Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Alcohol Cross-Coupling Reactions catalyzed by Ru and Ir Terpyridine complexes

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Supplementary Data

Optimization of reaction conditions:

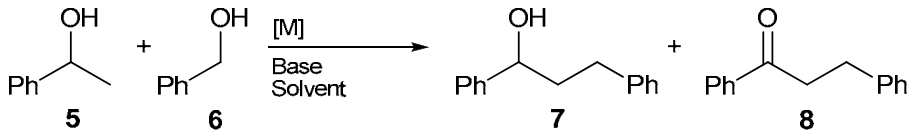
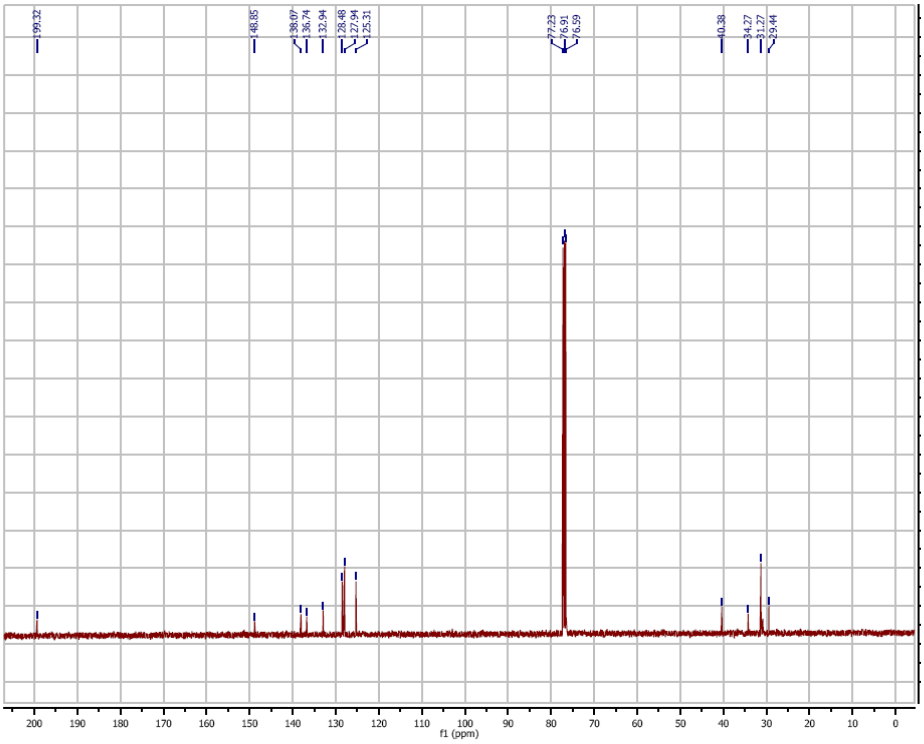


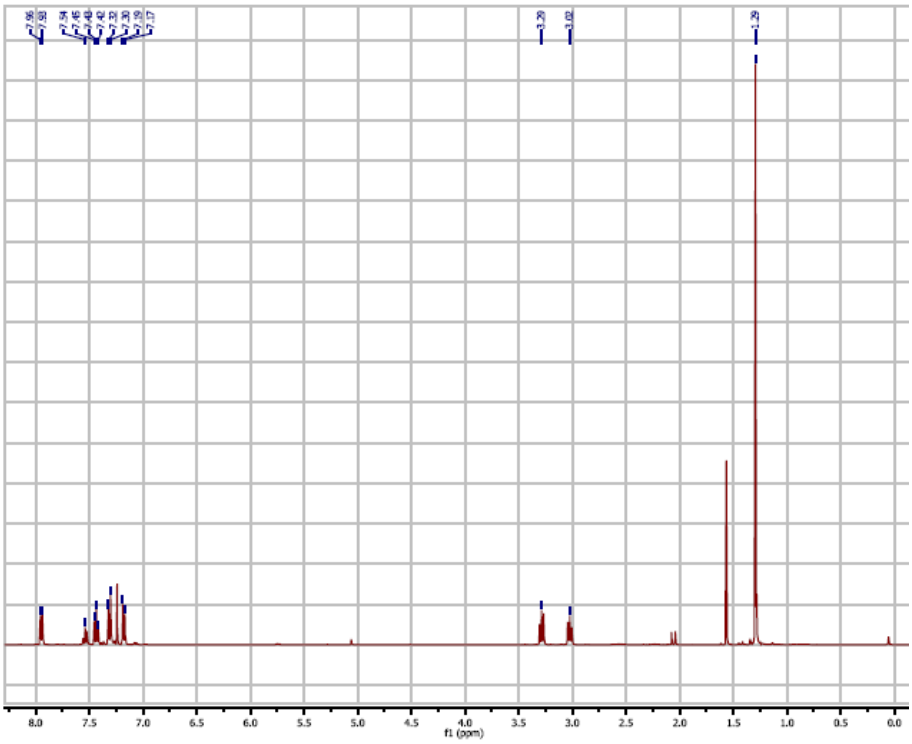
Table 1 Optimization of Conditions[a]

Entry	Base	Solvent	Conversion[b] (%)	Yield[c] (%)	product ratio **7** vs **8**
Catalyst **1**					
1	KOH (100%)	toluene	94	65	100:0
2	KOH (50%)	toluene	45	35	100:0
3	KOH (100%)	none	80	55	100:0
4	K_2CO_3 (100%)	toluene	-	-	-
5	KO*t*Bu (100%)	toluene	90	60	100:0
6	NaOH (100%)	toluene	85	71	90:10
7	$Ca(OH)_2$ (100%)	toluene	-	-	-
Catalyst **2**					
8	KOH (20%)	none[s]	99	99	89:11
9	KOH (20%)	toluene[s]	76	73	90:10
11	KOH (20%)	none[r] (1hr)	99	96	58:42
12	KOH (20%)	none[r] (3hr)	99	84	29:71
1	KOH(20%) 0.1% cata	none(12hr)[s]	87	77	74:26
13	NaOH (20%)	none[s]	97	80	85:15
14	KO*t*Bu	none[s]	>99	96	85:15

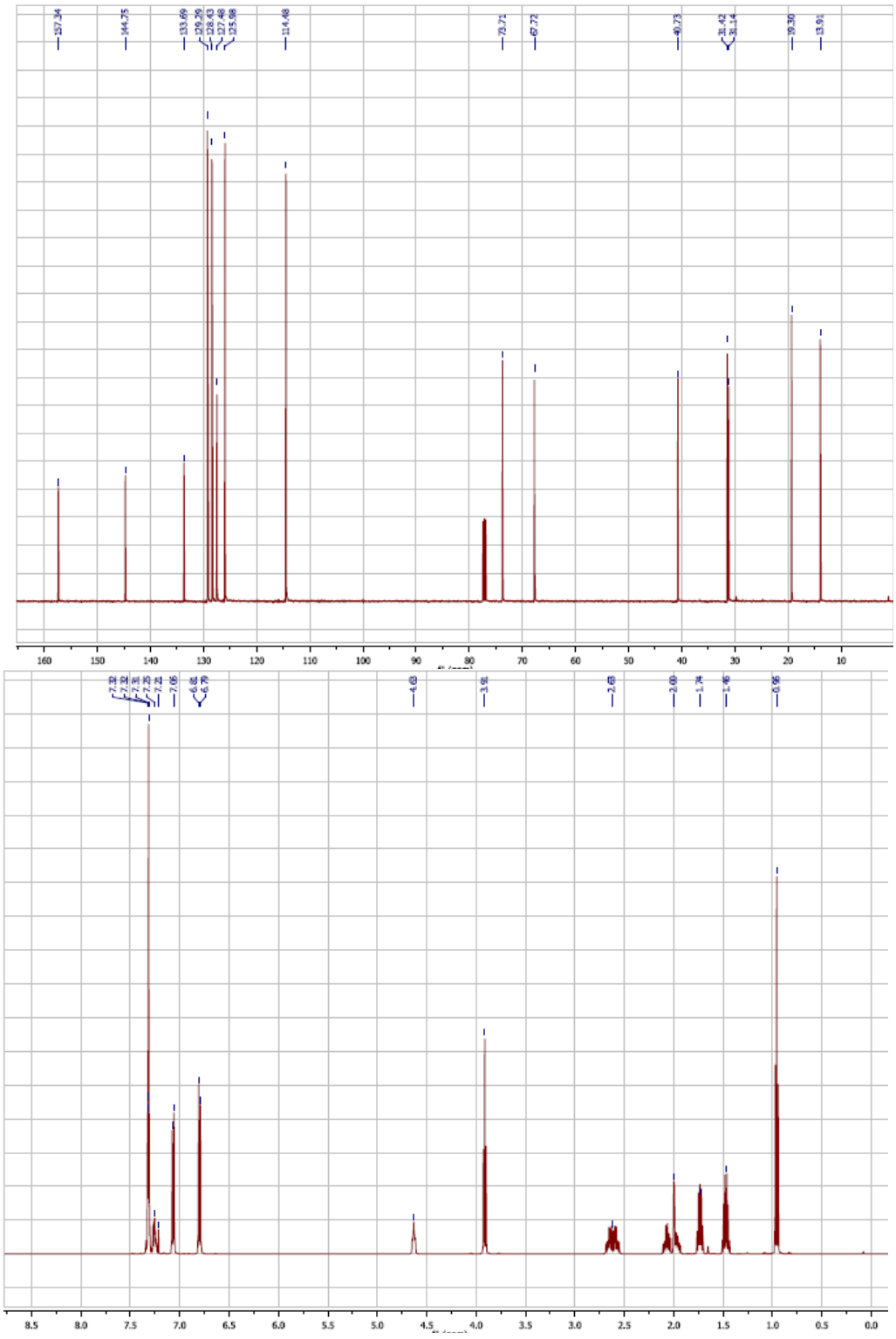
[a] Conditions: Catalyst **1**: 2.5 mmol of 1-phenylethanol and benzyl alcohol, base, 1 mol% catalyst in 0.5mL of toluene under aerobic conditions. Catalyst **2**: 2.5 mmol of 1-phenylethanol and benzyl alcohol, base, 1 mol% catalyst, neat at 120°C under N_2.
[b] Conversions were determined by the consumption of 2 alcohol.
[c] Yields were determined by ^{1}H NMR spectroscopy using 1,3,5-trimethoxybenzene as an internal standard.
[s] Conducted in a sealed vial.
[r] Conducted in a tube fitted with a reflux condenser, open to air.

^{1}H and ^{13}C NMR of **3-(4-tert-butylphenyl)-1-phenylpropan-1-one**

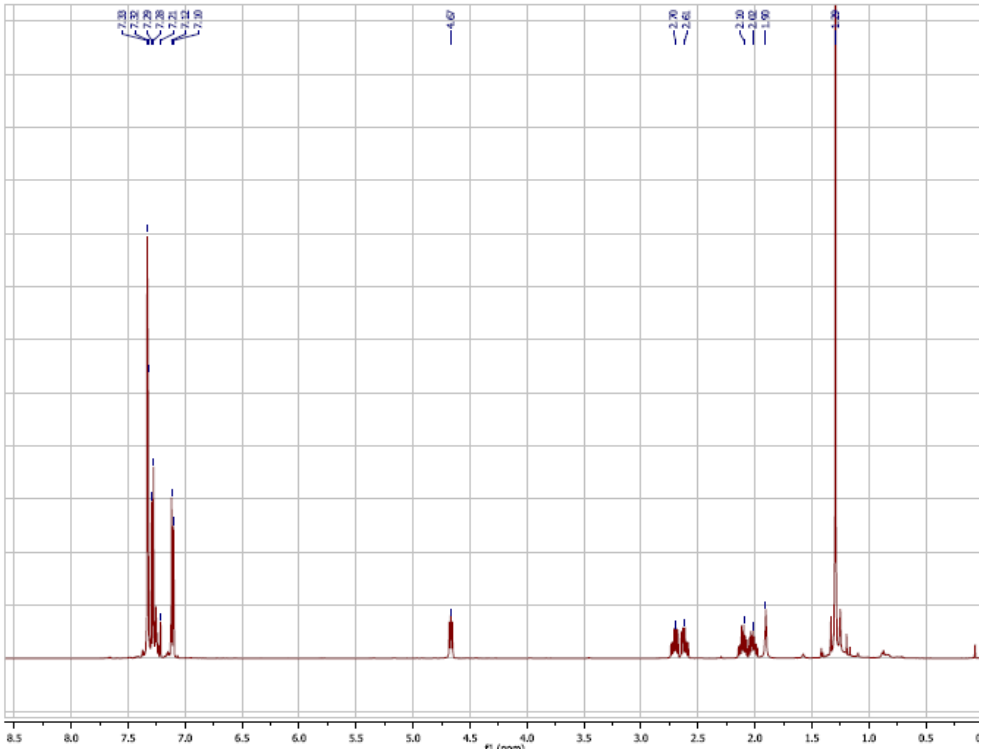


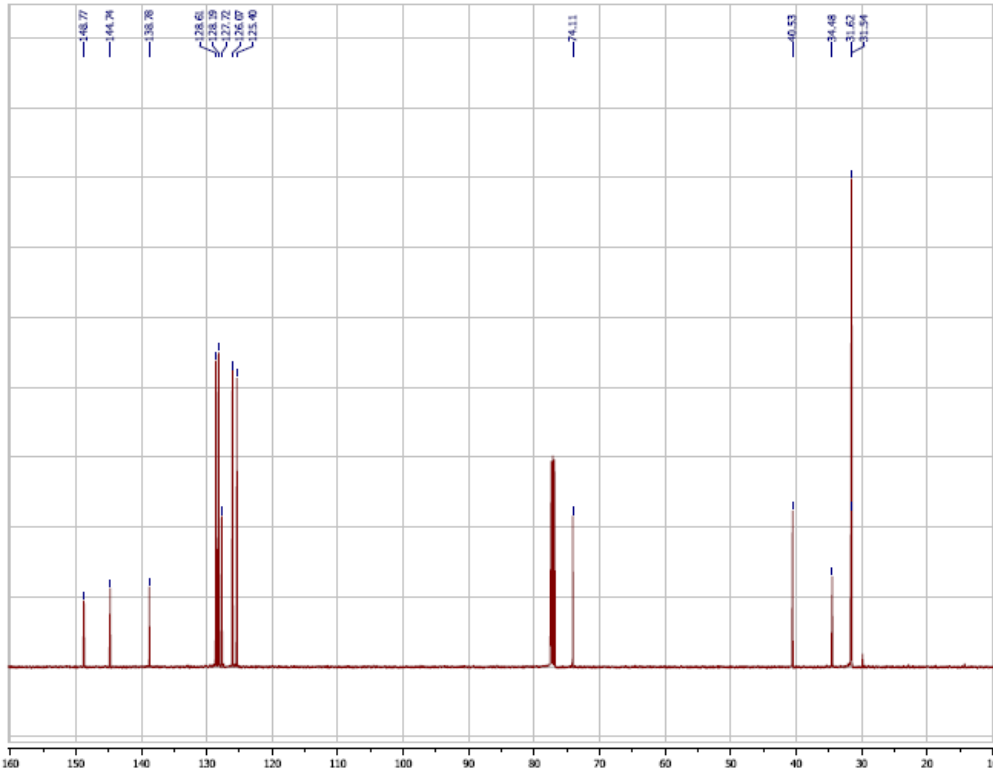


^{1}H and ^{13}C NMR of **3-(4-butoxyphenyl)-1-phenylpropan-1-ol**



^{1}H and ^{13}C NMR of **3-(4-tert-butylphenyl)-1-phenylpropan-1-ol**





^{1}H and ^{13}C NMR of **3-(4-butoxyphenyl)-1-phenylpropan-1-one**