Electronic Supporting Information

Cucurbit[7]uril host-guest complexes of cholines and phosphonium cholines in aqueous solution

Ian W. Wyman and Donal H. Macartney*

Department of Chemistry, Queen's University, 90 Bader Lane, Kingston, ON K7L 3N6 Canada. Fax: +1 613 533 6669; Tel: +1 613 533 2617; E-mail: donal@chem.queensu.ca

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Table S1. High resolution electrospray mass spectra data for the 1:1 host-guest complexes with CB[7] in water (X^- = Cl^- or Br^-)

Guest	$\{M•CB[7]-X\}^+$ (*m/z* observed)	$\{M•CB[7]-X\}^+$ (*m/z* calculated)
$(CH_3)_3N(CH_2)_2OH^+$	1266.4643	1266.4505 ($C_{47}H_{56}N_{29}O_{15}^+$)
$(CH_3)_3N(CH_2)_2O_2CCH_3^+$	1308.4684	1308.4611 ($C_{49}H_{58}N_{29}O_{16}^+$)
$(CH_3)_3NCH_2CH(CH_3)O_2CCH_3^+$	1322.4855	1322.4767 ($C_{50}H_{60}N_{29}O_{16}^+$)
$(CH_3)_3N(CH_2)_2O_2C(CH_2)_2CH_3^+$	1336.4994	1336.4942 ($C_{51}H_{62}N_{29}O_{16}^+$)
$(CH_3)_3NCH_2CH(OH)CH_2CO_2H^+$	1324.4600	1324.4560 ($C_{49}H_{58}N_{29}O_{17}^+$)
$(PhCH_2)(CH_3)_2N(CH_2)_2OH^+$	1342.5034	1342.4818 ($C_{53}H_{60}N_{29}O_{15}^+$)
$(CH_3CH_2)_3N(CH_2)_2OH^+$	1308.4975	1308.4974 ($C_{50}H_{62}N_{29}O_{15}^+$)
$(CH_3CH_2)_3N(CH_2)_4CH_3^+$	1334.5619	1334.5495 ($C_{53}H_{68}N_{29}O_{14}^+$)
$Quin(CH_2)_2OH^+$	1318.4766	1318.4818 ($C_{51}H_{60}N_{29}O_{15}^+$)
$(CH_3)_3P(CH_2)_4CH_3^+$	1309.4706	1309.4732 ($C_{50}H_{62}N_{28}PO_{14}^+$)
$(CH_3)_3P(CH_2)_2OH^+$	1283.4482	1283.4212 ($C_{47}H_{56}N_{28}PO_{15}^+$)
$(CH_3)_3P(CH_2)_2O_2CCH_3^+$	1325.4339	1325.4318 ($C_{49}H_{58}N_{28}PO_{16}^+$)
$(CH_3CH_2)_3P(CH_2)_4CH_3^+$	1351.5148	1309.5202 ($C_{53}H_{68}N_{28}PO_{14}^+$)
$(CH_3CH_2)_3P(CH_2)_2OH^+$	1325.4724	1325.4682 ($C_{50}H_{62}N_{28}PO_{15}^+$)
$(CH_3CH_2)_3P(CH_2)_2O_2CCH_3^+$	1367.4851	1367.4787 ($C_{52}H_{64}N_{28}PO_{16}^+$)

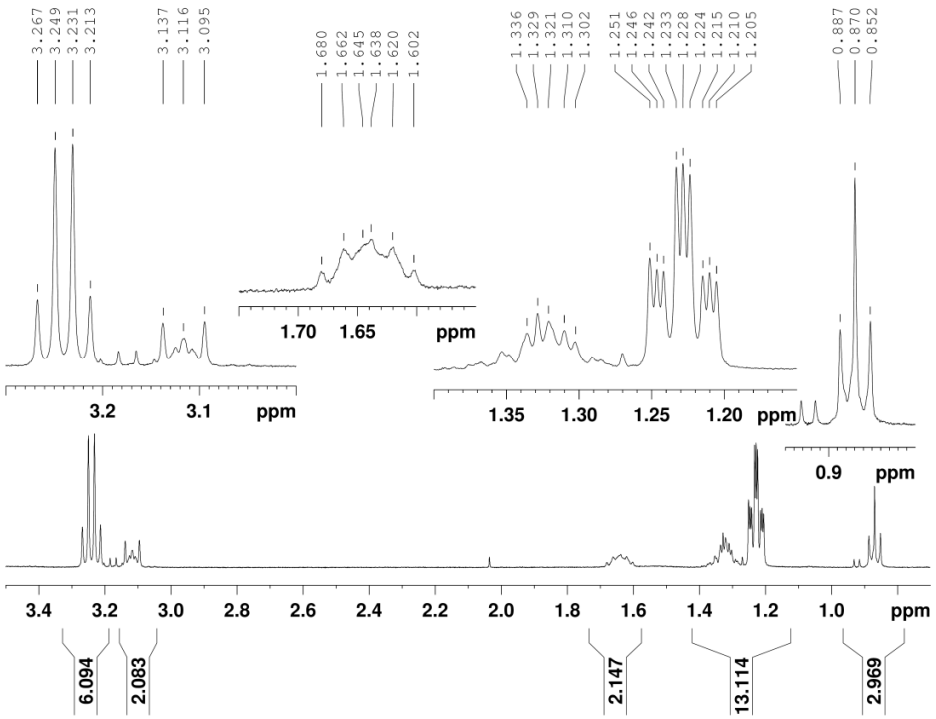

Figure S1. ^{1}H NMR spectrum (400 MHz) of triethylpentylammonium bromide in D_2O.

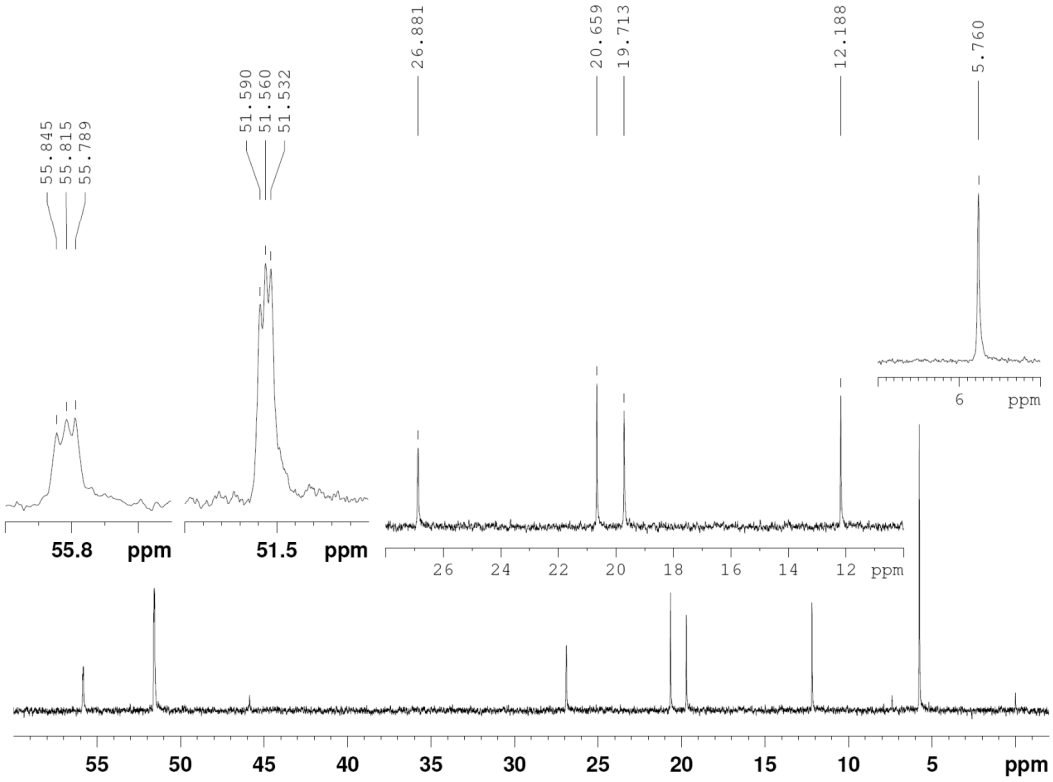

Figure S2. ^{13}C NMR spectrum (100 MHz) of triethylpentylammonium bromide in D_2O.

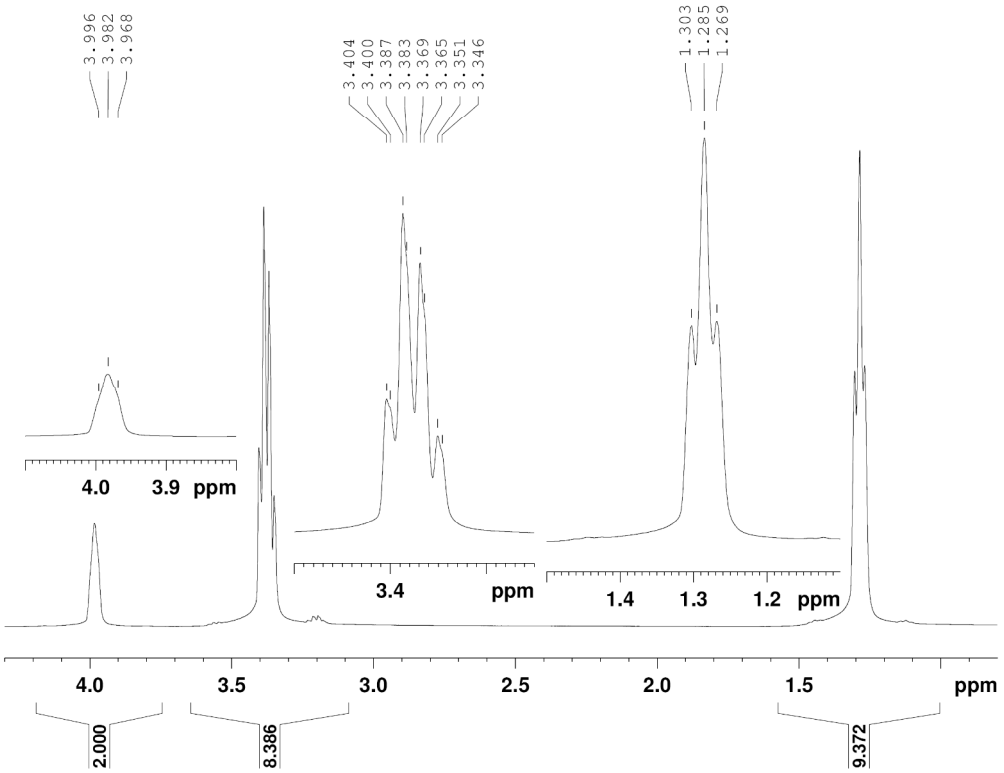

Figure S3. ^{1}H NMR spectrum (400 MHz) of (2-hydroxyethyl)triethylammonium bromide in D_2O.

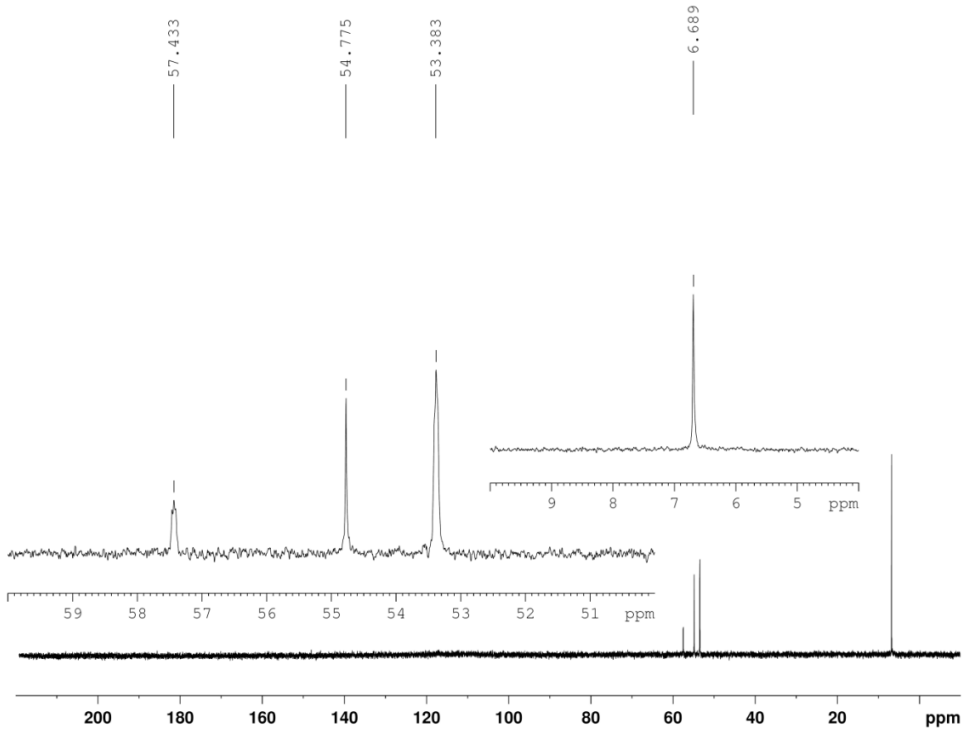

Figure S4. ^{13}C NMR spectrum (100 MHz) of (2-hydroxyethyl)triethylammonium bromide in D_2O.

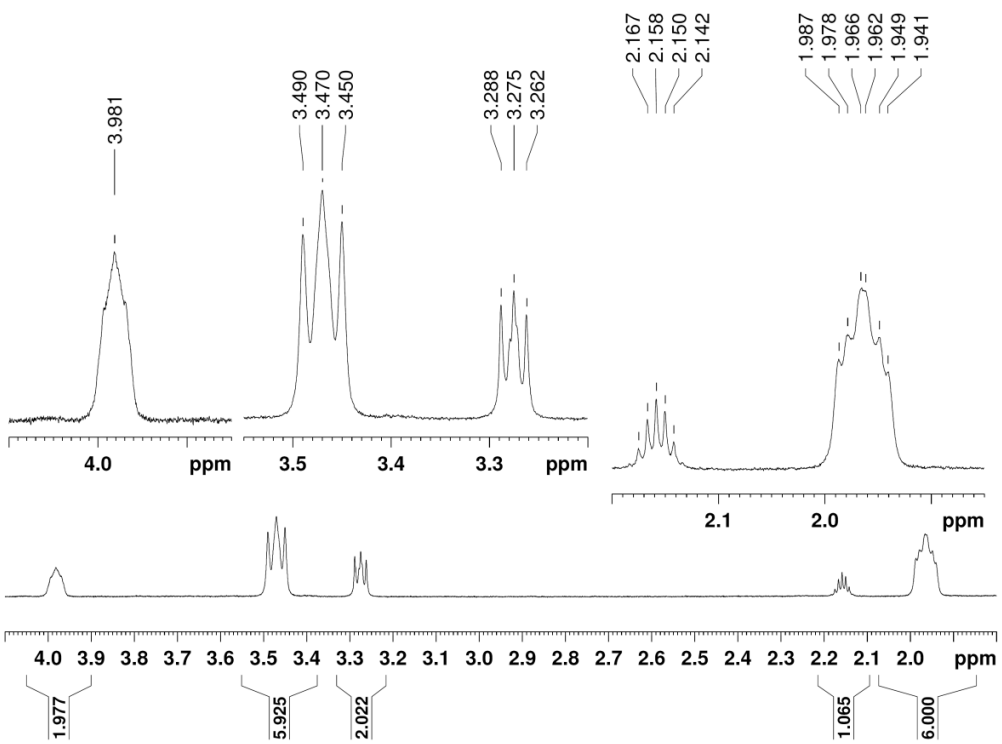

Figure S5. ^{1}H NMR spectrum (400 MHz) of 2-(hydroxyethyl)quinuclidinium bromide in D_2O.

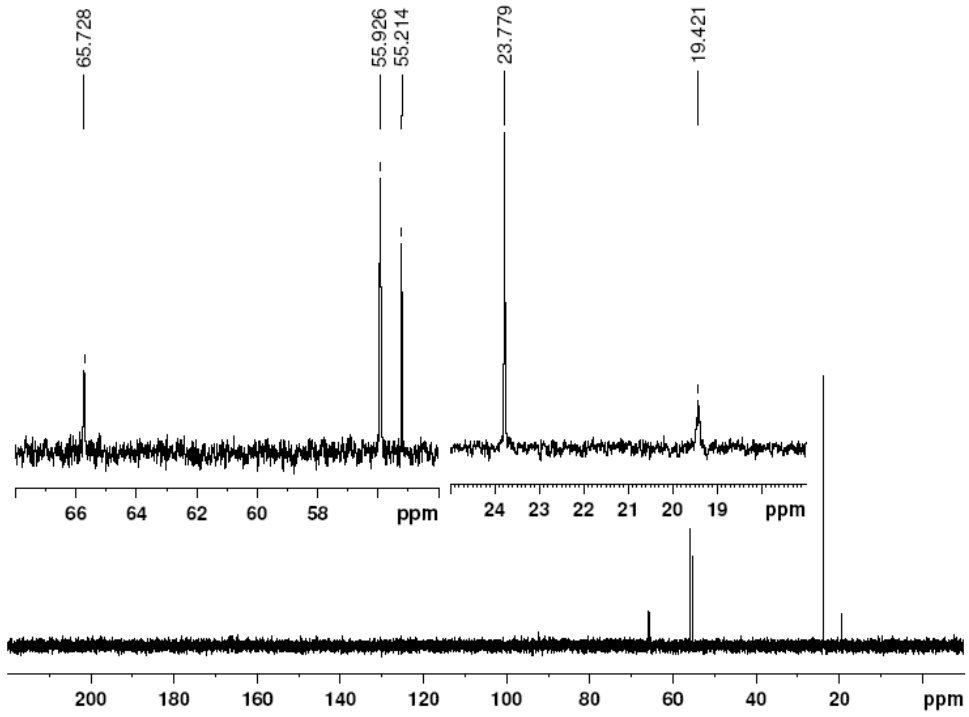

Figure S6. ^{13}C NMR spectrum (100 MHz) of 2-(hydroxyethyl)quinuclidinium bromide in D_2O.

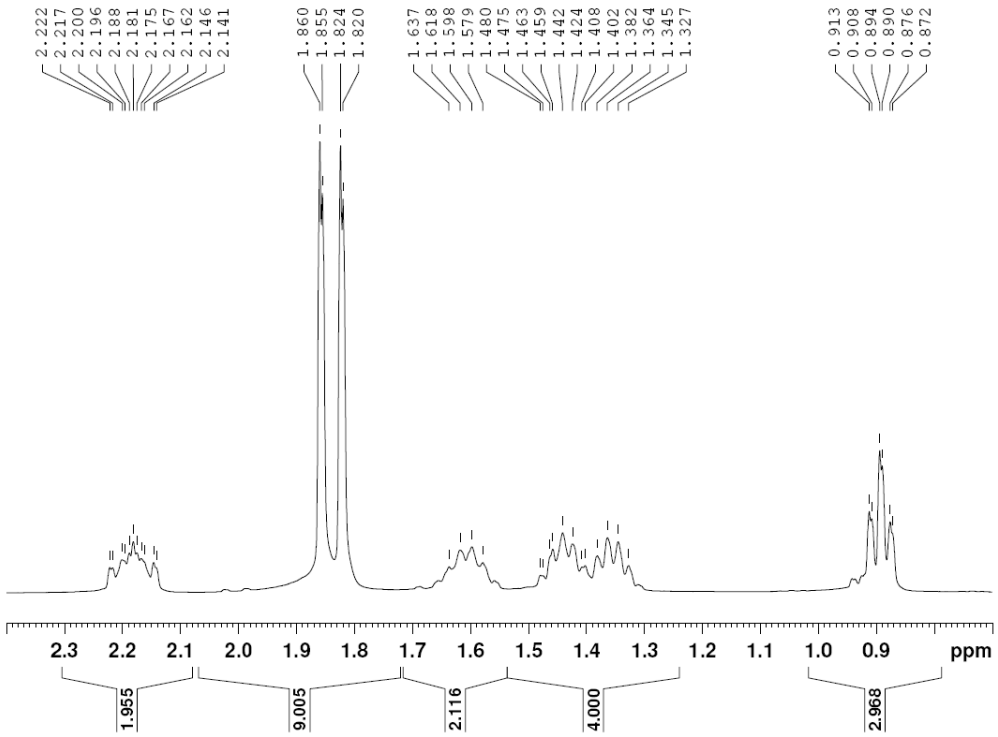

Figure S7. ^{1}H NMR spectrum (400 MHz) of trimethylpentylphosphonium bromide in D_2O.

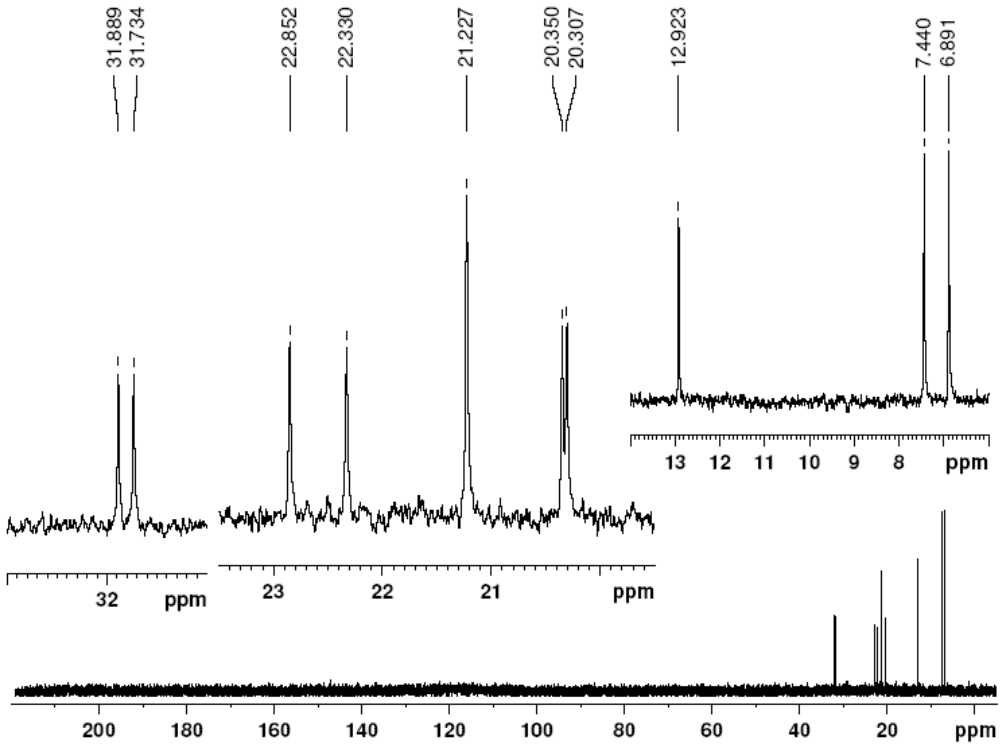

Figure S8. ^{13}C NMR spectrum (100 MHz) of trimethylpentylphosphonium bromide in D_2O.

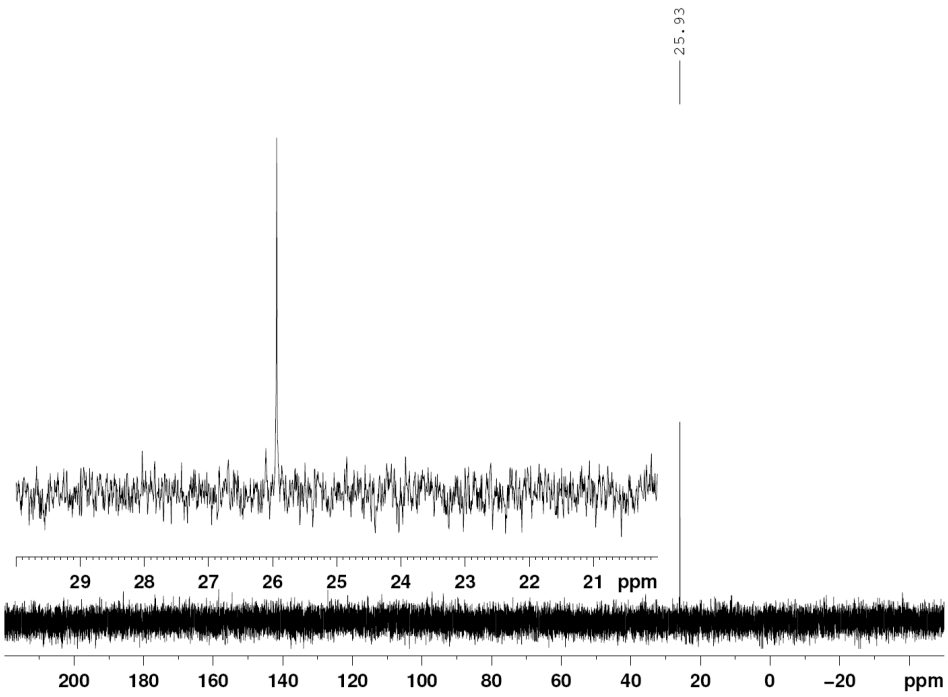

Figure S9. ^{31}P NMR spectrum (162 MHz) of trimethylpentylphosphonium bromide in D_2O.

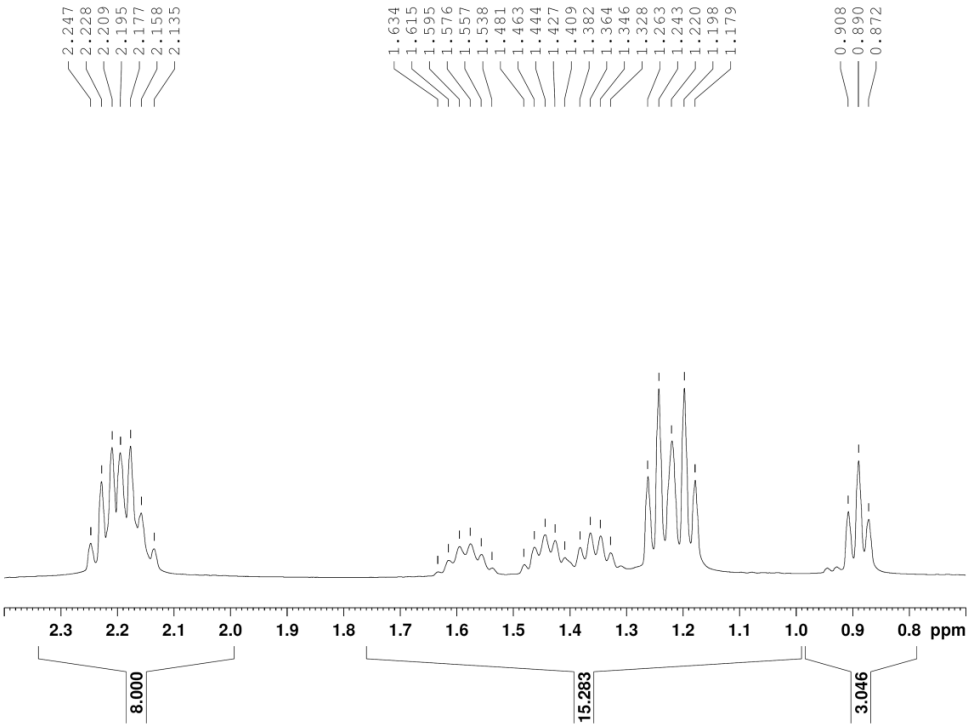

Figure S10. ^{1}H NMR spectrum (400 MHz) of triethylpentylphosphonium bromide in D_2O.

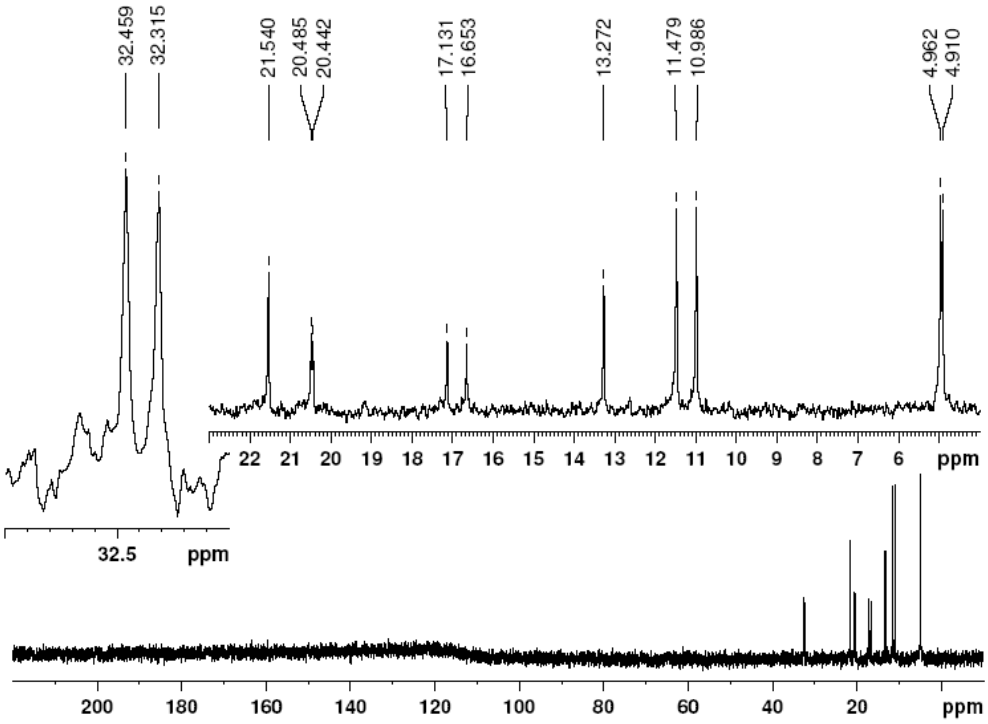

Figure S11. ^{13}C NMR spectrum (100 MHz) of triethylpentylphosphonium bromide in D_2O.

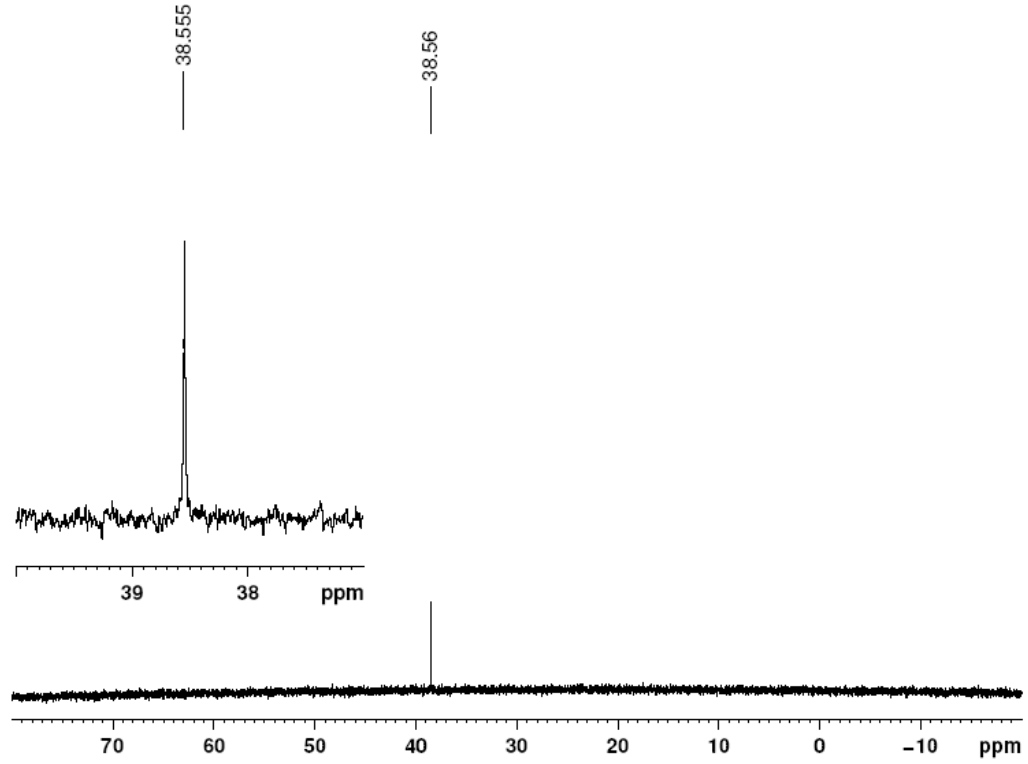

Figure S12. ^{31}P NMR spectrum (162 MHz) of triethylpentylphosphonium bromide in D_2O.

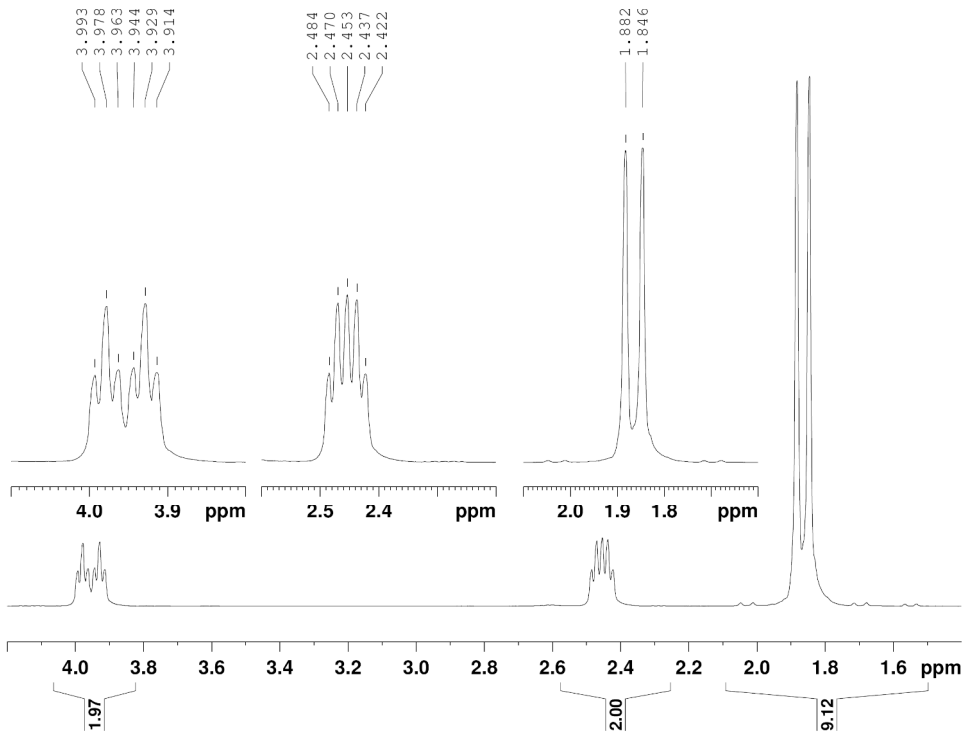

Figure S13. ^{1}H NMR spectrum (400 MHz) of (2-hydroxyethyl)trimethylphosphonium bromide in D_2O.

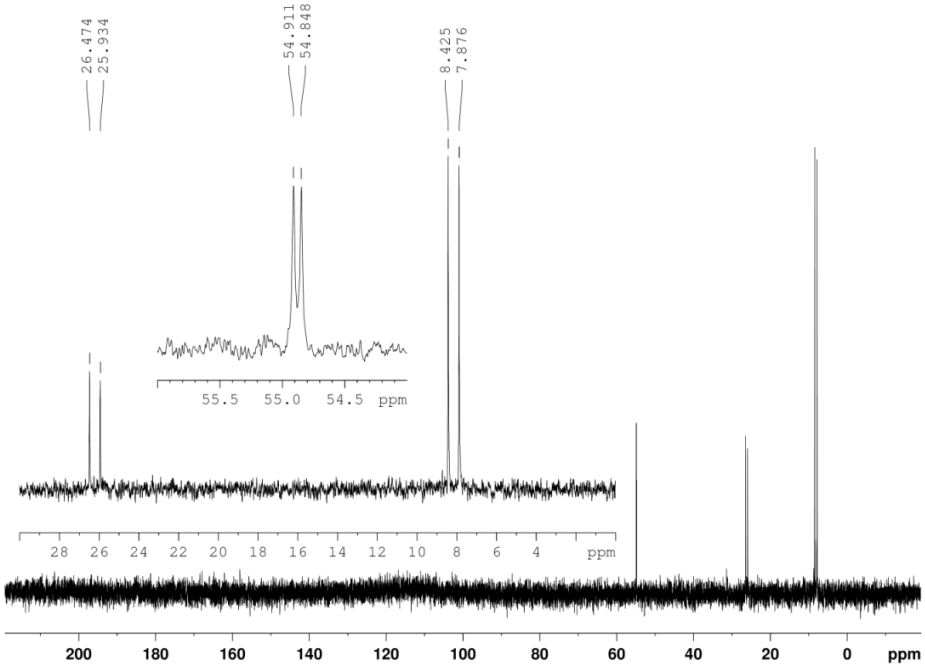

Figure S14. ^{13}C NMR spectrum (100 MHz) of (2-hydroxyethyl)trimethylphosphonium bromide in D_2O.

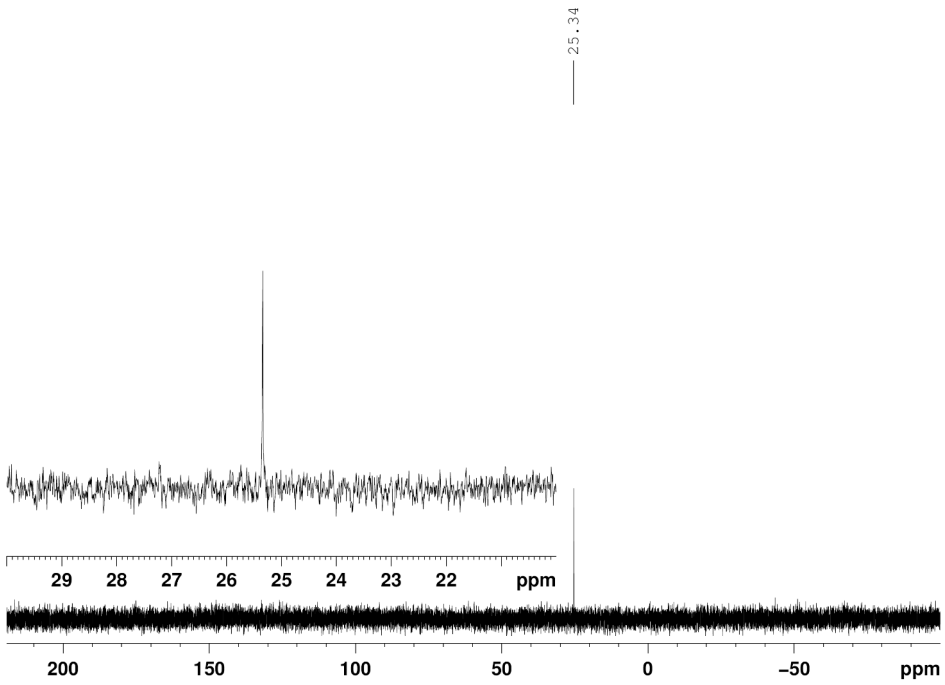

Figure S15. ^{31}P NMR spectrum (162 MHz) of (2-hydroxyethyl)trimethylphosphonium bromide in D_2O.

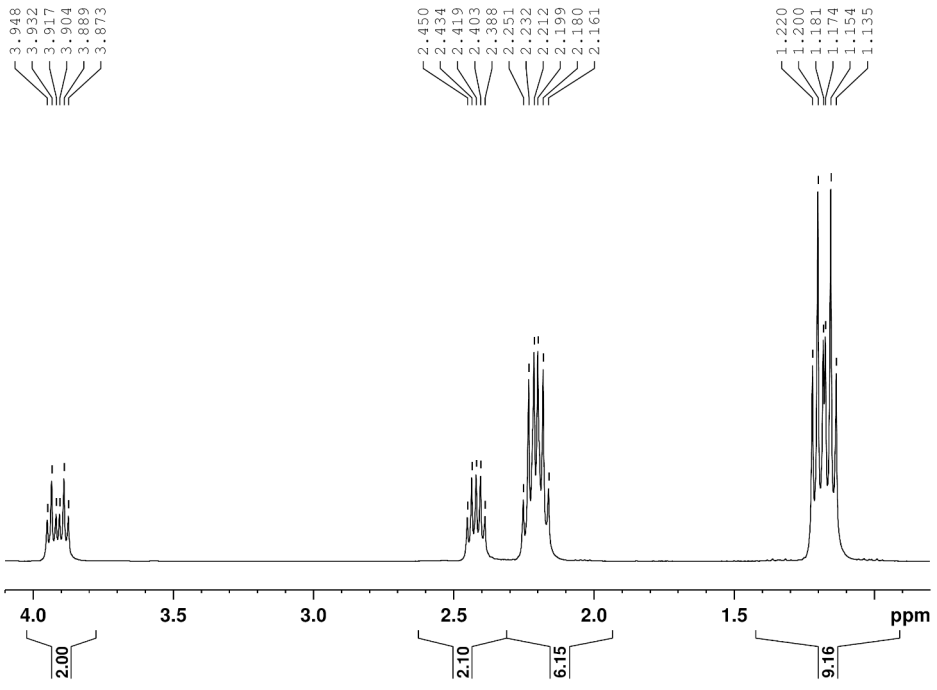

Figure S16. ^{1}H NMR spectrum (400 MHz) of (2-hydroxyethyl)triethylphosphonium bromide in D_2O.

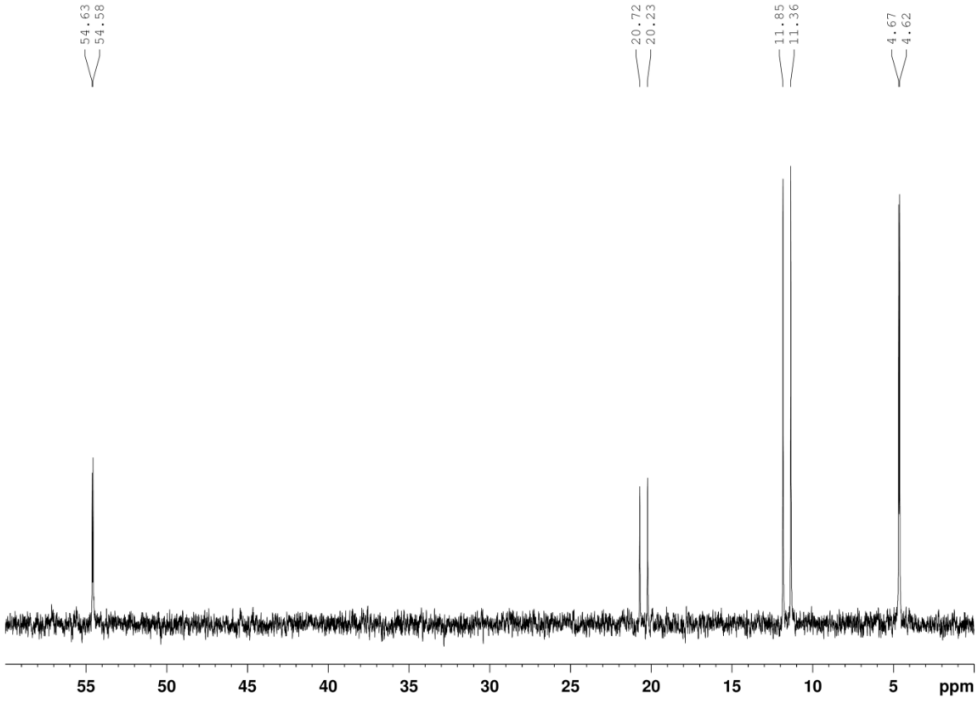

Figure S17. ^{13}C NMR spectrum (100 MHz) of (2-hydroxyethyl)triethylphosphonium bromide in D_2O.

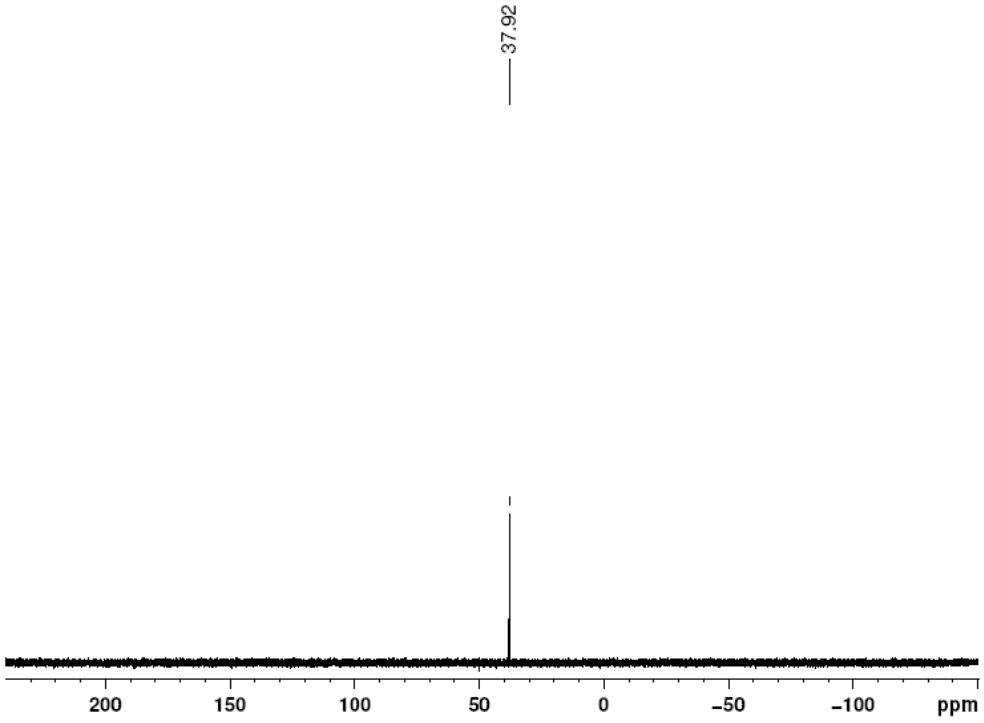

Figure S18. ^{31}P NMR spectrum (163 Mz) of (2-hydroxyethyl)triethylphosphonium bromide in D_2O.

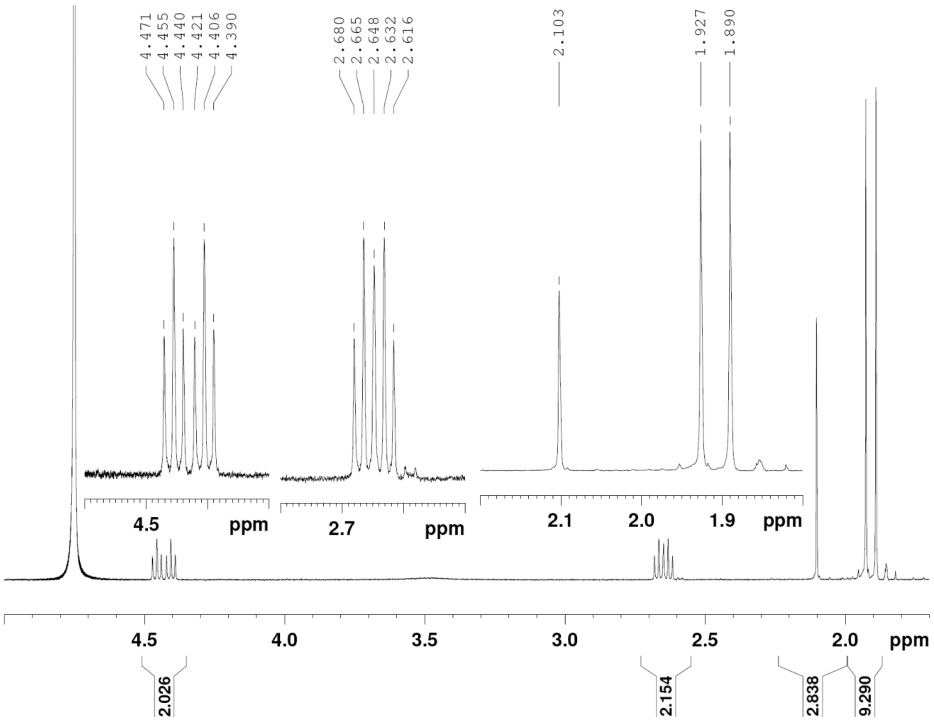

Figure S19. [1]H NMR spectrum (400 MHz) of (2-acetoxyethyl)trimethylphosphonium bromide in D_2O.

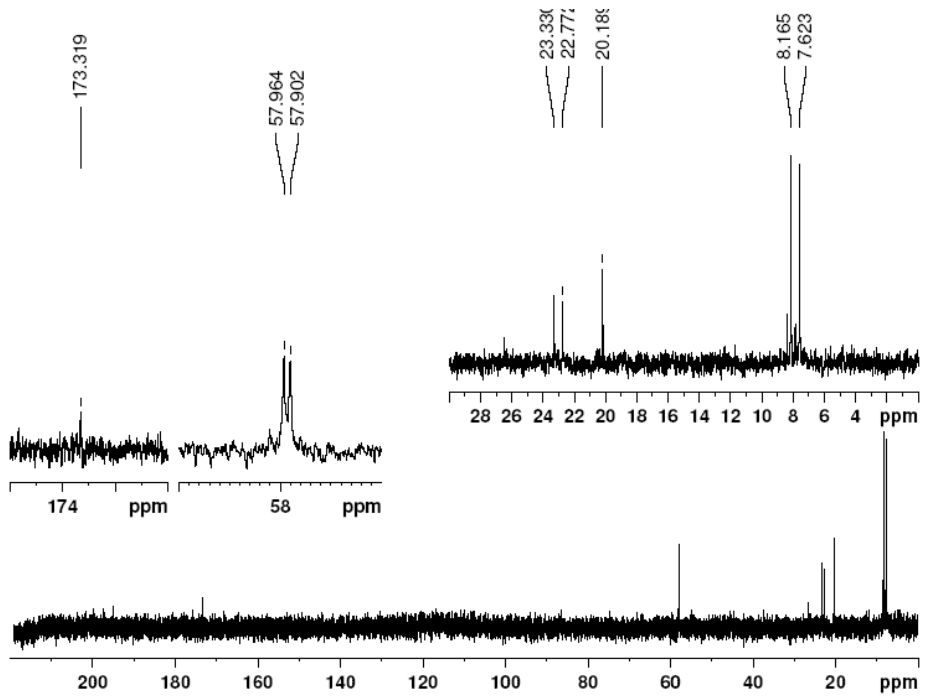

Figure S20. [13]C NMR spectrum (100 MHz) of (2-acetoxyethyl)trimethylphosphonium bromide in D_2O.

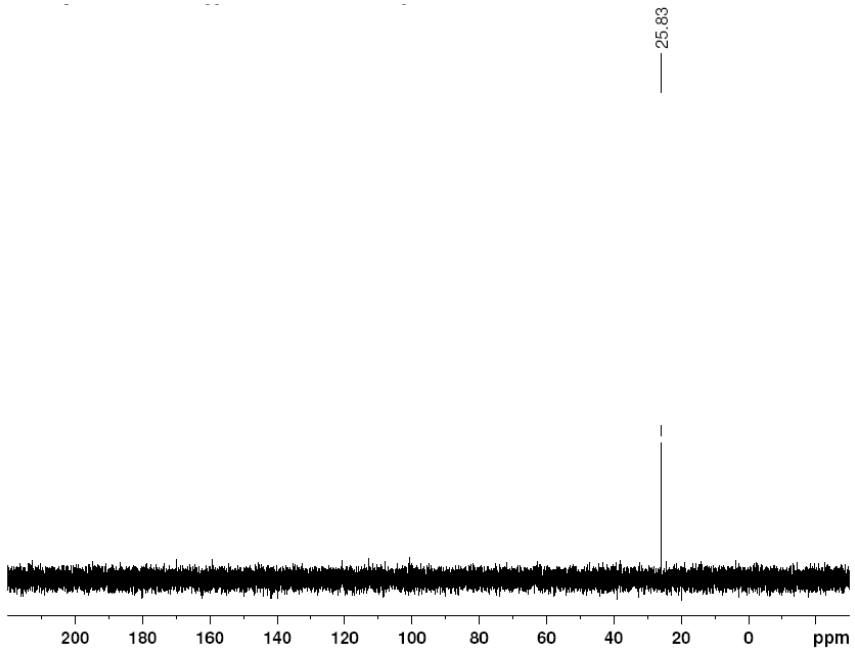

Figure S21. ^{31}P NMR spectrum (163 Mz) of (2-acetoxyethyl)trimethylphosphonium bromide in D_2O.

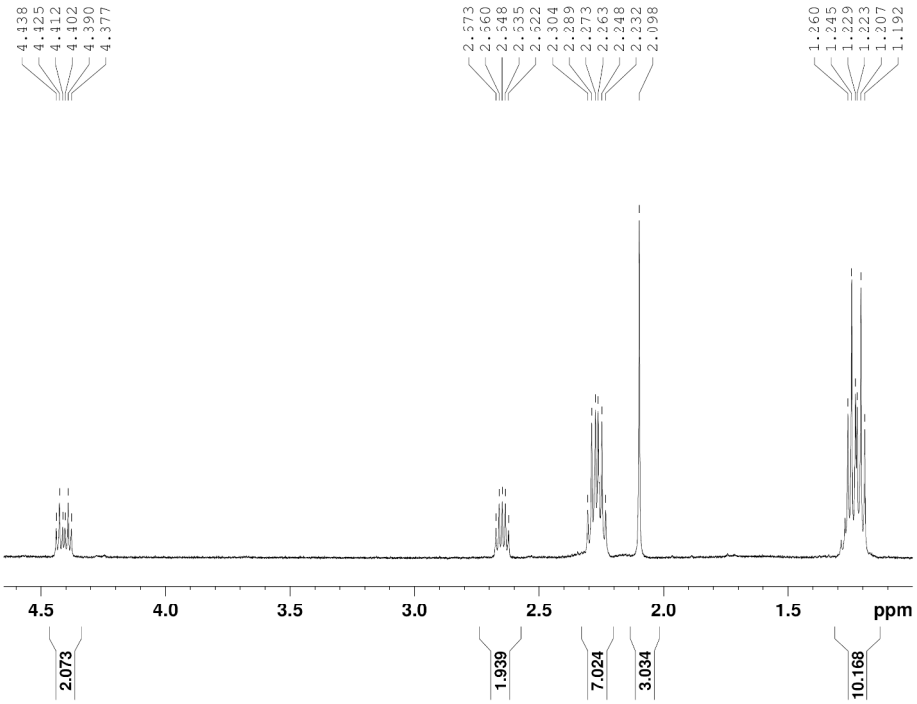

Figure S22. ^{1}H NMR spectrum (400 MHz) of (2-acetoxyethyl)triethylphosphonium bromide in D_2O.

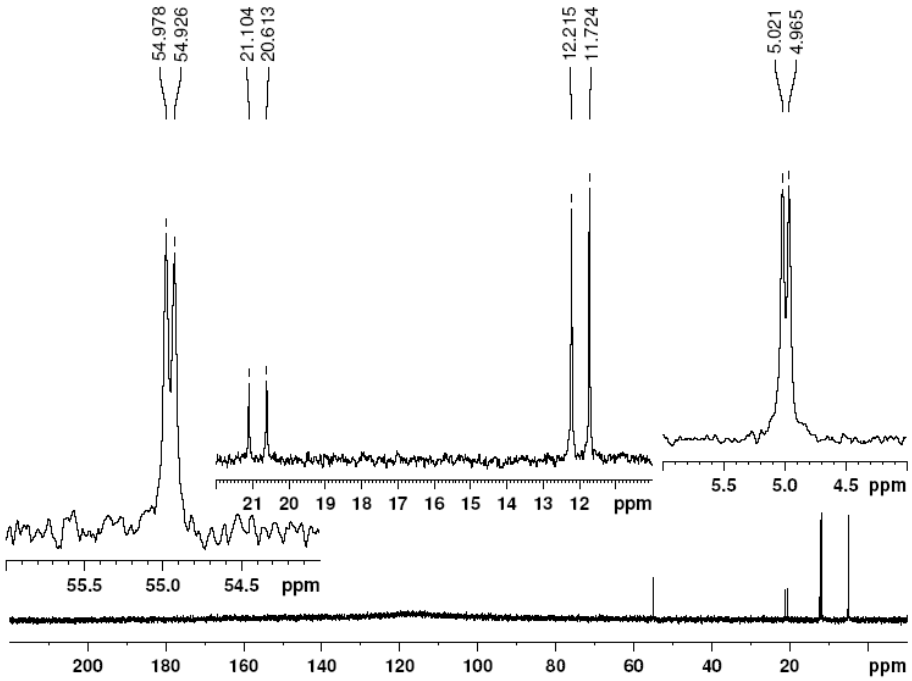

Figure S23. ^{13}C NMR spectrum (100 MHz) of (2-acetoxyethyl)triethylphosphonium bromide in D_2O.

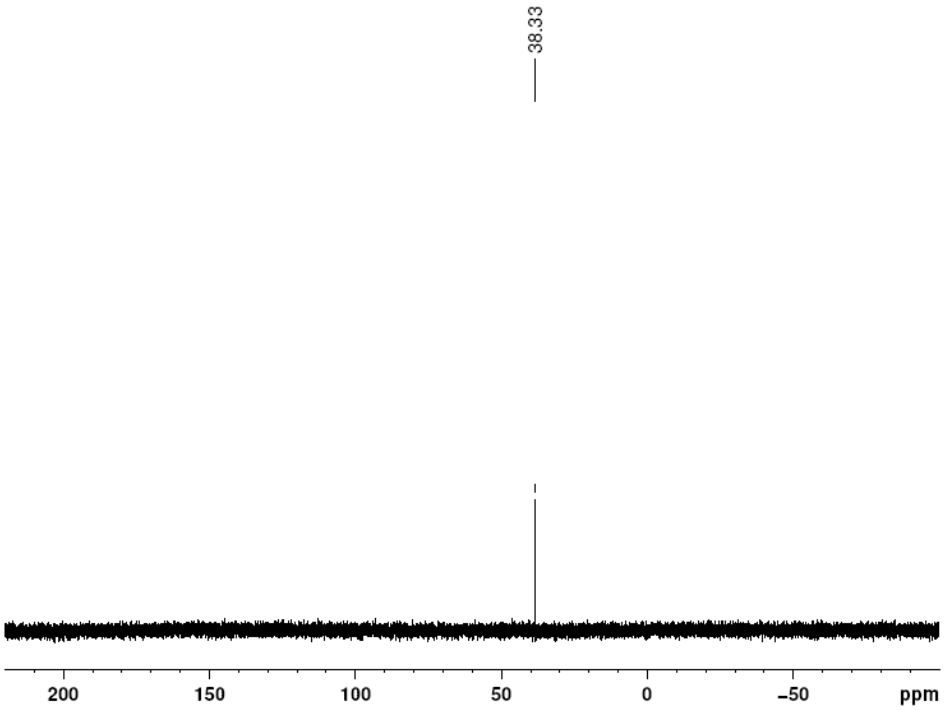

Figure S24. ^{31}P NMR spectrum (162 MHz) of (2-acetoxyethyl)triethylphosphonium bromide in D_2O.

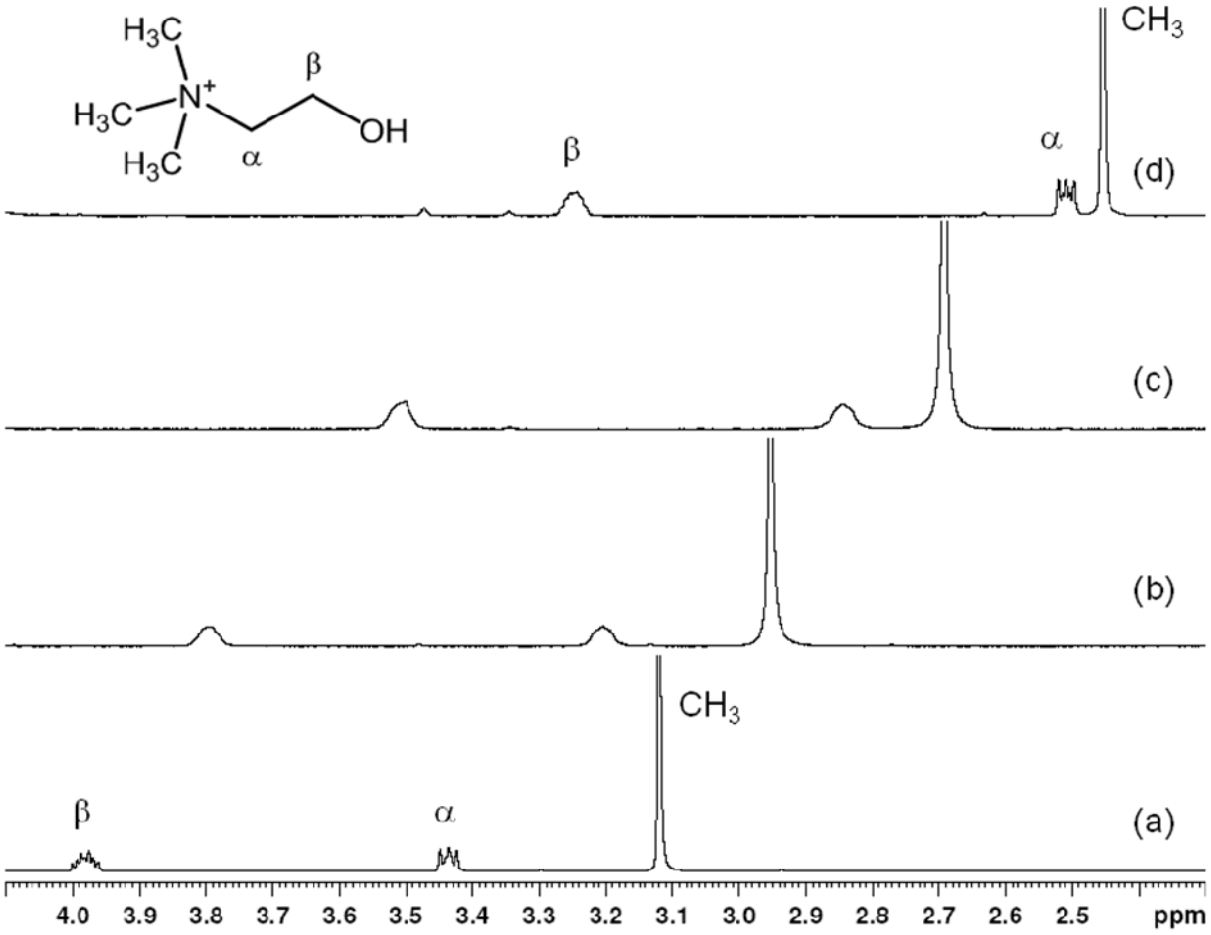

Figure S25. ^{1}H NMR spectra of choline (1.44 mmol dm^{-3}) in the (a) absence of CB[7] and the presence of (b) 0.25 equiv, (c) 0.65 equiv, and (d) 1.41 equiv of CB[7] in D_2O.

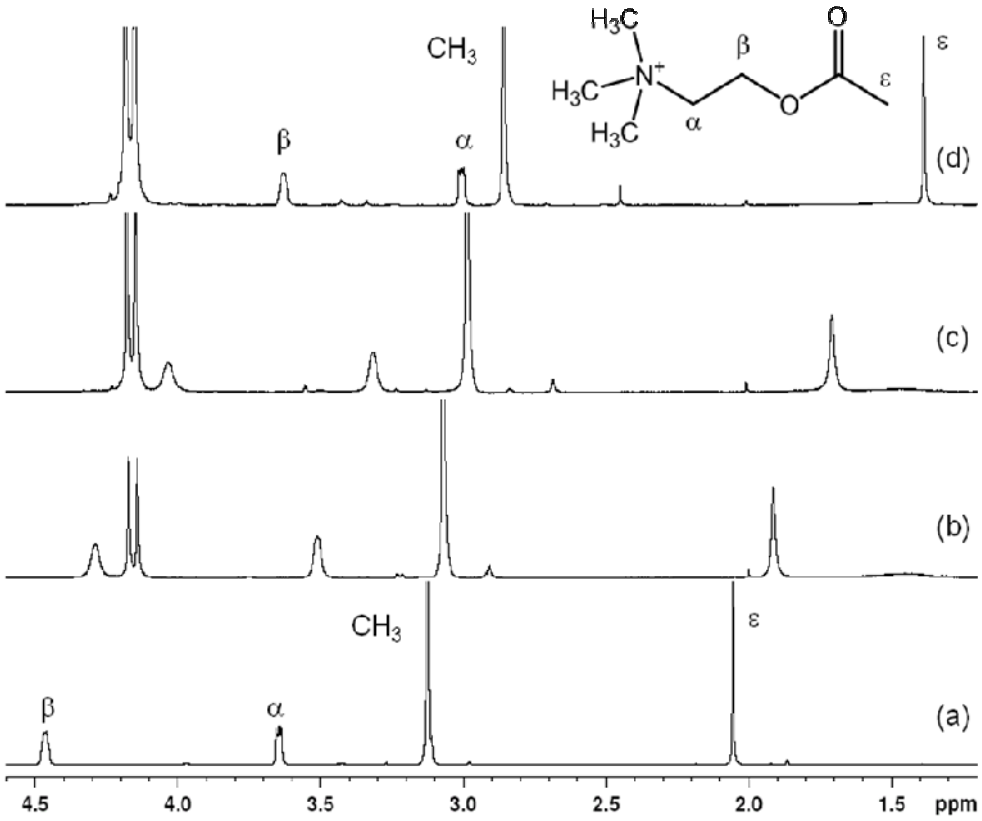

Figure S26. ^{1}H NMR spectra of acetylcholine (2.46 mmol dm^{-3}) in the (a) absence of CB[7] and the presence of (b) 0.23 equiv, (c) 0.56 equiv and (d) 1.43 equiv of CB[7] in D_2O.

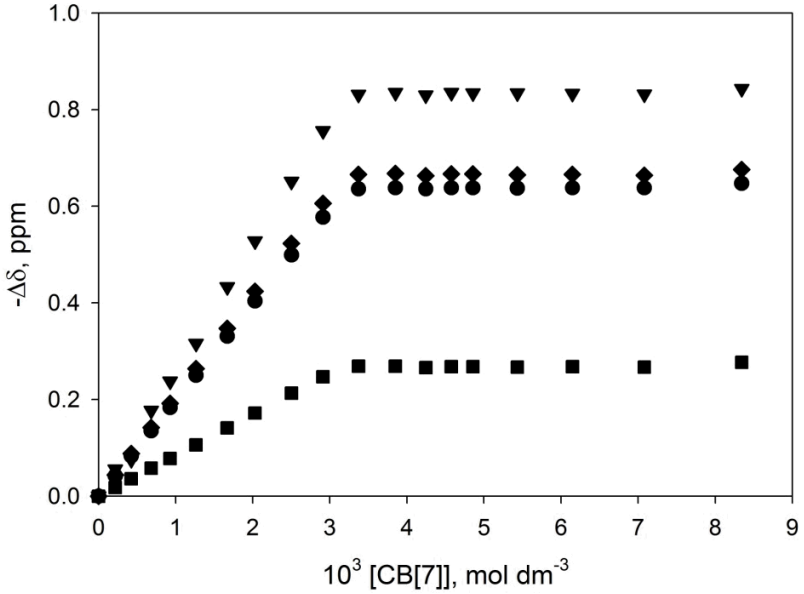

Figure S27. ^{1}H NMR titration of of acetylcholine with CB[7] in D_2O: (■) CH_3, (●) Hα (♦) Hε and (▼) Hβ.

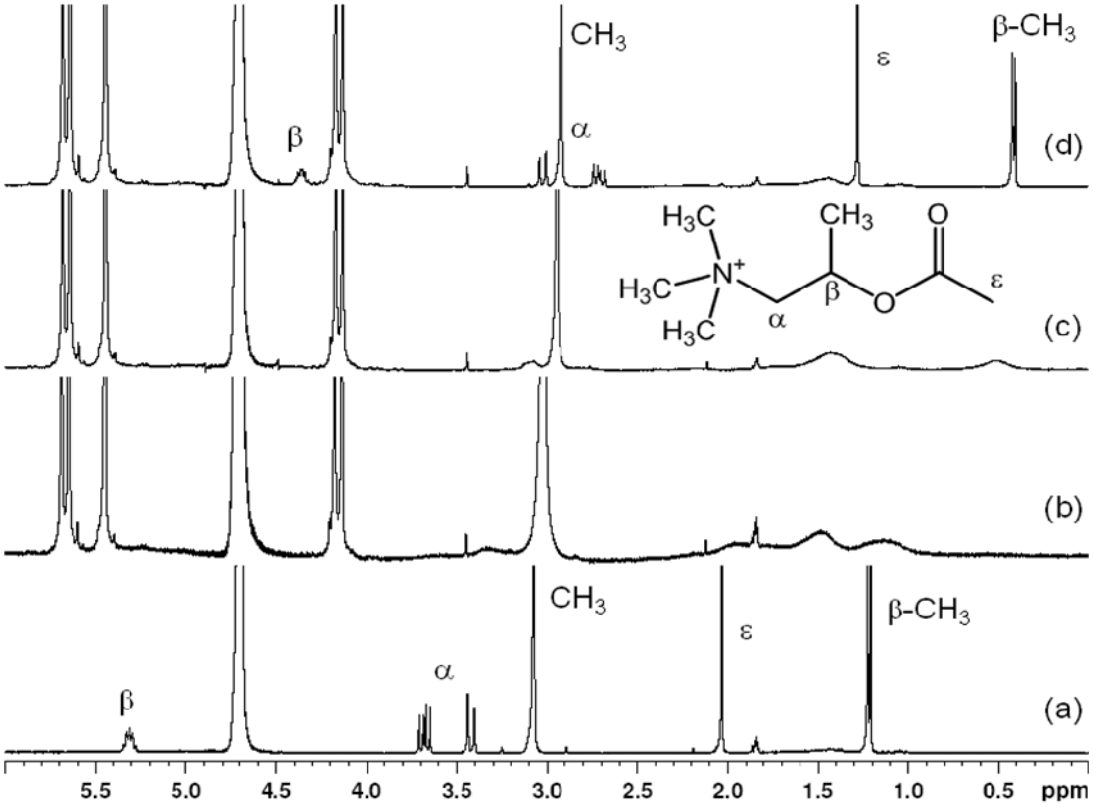

Figure S28. ^{1}H NMR spectra of β-methylacetylcholine (2.06 mmol dm^{-3}) in the (a) absence of CB[7] and the presence of (b) 0.40 equiv, (c) 1.08 equiv, and (d) 1.30 equiv of CB[7] in D_2O.

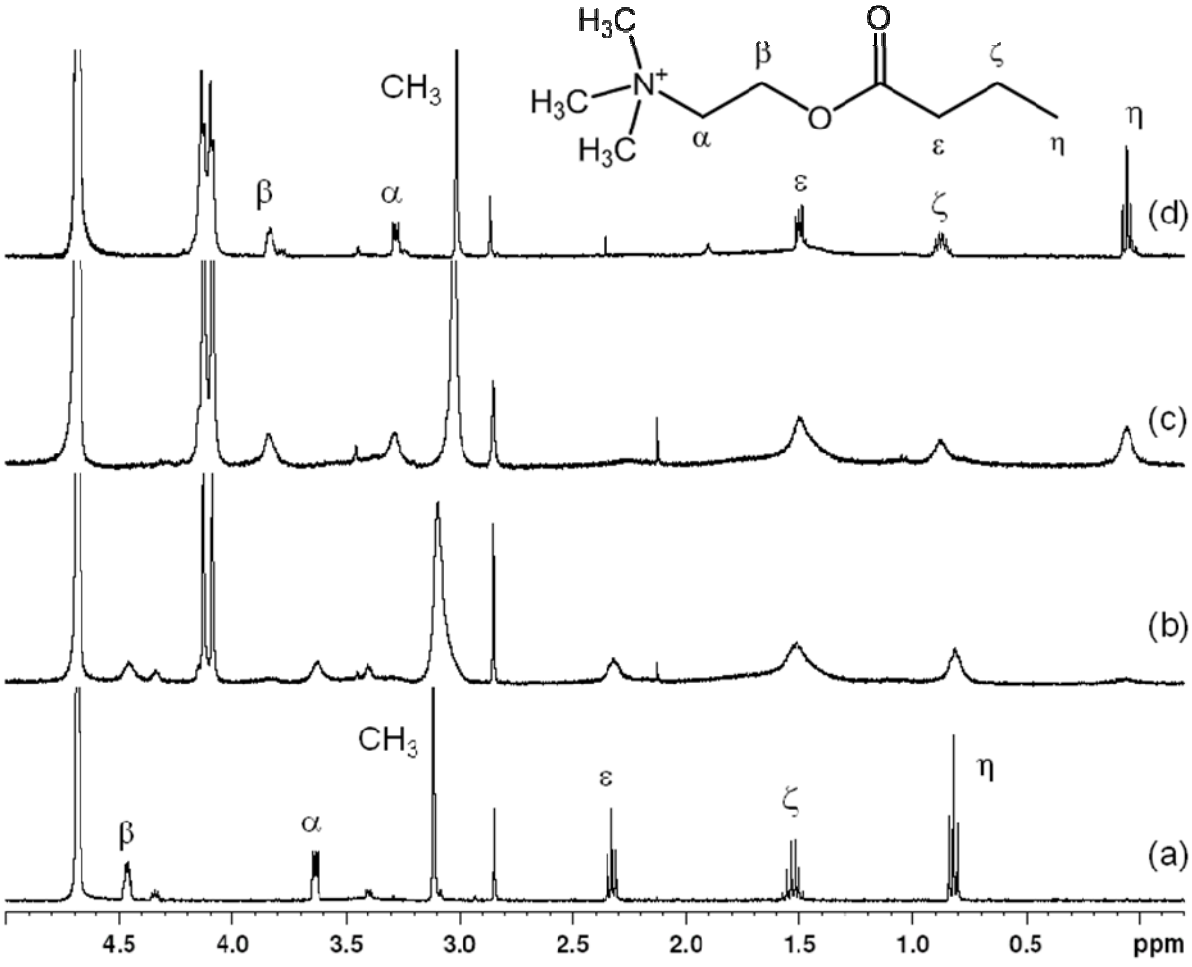

Figure S29. ^{1}H NMR spectra of butyrylcholine (1.51 mmol dm^{-3}) in the (a) absence of CB[7] and the presence of (b) 0.32 equiv, (c) 0.91 equiv, and (d) 1.68 equiv of CB[7] in D_2O.

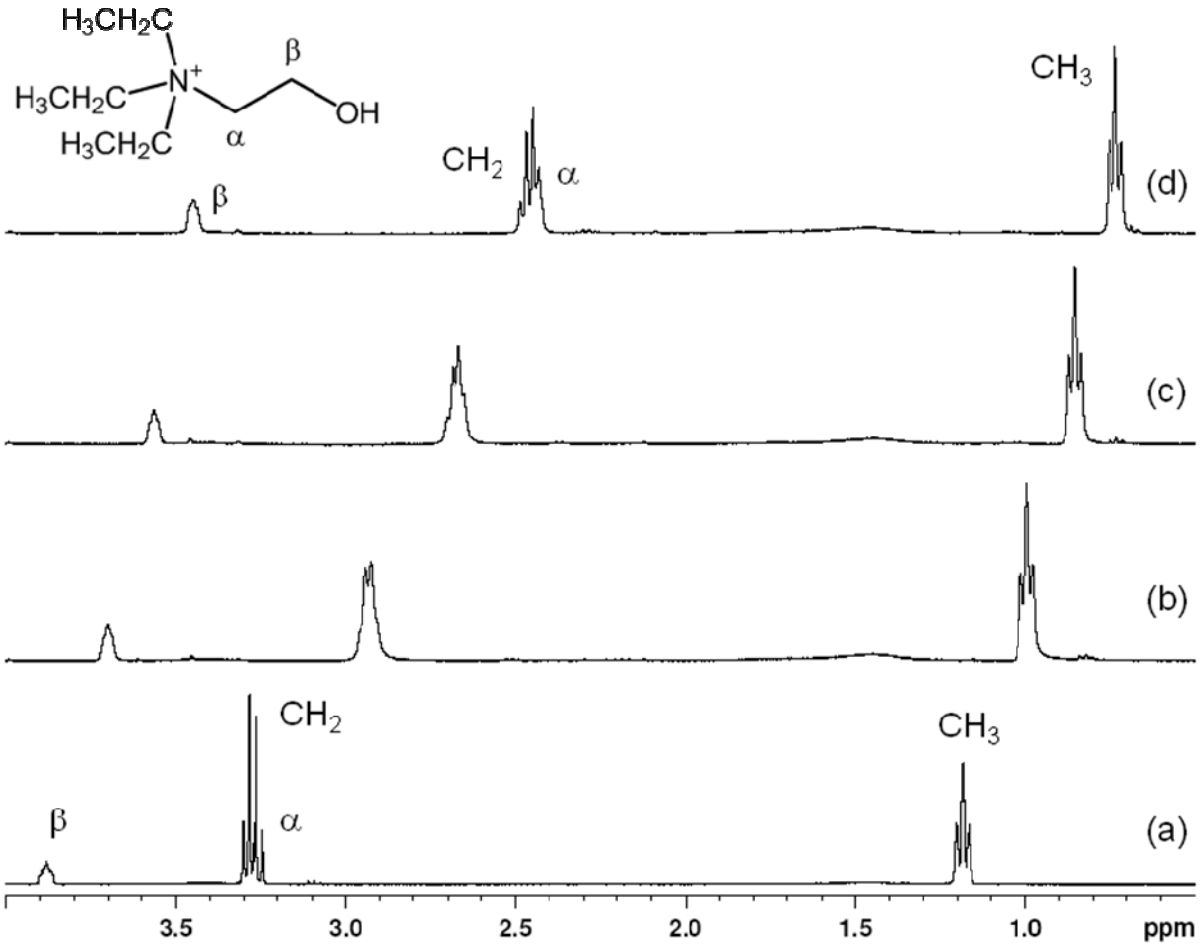

Figure S30. ^{1}H NMR spectra of (2-hydroxyethyl)triethylammonium bromide (1.49 mmol dm-3) in the (a) absence of CB[7] and the presence of (b) 0.31 equiv, (c) 0.76 equiv, and (d) 1.06 equiv of CB[7] in D_2O.

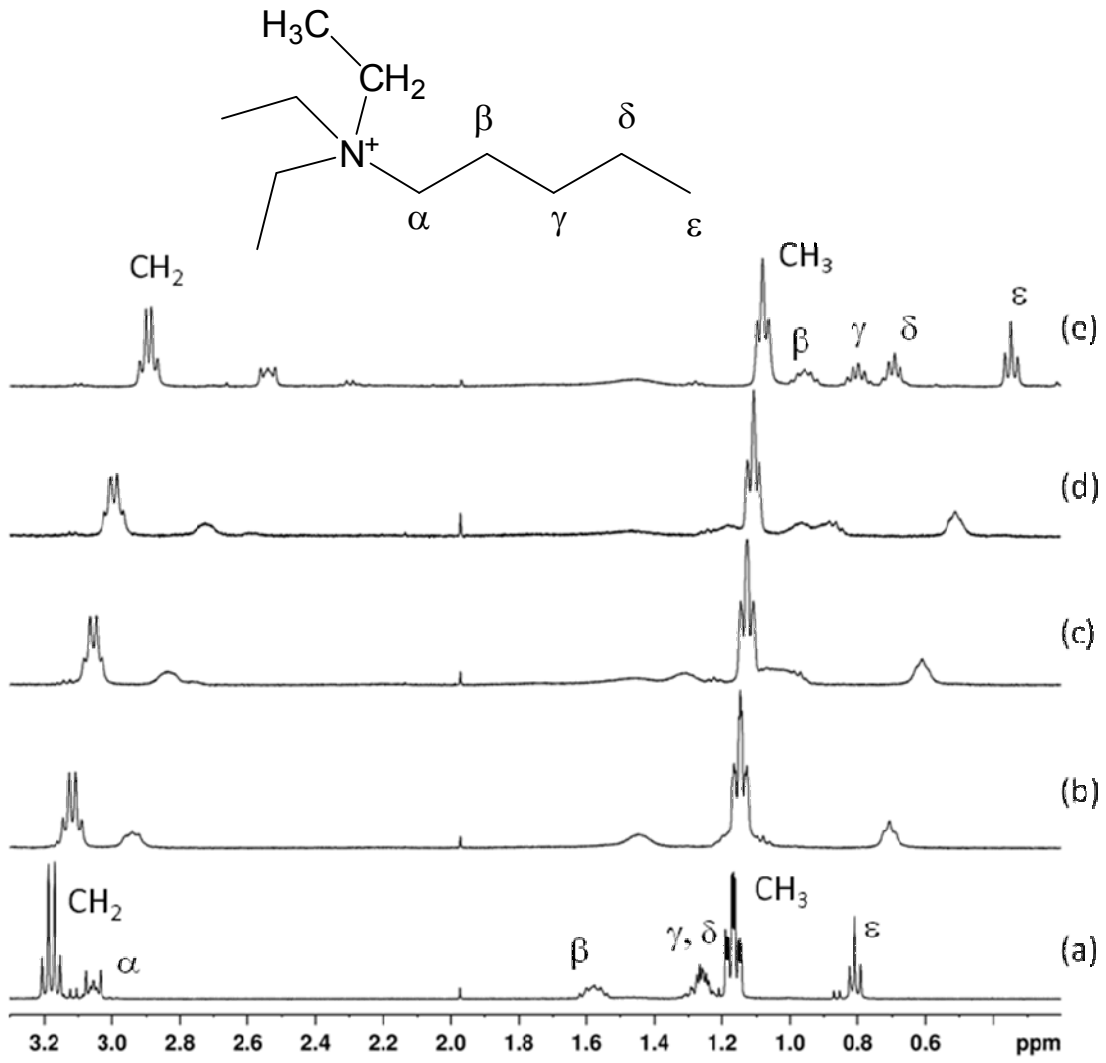

Figure S31. ^{1}H NMR spectra of triethylpentylammonium chloride (mmol dm^{-3}) in the (a) absence of CB[7] and the presence of (b) 0.26 equiv, (c) 0.52 equiv, (d) 0.76 equiv, and 1.44 equiv of CB[7] in D_2O.

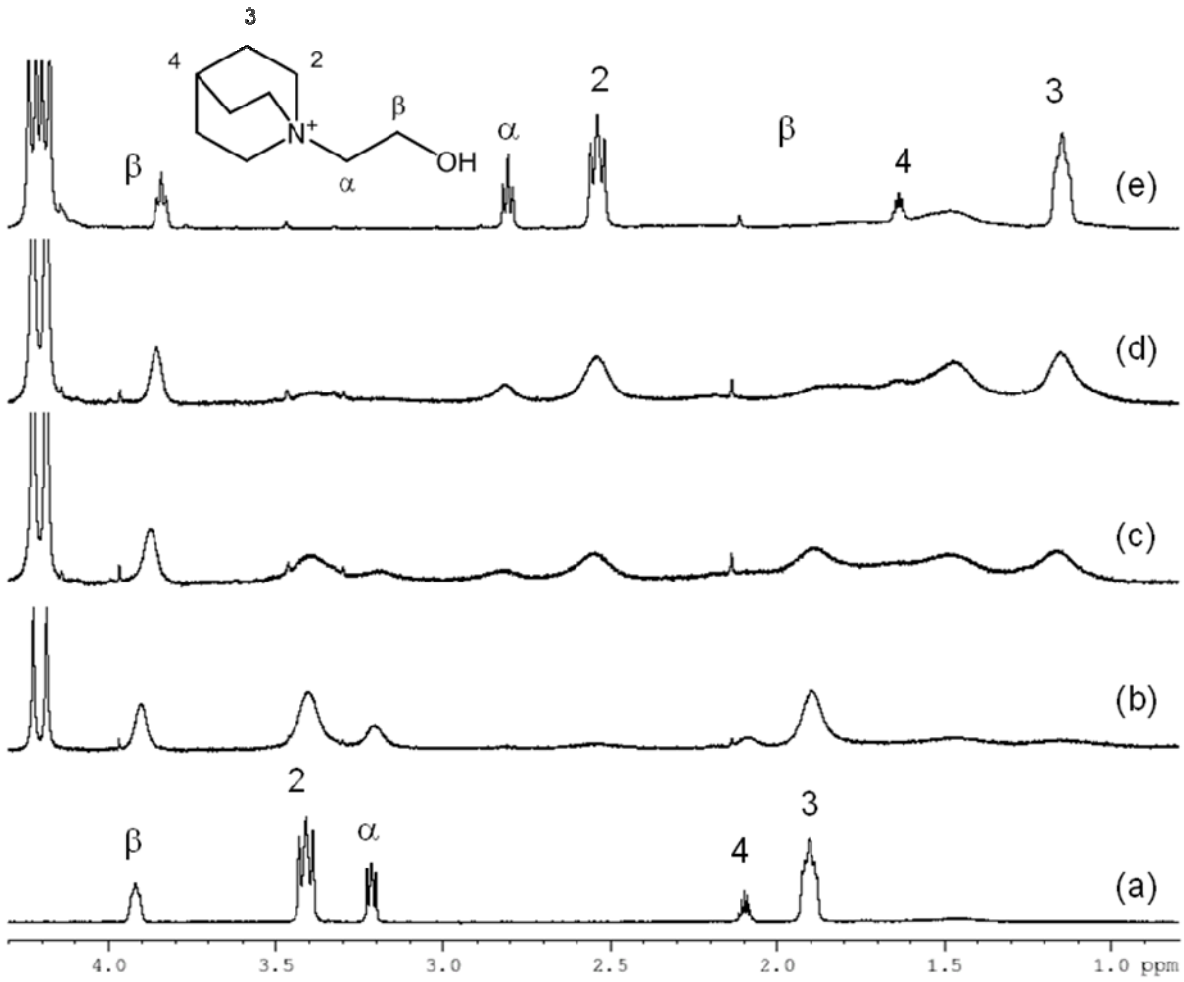

Figure S32. ^{1}H NMR spectra of (2-hydroxyethyl)quinuclidinium bromide (1.08 mmol dm^{-3}) in the (a) absence of CB[7] and the presence of (b) 0.22 equiv, (c) 0.53 equiv, (d) 0.71 equiv, and (e) 1.13 equiv of CB[7] in D_2O.

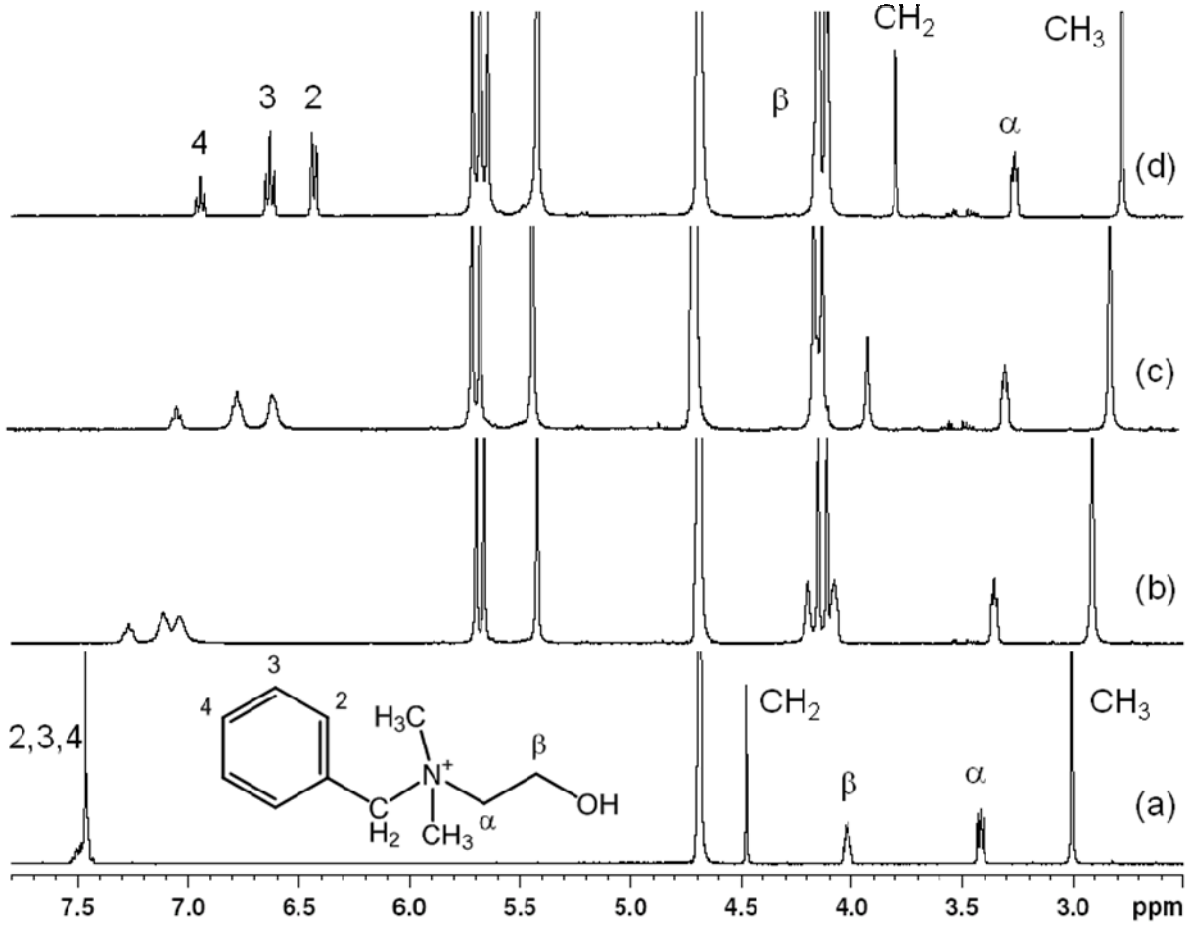

Figure S33. ^{1}H NMR spectra of (2-hydroxyethyl)benzyldimethylammonium bromide (1.90 mmol dm^{-3}) in the (a) absence of CB[7] and the presence of (b) 0.44 equiv, (c) 0.88 equiv, and (d) 1.11 equiv of CB[7] in D_2O.

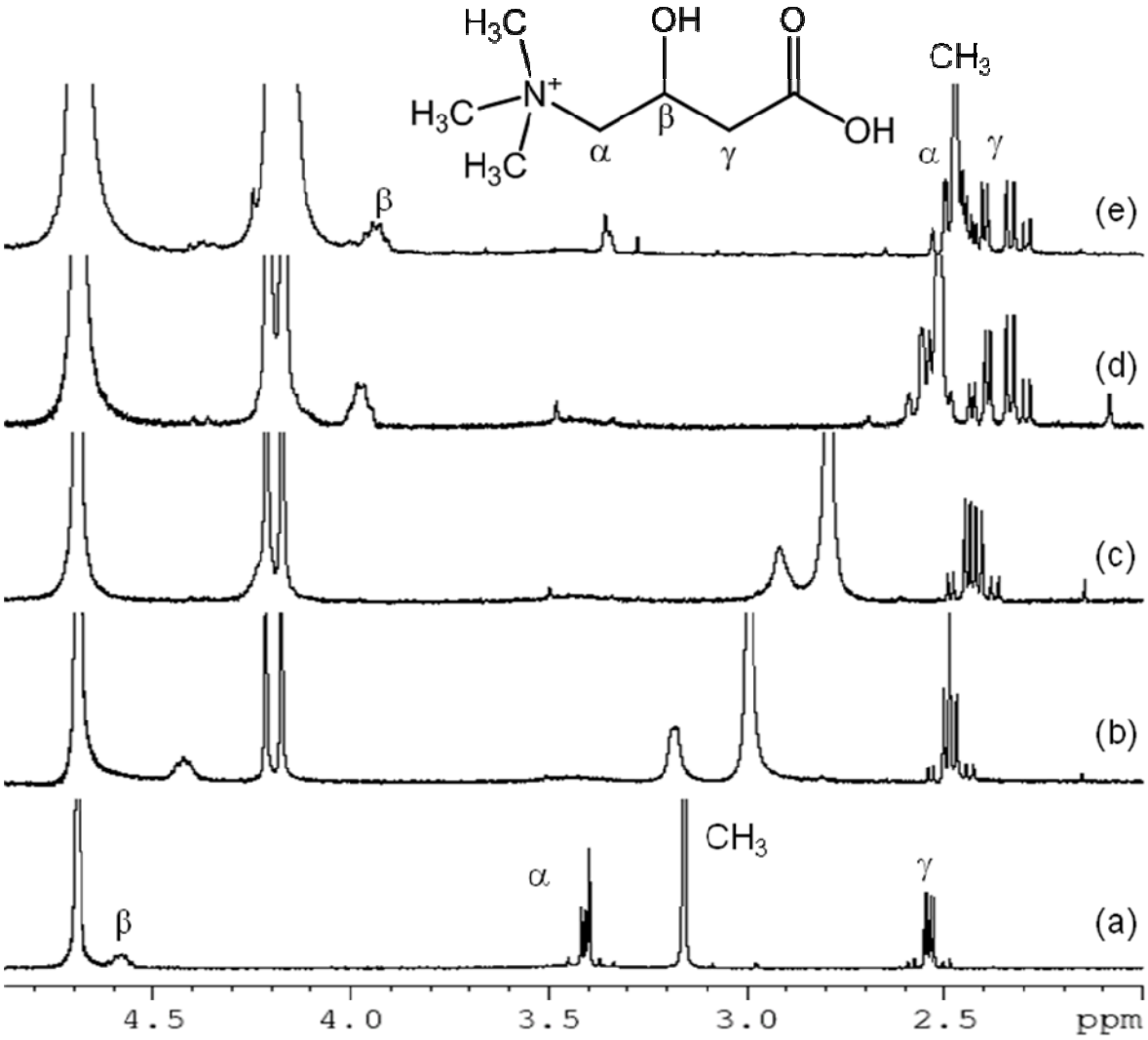

Figure S34. ^{1}H NMR spectra of carnitine (1.53 mmol dm^{-3}) in the (a) absence of CB[7] and the presence of (b) 0.25 equiv, (c) 0.56 equiv, (d) 1.06 equiv, and (e) 4.26 equiv of CB[7] in D_2O.

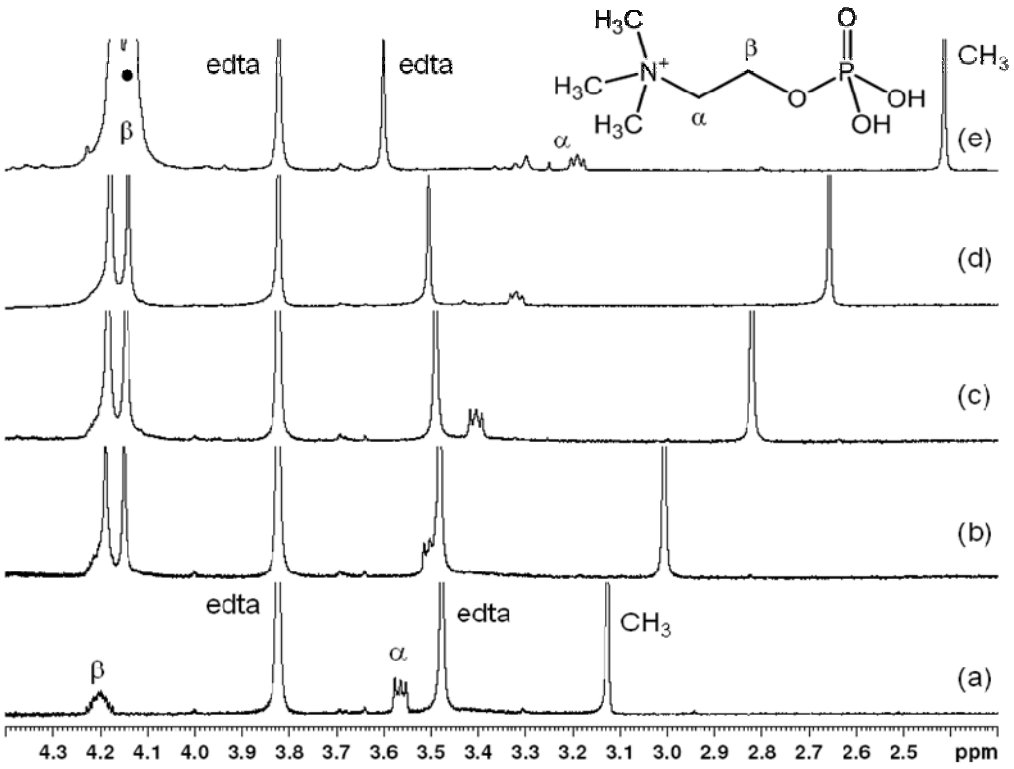

Figure S35. ^{1}H NMR spectra of calcium choline phosphate (0.542 mmol dm^{-3}) in the (a) absence of CB[7] and the presence of (b) 0.65 equiv, (c) 1.61 equiv, (d) 2.72 equiv, and (e) 12.87 equiv of CB[7] in D_2O containing 1.12 mmol dm^{-3} edta^{4-}. The β protons are overlapped by CH_2 protons of CB[7] (●).

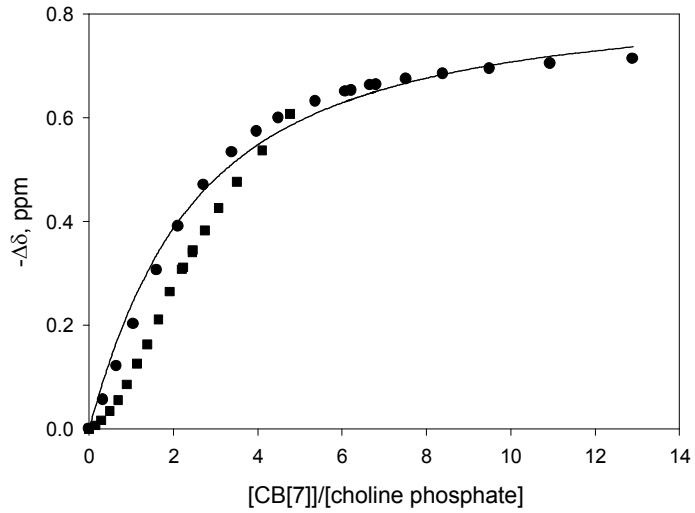

Figure S36. ^{1}H NMR chemical shift titrations of calcium choline phosphate with CB[7] in D_2O; (■) in the absence of $edta^{4-}$ and (●) 2.1 equiv $edta^{4-}$.

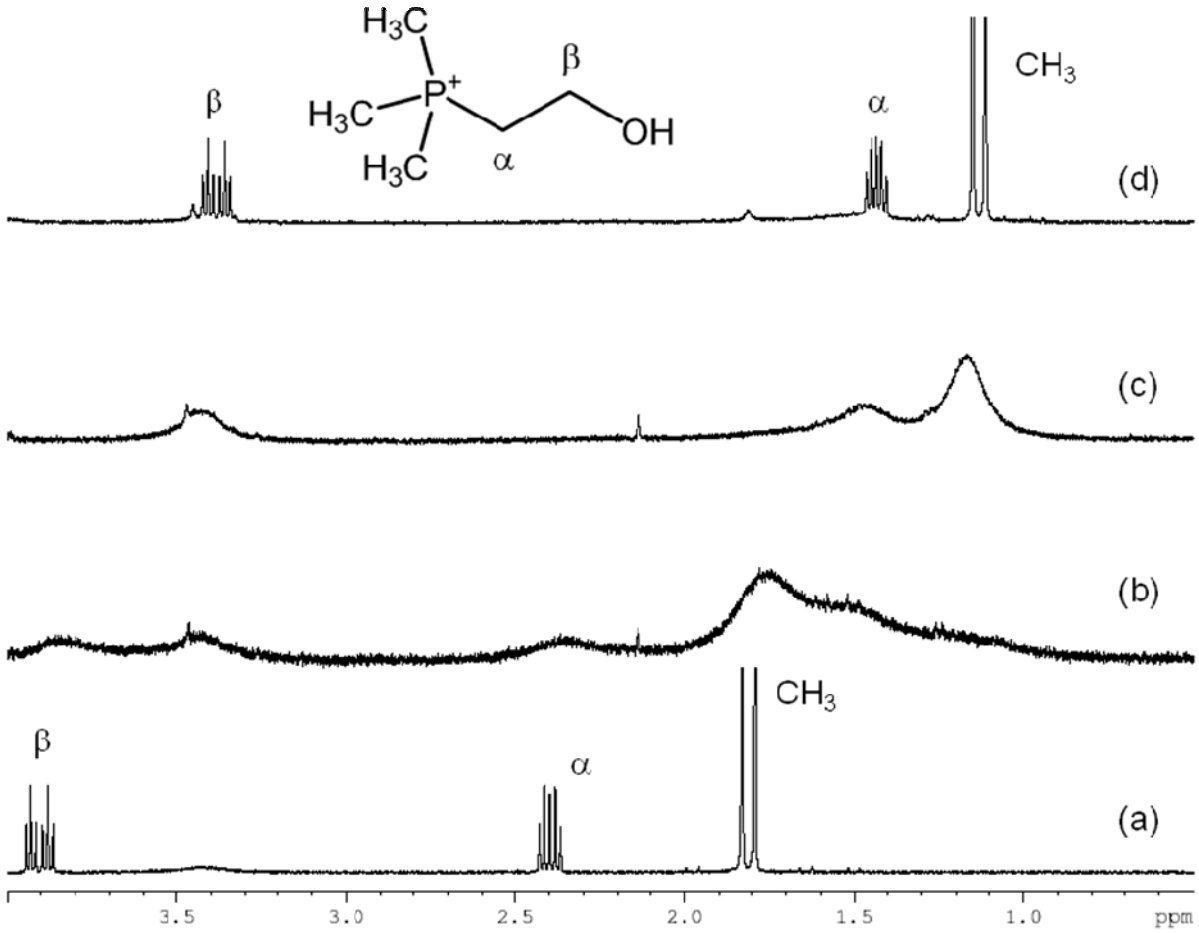

Figure S37. ^{1}H NMR spectra of (2-hydroxyethyl)trimethylphosphonium bromide (1.50 mmol dm^{-3}) in the (a) absence of CB[7] and the presence of (b) 0.29 equiv, (c) 0.74 equiv, and (d) 1.30 equiv of CB[7] in D_2O.

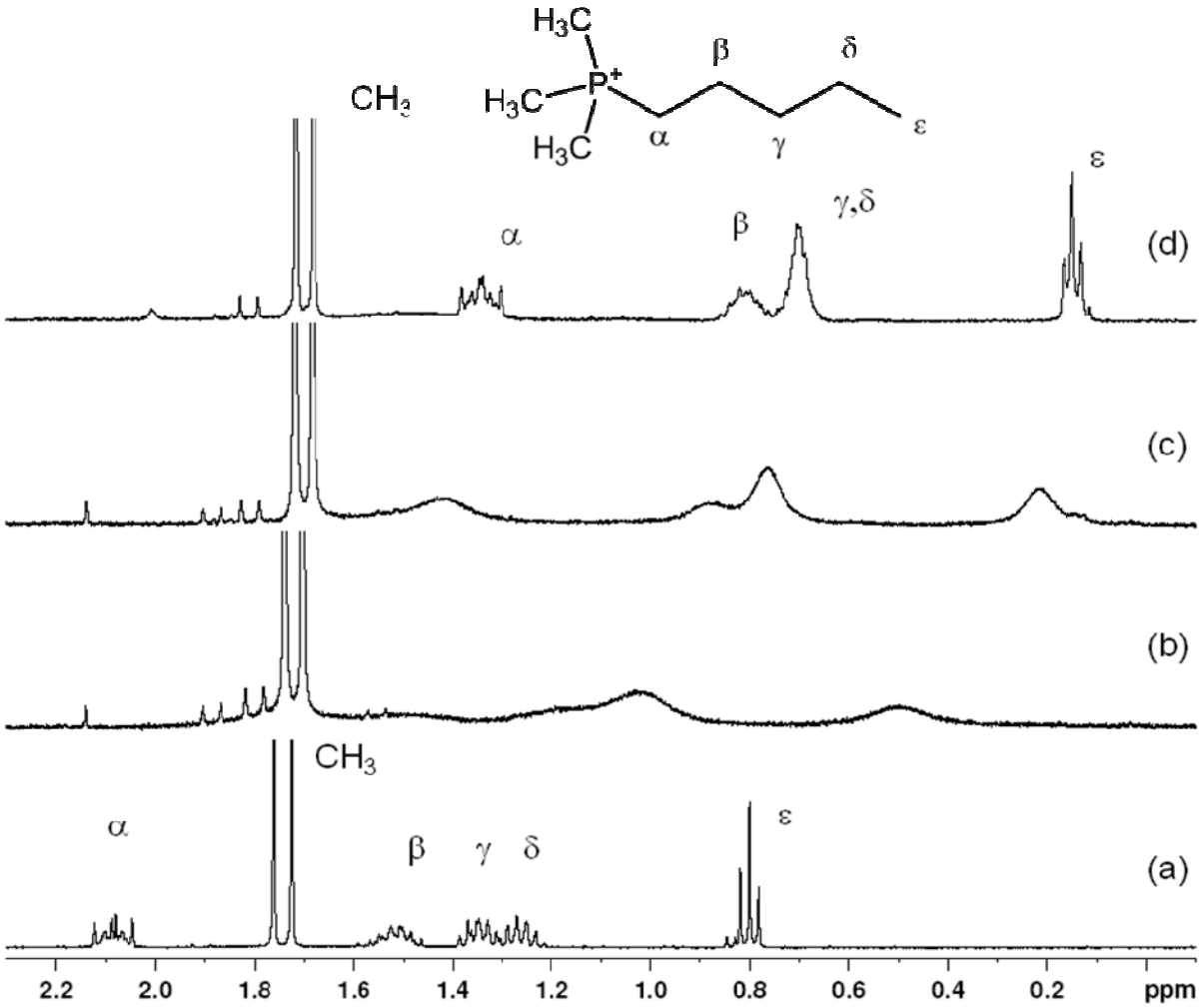

Figure S38. ^{1}H NMR spectra of trimethylpentylphosphonium (1.52 mmol dm^{-3}) in the (a) absence of CB[7] and the presence of (b) 0.54 equiv, (c) 0.99 equiv, and (d) 1.37 equiv of CB[7] in D_2O.

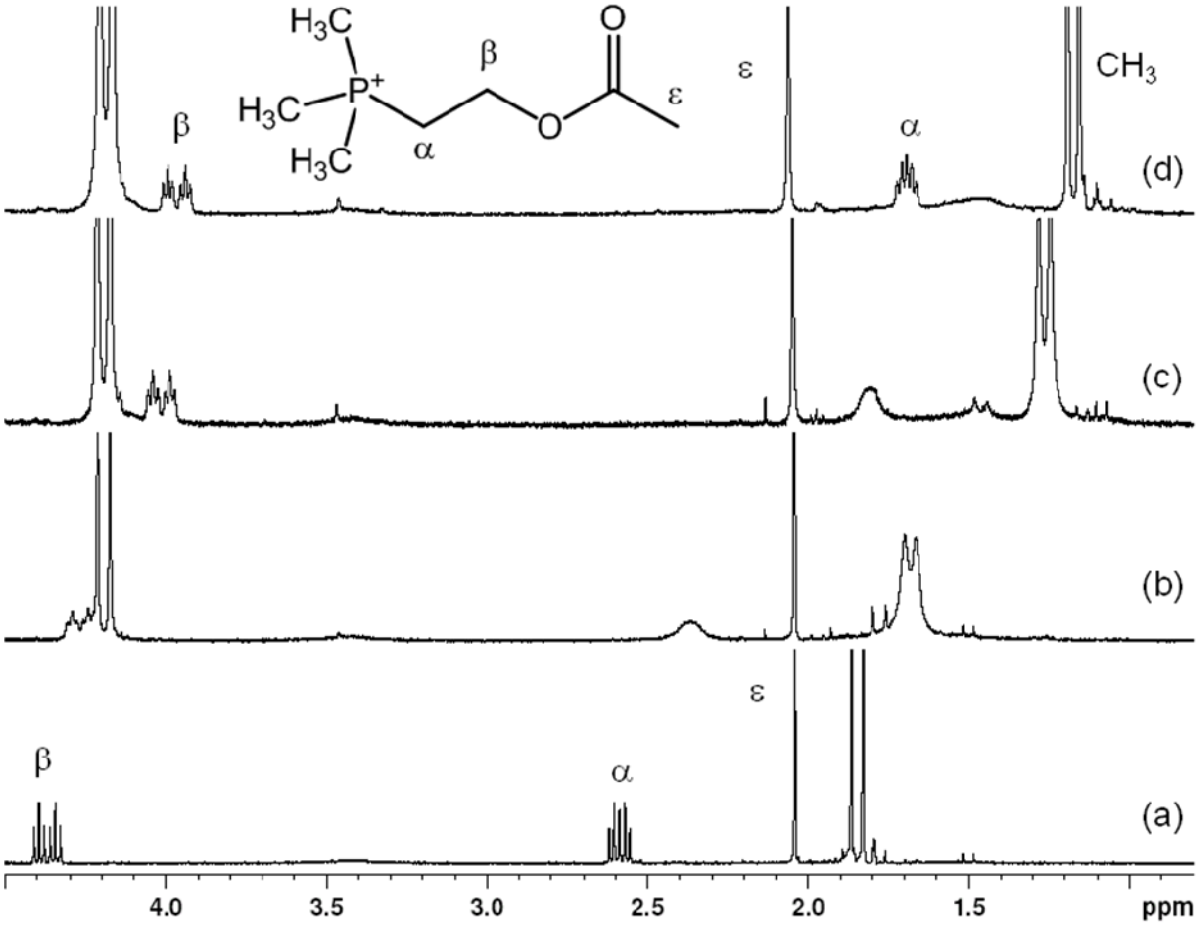

Figure S39. ^{1}H NMR spectra of (2-acetoxyethyl)trimethylphosphophonium bromide (1.52 mmol dm^{-3}) in the (a) absence of CB[7] and the presence of (b) 0.41 equiv, (c) 1.18 equiv, and (d) 1.75 equiv of CB[7] in D_2O.

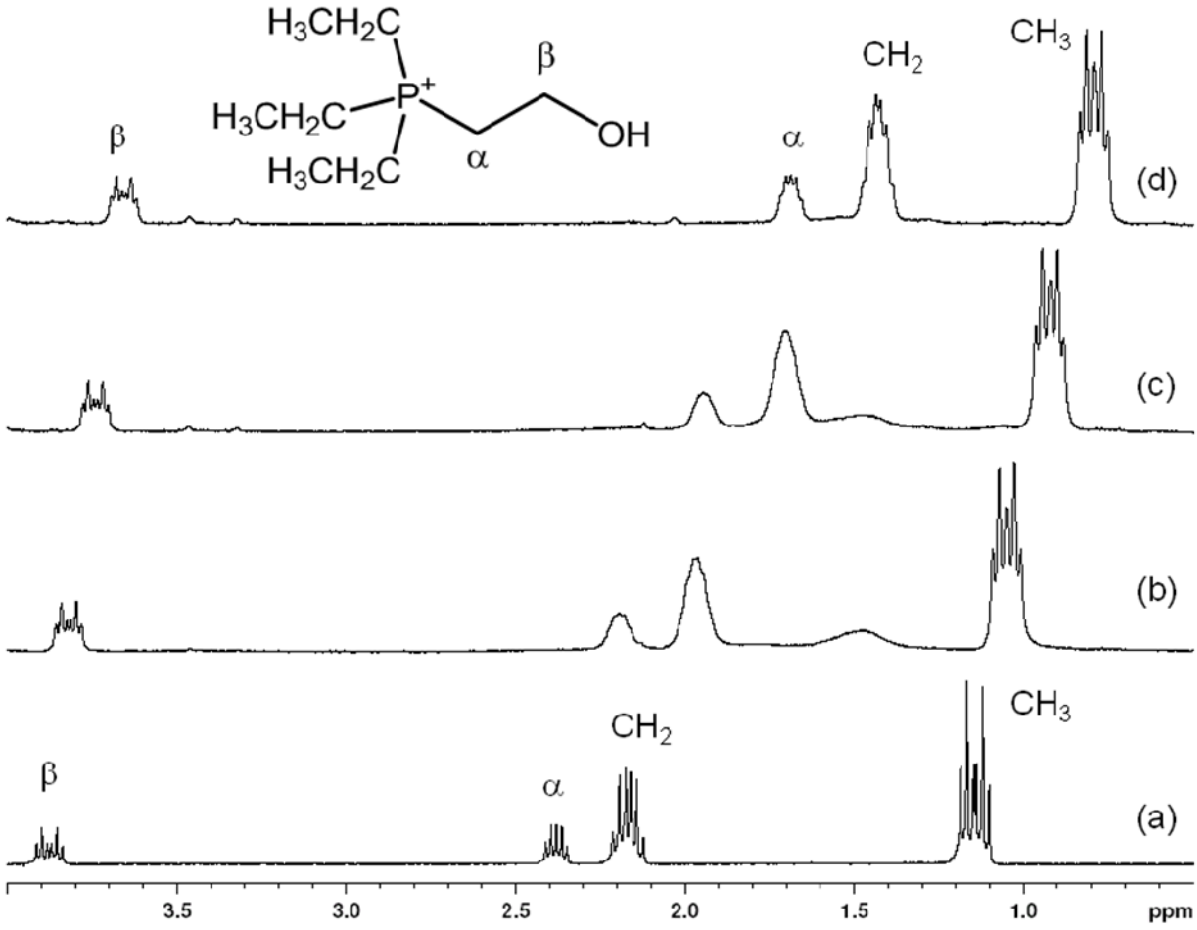

Figure S40. ^{1}H NMR spectra of (2-hydroxyethyl)triethylphosphophonium bromide (1.54 mmol dm^{-3}) in the (a) absence of CB[7] and the presence of (b) 0.30 equiv, (c) 0.70 equiv, and (d) 1.21 equiv of CB[7] in D_2O.

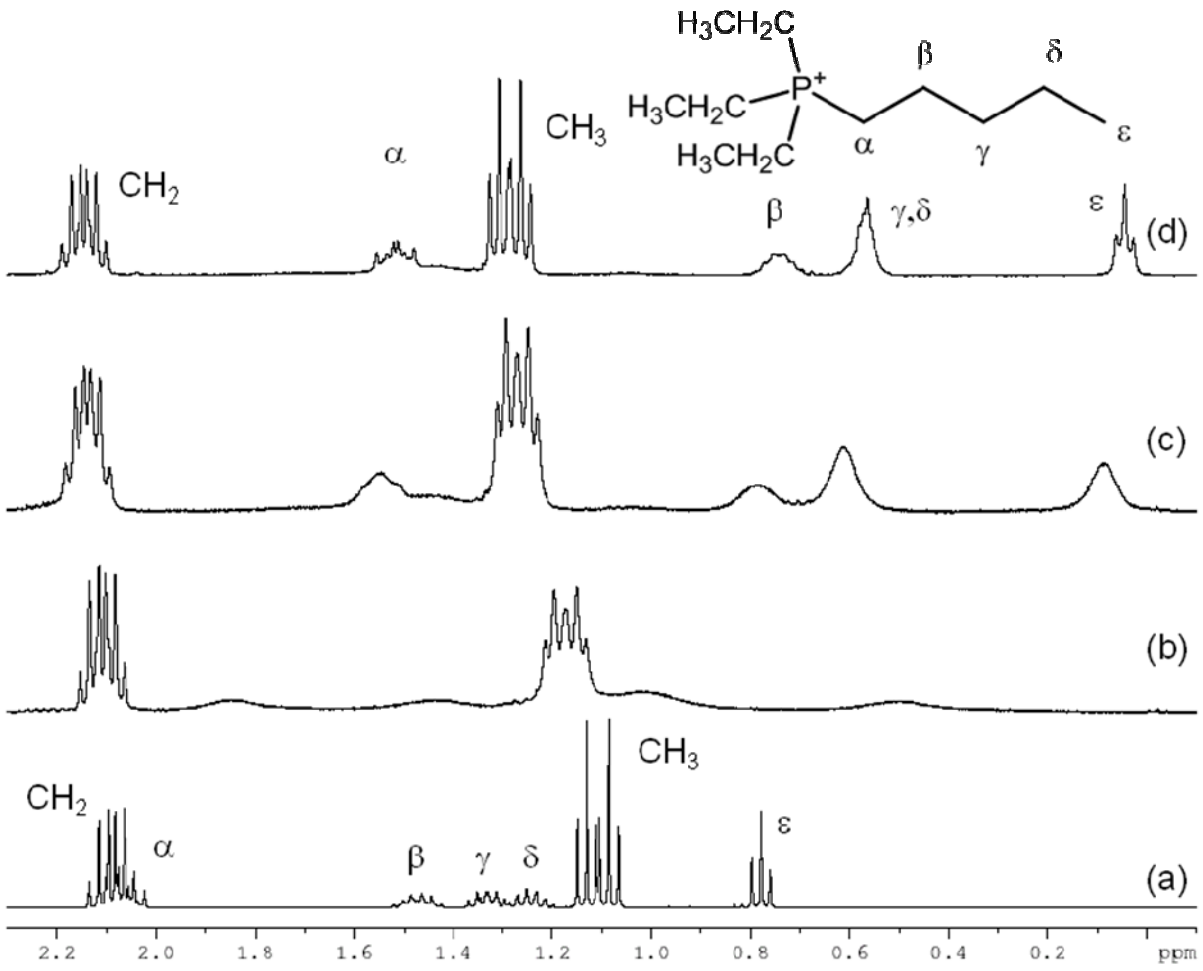

Figure S41. ^{1}H NMR spectra of triethylpentylphosphonium bromide (1.70 mmol dm^{-3}) in the (a) absence of CB[7] and the presence of (b) 0.53 equiv, (c) 1.27 equiv, and (d) 4.23 equiv of CB[7] in D_2O.

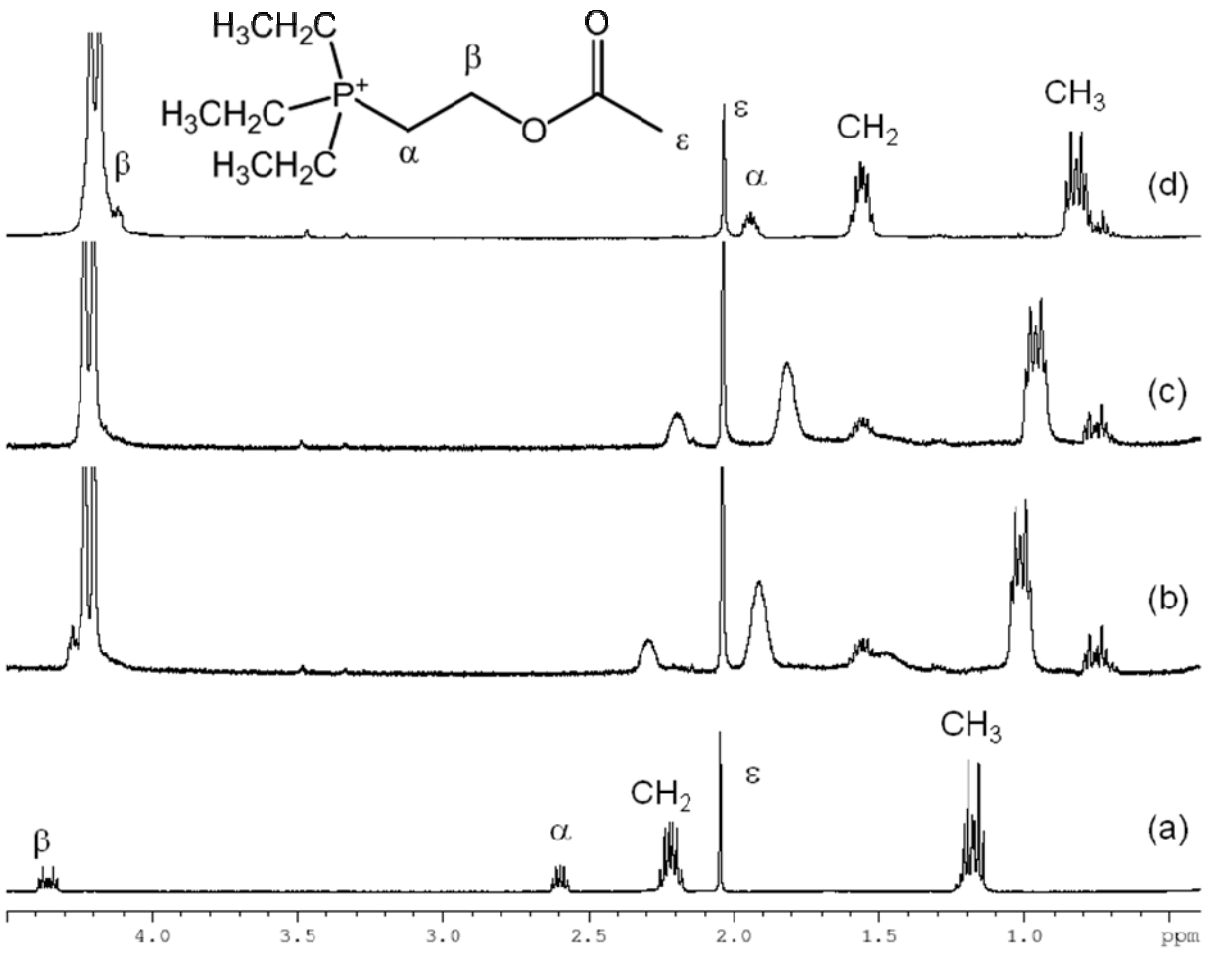

Figure S42. ^{1}H NMR spectra of (2-acetoxyethyl)triethylphosphophonium bromide (2.10 mmol dm^{-3}) in the (a) absence of CB[7] and the presence of (b) 0.76 equiv, (c) 0.93 equiv, and (d) 1.98 equiv of CB[7] in D_2O.