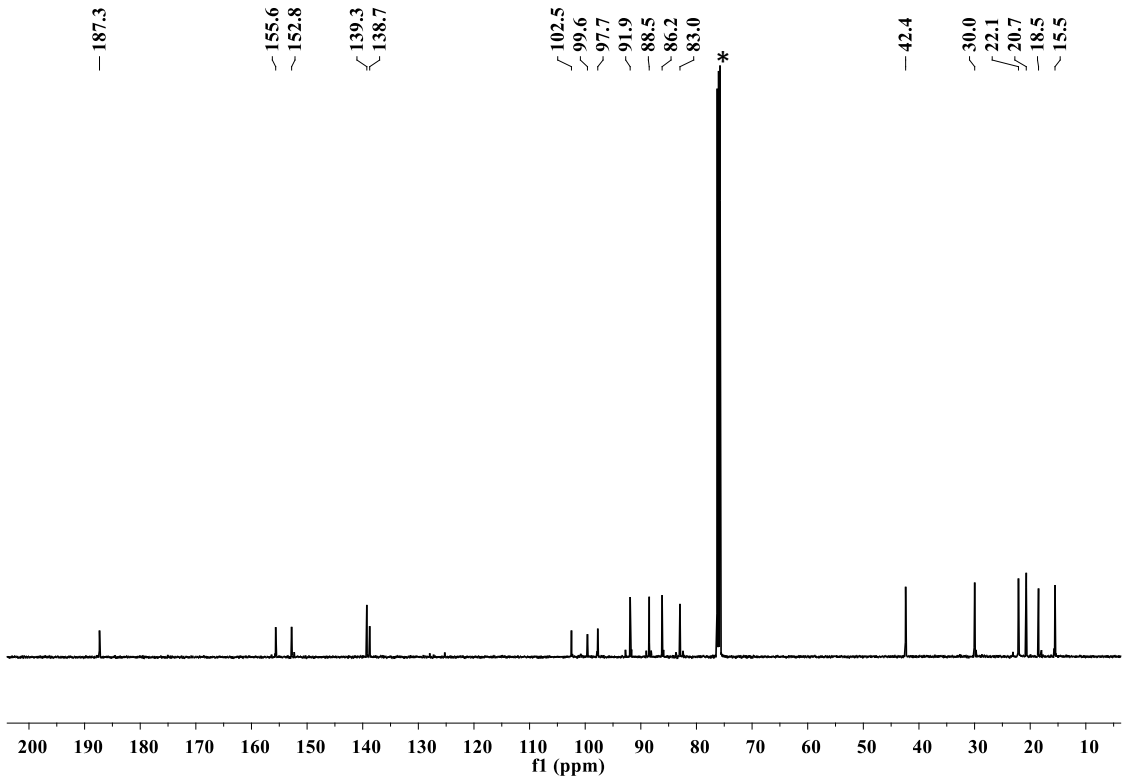


Figure S19. $^{13}C\{^{1}H\}$ NMR spectrum of **6** in $CDCl_3$ (*).

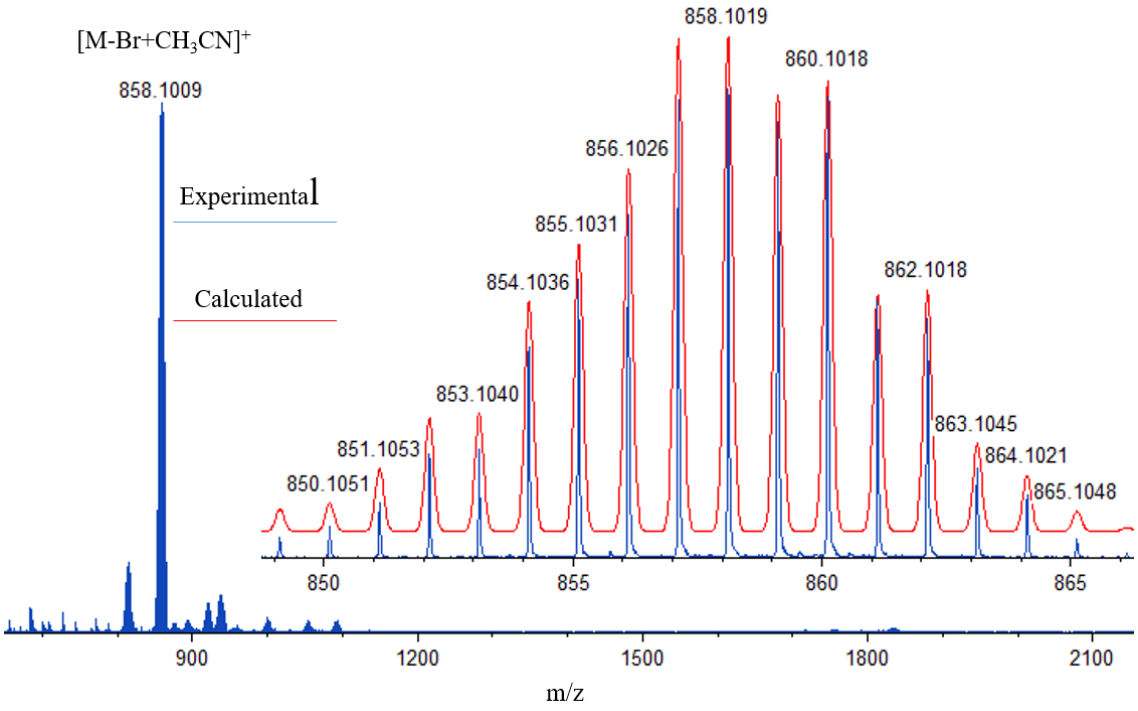


Figure S20. ESI-Mass spectrum of diorthometalated Ru(II)-NHC complex, **6**.

2. Crystallographic Data

Table S1. Crystallographic data for compounds [**L**-H_2]$(PF_6)_2$, **2** and [(**L**)$_2Ag_2$]$(PF_6)_2$, **3**.

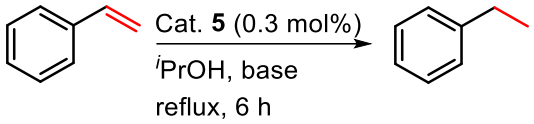
Parameter	**2**	**3**
Empirical formula	$C_{14}H_{18}F_{12}N_6P_2$	$C_{28}H_{32}Ag_2F_{12}N_{12}P_2$
Formula weight	560.28	1042.33
Crystal system	Triclinic	Monoclinic
Space group	P-1	$P2_1/c$
a (Å)	8.1345(3)	9.5672(4)
b (Å)	10.9351(4)	16.3601(7)
c (Å)	13.7618(5)	14.2120(6)
α (°)	109.328(2)	90.00
β (°)	104.605(2)	108.632(2)
γ (°)	98.266(2)	90.00
V(Å^3)	1082.65(7)	2107.88(16)
Z	2	2
D_{calc} (Mg/m^3)	1.719	1.642
F (000)	564	1032
μ (mm^{-1})	0.319	1.094
θ Range (°)	1.656-24.999	2.246-24.997
Crystal size (mm)	0.25 x 0.22 x 0.10	0.25 x 0.22 x 0.16
No. of total reflections	14152	14208
No. of unique reflections [I > 2σ(I)]	3803	3712
No. of parameters (Restraints)	421 (45)	272 (40)
Goodness-of-fit on F^2	1.079	1.038
Final R indices [I > 2σ(I)]	0.1825, 0.0694	0.0283, 0.0725
R indices (all data)	0.0942, 0.2060	0.0367, 0.0781

Table S2. Crystallographic data for the compounds $[(\mathbf{L})_2Cu_2](PF_6)_2$, **4** and **5**.

Parameter	**4**	**5**
Empirical formula	$C_{28}H_{32}Cu_2F_{12}N_{12}P_2$	$C_{34}H_{44}Ir_2N_6Br_2$
Formula weight	953.70	1080.97
Crystal system	Monoclinic	Triclinic
Space group	$P2_1/c$	P-1
a (Å)	8.986(2)	18.0475(6)
b (Å)	16.241(4)	18.9017(7)
c (Å)	14.337(3)	23.8803(9)
α (°)	90.0	77.667(1)
β (°)	106.984(10)	77.973(2)
γ (°)	90.0	89.973(2)
V($Å^3$)	2001.1(8)	7775.3(5)
Z	2	8
D_{calc} (Mg/m^3)	1.583	1.847
F (000)	960	4112
μ (mm^{-1})	1.192	8.924
θ Range (°)	1.944-24.991	1.104-25.00
Crystal size (mm)	0.20 x 0.18 x 0.15	0.20 x 0.15 x 0.10
No. of total reflections	11285	125576
No. of unique reflections [I > 2σ(I)]	3517	27352
No. of parameters (Restraints)	255 (0)	1567 (1778)
Goodness-of-fit on F^2	0.916	1.013
Final R indices [I > 2σ(I)]	0.0931, 0.2716	0.0586, 0.1186
R indices (all data)	0.1386, 0.3103	0.1592, 0.1504

3. Optimization studies for the catalytic reactions

Table S3. Base screening for the transfer hydrogenation reaction[a]



Entry	Base	Yield (%)
1	KOH	84
2	K^{t}BuO	92
3	Na^{t}BuO	100
4	K_2CO_3	Traces
5	None	-
6[b]	Na^{t}BuO	43

[a]**General conditions:** styrene (0.4 mmol), complex **5** (0.3 mol%), NaO^{t}Bu (20 mol%), ^{i}PrOH (4 mL), reflux temperature. Yield was determined by GC-MS analysis using mesitylene as internal standard. [b]Complex **6** was used.

Procedure for the time-dependent product distribution profile of the reaction between 1-phenylethanol and benzyl alcohol: In order to study the conversion and product selectivity at different time interval, four identical reactions were carried out parallelly under our standard reaction condition using 1-phenylethanol and benzyl alcohol as substrates at five different reaction durations (2 h, 4 h, 8 h, 12 h). The conversion and product distribution were determined by GC-MS analysis using mesitylene as internal standard.

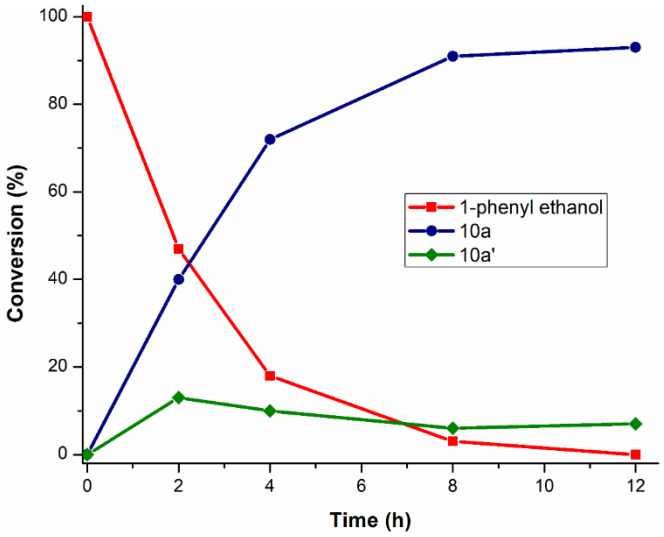
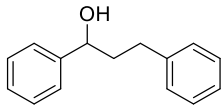


Figure S21. Course of the reaction progress showing the product distribution for the complex **6**-catalyzed *β*-alkylation of 1-phenylethanol with benzyl alcohol.

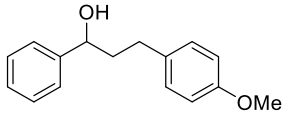
4. Characterization data of the isolated compounds from the catalytic run

1,3-diphenylpropan-1-ol[1]:



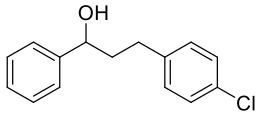
Pale yellow liquid (93 mg, 88%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37–7.31 (m, 4H), 7.30–7.22 (m, 3H), 7.21–7.14 (m, 3H), 4.66 (t, J = 5.9 Hz, 1H), 2.79–2.59 (m, 2H), 2.18–1.97 (m, 2H), 1.96 (s, 1H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.7, 141.9, 128.6, 128.6, 128.5, 127.8, 126.1, 126.0, 74.0, 40.6, 32.2 ppm.

3-(4-methoxyphenyl)-1-phenylpropan-1-ol[1,2]:



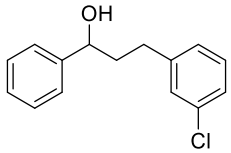
Yellow liquid (103 mg, 86%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37–7.22 (m, 5H), 7.08 (d, J = 8.0 Hz, 2H), 6.80 (d, J = 8.0 Hz, 2H), 4.63 (t, J = 5.9 Hz, 1H), 3.75 (s, 3H), 2.72–2.52 (m, 2H), 2.18 (s, 1H), 2.12–1.90 (m, 2H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.8, 144.7, 133.9, 129.4, 128.6, 127.66 (s), 126.0, 73.9, 55.3, 40.8, 31.2 ppm.

3-(4-Chlorophenyl)-1-phenylpropan-1-ol[1,2]:



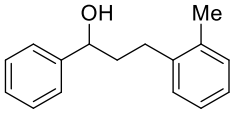
Yellow solid (91 mg, 74%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36–7.25 (m, 5H), 7.22 (d, J = 8.2 Hz, 2H), 7.08 (d, J = 7.8 Hz, 2H), 4.61 (t, J = 6.4 Hz, 1H), 2.73–2.53 (m, 2H), 2.19 (s, 1H), 2.00 (m, 2H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.5, 140.3, 131.6, 129.9, 128.7, 128.5, 127.8, 126.0, 73.8, 40.4, 31.4 ppm.

3-(3-Chlorophenyl)-1-phenylpropan-1-ol[3]:



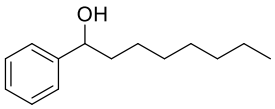
Yellow liquid (94 mg, 76%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27–7.14 (m, 5H), 7.10–7.01 (m, 3H), 6.93 (d, J = 6.6 Hz, 1H), 4.50 (t, J = 6.2 Hz, 1H), 2.64–2.41 (m, 2H), 2.19 (s, 1H), 2.04–1.77 (m, 2H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.4, 144.0, 134.2, 129.7, 128.7, 128.6, 127.8, 126.7, 126.1, 126.0, 73.7, 40.2, 31.8 ppm.

1-phenyl-3-(o-tolyl)propan-1-ol[2]:



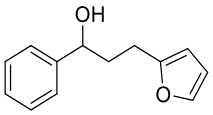
Yellow liquid (90 mg, 80%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 (m, 4H), 7.28 (s, 1H), 7.16–7.04 (m, 4H), 4.71 (s, 1H), 2.82–2.51 (m, 2H), 2.25 (s, 3H), 2.14–1.91 (m, 2H), 1.95 (s, 1H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.7, 140.1, 136.1, 130.3, 128.9, 128.7, 127.8, 126.1, 126.1, 126.0, 74.3, 39.3, 29.5, 19.3 ppm.

1-phenyloctan-1-ol[2,3a]:



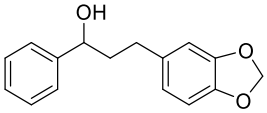
Colourless liquid (86 mg, 84%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46–7.14 (m, 5H), 4.63 (s, 1H), 2.02 (s, 1H), 1.83–1.65 (m, 2H), 1.40 (s, 1H), 1.27 (m, 8H), 0.97–0.82 (m, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.1, 128.5, 127.5, 126.0, 74.8, 39.2, 31.9, 29.6, 29.3, 25.9, 22.8, 14.2 ppm.

3-(furan-2-yl)-1-phenylpropan-1-ol[1]:



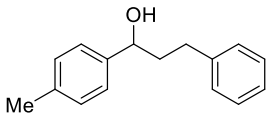
Pale yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.19 (m, 6H), 6.18 (s, 1H), 5.90 (s, 1H), 4.58 (t, J = 6.5 Hz, 1H), 2.62 (m, 2H), 2.09 (s, 1H), 1.97 (m, 2H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.6, 144.4, 141.0, 128.6, 127.8, 126.0, 110.2, 105.1, 73.7, 37.2, 24.5 ppm.

3-(Benzo[1,3]dioxol-5-yl)-1-phenylpropan-1-ol[3b]:



White crystalline solid (117 mg, 92%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44–7.16 (m, 5H), 6.72 (d, J = 7.9 Hz, 1H), 6.68 (s, 1H), 6.63 (d, J = 7.9 Hz, 1H), 5.90 (s, 1H), 4.66 (t, J = 6.1 Hz, 1H), 2.75–2.50 (m, 2H), 2.18–1.93 (m, 2H), 1.89 (d, J = 17.4 Hz, 1H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.7, 145.8, 144.7, 135.7, 128.7, 127.8, 126.0, 121.3, 109.1, 108.3, 100.9, 73.9, 40.9, 31.9 ppm.

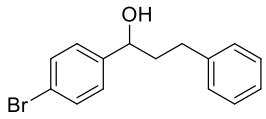
3-phenyl-1-(p-tolyl)propan-1-ol[1,2]:



Yellow liquid (97 mg, 86%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.15 (t, J = 7.4 Hz, 2H), 7.06 (dt, J = 12.8, 7.9 Hz, 7H), 4.47 (t, J = 6.3 Hz, 1H), 2.55 (m, 2H), 2.22 (s, 3H), 2.13 (s, 1H), 2.05–

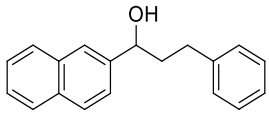
1.80 (m, 2H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.0, 141.7, 137.3, 129.2, 128.5, 128.4, 126.0, 125.9, 73.7, 40.4, 32.1, 21.2 ppm.

1-(4-bromophenyl)-3-phenylpropan-1-ol[1,3]:



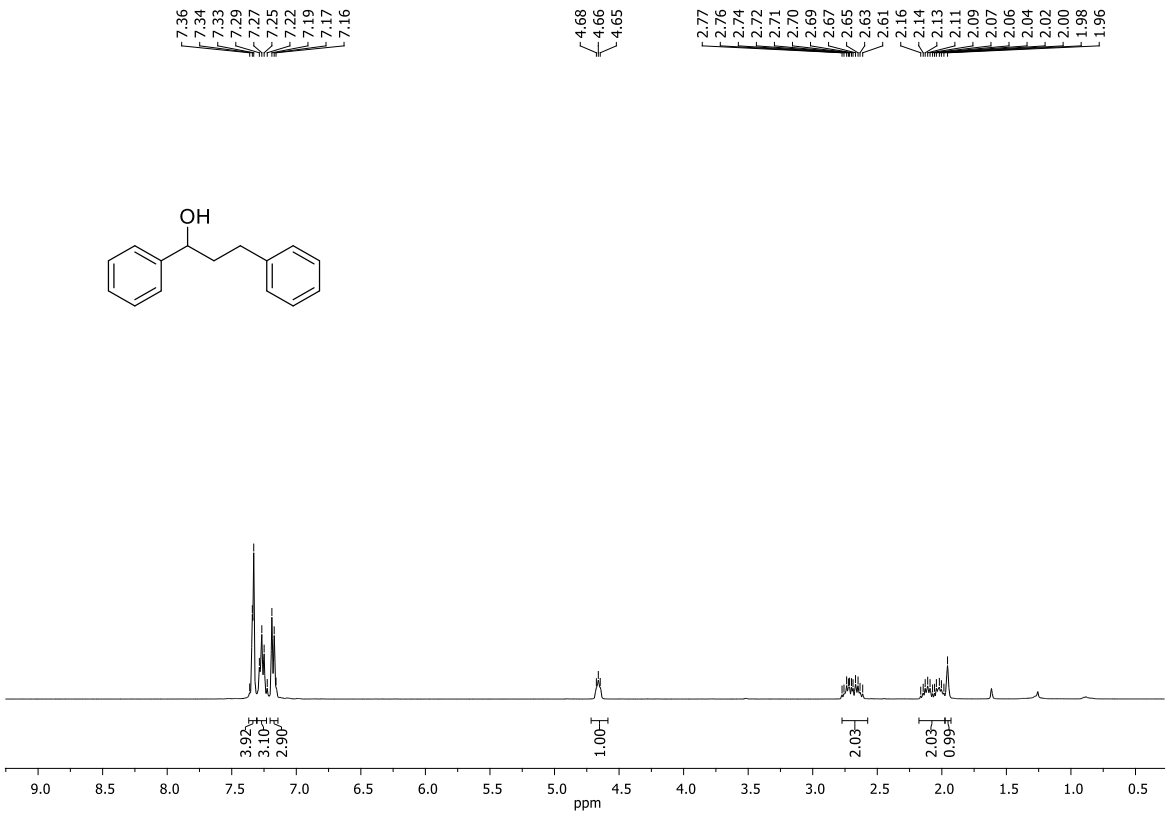
Colourless liquid (120 mg, 82%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, J = 7.4 Hz, 2H), 7.26 (q, J = 7.3 Hz, 2H), 7.18 (t, J = 8.9 Hz, 5H), 4.61 (s, 1H), 2.78–2.58 (m, 2H), 2.09 (s, 1H), 1.98 (m, 2H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.7, 141.6, 131.7, 128.6, 128.5, 127.9, 126.1, 121.4, 73.2, 40.5, 32.0 ppm.

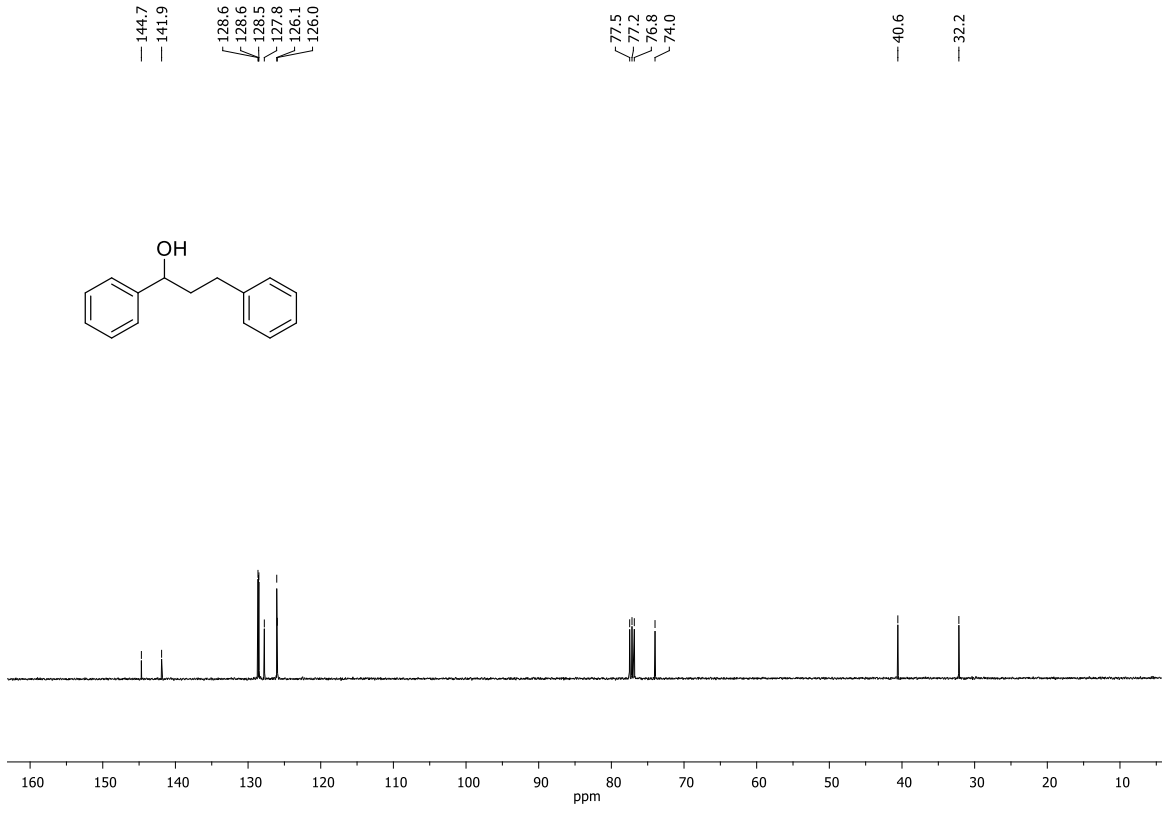
1-(Naphthalen-2-yl)-3-phenylpropan-1-ol[1,3]:

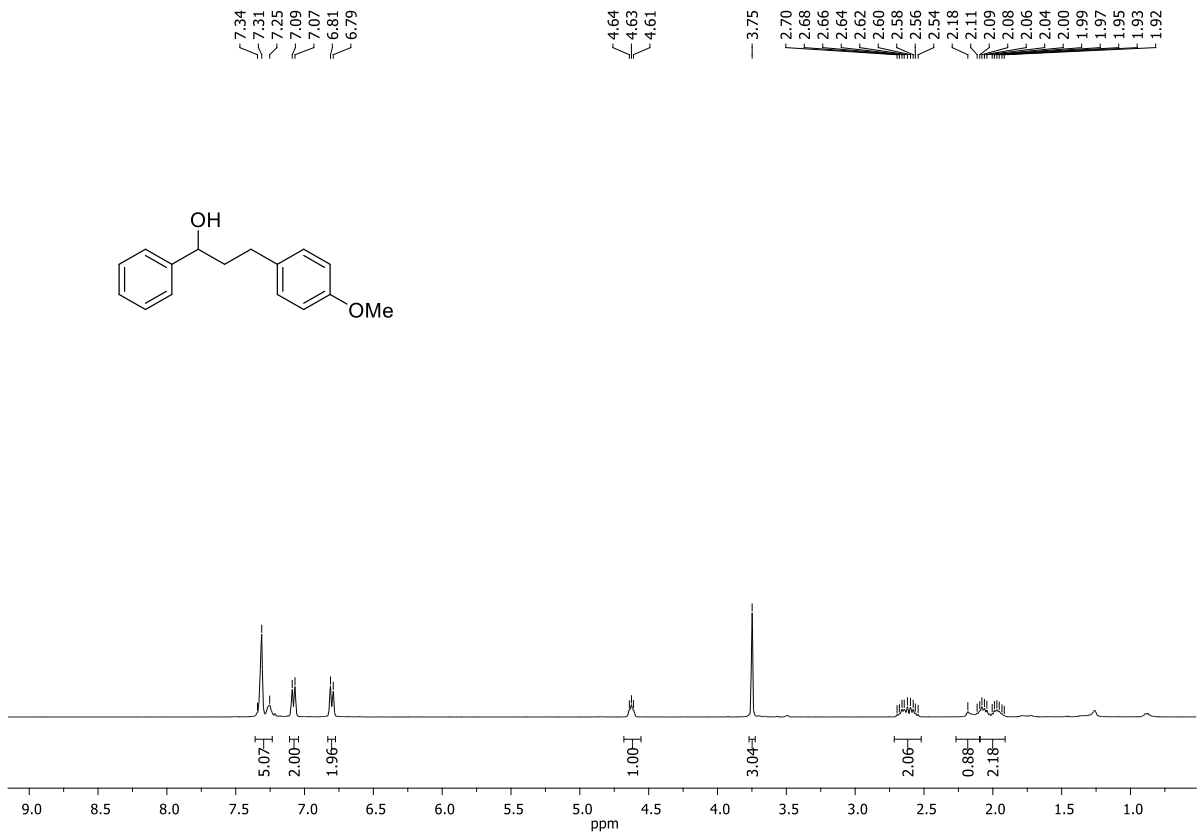


White solid (121 mg, 94%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, J = 7.5 Hz, 3H), 7.79 (s, 1H), 7.48 (t, J = 9.4 Hz, 3H), 7.29 (d, J = 7.5 Hz, 1H), 7.26 (d, J = 4.3 Hz, 1H), 7.22–7.16 (m, 3H), 4.86 (s, 1H), 2.84–2.64 (m, 2H), 2.29–2.04 (m, 2H), 1.96 (s, 1H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.0, 141.9, 133.4, 133.2, 128.6, 128.6, 128.1, 127.9, 74.2, 40.5, 32.2 ppm.

5. NMR spectra of the isolated alcohols from the catalytic run in $CDCl_3$



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4.64
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2.66
2.64
2.62
2.60
2.58
2.56
2.54
2.18
2.11
2.09
2.08
2.06
2.04
2.00
1.99
1.97
1.95
1.93
1.92
OH
OMe
5.07
2.00
1.96
1.00
3.04
2.06
0.88
2.18
9.0
8.5
8.0
7.5
7.0
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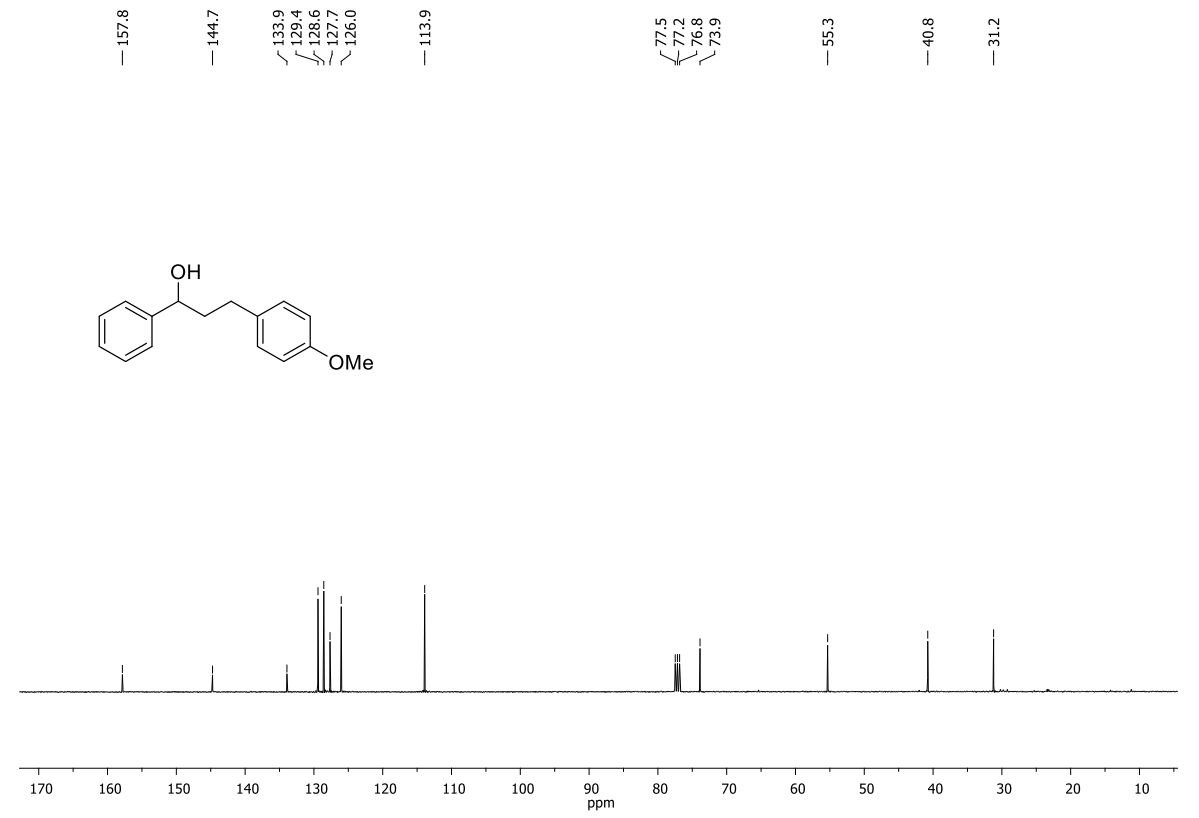
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127.7
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113.9
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77.2
76.8
73.9
55.3
40.8
31.2
OH
OMe
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150
140
130
120
110
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70
60
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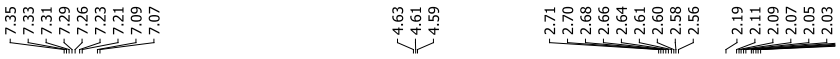
40
30
20
10
ppm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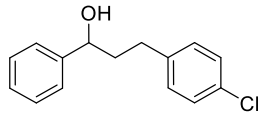
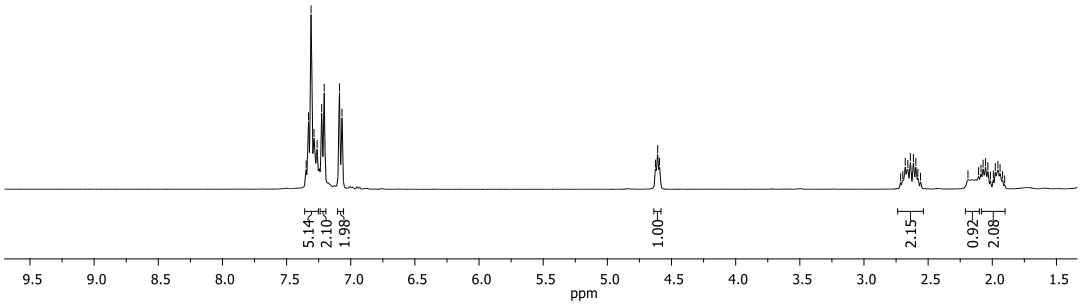
2.07
2.05
2.03


OH
Cl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6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm


144.5
140.3
131.6
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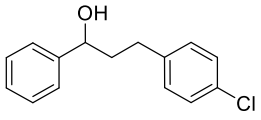
128.6
128.5
127.8
126.0
77.5
77.2
76.8
73.8
40.4
31.4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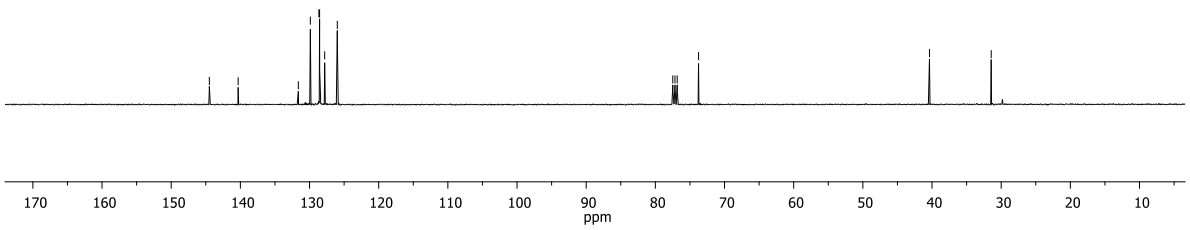
Cl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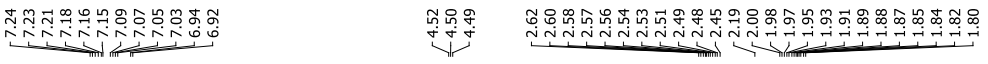
10
ppm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4.50
4.49
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2.60
2.58
2.57
2.56
2.54
2.53
2.51
2.49
2.48
2.45
2.19
2.00
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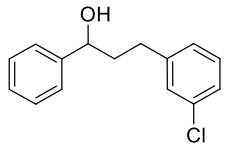
1.80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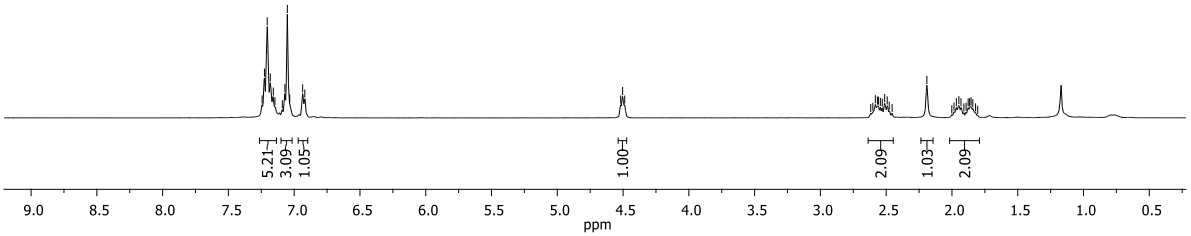
Cl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6.0
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5.0
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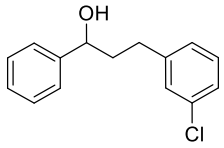
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm


144.4
144.0
134.2
129.7
128.7
128.6
127.8
126.7
126.1
126.0
77.5
77.2
76.8
73.7
40.2
31.8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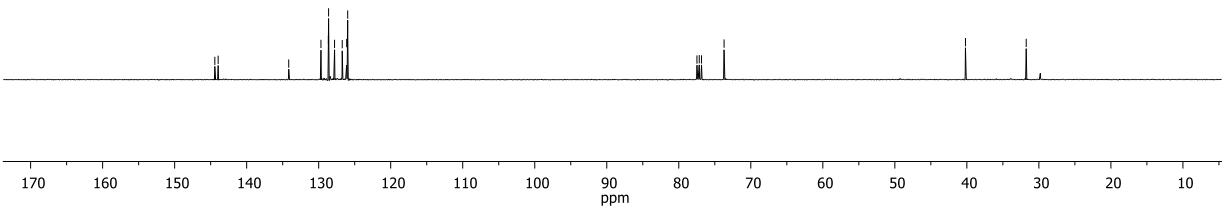
Cl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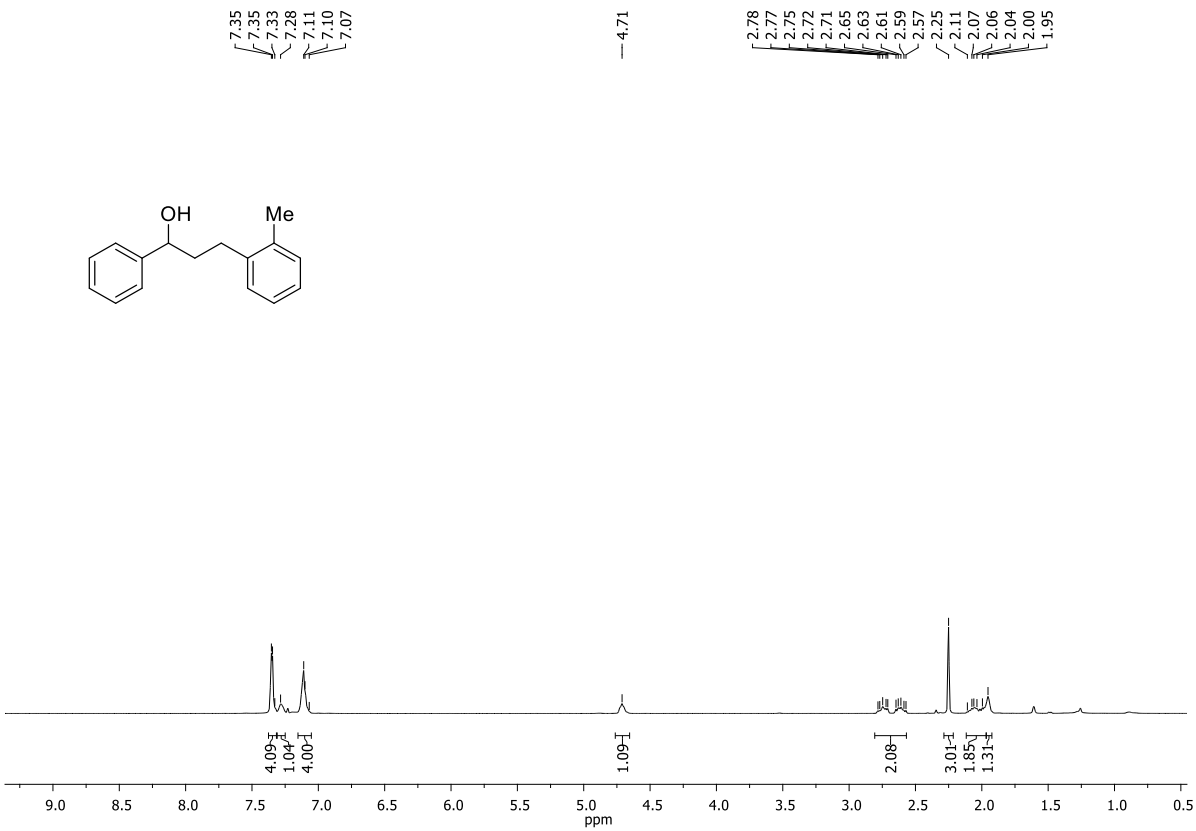
10
ppm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2.63
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2.59
2.57
2.25
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2.07
2.06
2.04
2.00
1.95
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Me
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4.00
1.09
2.08
3.01
1.85
1.31
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7.5
7.0
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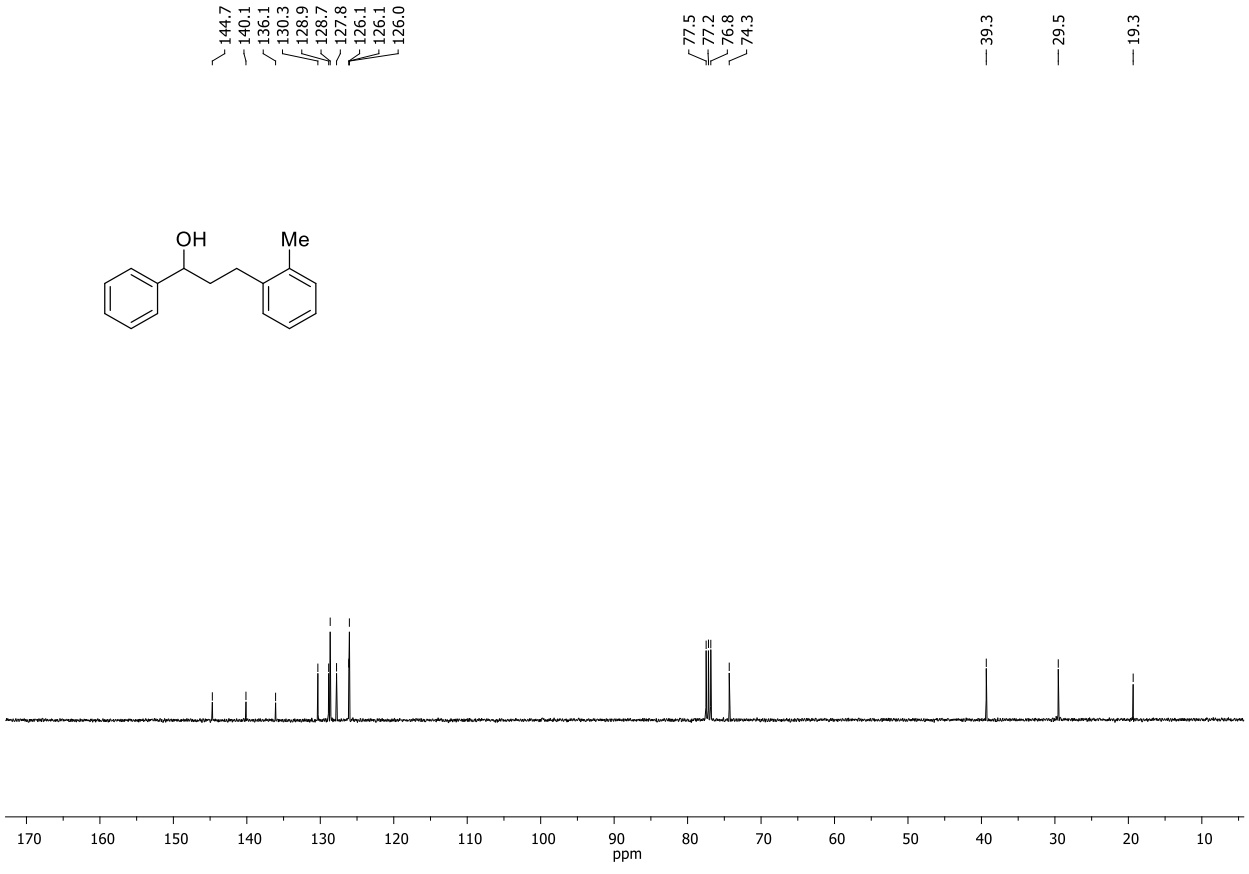
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126.1
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76.8
74.3
39.3
29.5
19.3
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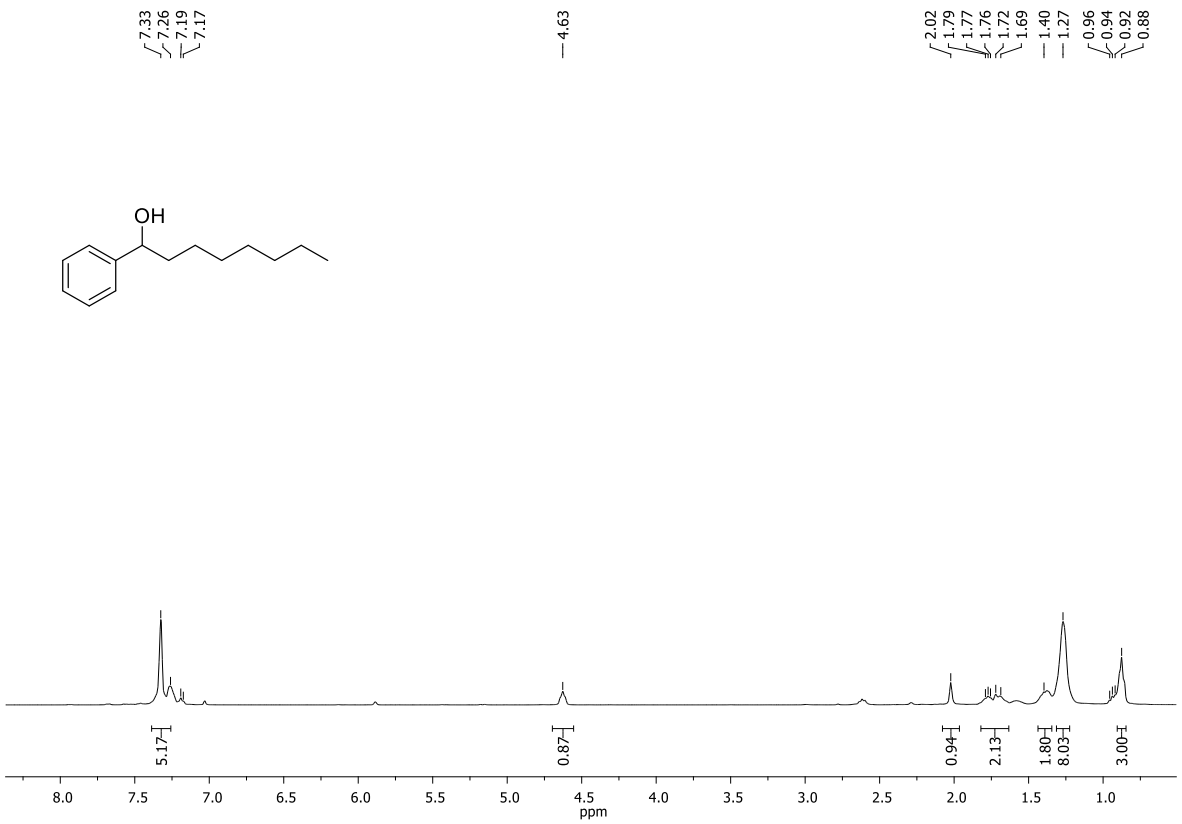
ppm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0.92
0.88
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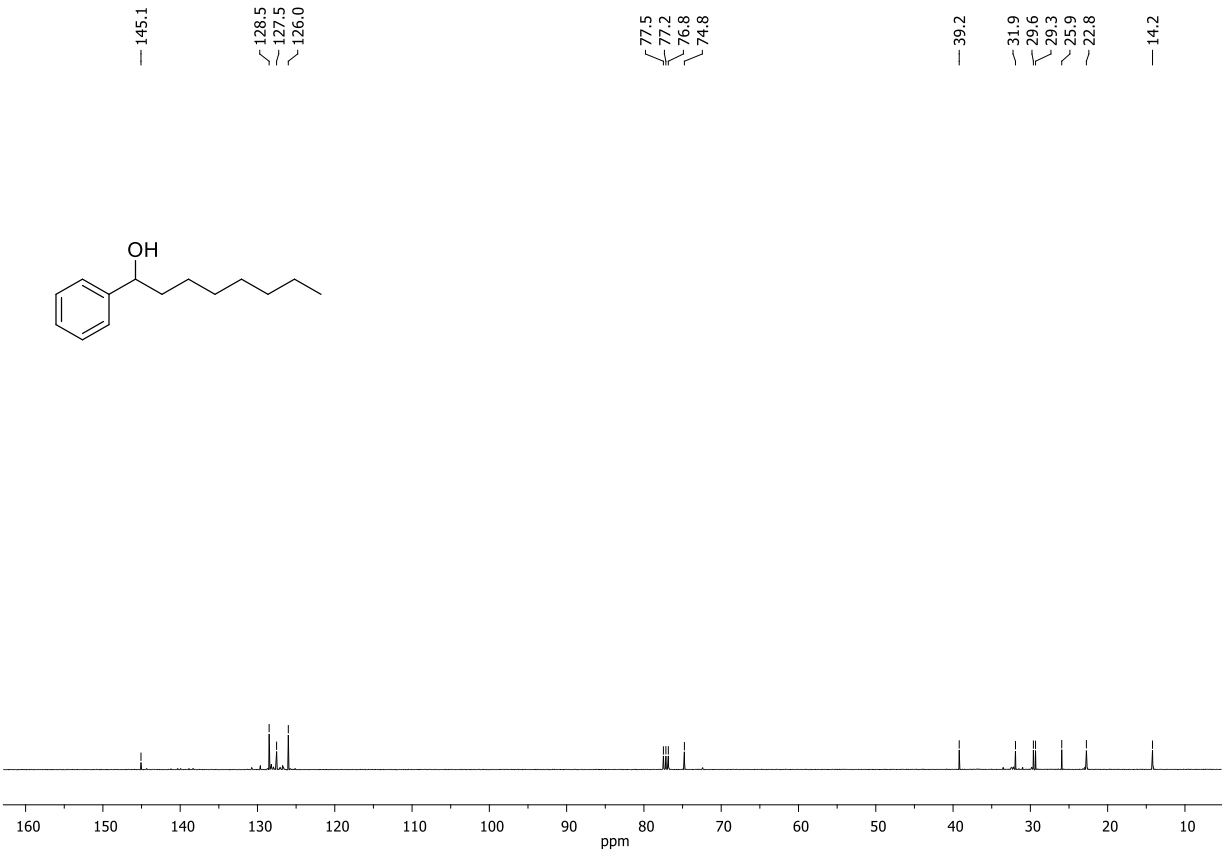
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22.8
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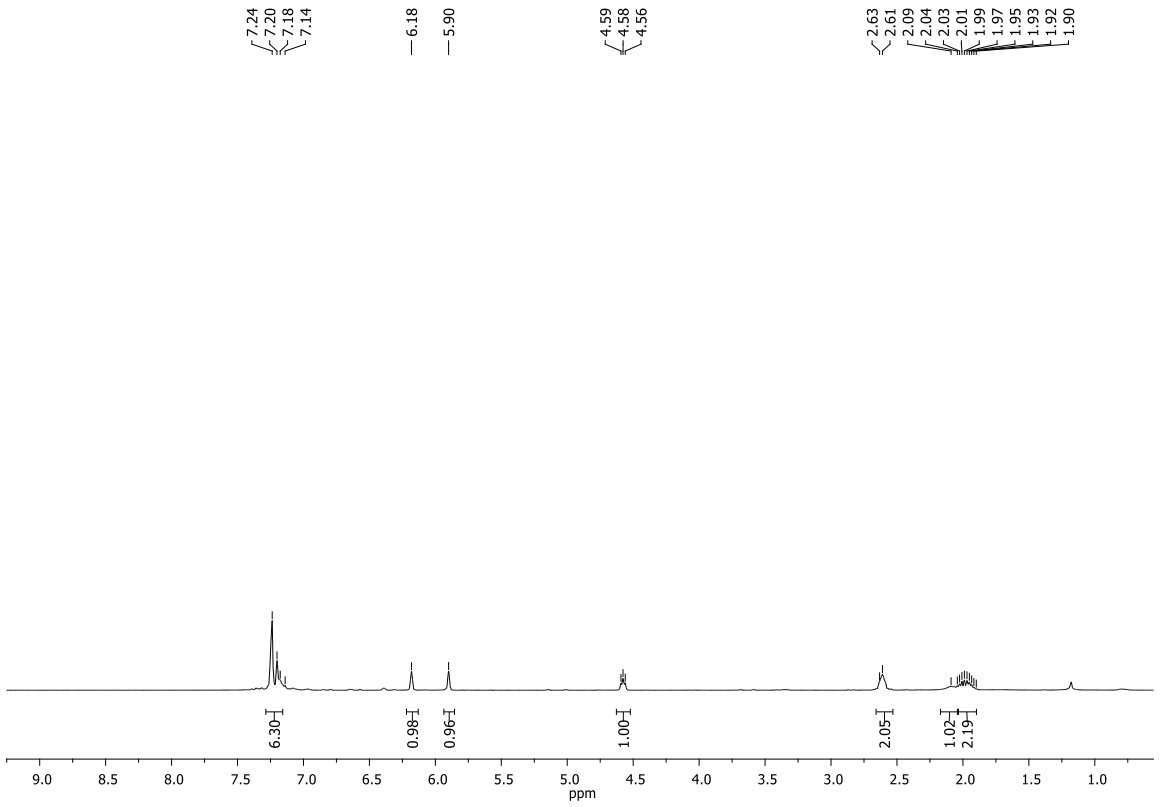
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1.90
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0.96
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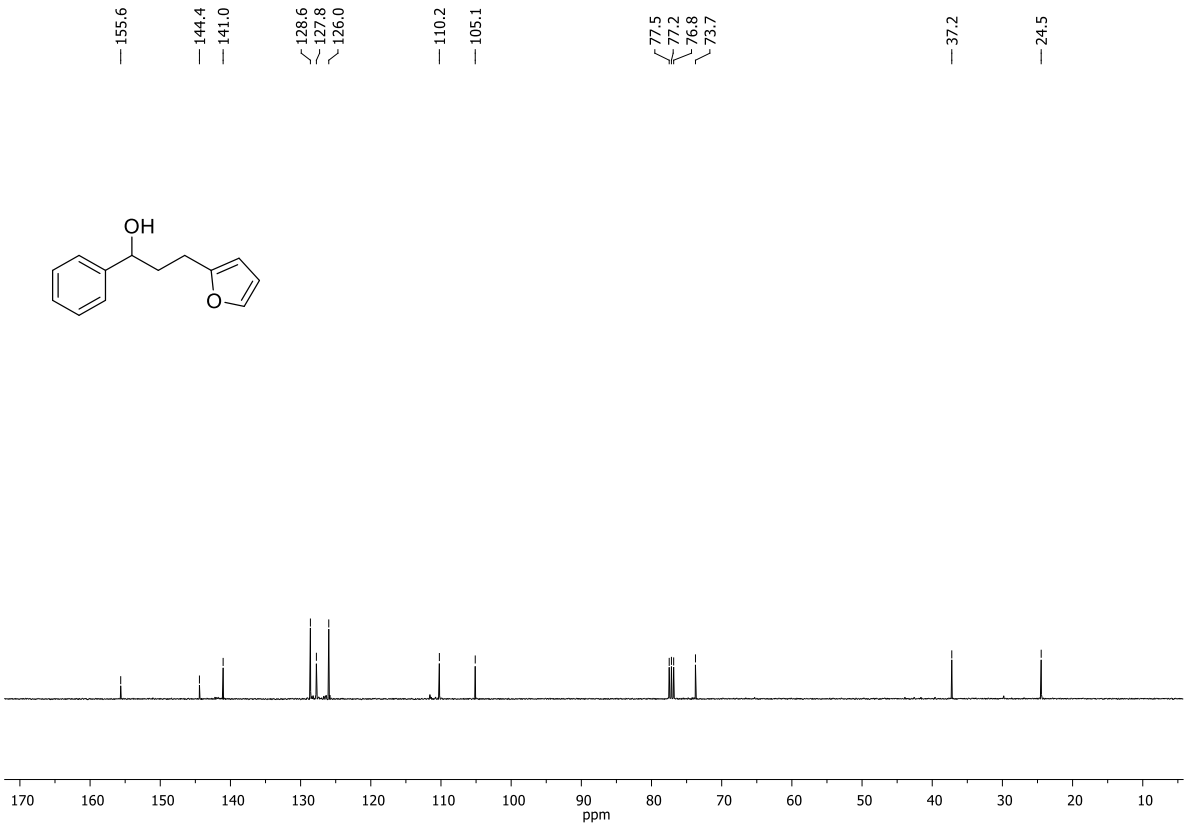
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24.5
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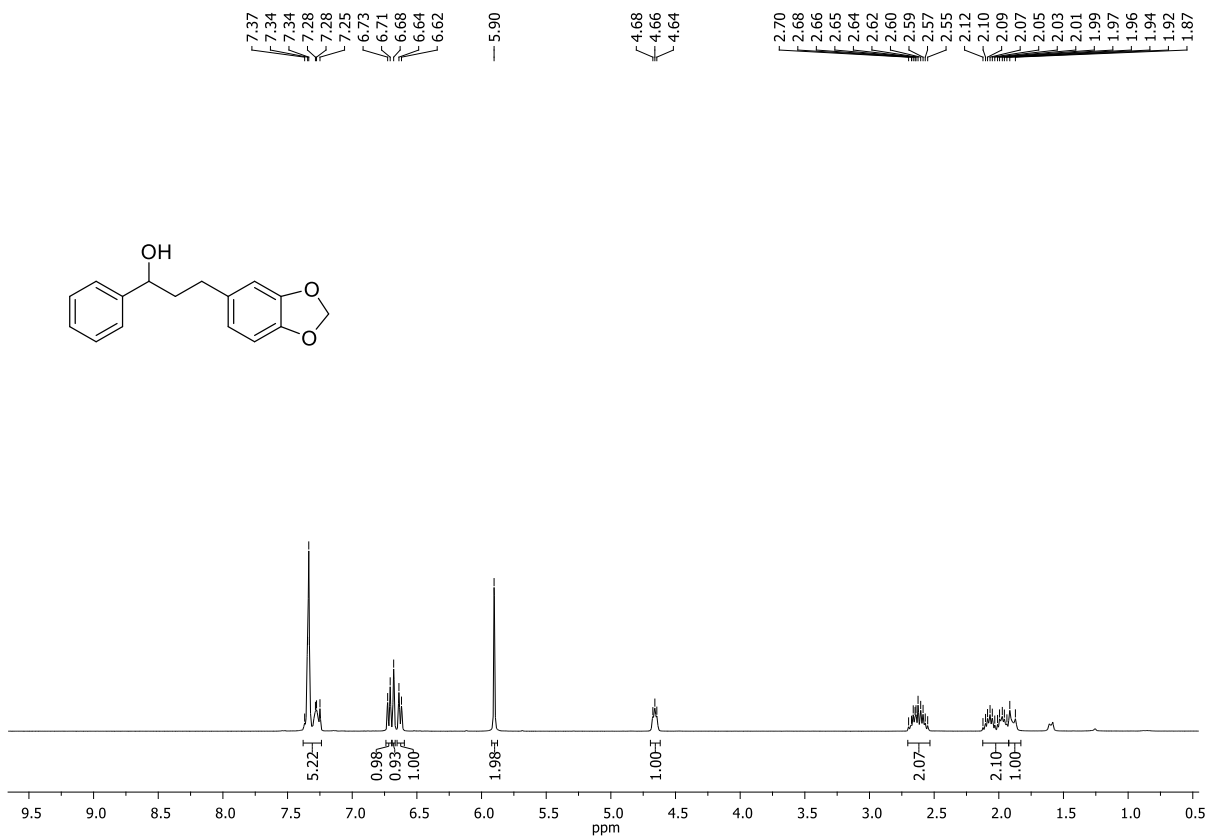
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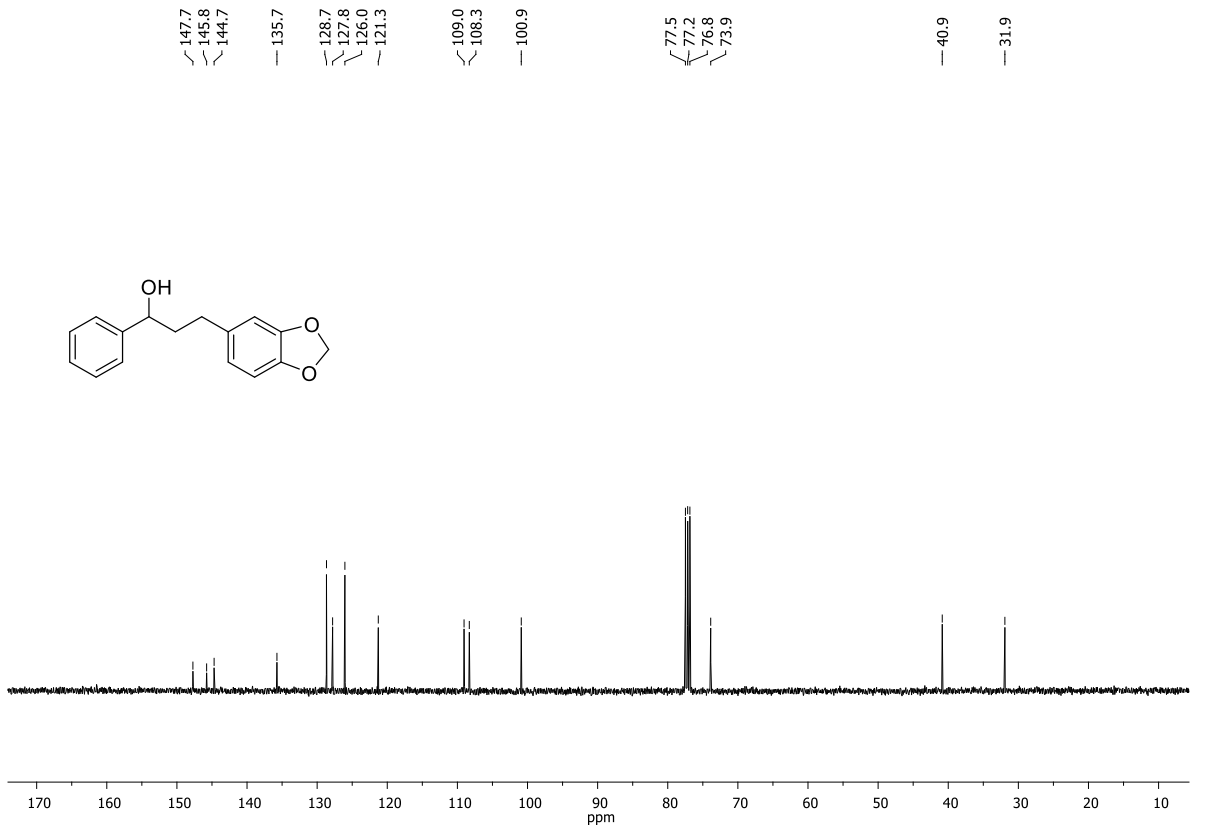
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77.2
76.8
73.9
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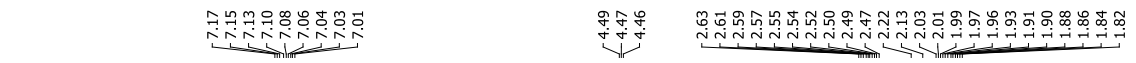
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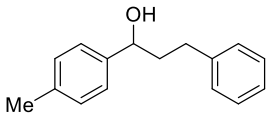
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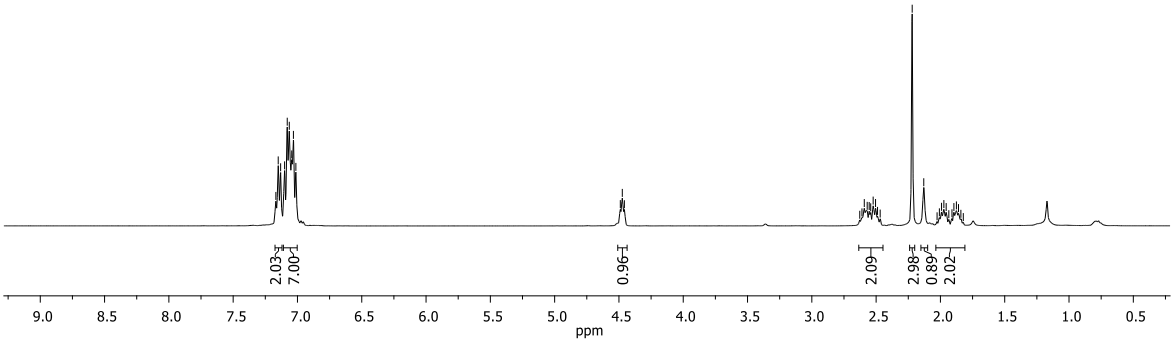
Me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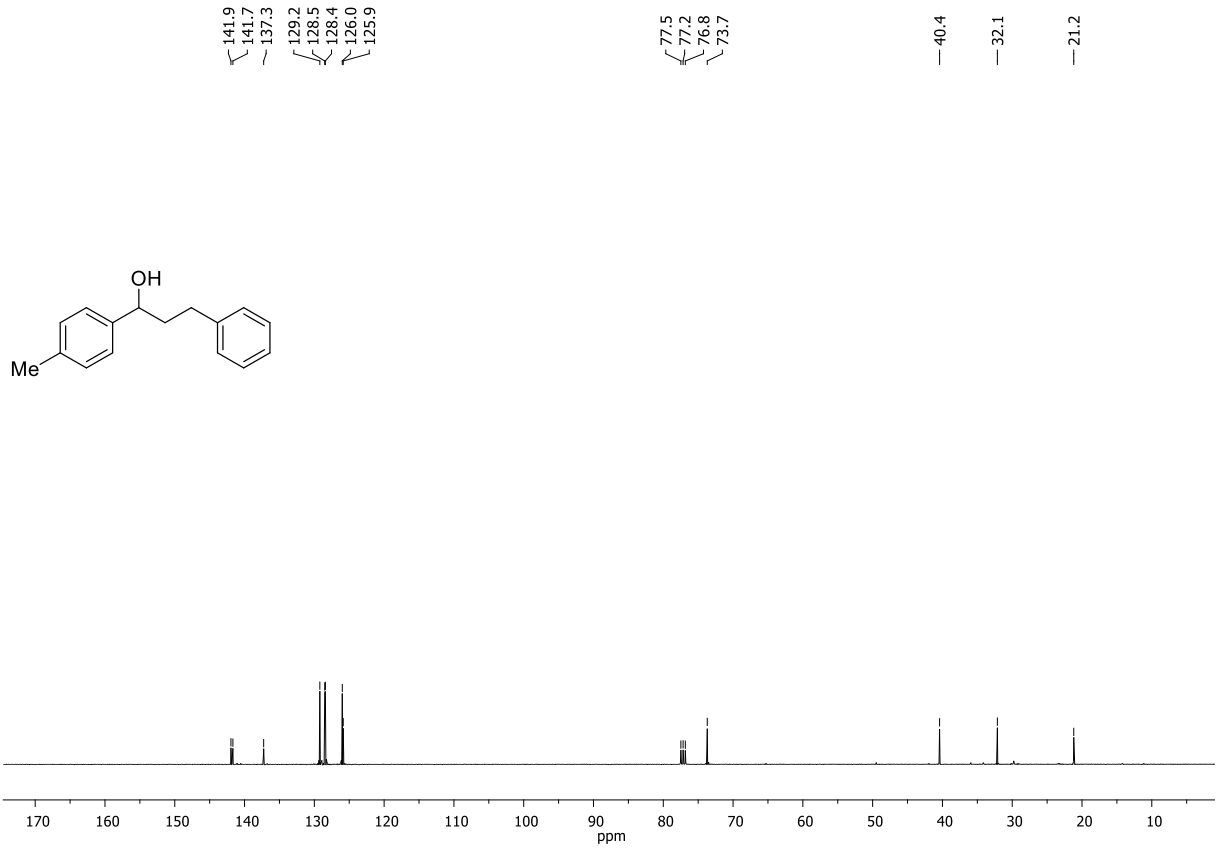
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128.4
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77.2
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73.7
40.4
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21.2
170
160
150
140
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100
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80
70
60
50
40
30
20
10
ppm

OH
Me


7.46
7.44
7.29
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7.20
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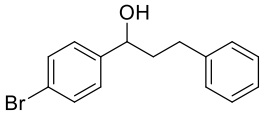
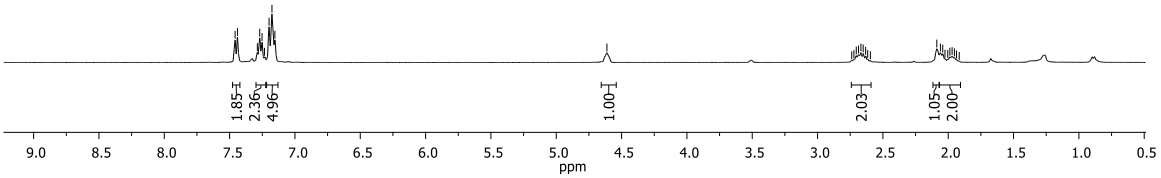
1.92


OH
Br


1.85
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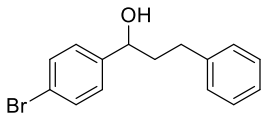
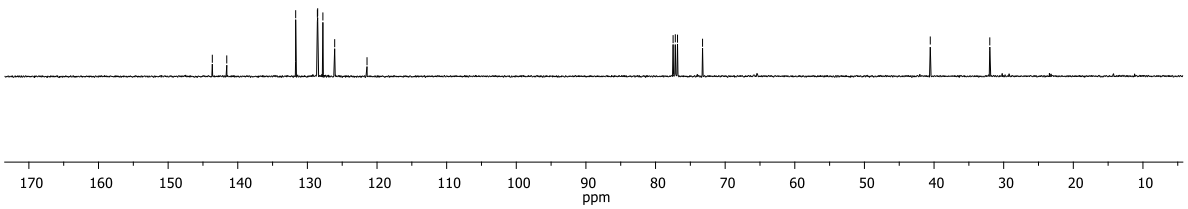
4.96
1.00
2.03
1.05
2.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm


143.7
141.6
131.7
128.6
128.5
127.8
126.1
121.4
77.5
77.2
76.8
73.2
40.5
32.0


OH
Br


170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.85
7.83
7.79
7.50
7.48
7.45
7.30
7.28
7.26
7.25
7.21
7.19
7.17
4.86
2.82
2.80
2.80
2.78
2.77
2.76
2.74
2.72
2.70
2.68
2.67
2.27
2.25
2.23
2.22
2.20
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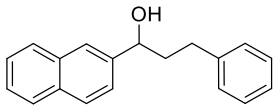
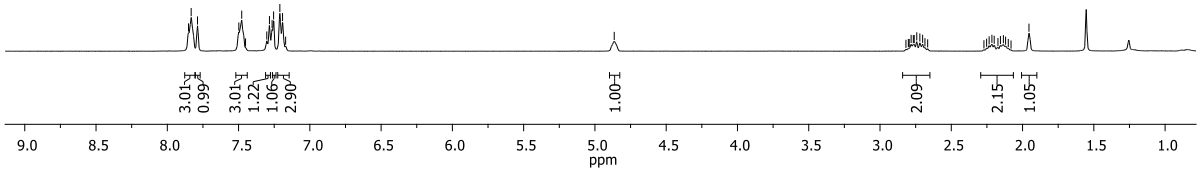
2.16
2.13
2.12
2.10
2.08
1.96


OH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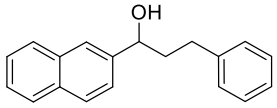
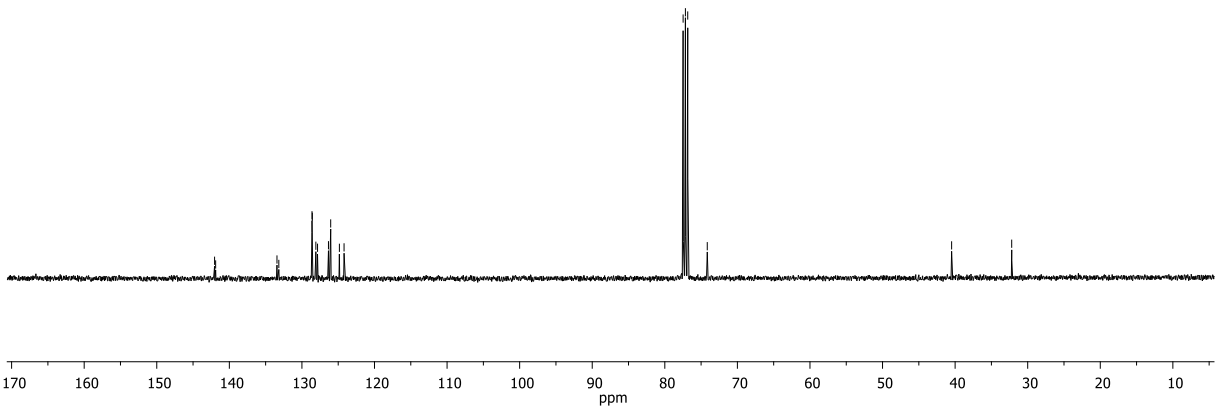
0.99
3.01
1.22
1.06
2.90
1.00
2.09
2.15
1.05
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm


142.0
141.9
133.4
133.2
128.6
128.6
128.1
127.8
126.3
126.0
124.8
124.2
77.5
77.2
76.8
74.2
40.5
32.2


OH


170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

6. References

1. Genç, S.; Arslan, B.; Gülcemal, S.; Günnaz, S.; Çetinkaya, B.; Gülcemal, D. Iridium(I)-catalyzed C−C and C−N bond formation reactions via the borrowing hydrogen strategy. *J. Org. Chem.* **2019**, *84*, 6286−6297.

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3. (a) Roy, B. C.; Debnath, S.; Chakrabarti, K.; Paul, B.; Maji, M.; Kundu, S. Orthoamino group functionalized 2,2′-bipyridine based Ru(II) complex catalysed alkylation of secondary alcohols, nitriles and amines using alcohols. *Org. Chem. Front.* **2018**, *5*, 1008−1018. (b) Shee, S.; Paul, B.; Panja, D.; Roy, B. C.; Chakrabarti, K.; Ganguli, K.; Das, A.; Das, G. K.; Kundu, S. Tandem cross coupling reaction of alcohols for sustainable synthesis of β-alkylated secondary alcohols and flavan derivatives. *Adv. Synth. Catal.* **2017**, *359*, 3888−3893.