SUPPORTING INFORMATION

Title: Selective Catalytic Hydration of Alkynes in the Presence of Au-Cavitands: A Study in Structure–Activity Relationships

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2) The stack of $^1$H NMR spectra (Figure S1) for representative procedure of hydration reactions of 2-octyne 7d (Table 2, entry 14), in which [D$_8$]toluene was used.

3) The data of HRMS (ESI) for 2•AuCl
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Compound 2 ($^{13}$C NMR spectrum in CDCl$_3$)
Compound 2 (\(^1\)H NMR spectrum in [D8]toluene)
Compound 5 (\(^1\)H NMR spectrum in CDCl\(_3\))
Compound 5 ($^{13}$C NMR spectrum in CDCl$_3$)
Compound 5 (^{1}H NMR spectrum in [D8]toluene)
Compound 6 (\(^1\text{H NMR spectrum in CDCl}_3\))
Compound 6 ($^{13}$C NMR spectrum in CDCl$_3$)
Compound 6 ($^1$H NMR spectrum in [D8]toluene)
Compound 3 (1H NMR spectrum in CDCl₃)
Compound 3 (\(^{13}\text{C} \) NMR spectrum in CDCl\(_3\))
Compound 3 (\textsuperscript{1}H NMR spectrum in [D8]toluene)
Compound 4 (\textsuperscript{1}H NMR spectrum in [D8]toluene)
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Compound 5•AuCl (¹H NMR spectrum in [D8]toluene)
Compound $6\cdot$AuCl ($^1$H NMR spectrum in CDCl$_3$)
Compound 6•AuCl ($^{13}$C NMR spectrum in CDCl$_3$)
Compound 6•AuCl (¹H NMR spectrum in [D8]toluene)
Compound 3•AuCl (¹H NMR spectrum in CDCl₃)
Compound 3•AuCl ($^{13}$C NMR spectrum in CDCl$_3$)
Compound 3•AuCl (¹H NMR spectrum in [D8]toluene)
2) The stack of $^1$H NMR spectra (Figure 1S) for representative procedure of hydration reactions of 2-octyne 7d (Table 2, entry 14), in which [D₈]toluene was used.

![NMR spectra](image)

**Figure S1.** Portions of $^1$H NMR spectra (400 MHz, toluene-$d_8$) for determination of NMR yields in Table 2, entry 14; the top, 2-octyne 7d; and the second and third from the top, the commercially available authentic samples of 3-octanone 8d and 2-octanone 9d; the bottom, the resultant product of 8d (12%) and 9d (88%).
3) The data of HRMS (ESI) for 2•AuCl.