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## **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

Contents

Page

Table S1. High resolution electrospray mass spectra data for the 1:1 host-guest	
complexes with CB[7] in water ( $X^{-} = Cl^{-}$ or Br <sup>-</sup> )	S4
<b>Figure S1.</b> <sup>1</sup> H NMR spectrum (400 MHz) of triethylpentylammonium bromide in $D_2O$ .	S5
<b>Figure S2.</b> <sup>13</sup> C NMR spectrum (100 MHz) of triethylpentylammonium bromide in $D_2O$ .	S5
<b>Figure S3.</b> <sup>1</sup> H NMR spectrum (400 MHz) of (2-hydroxyethyl)triethylammonium	96
bromide in $D_2O$ .	86
Figure S4. C NMR spectrum (100 MHz) of (2-nydroxyetnyi)trietnyiammonium	56
<b>Figure S5</b> <sup>1</sup> H NMR spectrum (400 MHz) of 2-(hydroxyethyl)aujnuclidinium bromide	30
in D <sub>2</sub> O	\$7
Figure S6 <sup>13</sup> C NMR spectrum (100 MHz) of 2 (hydroxyethyl)quinuclidinium bromide	57
in D <sub>2</sub> O	\$7
<b>Figure S7</b> <sup>1</sup> UNMP spectrum (400 MHz) of trimethylpentylphosphonium bromide in	57
<b>Figure 57.</b> If NMR spectrum (400 MHz) of trimethylpentylphospholinum bronnde in	60
$D_2 O$ . <b>Figure S9</b> <sup>13</sup> C NMD spectrum (100 MHz) of trimesthylaportulation because the provide in	20
Figure So. C NMK spectrum (100 MHz) of trimeuryipentyiphosphomum biomide in	00
$D_2 U$ . <b>E</b> : $D_2 U = 0$ (1(2) MHz) of this state has a finite interval of the set of	58
Figure S9. P NMR spectrum (162 MHZ) of trimethylpentylphosphonium bromide in	
$D_2 U_2$	89
Figure S10. 'H NMR spectrum (400 MHz) of triethylpentylphosphonium bromide in	
$D_2O$	<b>S</b> 9
Figure S11. <sup>13</sup> C NMR spectrum (100 MHz) of triethylpentylphosphonium bromide in	
$D_2O_2$	S10
Figure S12. <sup>31</sup> P NMR spectrum (162 MHz) of triethylpentylphosphonium bromide in	
D <sub>2</sub> O.	S10
<b>Figure S13.</b> <sup>1</sup> H NMR spectrum (400 MHz) of (2-hydroxyethyl)trimethylphosphonium	
bromide in $D_2O$ .	S11
<b>Figure S14.</b> <sup>13</sup> C NMR spectrum (100 MHz) of (2-hydroxyethyl)trimethylphosphonium	
bromide in $D_2O$ .	S11

Figure S15. <sup>1</sup> H NMR spectrum (400 MHz) of (2-hydroxyethyl)triethylphosphonium	
bromide in $D_2O_1$ .	S12
<b>Figure S16.</b> <sup>13</sup> C NMR spectrum (100 MHz) of (2-hydroxyethyl)triethylphosphonium	010
bromide in $D_2O_1$	812
Figure S17. "P NMR spectrum (163 Mz) of (2-hydroxyethyl)triethylphosphonium	~
bromide in $D_2O$ .	S13
Figure S18. 'H NMR spectrum (400 MHz) of (2-acetoxyethyl)trimethylphosphonium	
bromide in $D_2O_1$	S13
<b>Figure S19.</b> <sup>13</sup> C NMR spectrum (100 MHz) of (2-acetoxyethyl)trimethylphosphonium	
bromide in $D_2O$ .	S14
<b>Figure S20.</b> <sup>31</sup> P NMR spectrum (162 MHz) of (2-acetoxyethyl)trimethylphosphonium	
bromide in $D_2O$ .	S14
<b>Figure S21.</b> <sup>1</sup> H NMR spectrum (400 MHz) of 2-(acetoxyethyl)triethylphosphonium	
bromide in $D_2O$ .	S15
Figure S23. <sup>13</sup> C NMR spectrum (100 MHz) of (2-acetoxyethyl)triethylphosphonium	
bromide in $D_2O$ .	S15
Figure S24. <sup>31</sup> P NMR spectrum (162 MHz) of (2-acetoxyethyl)triethylphosphonium	
bromide in $D_2O$ .	S16
<b>Figure S25.</b> <sup>1</sup> H NMR spectra of choline (1.44 mmol dm <sup>-3</sup> ) 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 <sub>2</sub> O.	S17
Figure S26. <sup>1</sup> H NMR spectra of acetylcholine (2.46 mmol dm <sup>-3</sup> ) 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 <sub>2</sub> O.	S18
<b>Figure S27.</b> <sup>1</sup> H NMR titration of of acetylcholine with CB[7] in D <sub>2</sub> O: ( <b>a</b> ) CH <sub>3</sub> , ( <b>•</b> ) H $\alpha$ ,	
( $\blacklozenge$ ) H $\varepsilon$ and ( $\bigtriangledown$ ) H $\beta$ .	S19
<b>Figure S28.</b> <sup>1</sup> H NMR spectra of $\beta$ -methylacetylcholine (2.06 mmol dm <sup>-3</sup> ) in the	
(a) absence of $CB[7]$ and the presence of (b) 0.40 equiv, (c) 1.08 equiv, and (d) 1.30	<b>G2</b> 0
Equivor $CB[/]$ in $D_2O$ . Figure S20 <sup>1</sup> H NMR spectra of but vrylcholine (1.51 mmol dm <sup>-3</sup> ) in the (a) absence	520
of CB[7] and the presence of (b) 0.32 equiv. (c) 0.91 equiv. and (d) 1.68 equiv. of CB[7]	
in $D_2O_1$ .	S21
<b>Figure S30.</b> <sup>1</sup> H NMR spectra of triethylcholine (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 <sub>2</sub> O.	S22
<b>Figure S31.</b> <sup>1</sup> H NMR spectra of triethylpentylammonium chloride (mmol dm <sup>-3</sup> ) in the (a	ı)
absence of CB[7] and the presence of (b) $0.26$ equiv, (c) $0.52$ equiv, (d) $0.76$ equiv, and 1	.44
equivoi $CB[/]$ in $D_2O$ . Figure S32 <sup>1</sup> 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 <sub>2</sub> O.	S23
<b>Figure S33</b> . <sup>1</sup> H NMR spectra of (2-hydroxyethyl)benzyldimethyl bromide (1.90 mmol	
dm <sup>-3</sup> ) 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 <sub>2</sub> O.	S24

<b>Figure S34.</b> <sup>1</sup> H NMR spectra of carnitine (1.53 mmol dm <sup>-3</sup> ) 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 $D_2O$ . <b>Figure S35.</b> <sup>1</sup> H NMR spectra of calcium choline phosphate (0.542 mmol dm <sup>-3</sup> ) in the	S25
(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 <sub>2</sub> O containing 1.12 mmol dm <sup>-3</sup> edta <sup>4-</sup> .	S26
<b>Figure S36.</b> <sup>1</sup> H NMR chemical shift titrations of calcium choline phosphate with	
CB[7] in D <sub>2</sub> O; ( $\blacksquare$ ) in the absence of edta <sup>4-</sup> and ( $\bullet$ ) 2.1 equiv edta <sup>4-</sup> .	S26
<b>Figure S37.</b> <sup>1</sup> H NMR spectra of (2-hydroxyethyl)trimethylphosphonium bromide	
$(1.50 \text{ mmol dm}^{-3})$ 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 $D_2O$ .	S27
<b>Figure S38.</b> <sup>1</sup> H NMR spectra of trimethylpentylphosphonium bromide (1.52 mmol	
dm <sup><math>\circ</math></sup> ) in the (a) absence of CB[/] and the presence of (b) 0.54 equiv, (c) 0.99 equiv, and (d) 1.27 equiv. of CD[7] in D.O.	670
and (a) 1.57 equivor $CB[7]$ in $D_2O$ . Figure S30 <sup>1</sup> H NMP spectra of (2 acatoxyathyl)trimethylphosphonium bromide (1.52)	528
mmol dm <sup>-3</sup> ) 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 $D_2O$ .	S29
<b>Figure S40.</b> <sup>1</sup> H NMR spectra of (2-hydroxyethyl)triethylphosphonium bromide	
$(1.54 \text{ mmol } \text{dm}^{-3})$ 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 $D_2O$ .	S30
Figure S41. <sup>1</sup> H NMR spectra of triethylpentylphosphonium bromide $(1.70 \text{ mmol dm}^3)$	
In the (a) absence of $CB[7]$ and the presence of (b) 0.53 equiv, (c) 1.27 equiv, and (d) 4.22 equiv of $CB[7]$ in D O	G21
(a) 4.25 equiv of $CB[7]$ in $D_2O$ . Figure S42 <sup>-1</sup> H NMR spectra of (2-acetoxyethyl)trightylphosphonium bromide (2.10)	531
$mol dm^{-3}$ 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 $D_2O_2$ .	S32
1 / 1 LJ 2	

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

	1	1
Guest	$\{M \bullet CB[7] - X\}^{\top}$	$\{M \bullet CB[7] - X\}^+$
	(m/z  observed)	(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 <sub>3</sub> ) <sub>3</sub> NCH <sub>2</sub> CH(OH)CH <sub>2</sub> CO <sub>2</sub> H <sup>+</sup>	1324.4600	$1324.4560 (C_{49}H_{58}N_{29}O_{17}^{+})$
(PhCH <sub>2</sub> )(CH <sub>3</sub> ) <sub>2</sub> N(CH <sub>2</sub> ) <sub>2</sub> OH <sup>+</sup>	1342.5034	$1342.4818 (C_{53}H_{60}N_{29}O_{15}^{+})$
$(CH_3CH_2)_3N(CH_2)_2OH^+$	1308.4975	$1308.4974 (C_{50}H_{62}N_{29}O_{15}^{+})$
$(CH_{3}CH_{2})_{3}N(CH_{2})_{4}CH_{3}^{+}$	1334.5619	1334.5495 ( $C_{53}H_{68}N_{29}O_{14}^+$ )
Quin(CH <sub>2</sub> ) <sub>2</sub> OH <sup>+</sup>	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. <sup>1</sup>H NMR spectrum (400 MHz) of triethylpentylammonium bromide in D<sub>2</sub>O.



Figure S2. <sup>13</sup>C NMR spectrum (100 MHz) of triethylpentylammonium bromide in D<sub>2</sub>O.



**Figure S3.** <sup>1</sup>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<sub>2</sub>O.

**S6** 



Figure S5. <sup>1</sup>H NMR spectrum (400 MHz) of 2-(hydroxyethyl)quinuclidinium bromide in D<sub>2</sub>O.



**Figure S6.** <sup>13</sup>C NMR spectrum (100 MHz) of 2-(hydroxyethyl)quinuclidinium bromide in D<sub>2</sub>O.



Figure S7. <sup>1</sup>H NMR spectrum (400 MHz) of trimethylpentylphosphonium bromide in  $D_2O$ .



Figure S8. <sup>13</sup>C NMR spectrum (100 MHz) of trimethylpentylphosphonium bromide in  $D_2O$ .



Figure S9. <sup>31</sup>P NMR spectrum (162 MHz) of trimethylpentylphosphonium bromide in  $D_2O$ .



**Figure S10.** <sup>1</sup>H NMR spectrum (400 MHz) of triethylpentylphosphonium bromide in D<sub>2</sub>O.



Figure S11. <sup>13</sup>C NMR spectrum (100 MHz) of triethylpentylphosphonium bromide in  $D_2O$ .



Figure S12. <sup>31</sup>P NMR spectrum (162 MHz) of triethylpentylphosphonium bromide in D<sub>2</sub>O.



**Figure S13.** <sup>1</sup>H NMR spectrum (400 MHz) of (2-hydroxyethyl)trimethylphosphonium bromide in  $D_2O$ .



**Figure S14.** <sup>13</sup>C NMR spectrum (100 MHz) of (2-hydroxyethyl)trimethylphosphonium bromide in  $D_2O$ .



**Figure S15.** <sup>31</sup>P NMR spectrum (162 MHz) of (2-hydroxyethyl)trimethylphosphonium bromide in  $D_2O$ .

- 25.34



**Figure S16.** <sup>1</sup>H NMR spectrum (400 MHz) of (2-hydroxyethyl)triethylphosphonium bromide in  $D_2O$ .



**Figure S17.** <sup>13</sup>C NMR spectrum (100 MHz) of (2-hydroxyethyl)triethylphosphonium bromide in  $D_2O$ .



**Figure S18.** <sup>31</sup>P NMR spectrum (163 Mz) of (2-hydroxyethyl)triethylphosphonium bromide in  $D_2O$ .



**Figure S19.** <sup>1</sup>H NMR spectrum (400 MHz) of (2-acetoxyethyl)trimethylphosphonium bromide in  $D_2O$ .



**Figure S20.** <sup>13</sup>C NMR spectrum (100 MHz) of (2-acetoxyethyl)trimethylphosphonium bromide in  $D_2O$ .



**Figure S21.** <sup>31</sup>P NMR spectrum (163 Mz) of (2-acetoxyethyl)trimethylphosphonium bromide in  $D_2O$ .



**Figure S22.** <sup>1</sup>H NMR spectrum (400 MHz) of (2-acetoxyethyl)triethylphosphonium bromide in  $D_2O$ .



**Figure S23.** <sup>13</sup>C NMR spectrum (100 MHz) of (2-acetoxyethyl)triethylphosphonium bromide in  $D_2O$ .



**Figure S24.** <sup>31</sup>P NMR spectrum (162 MHz) of (2-acetoxyethyl)triethylphosphonium bromide in  $D_2O$ .



**Figure S25.** <sup>1</sup>H NMR spectra of choline (1.44 mmol dm<sup>-3</sup>) 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.** <sup>1</sup>H NMR spectra of acetylcholine (2.46 mmol dm<sup>-3</sup>) 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.** <sup>1</sup>H NMR titration of of acetylcholine with CB[7] in D<sub>2</sub>O: (**a**) CH<sub>3</sub>, (**•**) H $\alpha$  (**•**) H $\epsilon$  and (**V**) H $\beta$ .



**Figure S28.** <sup>1</sup>H NMR spectra of  $\beta$ -methylacetylcholine (2.06 mmol dm<sup>-3</sup>) 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<sub>2</sub>O.



**Figure S29.** <sup>1</sup>H NMR spectra of butyrylcholine (1.51 mmol dm<sup>-3</sup>) 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.** <sup>1</sup>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.** <sup>1</sup>H NMR spectra of triethylpentylammonium chloride (mmol dm<sup>-3</sup>) 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.** <sup>1</sup>H NMR spectra of (2-hydroxyethyl)quinuclidinium bromide (1.08 mmol dm<sup>-3</sup>) 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**. <sup>1</sup>H NMR spectra of (2-hydroxyethyl)benzyldimethylammonium bromide (1.90 mmol dm<sup>-3</sup>) 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.** <sup>1</sup>H NMR spectra of carnitine (1.53 mmol dm<sup>-3</sup>) 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.** <sup>1</sup>H NMR spectra of calcium choline phosphate (0.542 mmol dm<sup>-3</sup>) 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<sub>2</sub>O containing 1.12 mmol dm<sup>-3</sup> edta<sup>4-</sup>. The  $\beta$  protons are overlapped by CH<sub>2</sub> protons of CB[7] (•).



**Figure S36.** <sup>1</sup>H NMR chemical shift titrations of calcium choline phosphate with CB[7] in D<sub>2</sub>O; (**■**) in the absence of edta<sup>4-</sup> and (**●**) 2.1 equiv edta<sup>4-</sup>.



**Figure S37.** <sup>1</sup>H NMR spectra of (2-hydroxyethyl)trimethylphosphonium bromide (1.50 mmol dm<sup>-3</sup>) 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.** <sup>1</sup>H NMR spectra of trimethylpentylphosphonium (1.52 mmol dm<sup>-3</sup>) 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.** <sup>1</sup>H NMR spectra of (2-acetoxyethyl)trimethylphosphophonium bromide (1.52 mmol dm<sup>-3</sup>) 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.** <sup>1</sup>H NMR spectra of (2-hydroxyethyl)triethylphosphophonium bromide (1.54 mmol dm<sup>-3</sup>) 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.** <sup>1</sup>H NMR spectra of triethylpentylphosphonium bromide (1.70 mmol dm<sup>-3</sup>) 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.** <sup>1</sup>H NMR spectra of (2-acetoxyethyl)triethylphosphophonium bromide (2.10 mmol dm<sup>-3</sup>) 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  $D_2O$ .