Supporting information

Aluminum complexes based on pyridine substituted alcohols: synthesis, structure, catalytic application in ROP

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Fig. S1 $^1$H NMR spectrum for 3a (CDCl$_3$, rt).

Fig. S2 $^1$H NMR spectrum for 3a (CDCl$_3$+ 20 % DMSO-d$_6$, rt).
**Fig. S3** DOSY NMR spectrum for 3a (600 MHz, DMSO-d6, room temperature; the admixture of toluene is present).

The formula of MW calculation [Angew. Chem., Int. Ed. 2013, 52, 3199 – 3202]

\[ D = \frac{k_B T (\frac{3\alpha}{2} + \frac{1}{1+\alpha})}{6\pi\eta \sqrt{\frac{3MW}{4\pi\rho_{eff} N_A}}} \], where

\[ \alpha = 3\sqrt{\frac{MW_S}{MW}} \]

MW<sub>S</sub> – molecular weight of the solvent

MW – molecular weight of the solute
\( \rho_{\text{eff}} \) - the effective density of a small molecule

\( \eta \) - viscosity

\( N_A \) - the Avogadro number

\( k_B \) - Boltzmann constant

\( D \) – diffusion coefficient

\( T \) - temperature

Using known calculation algorithm the molecular weights of two particles was established:

\( M_1 = 820 \text{ g/mol, } D = 1.74 \times 10^{-10} \text{ m}^2/\text{s (M}_1\text{ (theor)} = 774.9), \) what corresponds to dimeric (3a)₂;

\( M_2 = 497.1 \text{ g/mol, } D = 2.19 \times 10^{-10} \text{ m}^2/\text{s (M}_1\text{ (theor)} = 465.6), \) what corresponds to adduct of monomer with DMSO.
Fig. S4 Molecular structure of complex 2c. Hydrogen atoms are omitted for clarity.

Fig. S5. MALDI-TOF mass spectrum of a PLA sample prepared with 2a (Table 2, entry 1) (solvent THF, HABA matrix, 2,5-dihydroxybenzoic acid).
Fig. S6. $^1$H NMR spectra (CDCl$_3$) for BnO-PLLA, prepared with 2a (75 % conversion).
Fig. S7. $^1$H NMR spectra (CDCl$_3$) for MeO-PLLA, prepared with 2c (100 % conversion).

Fig. S8. Homodecoupled $^1$H NMR spectra (CDCl$_3$) for BnO-PLLA.
Fig. S9. $\ln([LA]/[LA])$ versus time plot for $L$-lactide polymerization with 2a-4a.

Fig. S10. $M_n$ versus conversion plot for $L$-lactide polymerization with 3a.
Fig. S11. Ln([M]_0/[M]) vs. time plots for the polymerization of L-lactide in the presence of catalytic complex 4a (100:1:1) at 80 °C; [LA]/[initiator]= 100.

Fig. S12. ^1^H NMR spectrum (CDCl₃, rt) for PLLA (the sample contains the polymer, [(3)(PLLA)], with ligand fragment).
Figure S13. $^1$H NMR spectrum (CDCl$_3$, rt) of complex 2a.

Figure S14. $^{13}$C NMR spectrum (CDCl$_3$, rt) of complex 2a.
Figure S15. $^1$H NMR spectrum (CDCl$_3$, rt) of complex 3a.

Figure S16. $^{13}$C NMR spectrum (CDCl$_3$, rt) of complex 3a.
Figure S17. $^1$H NMR spectrum (CDCl$_3$, rt) of complex 4a.

Figure S18. $^{13}$C NMR spectrum (CDCl$_3$, rt) of complex 4a.
Figure S19. $^{13}$C NMR spectrum (CDCl$_3$, rt) of complex 3b.

Figure S20. $^{13}$C NMR spectrum (CDCl$_3$, rt) of complex 3b.
Figure S21. $^1$H NMR spectrum (CDCl$_3$, rt) of complex 4b.

Figure S22. $^{13}$C NMR spectrum (CDCl$_3$, rt) of complex 4b.
Figure S23. $^1$H NMR spectrum (CDCl$_3$, rt) of complex 2c.

Figure S24. $^{13}$C NMR spectrum (CDCl$_3$, rt) of complex 2c.
Figure S25. $^1$H NMR spectrum (CDCl$_3$, rt) of complex 3c.

Figure S26. $^{13}$C NMR spectrum (CDCl$_3$, rt) of complex 3c.
Figure S27. $^1$H NMR spectrum (CDCl$_3$, rt) of complex 4c.

Figure S28. $^1$H NMR spectrum (C$_6$D$_6$, rt) of complex 2d.
Figure S29. $^{13}$C NMR spectrum (C$_6$D$_6$, rt) of complex 2d.