Supplementary Material

Enhanced Activity in the Tosylation of Tolanophanes via Supramolecular HgCl₂ Recognition


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Fig S1. ^1H NMR spectrum of isomeric mixture of 5a (E/Z = 95:5).
Fig S2. $^1$H NMR spectrum of 5a (E/Z = 95:5).

Fig S3. $^{13}$C NMR spectrum of 5a
Fig S4. $^1$H NMR spectrum of 5b ($E/Z = 75:25$).

Fig S5. $^1$H NMR spectrum of 5b ($E/Z = 75:25$).
Fig S6. $^{13}$C NMR spectrum of 5b.

Fig S7. $^1$H NMR spectrum of 5c (E/Z = 40:60).
Fig S8. $^1$H NMR spectrum of 5c (E/Z = 40:60).
Fig S9. Mass spectrum and LC-Mass spectrum of 5a
Fig S10. Mass spectrum and LC-Mass spectrum of 5b
Fig S11. Mass spectrum and LC-Mass spectrum of 5c

Fig S12. $^{13}$C NMR spectrum of 1b
Fig S13. $^{13}$C NMR spectrum of 1b@HgCl$_2$.

Fig S14. UV–vis spectrum of 1a upon addition of HgCl$_2$ in CH$_3$CN. Above inset: the changes in absorbance intensity of the solution. Below inset: Job Plot.
**Fig S15.** UV−vis spectrum of 1c upon addition of HgCl$_2$ in CH$_3$CN. Above inset: the changes in absorbance intensity of the solution. Below inset: Job Plot.

**Scheme S1.** Plausible mechanism of hydration of alkyne.

**Scheme S2.** Proposed mechanism for HgCl$_2$-catalyzed synthesis of 5.
Fig S16. $^1$H-NMR spectrum of 4b
Fig S17. $^{13}$C-NMR spectrum of 4b
Fig S18. HH-COSY spectrum of 4b
Fig S19. HSQC spectrum of 4b
Fig S20. Mass spectrum of 4b

Fig S21. $^1$HNMR spectrum of 4c
Fig S22. $^{13}$CNMR spectrum of 4c

Fig S23. Mass spectrum of 4c
**Fig S24.** The reaction rate ($K_2 / K_1$) of 1 at 50 °C (blue) and room temperature (red) conditions (The first run).

**Fig S25.** The reaction rate ($K_2 / K_1$) of 1 at 50 °C (blue) and room temperature (red) conditions (The second run).
**Fig S26.** The reaction rate \((K_2 / K_1)\) of 1 at 50 ºC (blue) and room temperature (red) conditions (The third run).

**Fig S27.** The comparison of three runs and their average reaction rate \((K_2 / K_1)\) of 1 at 50 ºC.
The comparison of three runs and their average reaction rate ($K_2 / K_1$) of 1 at room temperature.

**Fig S28.** The comparison of three runs and their average reaction rate ($K_2 / K_1$) of 1 at room temperature.