

Supporting Information

Dimeric iminophenoxide copper complexes in *rac*-Lactide polymerization

Pargol Daneshmand, Leena Pinon, Frank Schaper*

Centre in Green Chemistry and Catalysis, Department of chemistry, Université de Montréal, C. P. 6128 Succ. Centre-Ville, Montréal, QC, H3T 3J7, Canada. *Email:* Frank.Schaper@umontreal.ca

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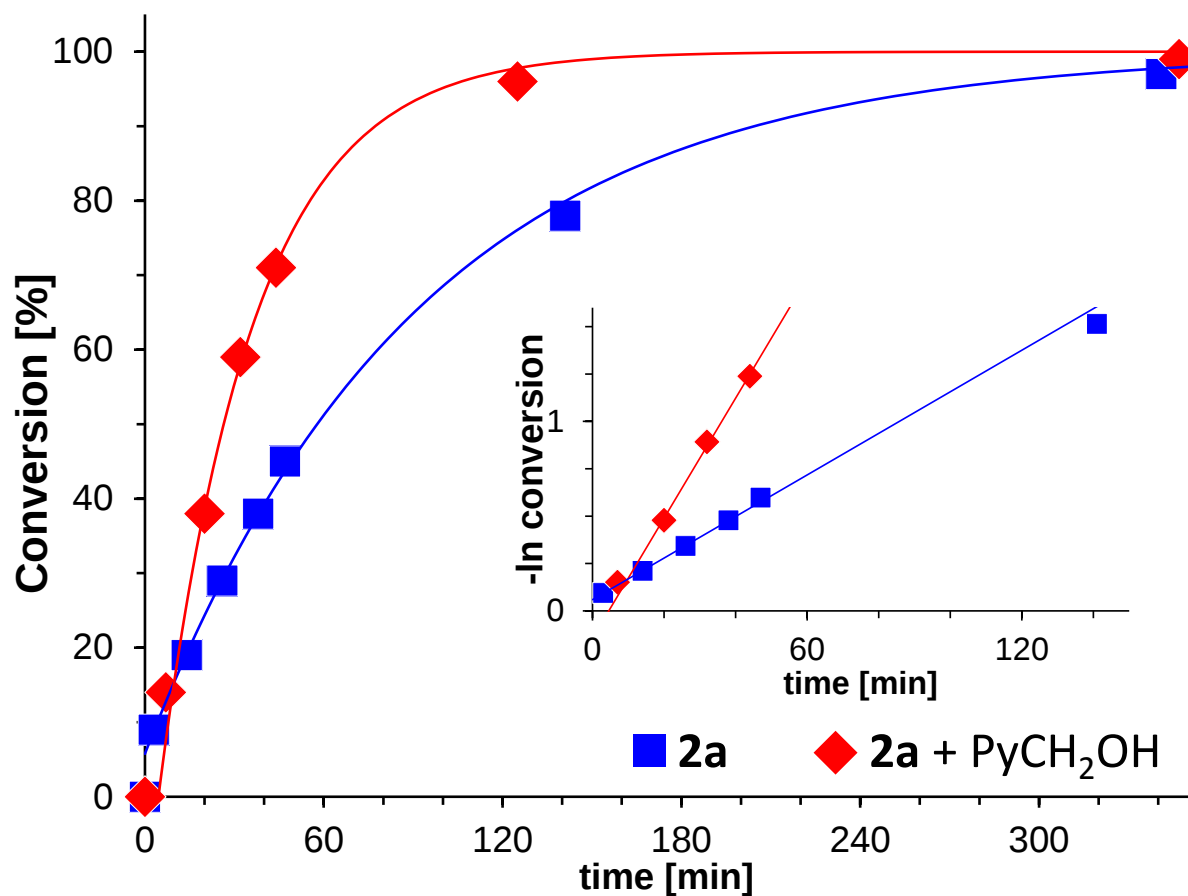


Figure S1. Kinetics of *rac*-lactide polymerization with **2a** without (blue squares) and with addition of 1 equiv pyridylmethanol (red diamonds). Linear regression provided $k_{\text{app}} = 0.69(2) \text{ h}^{-1}$ and $t_0 = -4 \text{ min}$ (**2a**) and $k_{\text{app}} = 1.9(1) \text{ h}^{-1}$ and $t_0 = 5 \text{ min}$ (**2a**/PyCH₂OH). Conditions: C₆D₆, RT, [lactide] = 200 mM, [L₂Cu₂(OR)₂] = 2 mM.

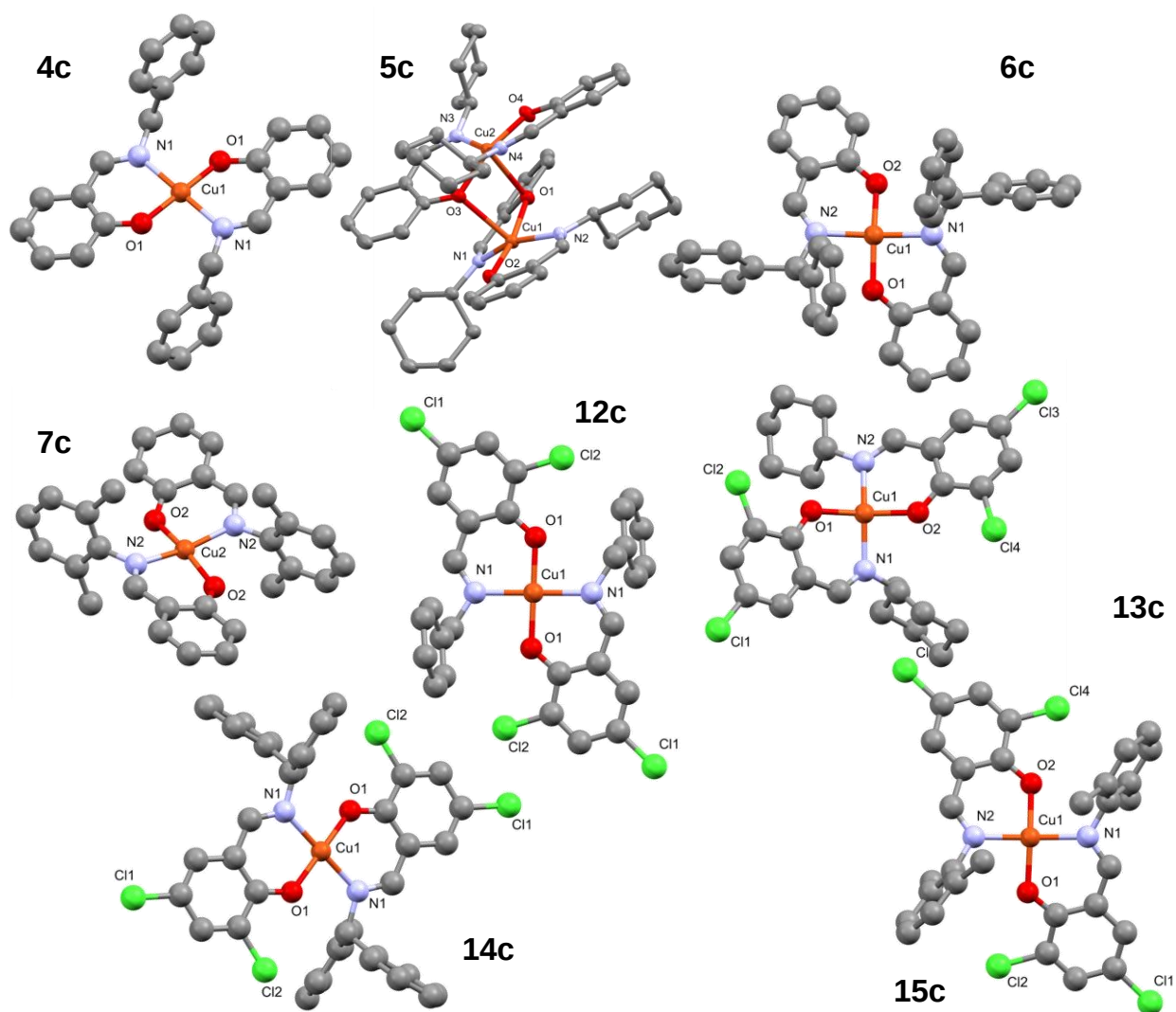


Figure S2. X-ray structures of homoleptic bis(iminoaryloxy) copper complexes **4c-7c** and **12c-15c**.

The structure of **5c** has been reported before.¹ Complex **5c**, the only dimeric complex, is also the only crystal with a green colour. All other crystals have brownish colours. For **4c**² and **6c**³, the structure of a polymorph has been reported.

Table S1. Experimental details of X-ray diffraction studies of the homoleptic complexes.

	4c	5c	6c	7c	12c	13c	14c	15c
Formula	C ₂₈ H ₂₄ CuN ₂ O ₂	C ₂₆ H ₃₂ CuN ₂ O ₂	C ₄₀ H ₃₂ CuN ₂ O ₂	C ₃₀ H ₂₈ CuN ₂ O ₂	C ₂₈ H ₂₀ Cl ₄ CuN ₂ O ₂	C ₂₆ H ₂₈ Cl ₄ CuN ₂ O ₂	C ₄₀ H ₂₈ Cl ₄ CuN ₂ O ₂	C ₃₇ H ₃₂ Cl ₄ CuN ₂ O ₂
<i>M_w</i> (g/mol)	484.03	468.07	636.21	512.08	621.80	605.84	773.98	741.98
<i>T</i> (K); F(000)	150; 502	100; 1976	110; 1324	100; 1068	150; 630	130; 1244	150; 395	150; 762
Crystal System	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Triclinic	Monoclinic
Space Group	<i>P</i> 2 ₁ /n	<i>P</i> 2 ₁ /n	<i>P</i> 2 ₁ /n	<i>P</i> 2/n	<i>P</i> 2 ₁ /c	<i>P</i> 2 ₁ /c	<i>P</i> (-1)	<i>P</i> 2 ₁
Unit Cell: <i>a</i> (Å)	10.1218(3)	21.3119(6)	17.4037(5)	14.3106(5)	10.5290(4)	14.7942(4)	8.4189(3)	11.0291(3)
<i>b</i> (Å)	9.0847(2)	9.3432(3)	10.2071(3)	12.1062(5)	6.0011(2)	12.6835(4)	8.9201(3)	9.5222(3)
<i>c</i> (Å)	12.4074(3)	23.0794(7)	18.7364(5)	14.6604(6)	20.1597(8)	14.0429(4)	12.4839(4)	16.5393(5)
<i>α</i> (°)	90	90	90	90	90	90	72.893(1)	90
<i>β</i> (°)	107.042(1)	99.239(1)	111.805(1)	96.816(2)	99.976(1)	91.930(1)	72.331(1)	96.603(1)
<i>γ</i> (°)	90	90	90	90	90	90	87.649(1)	90
<i>V</i> (Å ³)	1090.81(5)	4536.0(2)	3090.2(2)	2521.9(2)	1254.54(8)	2633.6(1)	852.56(5)	1725.46(9)
<i>μ</i> (mm ⁻¹); <i>Z</i>	5.555; 2	1.549; 8	4.012; 4	4.824; 4	7.436; 2	7.067; 4	5.553; 1	5.467; 2
<i>θ</i> (°); completeness	3.2-60.6; 1.0	5.1-71.9; 1.0	2.2-60.8; 0.99	3.6-60.6; 1	3.7-60.7; 1.0	2.6-54.2; 0.95	3.4-60.7; 1.0	3.5-60.6; 0.77
collected reflections; <i>R_σ</i>	27675; 0.026	122428; 0.018	68961; 0.024	43808; 0.038	18642; 0.022	19086; 0.034	20783; 0.036	87742; 0.019
unique reflections; <i>R_{int}</i>	2492; 0.052	8881; 0.040	7097; 0.045	5818; 0.060	2879; 0.042	4639; 0.034	3881; 0.060	6152; 0.030
<i>R</i> 1(<i>F</i>) (<i>I</i> > 2σ(<i>I</i>))	0.080	0.035	0.047	0.051	0.032	0.047	0.044	0.025
w <i>R</i> (<i>F</i> ²) (all data)	0.253	0.100	0.134	0.130	0.086	0.123	0.124	0.066
Go <i>F</i> (<i>F</i> ²); Flack- <i>x</i>	1.068; -	1.034; -	1.052; -	1.054; -	1.099; -	1.040; -	1.080; -	1.13; -0.011(3)
Residual electron density	0.80; -1.54	0.42; -0.43	0.68; -0.60	1.08; -0.52	0.26; -1.08	0.41; -0.80	0.48; -1.11	0.24; -0.56

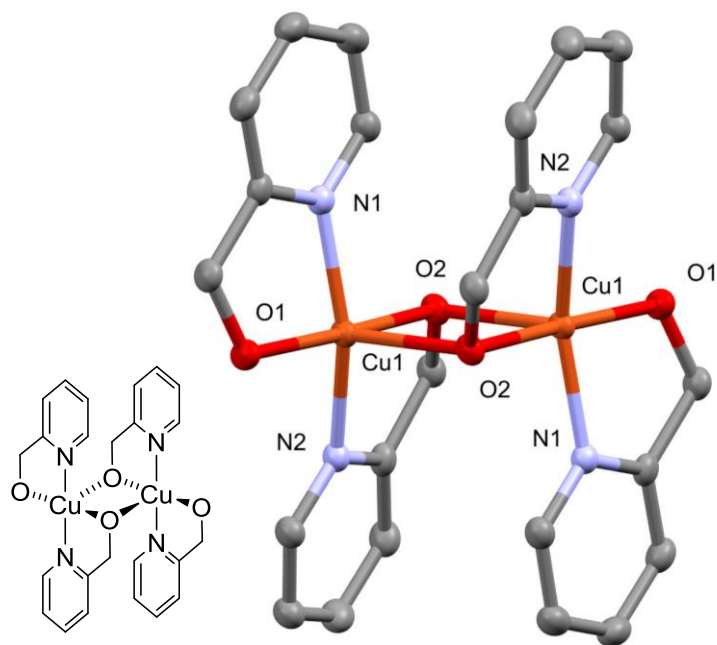


Figure S3. X-ray structure of bis(pyridylmethoxide)copper. Thermal displacements are shown at the 50% probability level. Hydrogen atoms were omitted for clarity.

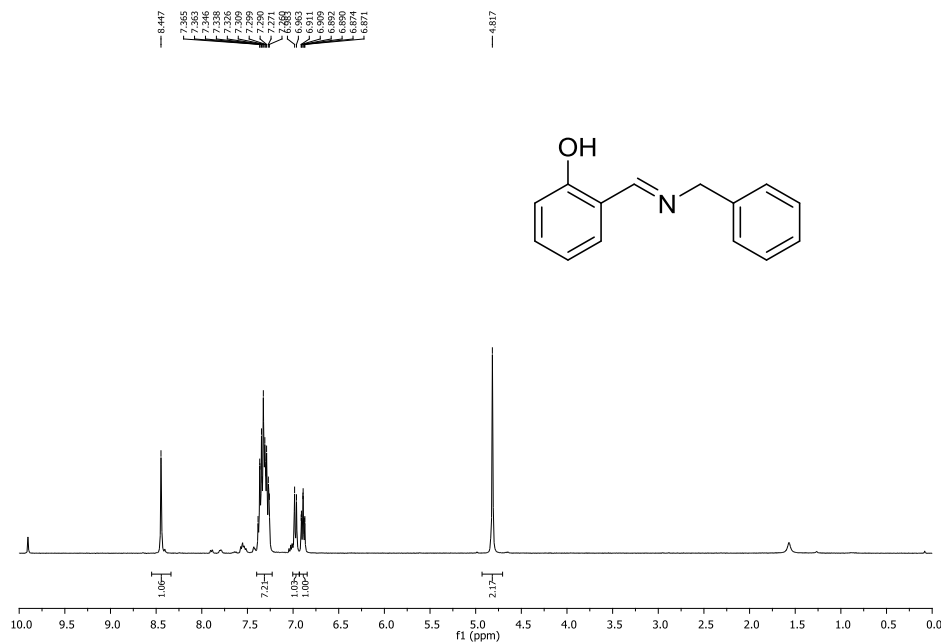


Figure S4. ¹H-NMR spectra of L4H in CDCl₃ (400 MHz).

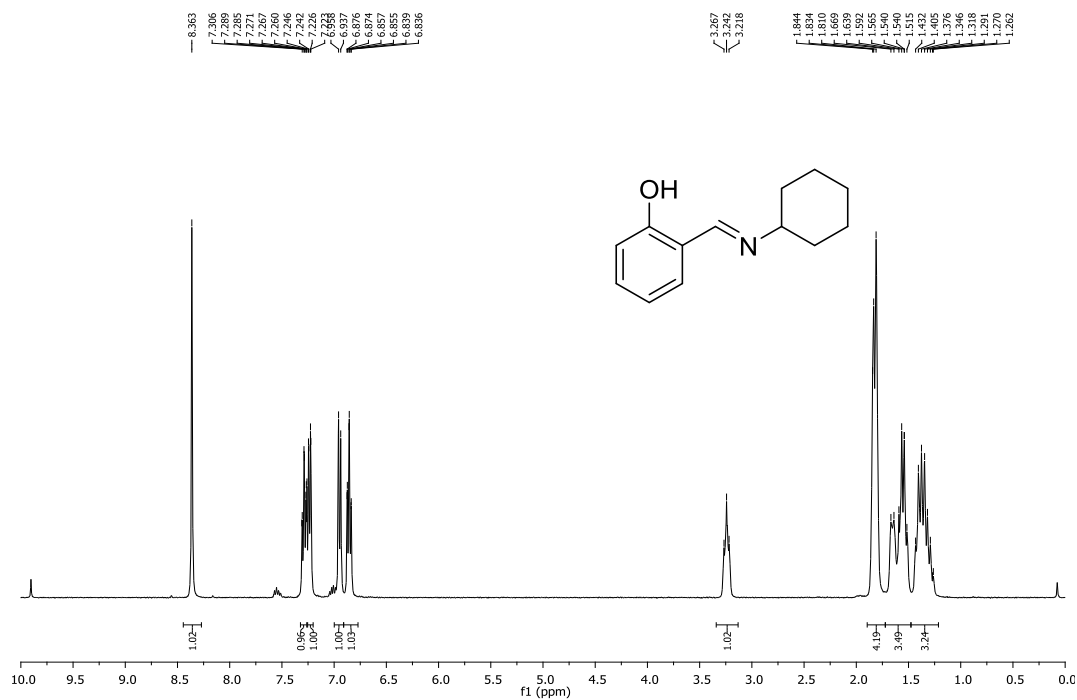


Figure S5. ¹H-NMR spectra of L5H in CDCl₃ (400 MHz).

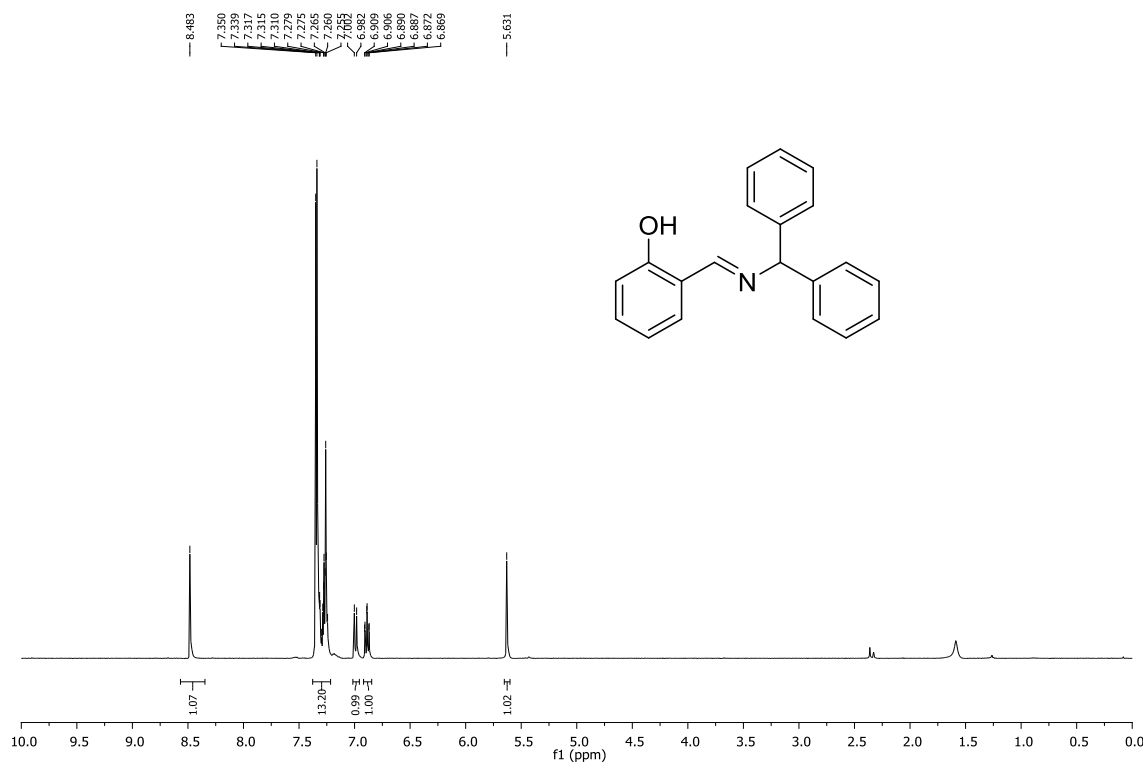


Figure S6. ¹H-NMR spectra of L6H in CDCl₃ (400 MHz).

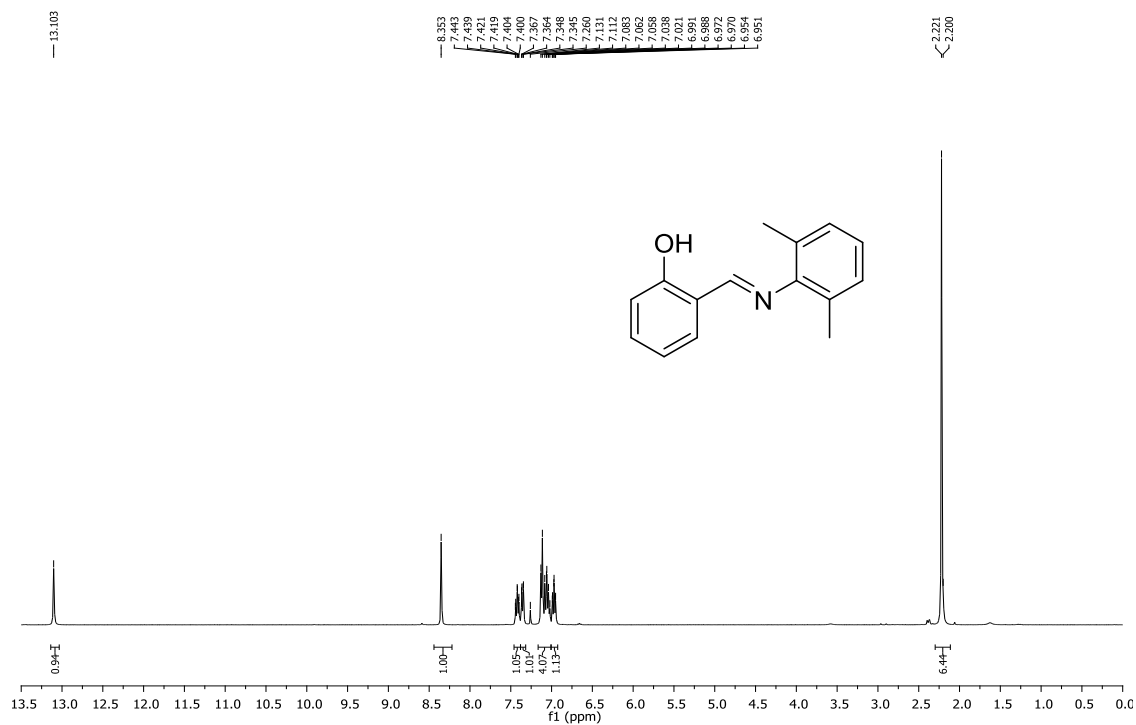


Figure S7. ^1H -NMR spectra of **L7H** in CDCl_3 (400 MHz).

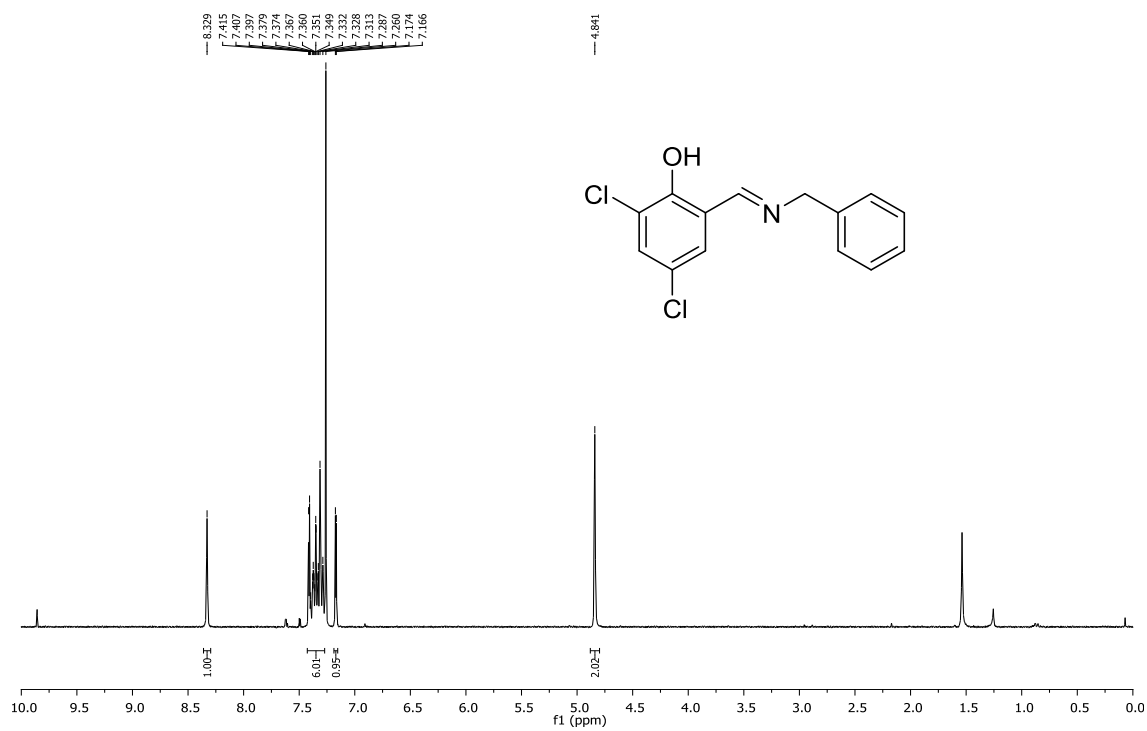


Figure S8. ^1H -NMR spectra of **L12H** in CDCl_3 (400 MHz).

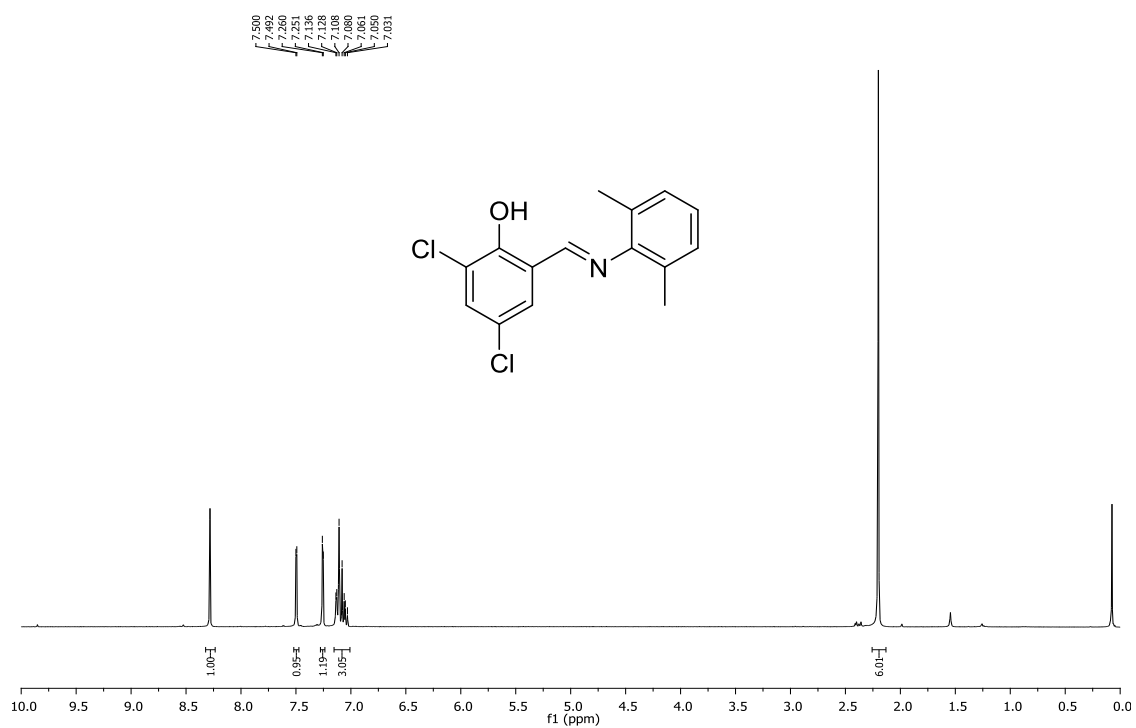


Figure S11. ¹H-NMR spectra of **L15H** in CDCl₃ (400 MHz).

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2. J. M. Fernández-G, J. Xochitiotzi-Flores, S. Hernández-Ortega, V. Gómez-Vidales and M. Del Rocío Patiño-Maya, *J. Coord. Chem.*, 2010, **63**, 2132.
3. J. M. Fernández-G, O. L. Ruíz-Ramírez, R. A. Toscano, N. Macías-Ruvalcaba and M. Aguilar-Martínez, *Transition Metal Chemistry*, 2000, **25**, 511.