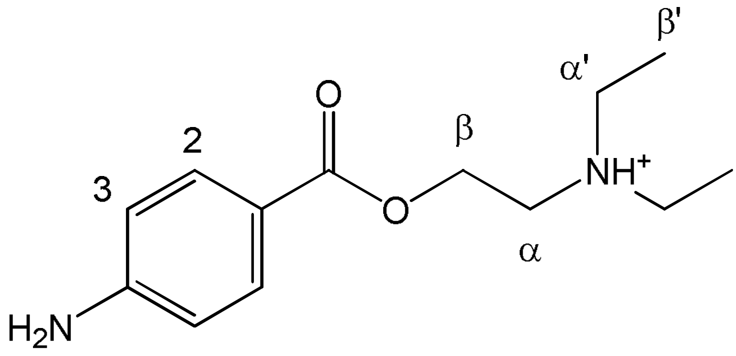
Electronic Supporting Information

Host-guest complexations of local anaesthetics by cucurbit[7]uril in aqueous solution

Ian W. Wyman and Donal H. Macartney*
Department of Chemistry, Queen's University, 90 Bader Lane, Kingston, Ontario K7L 3N6, Canada.
Fax: +1 613 533 6669; Tel: +1 613 533 2617; E-mail: donal@chem.queensu.ca

Contents | Page



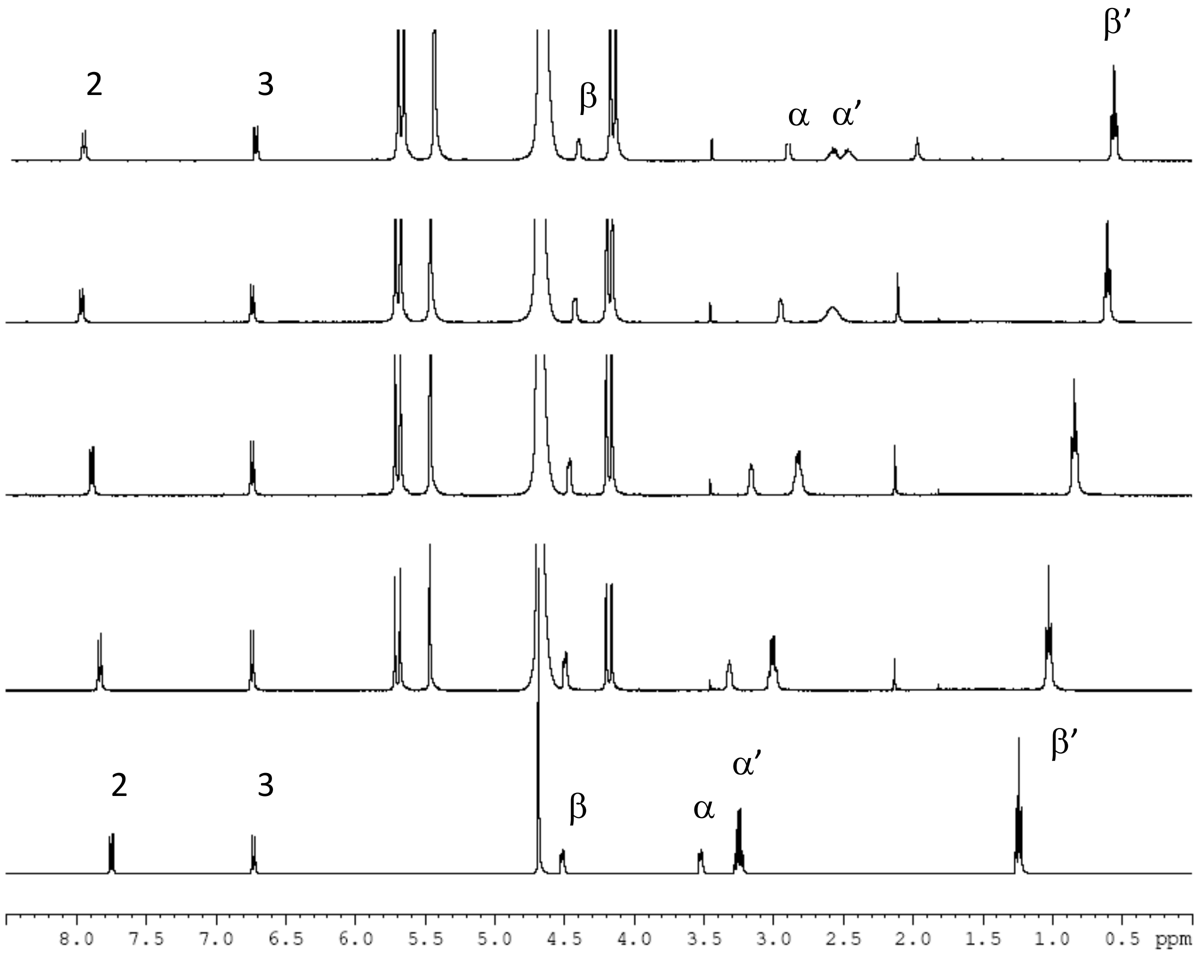


Figure S1. ^{1}H NMR titration of procaine (1.02 mmol dm^{-3}) with CB[7] in D_2O. (a) 0.0 equiv, (b) 0.30 equiv, (c) 0.57 equiv, (d) 0.96 equiv, and (e) 1.18 equiv of CB[7].

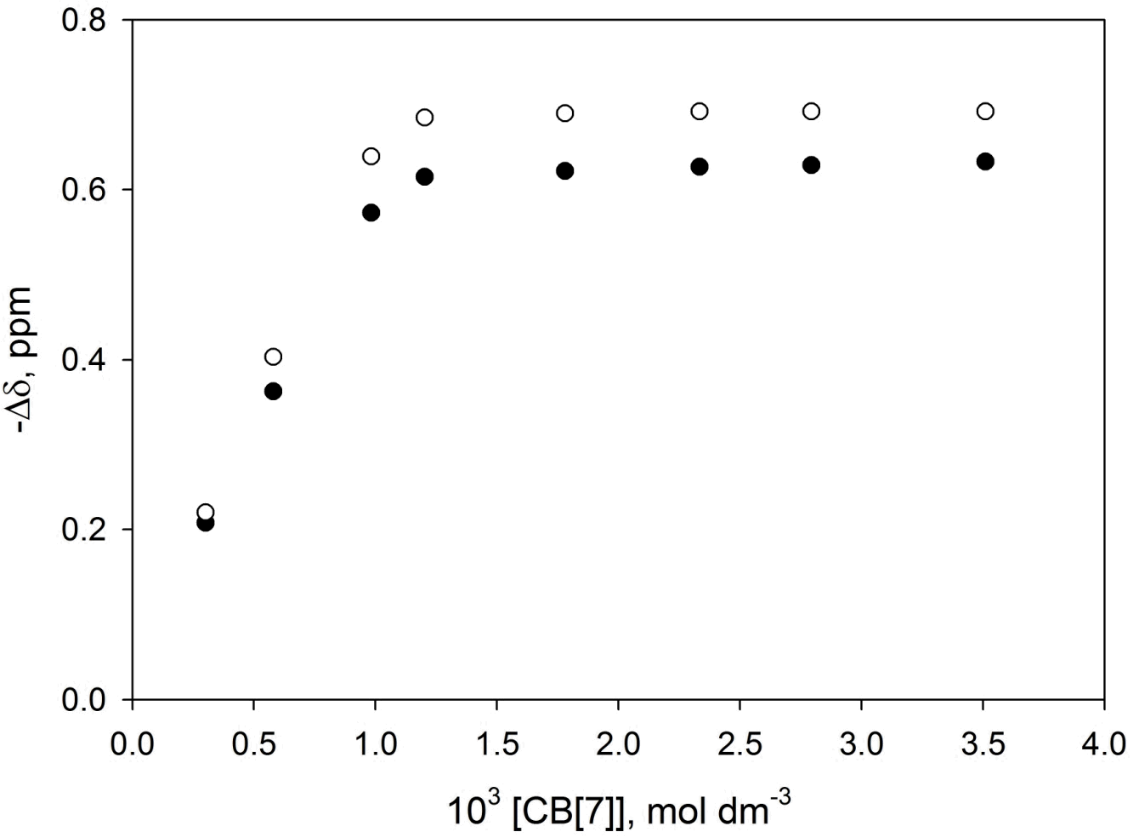
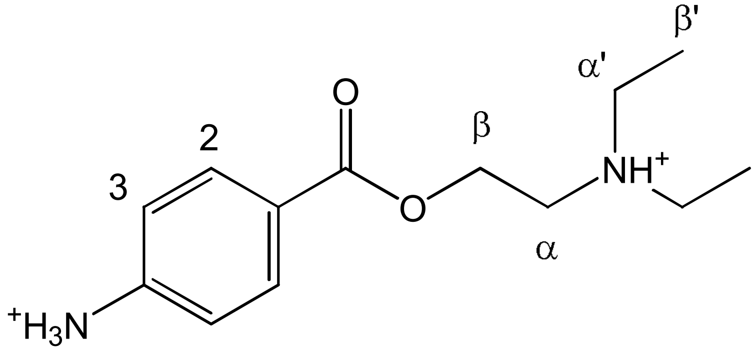


Figure S2. ^{1}H NMR chemical shift titration of procaine (1.02 mmol dm^{-3}) with CB[7] in D_2O. (•) Hα and (○) Hβ'.



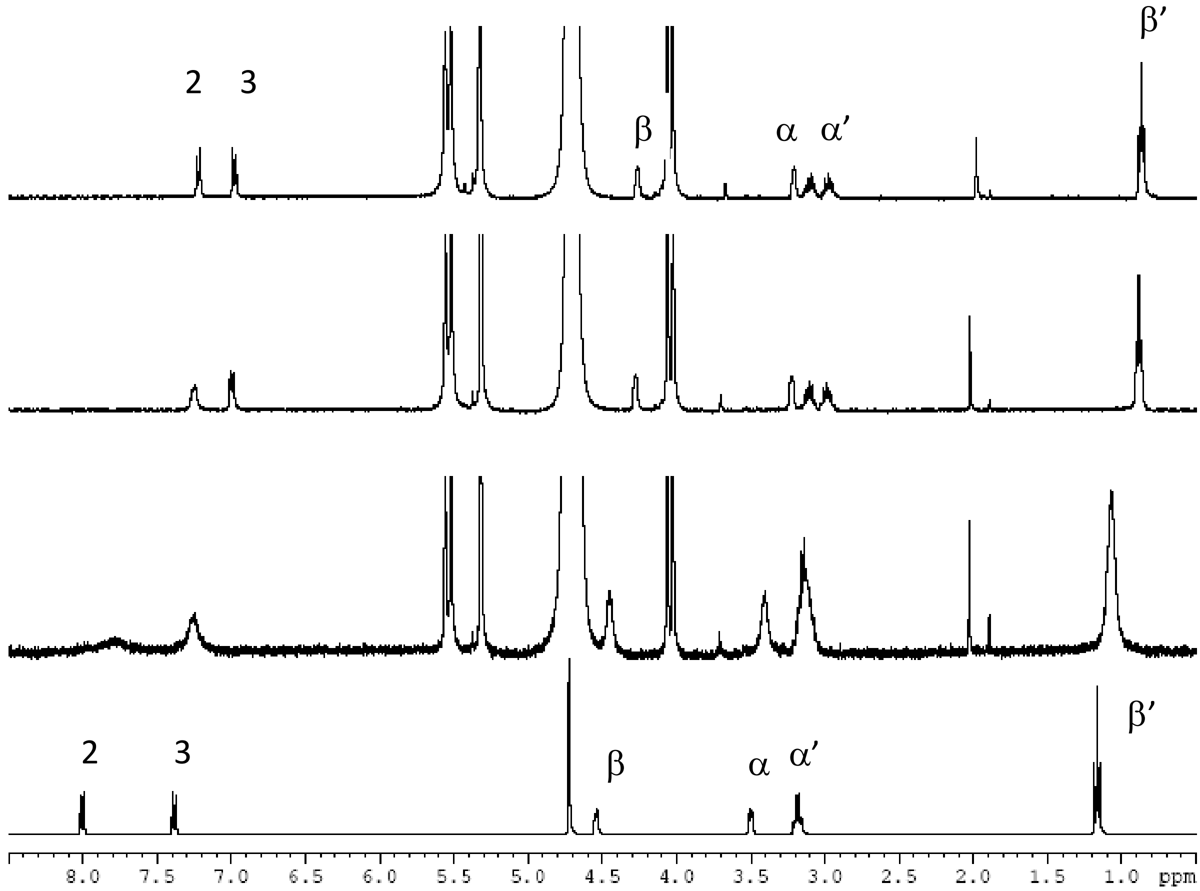


Figure S3. ^{1}H NMR titration of procaine (1.02 mmol dm^{-3}) with CB[7] in D_2O/0.10 mol dm^{-3} DCl. (a) 0.0 equiv, (b) 0.33 equiv, (c) 0.92 equiv, and (d) 1.28 equiv of CB[7].

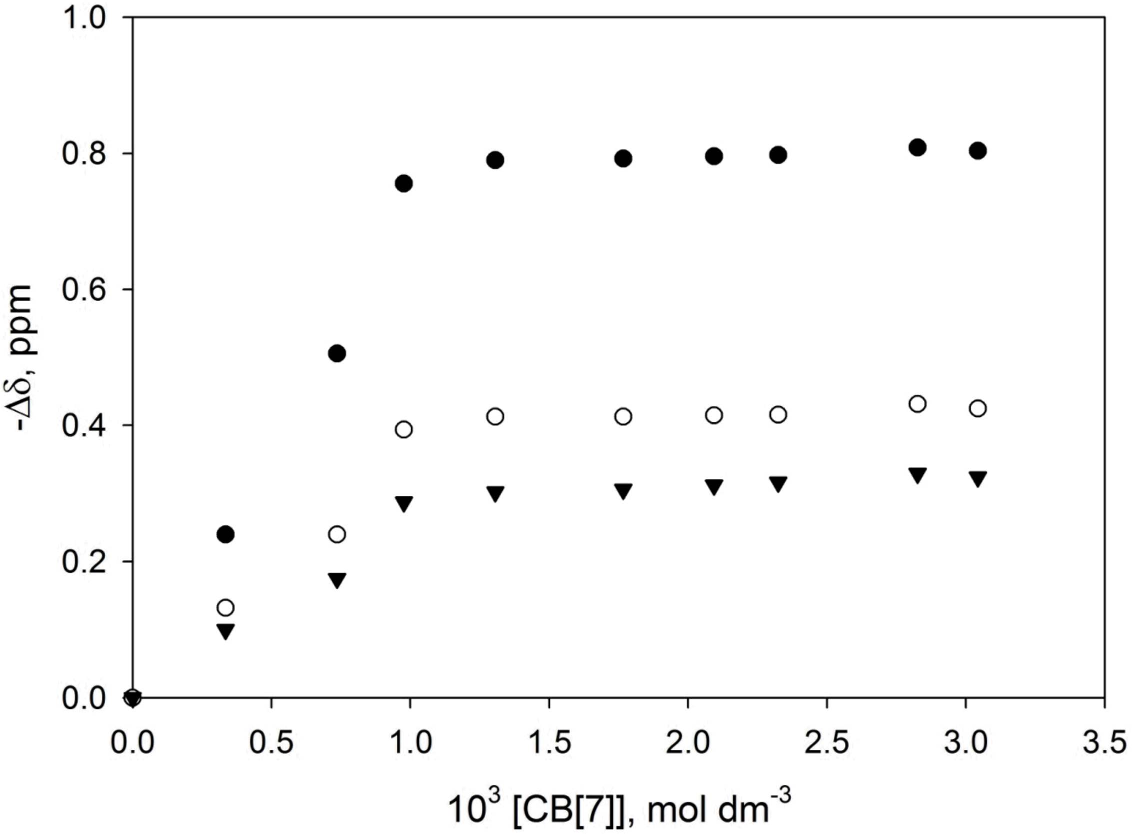
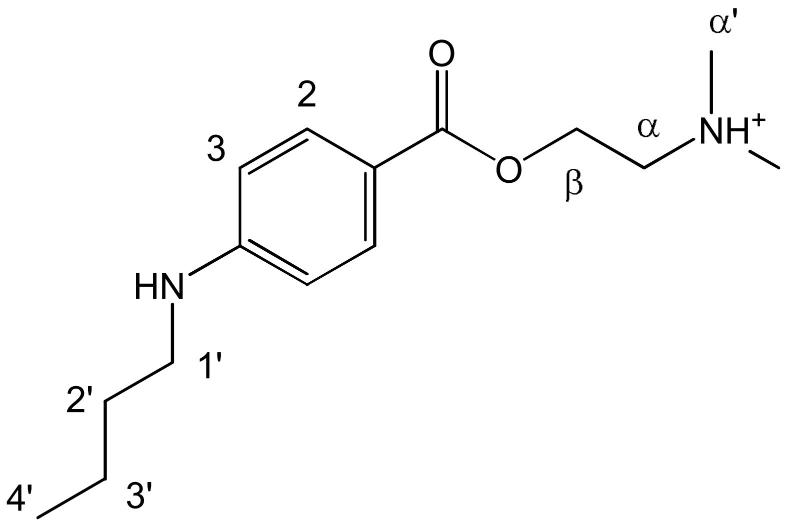


Figure S4. ^{1}H NMR chemical shift titration of procaine (1.02 mmol dm^{-3}) with CB[7] in D_2O containing 0.10 M DCl. (•) H2, (○) H3, and (▼) Hβ'.



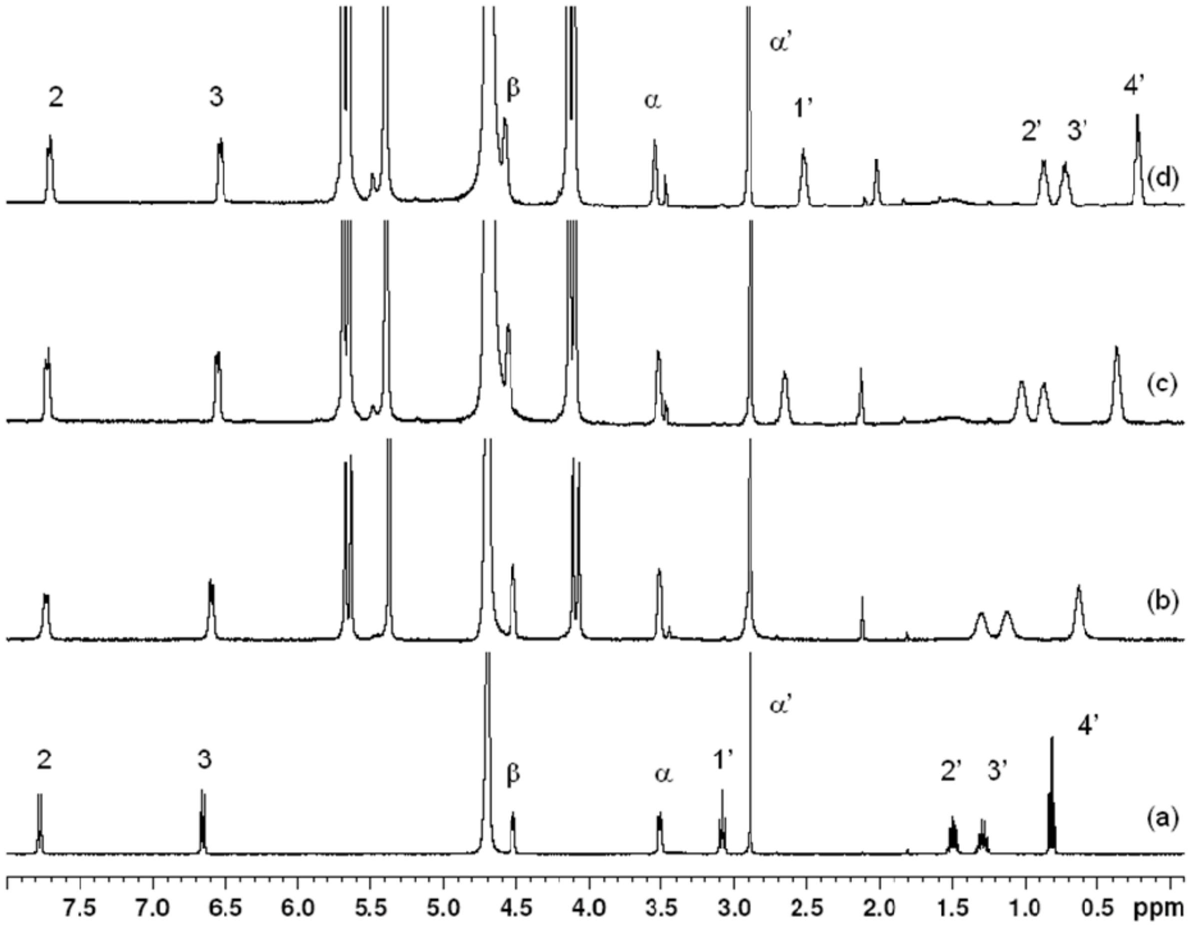


Figure S5. ^{1}H NMR titration of tetracaine (1.33 mmol dm^{-3}) with CB[7] in D_2O. (a) 0.0 equiv, (b) 0.40 equiv, (c) 0.84 equiv, and (d) 1.29 equiv of CB[7].

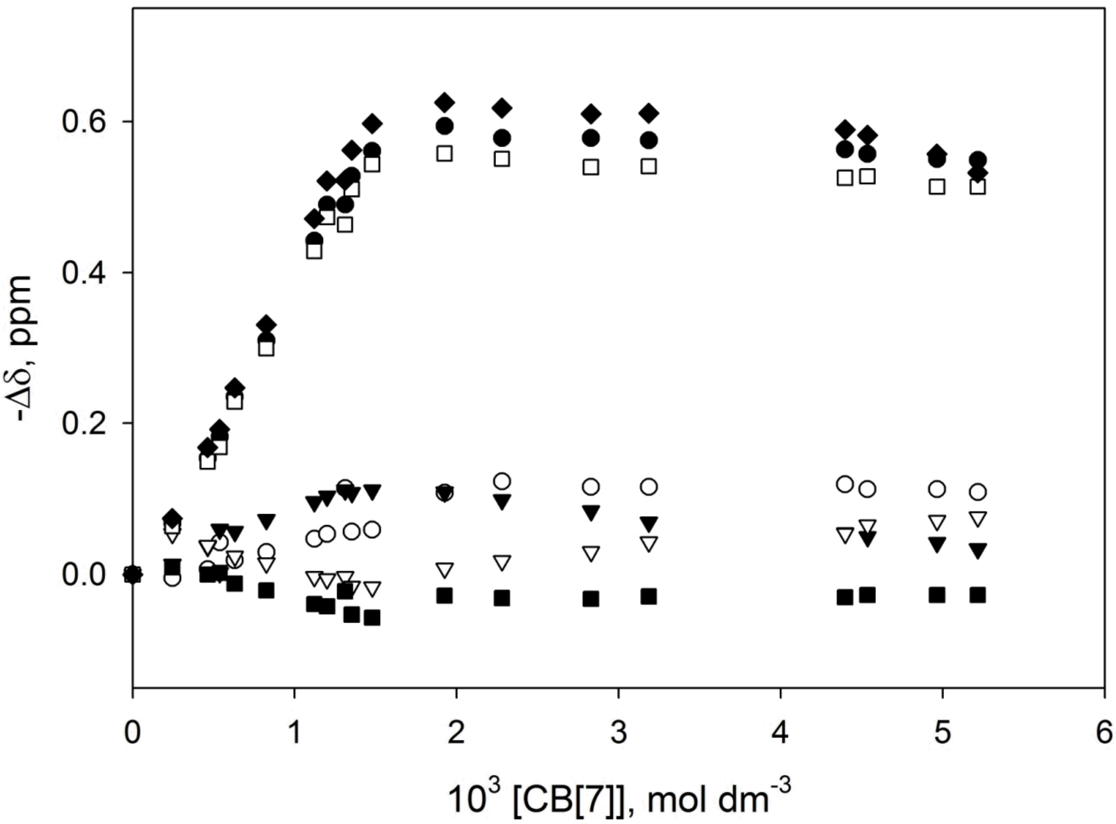
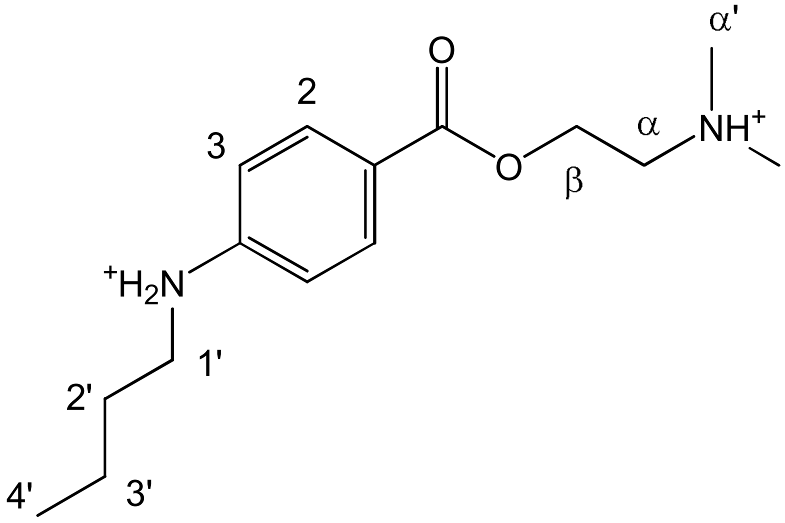


Figure S6. [1]H NMR chemical shift titration of tetracaine (1.33 mmol dm^{-3}) by CB[7] in D_2O. (●) H4’, (○) H2, (▼) H3, (∇) Hα’, (■) Hβ, (□) H3’, and (♦) H2’.



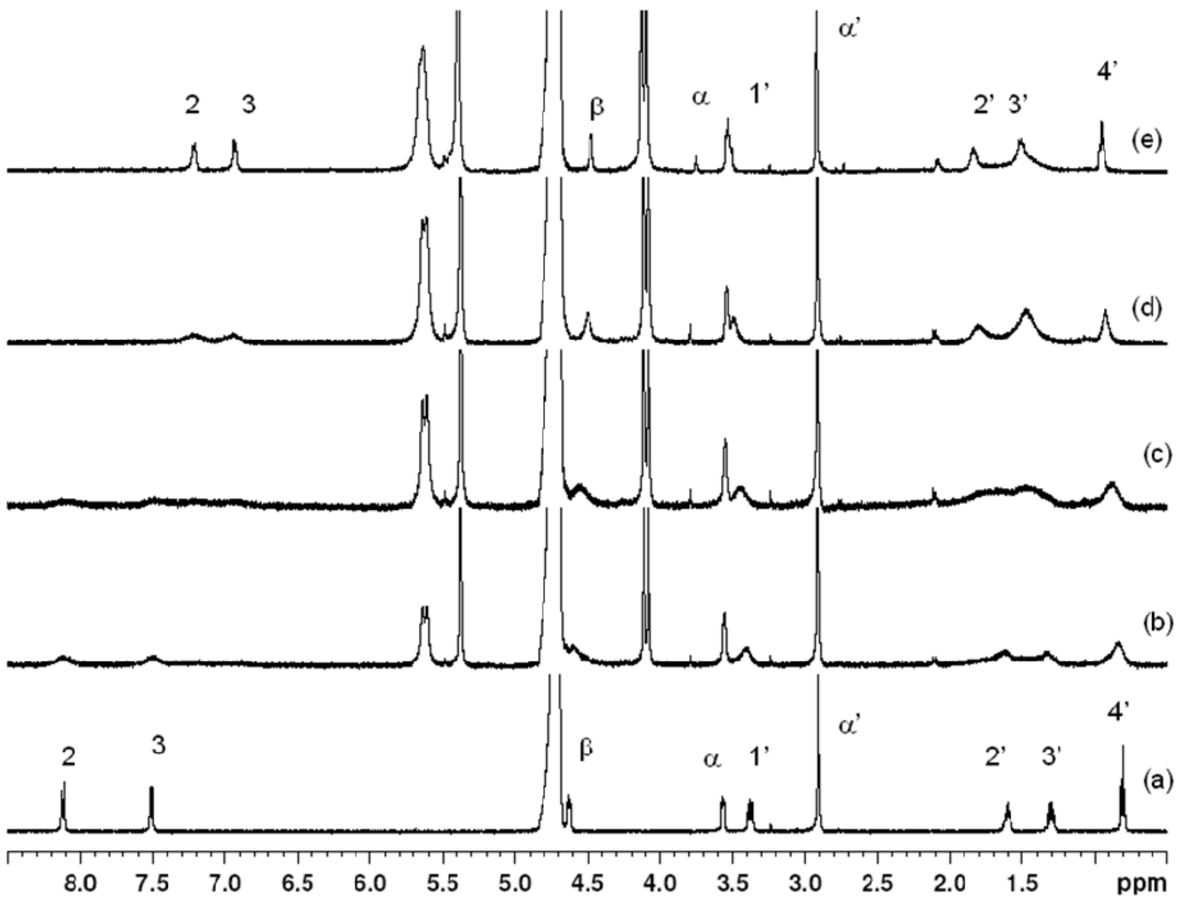


Figure S7. ^{1}H NMR titration of tetracaine (1.03 mol dm^{-3}) with CB[7] in D_2O containing 0.10 mol dm^{-3} DCl. (a) 0.0 equiv, (b) 0.29 equiv, (c) 0.49 equiv, (d) 0.78 equiv, and (e) 1.18 equiv of CB[7].

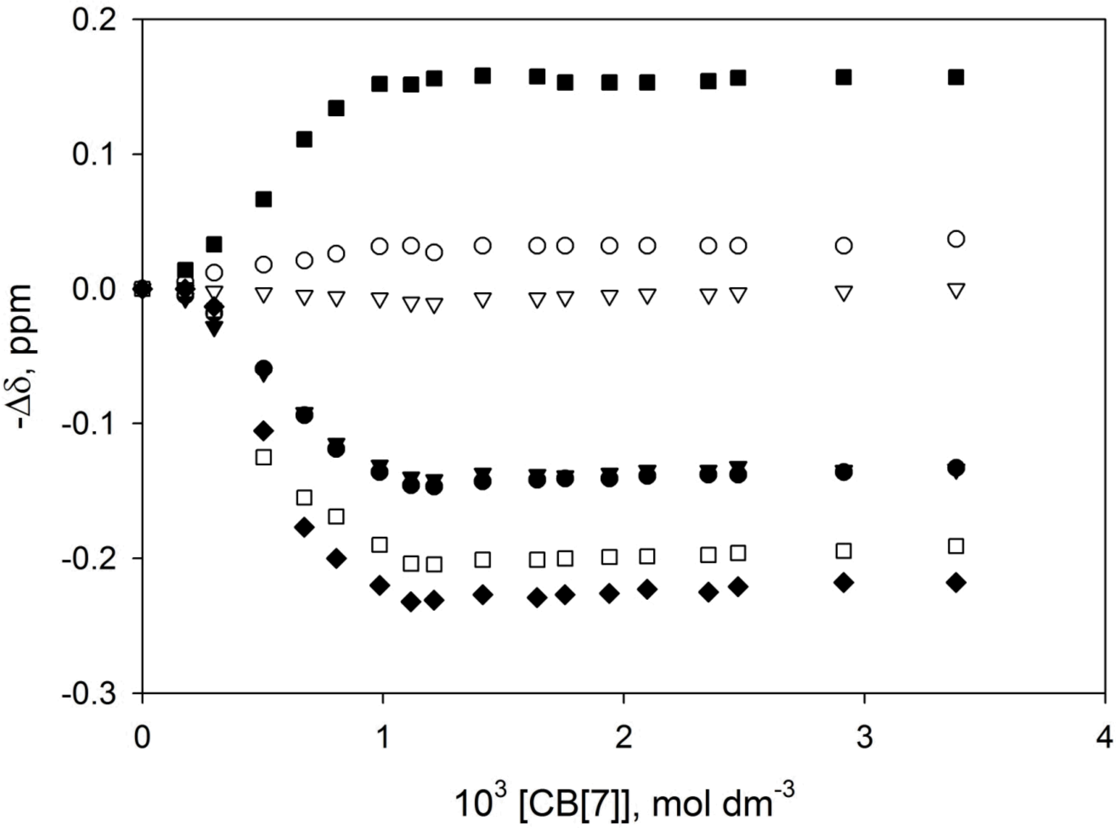


Figure S8. ^{1}H NMR chemical shift titration of tetracaine (1.33 mmol dm^{-3}) by CB[7] in D_2O containing 0.10 mol dm^{-3} DCl. (●) H4', (○) H2, (▼) Hα, (∇) H1', (■) Hβ, (□) H3', and (♦) H2'.

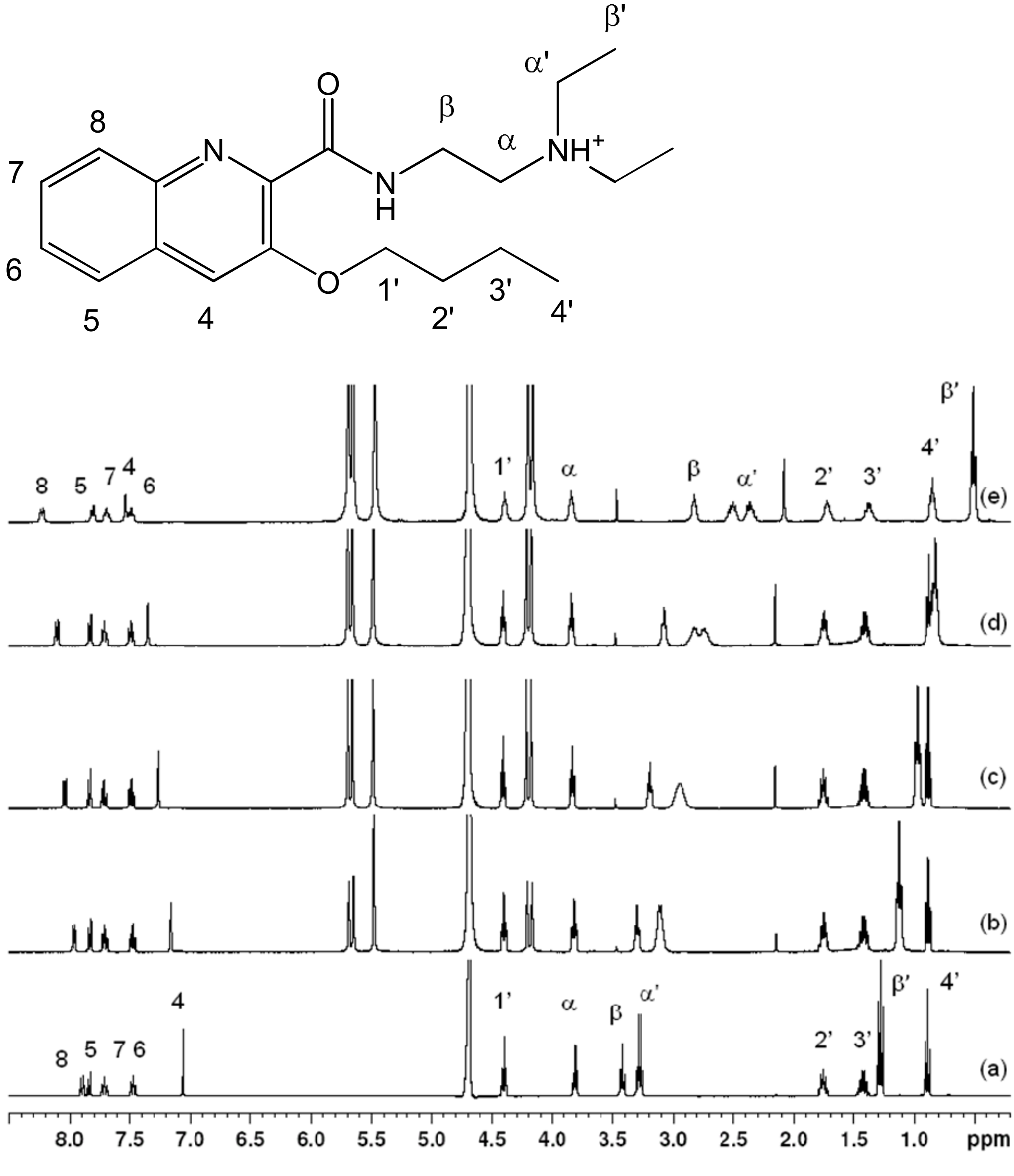


Figure S9. ^{1}H NMR titration of dibucaine (1.01 mmol dm^{-3}) with CB[7] in D_2O. (a) 0.0 equiv, (b) 0.21 equiv, (c) 0.44 equiv, (d) 0.68 equiv and (e) 1.37 equiv of CB[7].

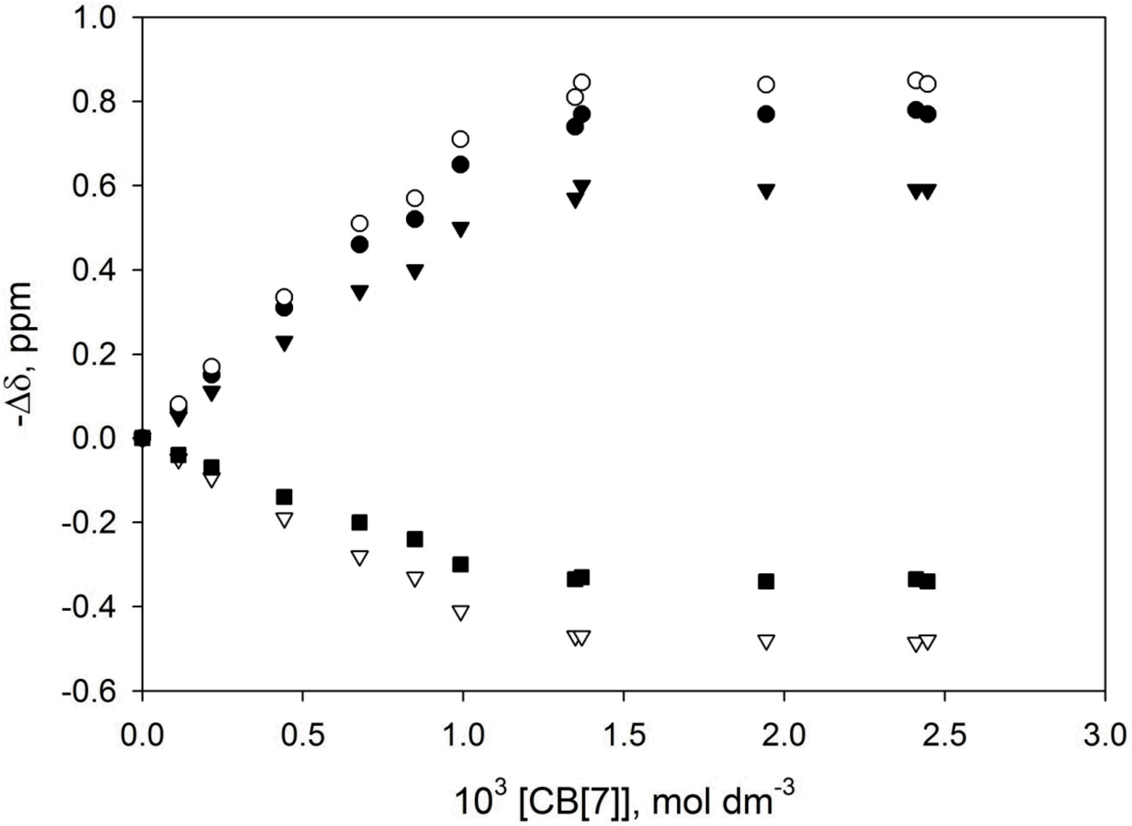
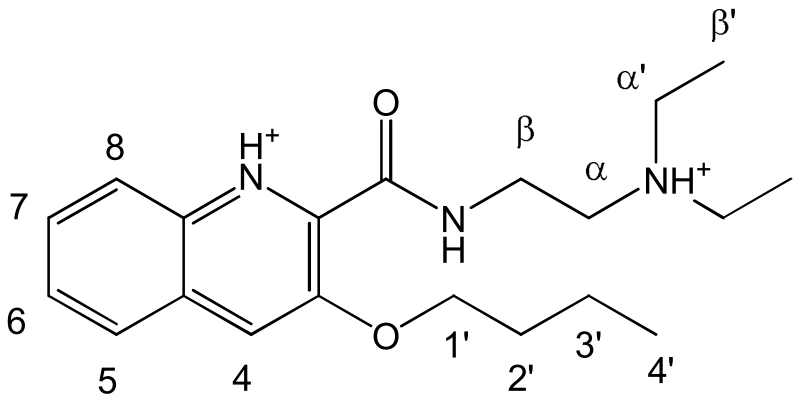


Figure S10. ^{1}H NMR chemical shift titration of dibucaine (1.01 mmol dm^{-3}) by CB[7] in D_2O. (●) Hb', (○) Hα', (▼) Hα, (∇) H4, and (■) H8.



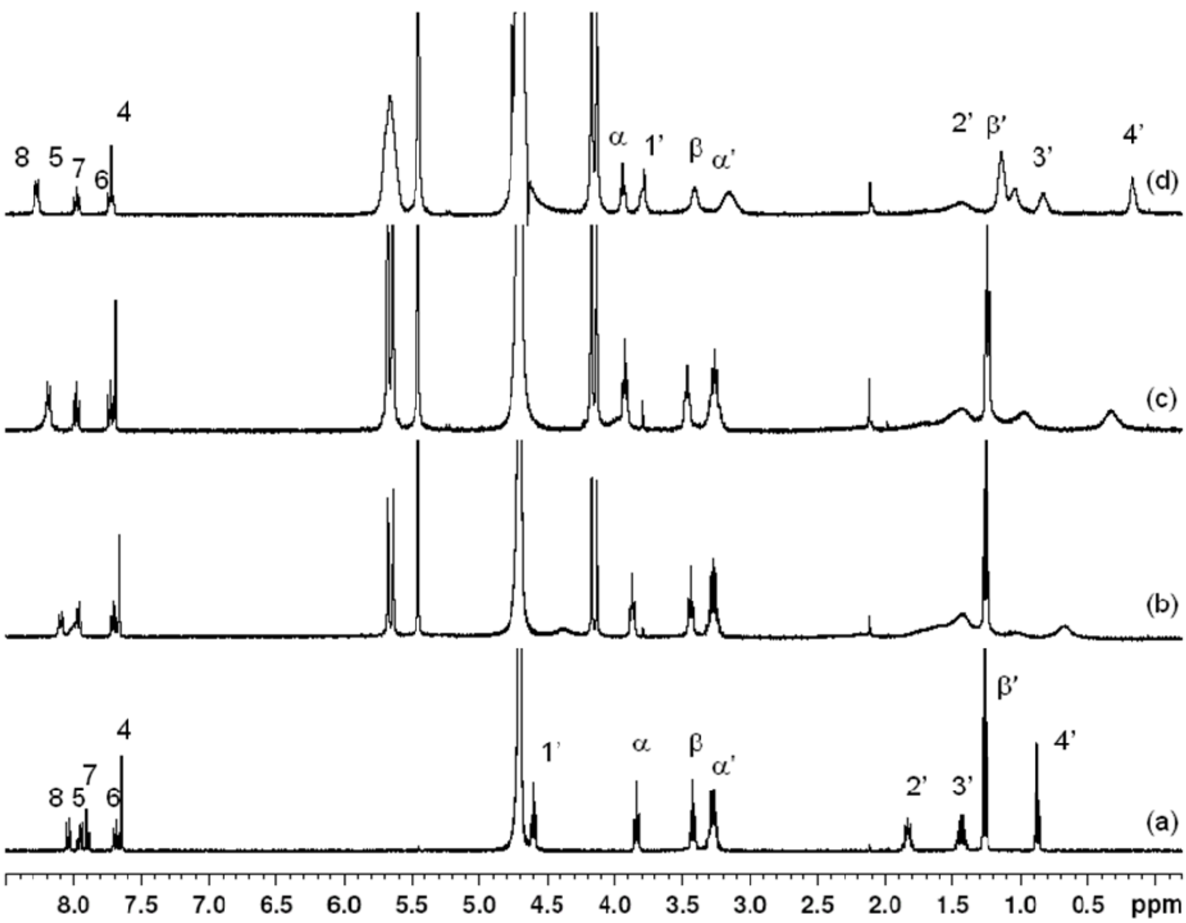


Figure S11. [1]H NMR titration of dibucaine (1.02 mmol dm^{-3}) with CB[7] in D_2O containing 0.10 mol dm^{-3} DCl. (a) 0.0 equiv, (b) 0.31 equiv, (c) 0.78 equiv, and (d) 1.24 equiv of CB[7].

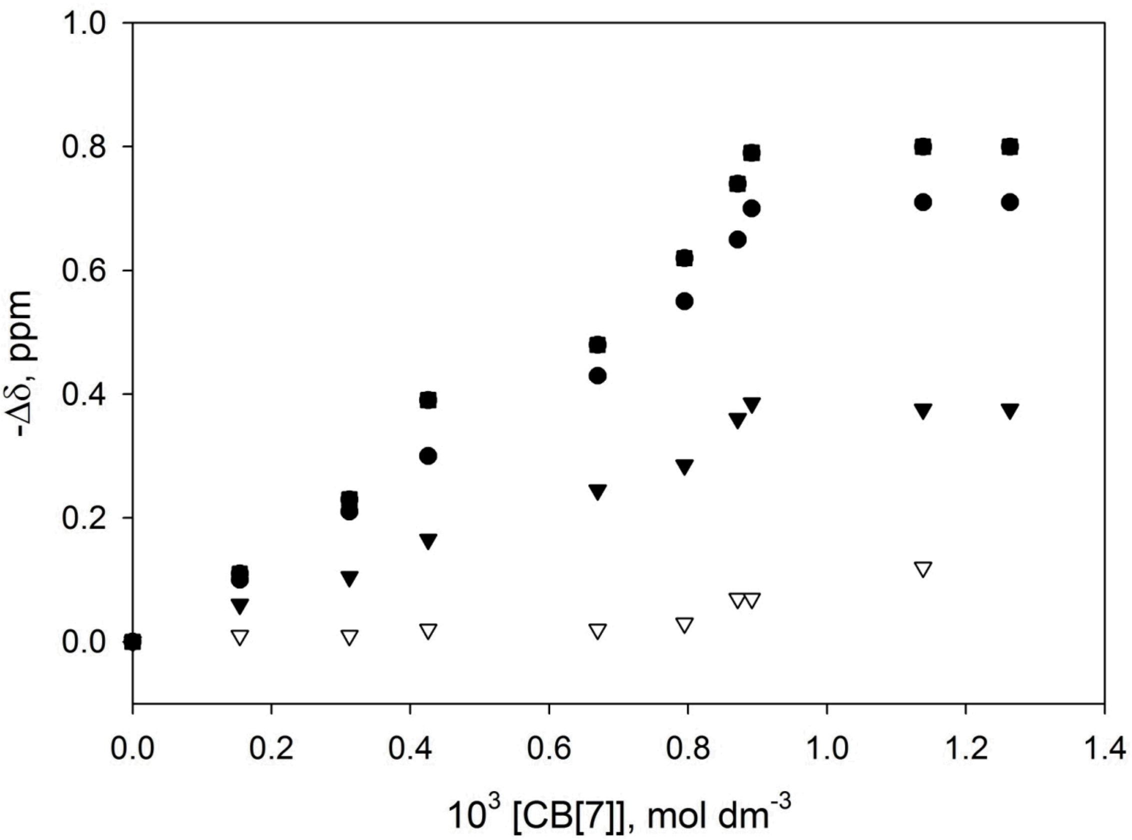
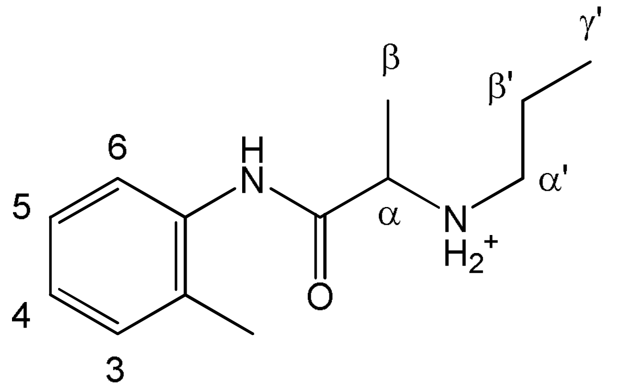


Figure S12. ^{1}H NMR chemical shift titration of dibucaine (1.02 mmol dm^{-3}) by CB[7] in D_2O containing 0.10 mol dm^{-3} DCl. (●) H', (○) H2, (▼) Hα, (∇) H1', (■) Hβ, (□) H3', and (♦) H2'.



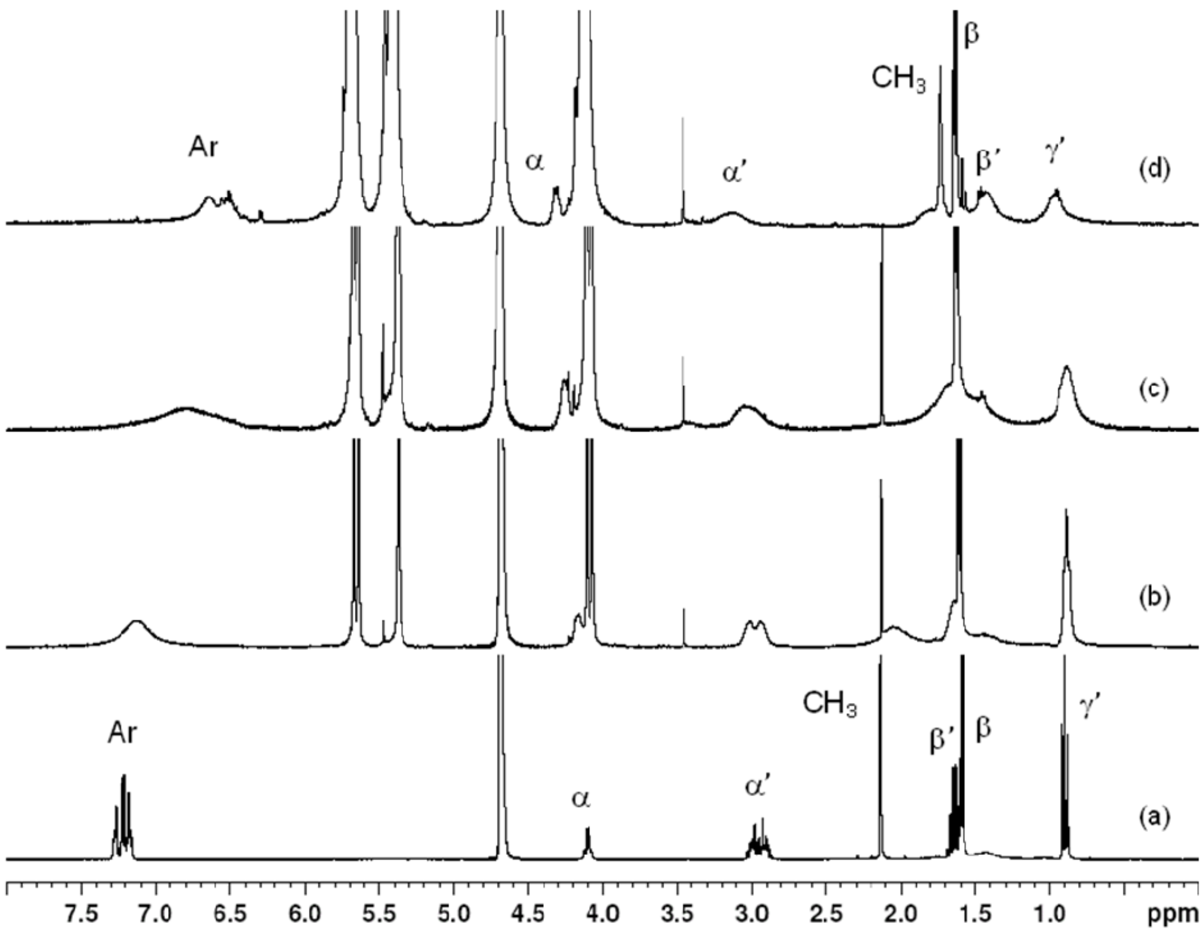


Figure S13. ^{1}H NMR spectra of prilocaine (1.27 mmol dm^{-3}) in D_2O. (a) 0.0 equiv, (b) 0.31 equiv, (c) 0.68 equiv, and (d) 1.80 equiv of CB[7].

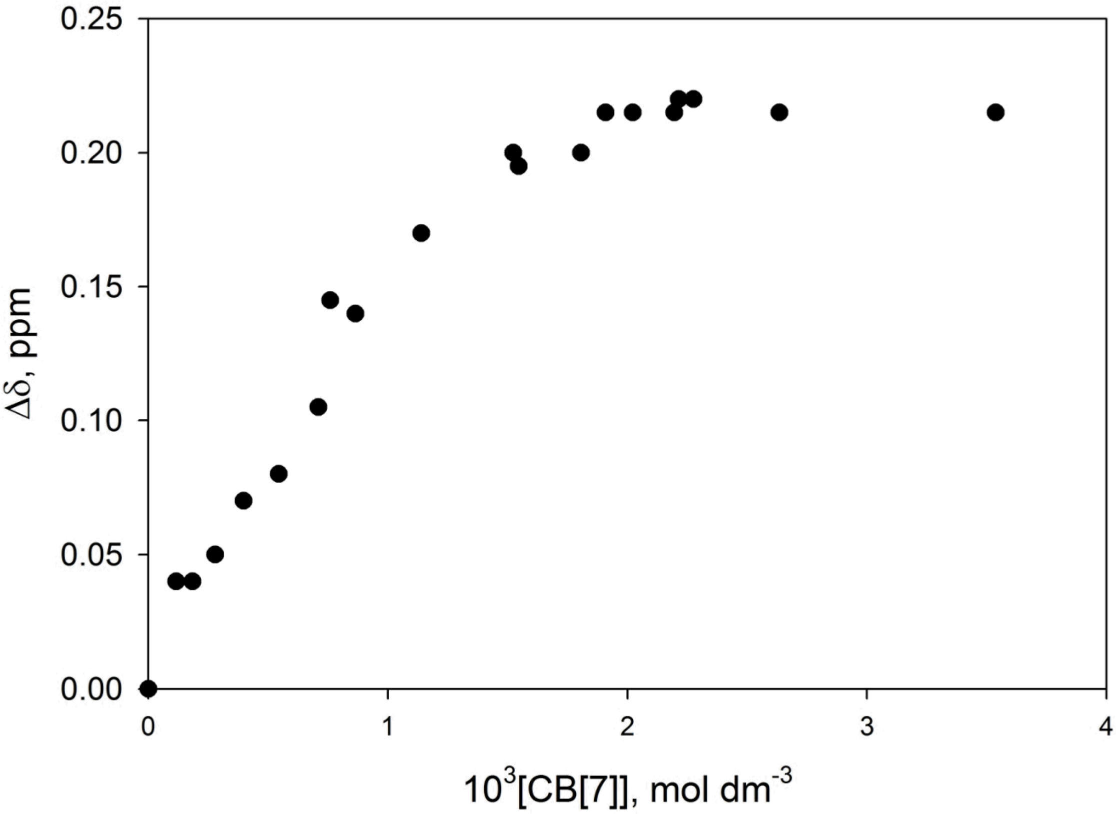
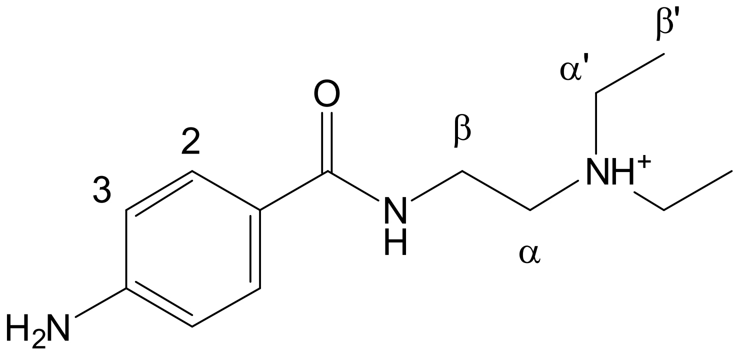


Figure S14. ^{1}H NMR chemical shift titration of prilocaine (1.27 mmol dm^{-3}) with CB[7] in D_2O. (●) Hα.



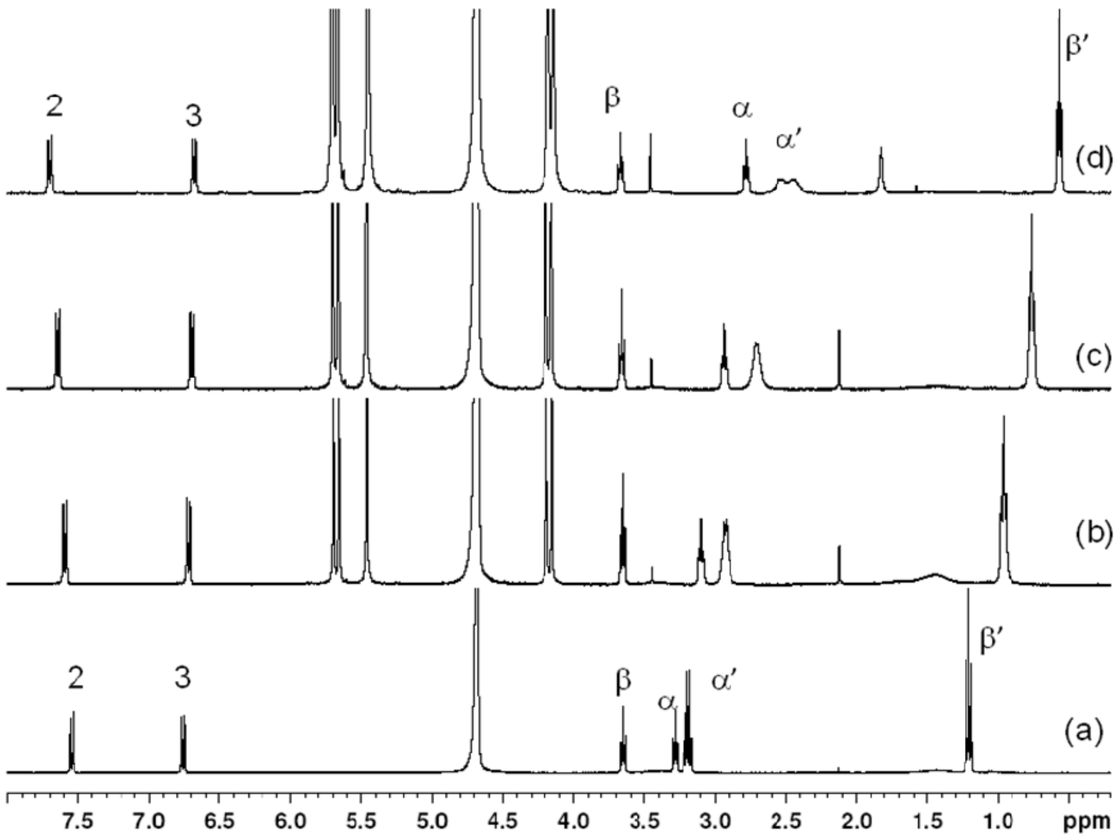


Figure S15. ^{1}H NMR spectra of procainamide (1.10 mmol dm^{-3}) with (a) 0.0 equiv, (b) 0.39 equiv, (c) 0.72 equiv, and (d) 1.88 equiv of CB[7] in D_2O.

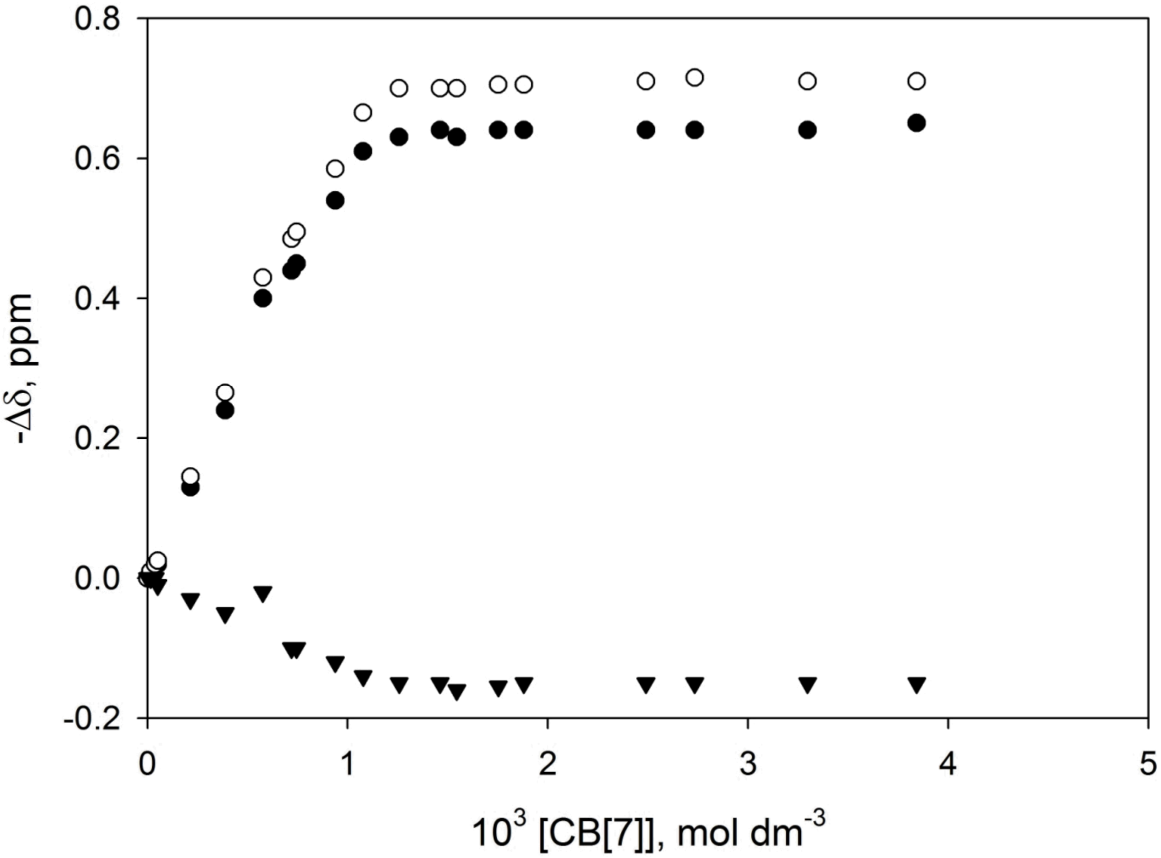
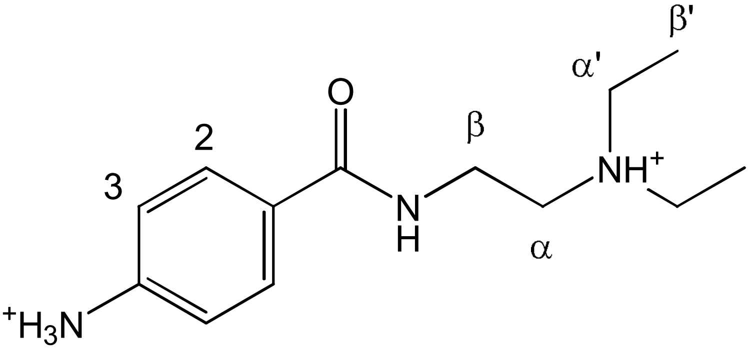


Figure S16. ^{1}H NMR chemical shift titration of procainamide (1.01 mM) with CB[7] in D_2O. (●) Hβ', (○) Hα', and (▼) H2.



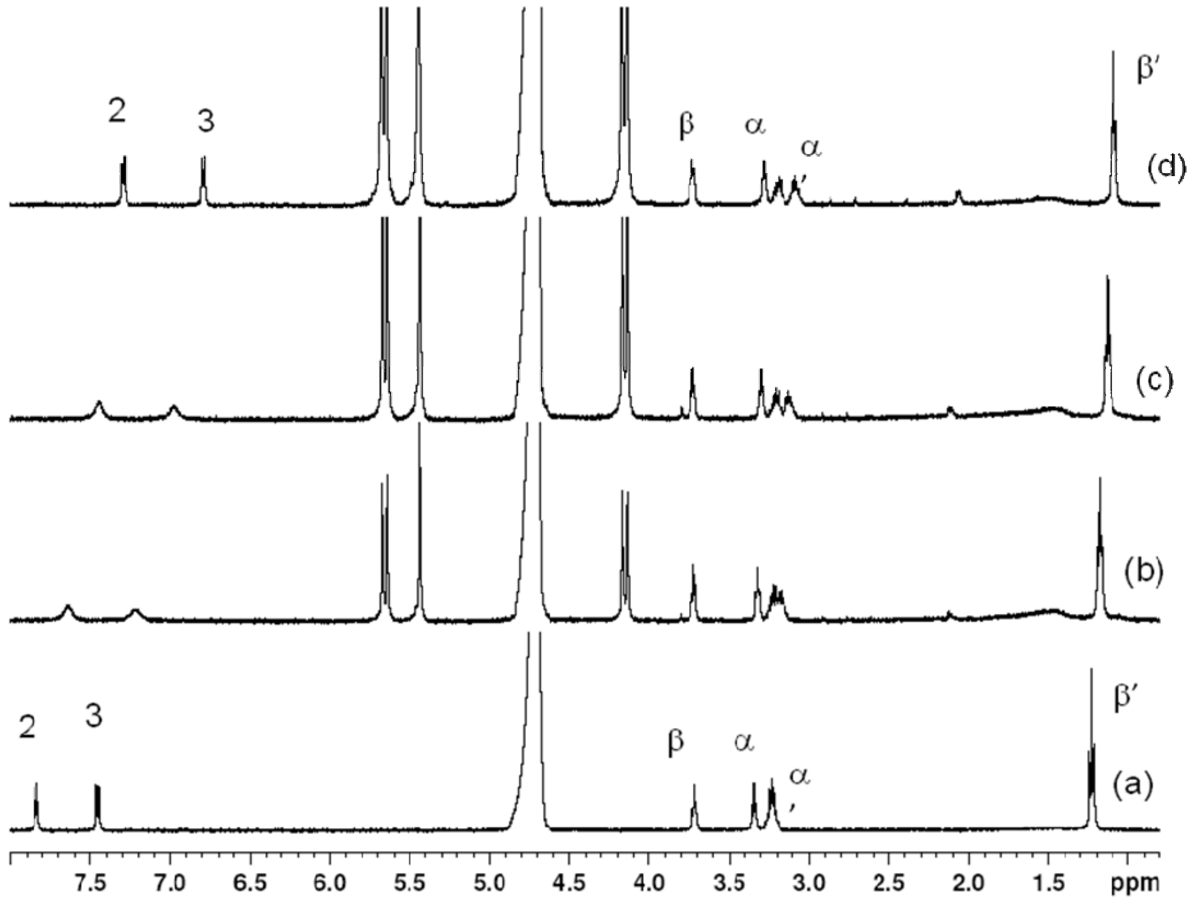


Figure S17. ^{1}H NMR spectra of procainamide (1.01 mmol dm^{-3}) with (a) 0.0 equiv, (b) 0.39 equiv, (c) 0.79 equiv, and (d) 1.53 equiv of CB[7] in D_2O in the presence of 0.10 mol dm^{-3} DCl.

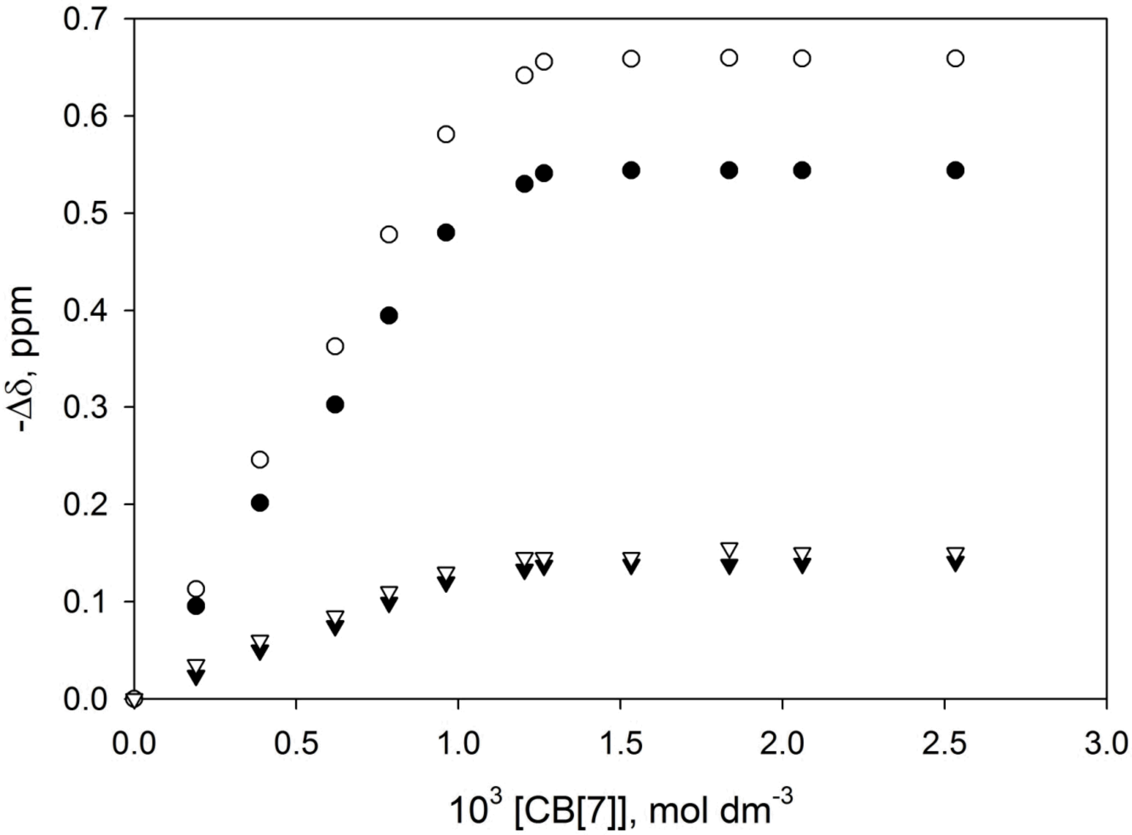


Figure S18. ^{1}H NMR chemical shift titration of procainamide (1.01 mM) with CB[7] in D_2O containing 0.10 mol dm^{-3} DCl . (●) H2, (○) H3, (▼) Hβ', and (∇) Hα'.

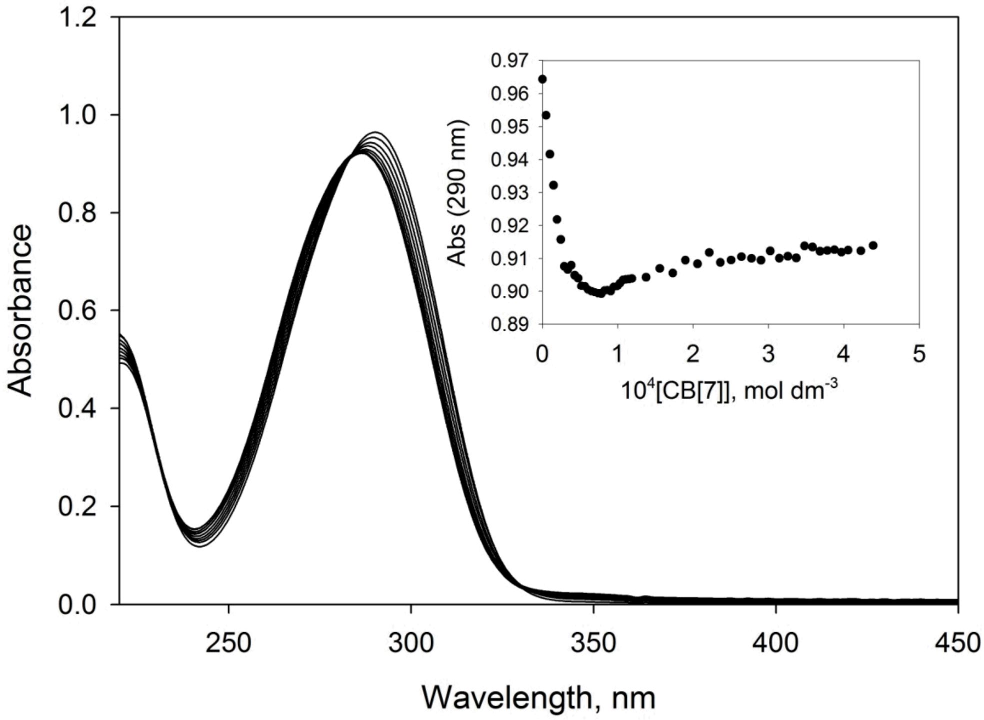


Figure S19. UV titration of procaine (50 μmol dm^{-3}) with CB[7] in H_2O. Inset: Dependence of absorbance at 290 nm on the concentration of CB[7].

Table S1. Mass spectral data for the 1:1 and 2:1 CB[7] host-guest complexes with the local anaesthetic guests in water.

Guest	1:1 Host-guest complex	2:1 Host-guest complex*
procaine	700.2551 (M•CB[7]-Cl+H}$^{2+}$ (700.2553 for $C_{55}H_{64}N_{30}O_{16}{}^{2+}$) 711.2382 (M•CB[7]-Cl+Na}$^{2+}$ (711.2465 for $C_{55}H_{63}N_{30}NaO_{16}{}^{2+}$)	1292.4687 (M•2CB[7]-Cl+Na}$^{2+}$ (1292.4180 for $C_{97}H_{105}N_{58}NaO_{30}{}^{2+}$)
tetracaine	714.2717 (M•CB[7]-Cl+H}$^{2+}$ (714.2709 for $C_{57}H_{68}N_{30}O_{16}{}^{2+}$) 725.2762 (M•CB[7]-Cl+Na}$^{2+}$ (725.2642 for $C_{57}H_{67}N_{30}NaO_{16}{}^{2+}$)	1295.4767 (M•2CB[7]-Cl+H}$^{2+}$ (1295.4427 for $C_{99}H_{110}N_{58}O_{30}{}^{2+}$)
procainamide	699.7661 (M•CB[7]-Cl+H}$^{2+}$ (699.7632 for $C_{55}H_{65}N_{31}O_{15}{}^{2+}$)	1291.9526 (M•2CB[7]-Cl+Na}$^{2+}$ (1291.7601 for $C_{97}H_{106}N_{59}NaO_{29}{}^{2+}$)
dibucaine	753.8056 (M•CB[7]-Cl+H}$^{2+}$ (753.7920 for $C_{62}H_{73}N_{31}O_{16}{}^{2+}$)	1334.9858 (M•2CB[7]-Cl+H}$^{2+}$ (1334.9643 for $C_{104}H_{115}N_{59}O_{30}{}^{2+}$) 1345.980 (M•2CB[7]-Cl+Na}$^{2+}$ (1345.9553 for $C_{104}H_{114}N_{59}NaO_{30}{}^{2+}$)
prilocaine	703.2593 (M•CB[7]-Cl+Na}$^{2+}$ (703.2488 for $C_{55}H_{63}N_{30}NaO_{15}{}^{2+}$) 1383.5430 (M•CB[7]-Cl}$^{+}$ (1383.5084 for $C_{55}H_{63}N_{30}O_{15}{}^{+}$)	1284.4416 (M•2CB[7]-Cl+Na}$^{2+}$ (1284.4206 for $C_{104}H_{115}N_{59}NaO_{30}{}^{2+}$)

*The peaks for the 2:1 host-guest complexes are ~1-2% the intensity of the peaks for the 1:1 host-guest complexes.