Electronic Supplementary Material (ESI) for Chemical Communications

Supporting Information

Synthetic chloride transporters with the binding mode observed in a ClC chloride channel

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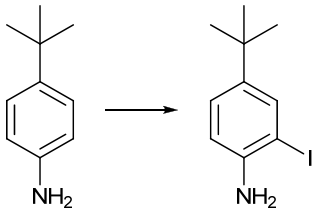
Contents

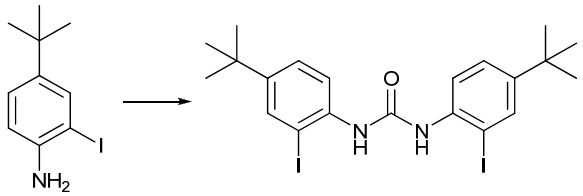
General: All reagents were purchased from commercial suppliers and used without further purification. If it is necessary, anhydrous reagents were purchased. CH_2Cl_2 was purified by drying over CaH_2 followed by distillation. Thin layer chromatography (TLC) was performed on Merck (silica gel 60, F-254, 0.25 mm). Silica gel 60 (230 ~ 240 mesh, Merck) was used for column chromatography. Melting points were determined with a Barnsted Electrochemical (IA9100). The NMR (Bruker Avance II spectrometer) chemical shifts were reported in ppm downfield relative to the residual protonated solvent peaks (for ^{1}H NMR spectra: CD_3CN 1.94 ppm; DMSO-d_6 2.50 ppm, for ^{13}C NMR spectra: CD_3CN 1.32 ppm; DMSO-d_6 39.52 ppm). Routine mass analyses were performed with photodiode array detector using electron spray ionization (ESI) or atmospheric pressure chemical ionization (APCI). Fluorescence spectra were measured with HITACHI-F4500. The elemental analysis data were obtained from Organic Chemistry Research Center at Sogang University.

1. Synthesis and characterization of new compounds



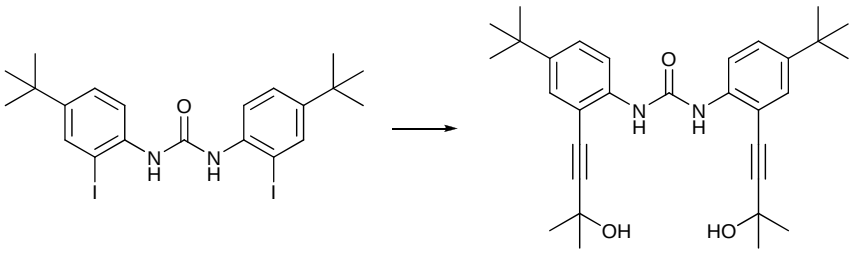
1a **2a**

2a: I_2 (6.8 g, 1 equiv) diluted in EtOH (100 ml) was dropwise added to a round bottom flask charged with 4-*t*-butylaniline (4 g, 27 mmol), Ag_2SO_4 (8.4 g, 1 equiv) and EtOH (100 ml). The solution was stirred vigorously for 4 h at room temperature. The reaction mixture was filtered through Celite and the organic solvent was evaporated. The concentrated mixture was dissolved in CH_2Cl_2 and was washed with saturated $NaHCO_3$ solution and brine, dried over anhydrous Na_2SO_4 and concentrated. The reaction mixture was purified by column chromatography (silica gel, 1:3 (v/v) ethyl acetate in hexane) to give **2a** as brown liquid. (6.9 g, 75%); ^{1}H NMR (400 MHz, DMSO–d_6) δ 7.47 (s, 1H), 7.12 (d, J = 8.5 Hz, 1H), 6.70 (d, J = 8.4 Hz, 1H), 4.98 (s, 2H, NH), 1.19 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.2, 143.2, 135.6, 126.5, 114.4, 84.5, 33.8, 31.4 ppm; HR-MS(ESI) m/z Calcd for $C_{10}H_{14}IN$ 275.0171, found : 275.0177.



2a **3a**

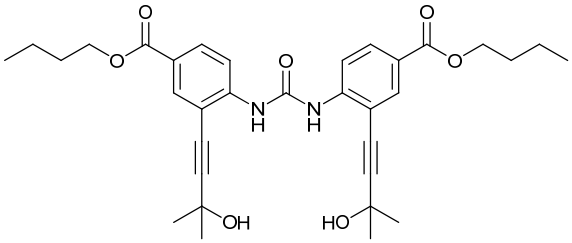
3a: **2a** (4.8 g, 17 mmol) in CH_2Cl_2 (100 ml, 0.17 M) and saturated $NaHCO_3$ aqueous solution (100 ml) was stirred and triphosgene (5.2 g, 1 equiv) was added in several portions. The reaction mixture was vigorously stirred at room temperature. The resulting suspension was washed with saturated $NaHCO_3$ solution and brine, dried over anhydrous Na_2SO_4 and concentrated. The residue was recrystallized with MeOH to give **3a** (6.2 g, 62%) as white solid. mp > 250 ºC (dec); ^{1}H NMR (400 MHz, DMSO–d_6) δ 8.44 (s, 2H, NH), 7.77 (s, 2H), 7.59 (d, J = 8.6 Hz, 2H), 7.39 (d, J = 8.4 Hz, 2H), 1.26 (s, 18H); ^{13}C NMR (100 MHz, DMSO–d_6) δ 153.0, 148.2, 137.5, 135.3, 125.7, 124.1, 92.8, 33.9, 31.0; Anal. Calcd for $C_{21}H_{26}I_2N_2O$: C, 43.8; H, 4.55; N, 4.9, found: C, 43.7; H, 4.55; N, 5.0%



3a **4a**

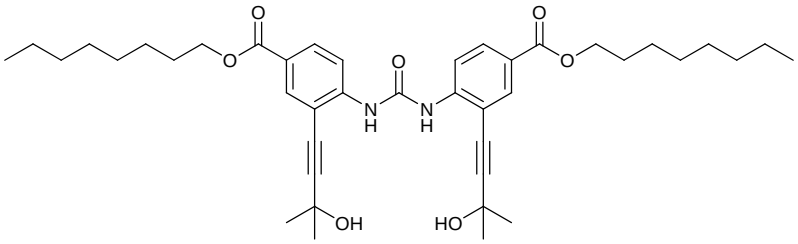
4a: A Schlenk flask charged with **3a** (1 g, 1.7 mmol), CuI (3.3 mg, 0.01 equiv) and $Pd(PPh_3)_2Cl_2$ (12.2 mg, 0.01 equiv) were evacuated under vacuum and back filled with nitrogen (two times). Anhydrous THF (10 ml), TEA (10 ml) and 3-methyl-1-butyn-3-ol (0.51 ml, 3 equiv) were added, the solution was degassed, refilled with N_2, and stirred at 55-58 ^{o}C for 19 h. The mixture was cooled down to room temperature, filtered through Celite and organic solvent was evaporated. The residue was dissolved in CH_2Cl_2, washed with saturated $NaHCO_3$ aqueous solution and brine, dried over anhydrous Na_2SO_4 then concentrated. The mixture was purified by short column chromatography (CH_2Cl_2) to get **4a (**0.7 g, 83%) as white solid.; mp > 197 ºC (dec); ^{1}H NMR (400 MHz, DMSO–d_6) δ 8.44 (s, 2H, NH), 7.87 (d, J = 8.8 Hz, 2H), 7.36 (d, J = 8.6 Hz, 2H), 7.30 (s, 2H), 5.44 (s, 2H, OH), 1.48 (s, 12H), 1.26 (s, 18H); ^{13}C NMR (100 MHz, DMSO–d_6) δ 157.7, 150.3, 142.3, 133.8, 131.3, 126.5, 118.2, 106.3, 82.5, 69.1, 39.1, 36.8, 36.2.; HR-MS-FAB (m/z) Calcd for $C_{31}H_{40}N_2O_3$: 488.3039, found: 488.3038; Anal. Calcd for $C_{31}H_{40}N_2O_3$: C, 76.2; H, 8.25; N, 5.7, found: C, 76.0; H, 8.0; N, 5.9%

Compound **4b-h** were prepared following the procedures described above for the synthesis of **4a**.



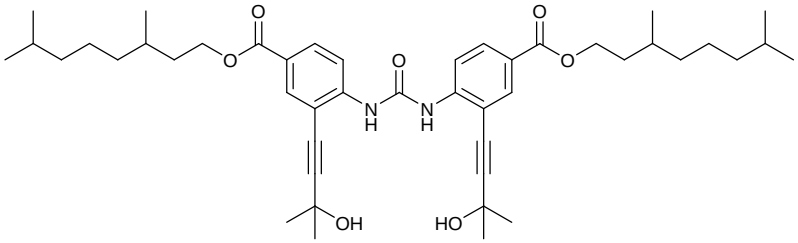
4b

4b: Mp 174 ~ 178 °C; ^{1}H NMR (400 MHz, DMSO–d_6) δ 9.13 (s, 2H, NH), 8.24 (d, J = 9.2 Hz, 2H), 7.90 (overlapped, 4H), 5.53 (s, 2H, OH), 4.26 (t, J = 6.6 Hz, 4H), 1.69 (qn, J = 6.8 Hz, 4H), 1.52 (s, 12H), 1.41 (m, 4H), 0.96 (t, J = 7.0 Hz ,6H); ^{13}C NMR (100 MHz, DMSO–d_6) δ : 164.7, 151.6, 143.2, 133.4, 129.8, 123.9, 120.2, 112.7, 102.8, 75.7, 64.4, 63.9, 31.3, 30.2, 18.7, 13.6; LR-MS(ESI) m/z Calcd for $C_{33}H_{40}N_2O_7$ [M-H$^+$]: 575.28, found: 575.26; Anal. Calcd for $C_{33}H_{40}N_2O_7$: C, 68.8; H, 7.0; N, 4.9. Found: C, 68.8; H, 7.0, N, 4.9%



4c

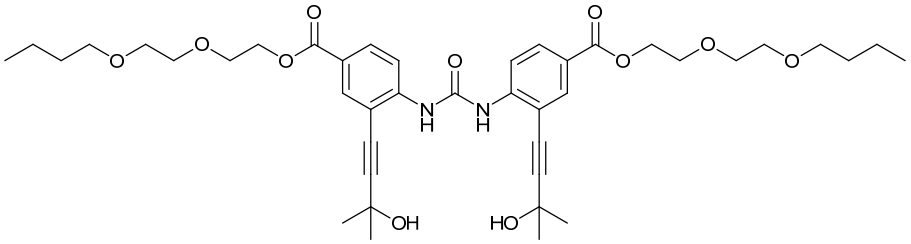
4c: Mp 139 ~ 143 °C; ^{1}H NMR (400 MHz, DMSO–d_6) δ 9.26 (s, 2H), 8.23 (d, J = 9.6 Hz, 2H), 7.91 (overlapped, 4H), 5.61 (s, 2H), 4.25 (t, J = 6.4 Hz, 4H), 1.70 (qn, J = 6.8 Hz, 4H), 1.51 (s, 12H), 1.26 ~ 1.39 (overlapped, 20H), 0.87 (t, J = 6.4 Hz, 6H); ^{13}C NMR (100 MHz, DMSO–d_6) δ 164.7, 151.6, 143.2, 133.4, 129.8, 123.9, 120.1, 112.65, 102.8, 75.7, 64.7, 64.0, 31.3, 31.2, 28.6, 28.5, 28.1, 25.4, 22.0, 13.9; LR-MS(ESI) m/z Calcd for $C_{41}H_{56}N_2O_7$ [M-H$^+$]: 687.40, found: 687.34; Anal. Calcd for $C_{41}H_{56}N_2O_7$: C, 71.5; H, 8.2; N, 4.0. Found: C, 71.5; H, 8.2; N, 4.0%



4d

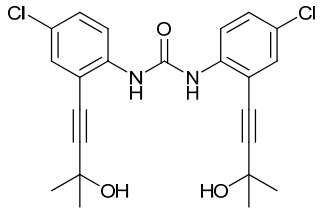
4d: Mp 102 ~105 °C; ^{1}H NMR (250 MHz, DMSO–d_6) δ 9.06 (s, 2H), 8.24 (d, J = 8.5 Hz, 2H), 7.87 (overlapped, 4H), 5.47 (s, 2H), 4.26 (t, J = 6.5, 4H), 1.72 ~ 1.10 (overlapped, 32 H), 0.89 (d, J = 5.5Hz, 6H), 0.81 (d, J = 6.7 Hz, 12H); ^{13}C NMR (100 MHz, DMSO–d_6) δ 165.1, 152.0, 146.7, 133.9, 130.2, 124.4, 120.5, 113.0, 103.2, 76.2, 64.4, 63.5, 36.9, 35.4, 31.8, 19.8, 27.8, 24.4, 22.9, 22.8, 19.8.;

LR-MS(ESI) m/z Calcd for $C_{45}H_{64}N_2O_7$ [M-H$^+$]: 743.46, found : 743.47; Anal. Calcd for $C_{45}H_{64}N_2O_7$: C, 72.55; H, 8.7; N, 3.8. found: C, 72.55; H, 9.2; N, 3.8%



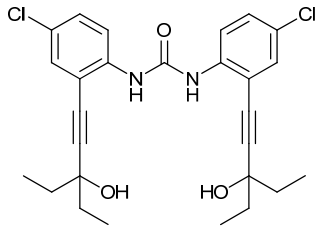
4e

4e: Mp: 83 ~ 87 °C; ^{1}H NMR (250 MHz, DMSO–d_6) δ 9.09 (s, 2H, NH), 8.25 (d, J = 9.2 Hz, 2H), 7.92 (overlapped, 4H), 5.49 (s, 2H, OH), 4.37 (t, J = 3.7 Hz, 4H), 3.73 (t, J = 4.5 Hz, 4H), 3.56 (t, J = 4.0 Hz, 4H), 3.48 (t, J = 3.3 Hz, 4H), 3.35 (t, J = 6.5, 4H), 1.51 (s, 12H), 1.44 (qn, J = 4.0 Hz, 4H), 1.33 (m, 4H), 0.83 (t, J = 7.2 Hz, 6H); ^{13}C NMR (100 MHz, DMSO–d_6) δ 165.1, 152.0, 143.8, 134.0, 130.4, 124.2, 120.6, 113.1, 103.3, 76.2, 70.5, 70.3, 69.9, 68.8, 64.5, 64.4, 31.8, 31.7, 19.3, 14.2 ; LR-MS(ESI) m/z Calcd for $C_{41}H_{56}N_2O_{11}$ [M-H$^+$]: 751.38, found : 751.36 ; Anal. Calcd for $C_{41}H_{56}N_2O_{11}$: C, 65.4; H, 7.5; N, 3.7, found: C, 65.5; H, 7.5; N, 3.7%



4f

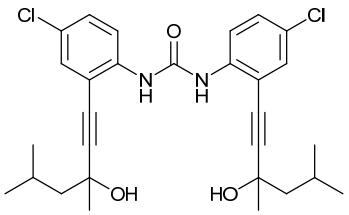
4f: Mp 149 ~ 152 °C; ^{1}H NMR (400 MHz, DMSO–d_6) δ 8.73 (s, 2H, NH), 7.99 (d, J = 9.6, 2H), 7.39 (d, J = 7.6, 2H), 7.38 (s, 2H), 5.48 (s, 2H, OH), 1.49 (s, 12H); ^{13}C NMR (100 MHz, DMSO–d_6) δ 152.0, 138.3, 131.3, 128.8, 126.5, 122.8, 115.1, 103.0, 75.5, 63.9, 31.4; Anal. Calcd for $C_{23}H_{22}Cl_2N_2O_3$: C, 62.0; H, 5.0; N, 6.3. Found: C, 62.0; H, 4.9; N, 6.3%



4g

4g: Mp:114 ~ 117 °C; ^{1}H NMR (400 MHz, DMSO–d_6) δ 8.54 (s, 2H, NH), 7.92 (d, J = 8.4, 2H), 7.41 (s, 2H), 7.39 (d, J = 9.0, 2H), 5.15 (s, 2H, OH), 1.65 (t, J = 6.8, 8H), 0.96 (t, J = 7.2, 12H); ^{13}C NMR (100 MHz, DMSO–d_6) δ 152.0, 138.2, 131.3, 128.8, 126.7, 123.0, 115.7, 100.9, 77.8, 70.7, 33.6, 8.5;

LR-MS(ESI) m/z Calcd for $C_{27}H_{30}Cl_2N_2O_3$ [M-H$^+$]: 499.16, found : 499.07; Anal. Calcd for $C_{27}H_{30}Cl_2N_2O_3$: C, 64.6; H, 6.0; N, 5.5. Found: C, 64.7; H, 6.0, N, 5.6%



4h

4h: Mp 70 ~ 72 °C; ^{1}H NMR (400 MHz, DMSO–d_6) δ 8.78 (s, 2H, NH), 7.94 (d, J = 8.8, 2H), 7.38 (m, 4H), 5.44 (s, 2H, OH), 1.93 (m, 2H), 1.57 (d, J = 6.0, 4H), 1.57 (s, 6H), 0.94 (d, J = 6.8, 12H), ^{13}C NMR (100 MHz, DMSO–d_6) δ 152.0, 138.2, 131.1, 128.8, 126.6, 122.9, 115.5, 102.5, 76.8, 66.7, 51.6, 30.6, 34.4, 24.2, 24.1; LR-MS(ESI) m/z Calcd for $C_{29}H_{34}Cl_2N_2O_3$ [M-H$^+$]: 527.19, found : 527.12; Anal. Calcd for $C_{29}H_{34}Cl_2N_2O_3$: C, 66.8; H, 6.5; N, 5.2. Found: C, 65.8; H, 6.5, N, 5.3%

2. X-ray crystallographic analysis

Complex 4f• TBA$^+$Cl$^-$: Single crystals were grown as follow: **4f** (10 mg) and TBA$^+$Cl$^-$ (3 equiv) were dissolved in 50:1 (v/v) toluene/CH_2Cl_2 (10 ml) and *n*-heptane was added to the solution until no precipitate was formed. Slow diffusion of *n*-heptane into a toluene/CH_2Cl_2 solution over a few days yielded single crystals suitable for the X-ray diffraction.

A crystal of complex **4f** •TBA$^+$Cl$^-$ was coated with paratone oil and the diffraction data measured at 193 K with Mo Kα radiation on an X-ray diffraction camera system using an imaging plate equipped with a graphite crystal incident beam monochromator. The RapidAuto software [S1] was used for data collection and data processing. Structure was solved by direct method and refined by full-matrix least-squares calculation with the SHELXTL software package.[S2]

One ligand, one chloride anion and one tetrabutylammonium cation were observed as an asymmetric unit. A terminal methyl residue of the tetrabutylammonium cation is statistically disordered. All non-hydrogen atoms are refined anisotropically; the hydrogen atoms were assigned isotropic displacement coefficients U(H) = 1.2U (C) and 1.5U (C_{methyl}), and their coordinates were allowed to ride on their respective atoms. All hydrogen atoms involved in hydrogen bonding interaction with the chloride anion are found in difference Fourier map and refined with isotropic

[S1] Rapid Auto software, R-Axis series, Cat. No. 9220B101, Rigaku Corporation.
[S2] G. M. Sheldrick, *SHELXTL-PLUS, Crystal Structure Analysi Package*; Bruker Analytical X-Ray; Madison, WI, USA, 1997.

displacement coefficients.

Final least-squares refinement of the structure converged at a final $R1$ = 0.0497 and $wR2$ = 0.1120 for 4808 reflections with $I > 2\sigma(I)$; $R1$ = 0.1247 and $wR2$ = 0.1503 for all 9561 reflections. The largest different peak and hole were 0.390 and –0.417 e·Å^{-3}, respectively.

A summary of the crystal and some crystallography data is given in Table S1. CCDC-875574 contains the supplementary crystallographic data for this paper. The data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html or from the Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB2 1EZ, UK.

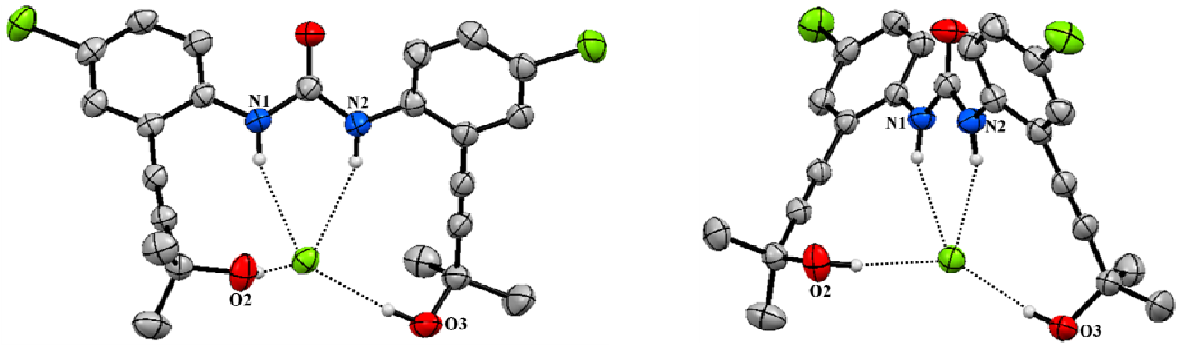


Figure S1. Top view (left) and side view (right) of ORTEP plots for the crystal structure of **4f•** TBA^+Cl^- with 50% probability ellipsoids. The counter cation and CH hydrogen atoms were all omitted for clarity.

Table S1. Crystal data and structure refined for **4f•** TBA^+Cl^-.

Identification code	o11_15mo	
Empirical formula	$C_{39}H_{58}N_3O_3Cl_3$	
Formula weight	723.23	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 13.590(3) Å	□□= 90°
b = 19.104(4) Å	□= 110.86(3)°	
c = 17.224(3) Å	□ = 90°	
Volume	4178.6(14) Å^3	
Z	4	
Density (calculated)	1.150 Mg/m^3	

Absorption coefficient	0.256 mm^{-1}
F(000)	1552
Crystal size	0.29 x 0.22 x 0.16 mm^3
Theta range for data collection	3.18 to 27.48°.
Index ranges	-17<=h<=17, -24<=k<=24, -22<=l<=21
Reflections collected	40579
Independent reflections	9561 [R(int) = 0.0806]
Completeness to theta = 27.48°	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9602 and 0.9294
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9561 / 0 / 469
Goodness-of-fit on F^2	1.056
Final R indices [I>2sigma(I)]	R1 = 0.0497, wR2 = 0.1120
R indices (all data)	R1 = 0.1247, wR2 = 0.1503
Extinction coefficient	0.0037(5)
Largest diff. peak and hole	0.390 and -0.417 e.$Å^{-3}$

Table S2. Hydrogen bonds length and bonds angles for **4f•** TBA^+Cl^- [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(2N)...Cl(1)	0.89(3)	2.52(3)	3.358(3)	156(3)
N(1)-H(1N)...Cl(1)	0.88(3)	2.51(3)	3.321(3)	154(3)
O(3)-H(3O)...Cl(1)	0.95(4)	2.27(5)	3.221(2)	171(4)
O(2)-H(2O)...Cl(1)	0.95(4)	2.18(4)	3.121(2)	170(3)

3. Binding study

^{1}H NMR titrations: Each stock solution of receptor (5.0×10^{-4} M) and TBA$^+$Cl$^-$ (5.0×10^{-3} M) was prepared in 1% (v/v) H_2O/CD_3CN (5.0×10^{-4} M) at 24 ± 1 °C. The ^{1}H NMR spectrum of receptor (500 μL) was taken first to determine the chemical shift of free host, and then aliquots of TBA$^+$Cl$^-$ (at first 10 μL and finally 200 μL) were added to the receptor stock solution and the spectrum was recorded after each addition. The association constant (K_a, M^{-1}) was determined by non-linear least square fitting of the titration curve[S3] as show below.

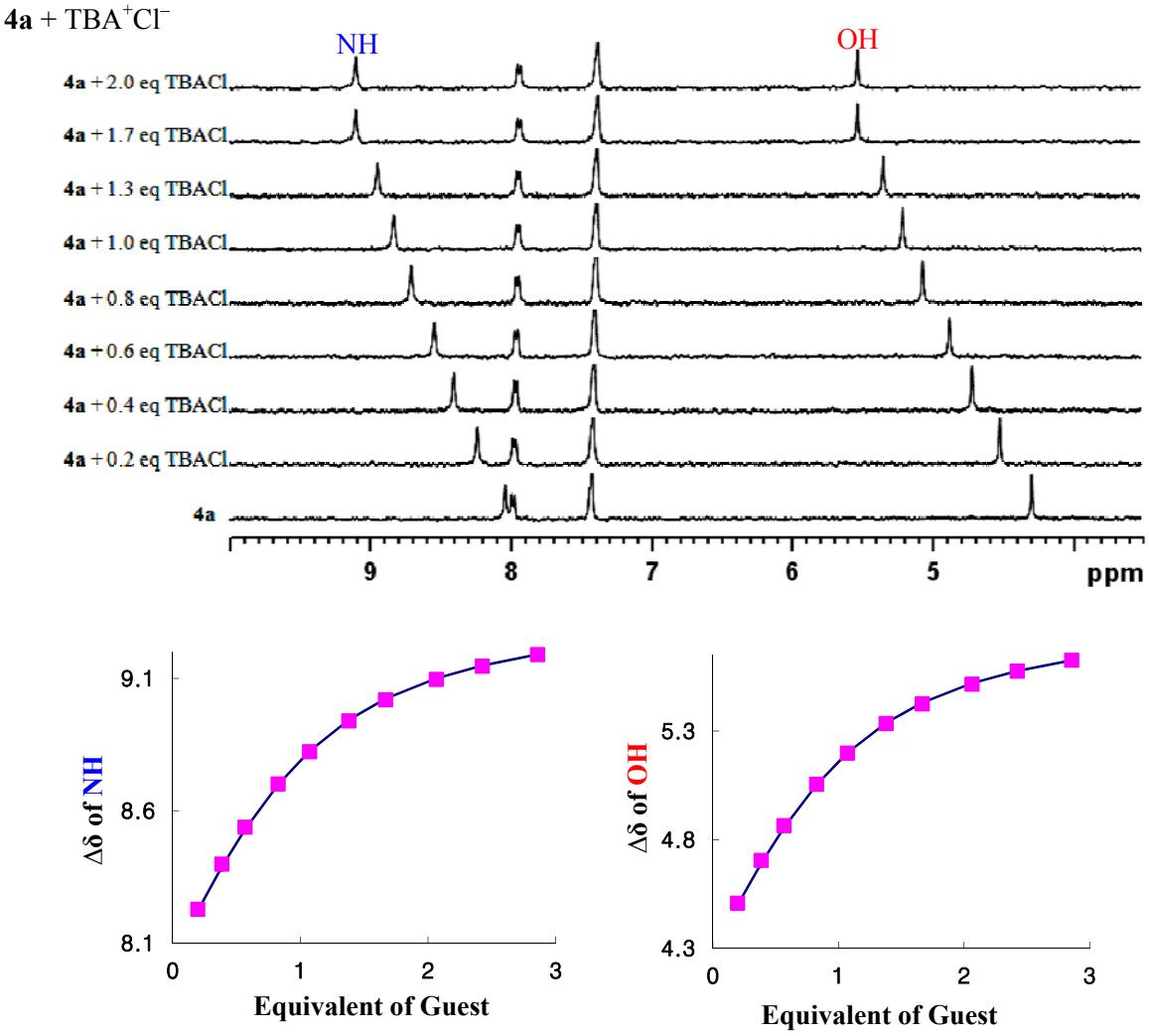


Figure S2. ^{1}H NMR spectral changes of **4a** upon addition of TBA$^+$Cl$^-$ (top), and titration curves (bottom) plots for NH (left) and OH (right): the experimental data (dots) are fitted to theoretical ones (lines) with the association constant, $K_a = (5.1 \pm 0.6) \times 10^3$ M^{-1}.

[S3](a) Connors, K. A. *Binding Constants*; John Wiley & Sons: New York, 1987. (b) R. S. Macomber, *J. Chem. Educ.*, 1992, **69**, 375. (c) P. Thordarson, *Chem. Soc. Rev.*, 2011, **40**, 1305.

4b + TBA^+Cl^-

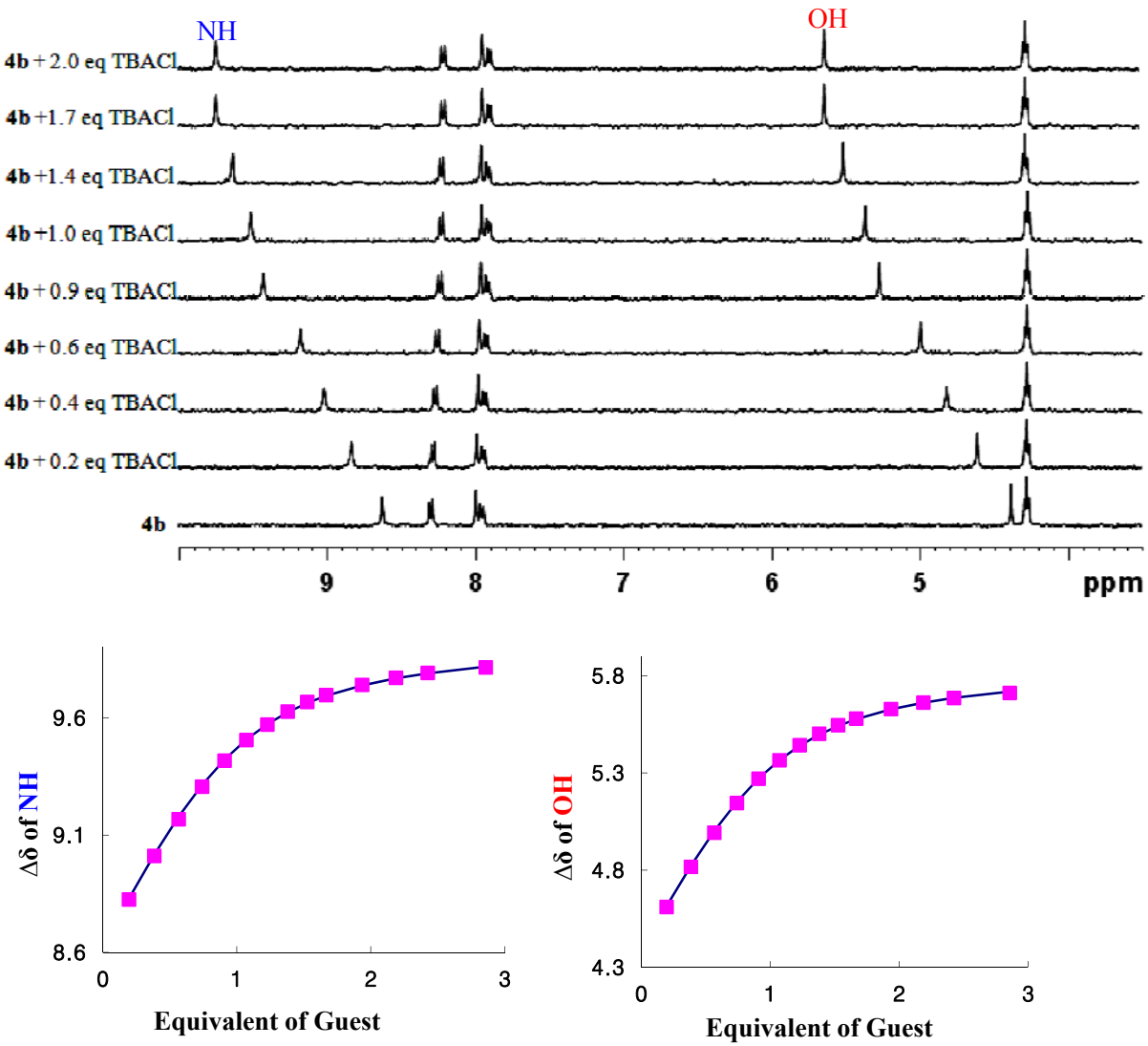


Figure S3. ^{1}H NMR spectral changes of **4b** upon addition of TBA^+Cl^- (top), and titration curves (bottom) plots for NH (left) and OH (right): the experimental data (dots) are fitted to theoretical ones (lines) with the association constant, $K_a = (8.5 \pm 0.2) \times 10^3\ M^{-1}$.

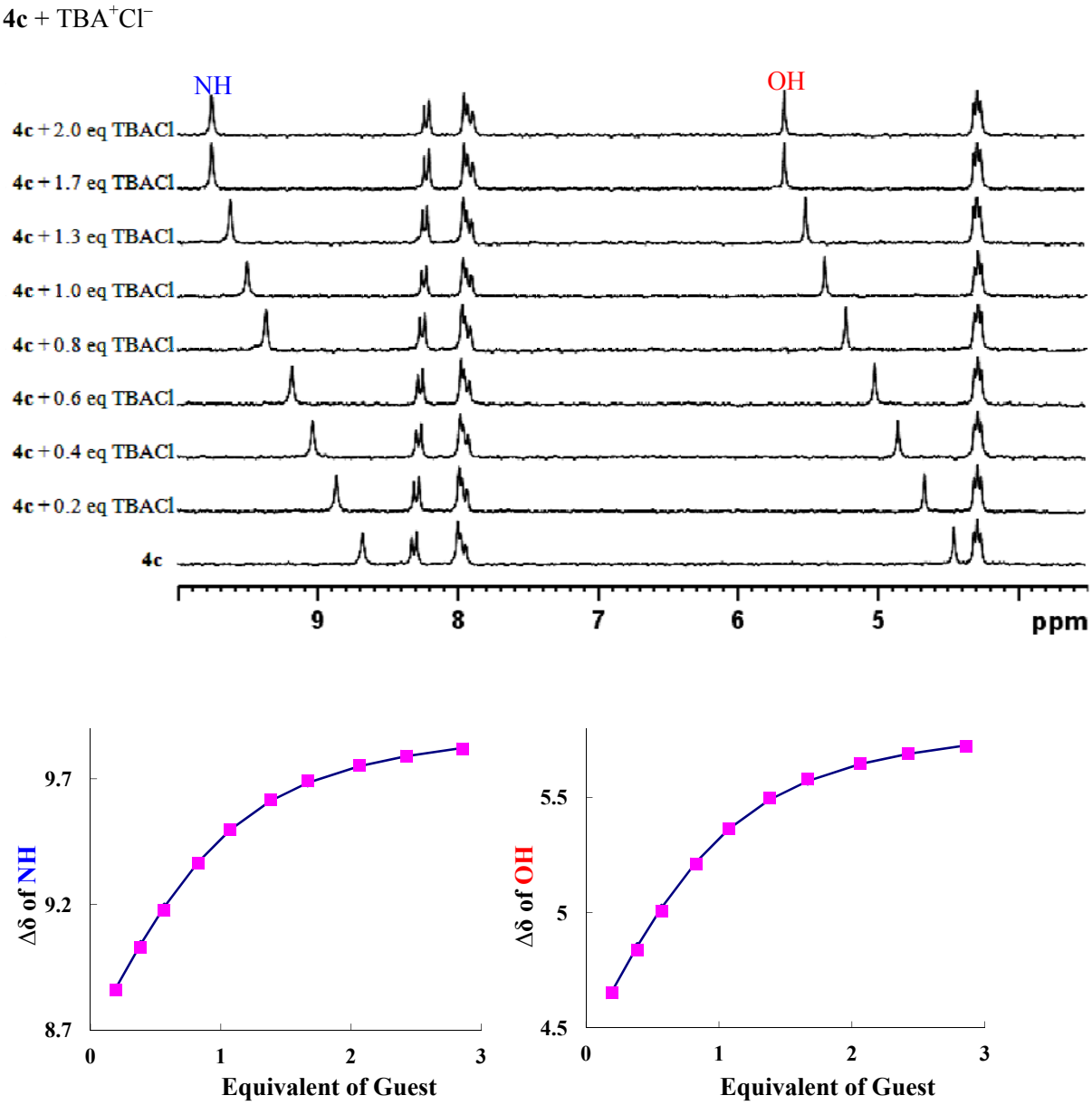


Figure S4. ^{1}H NMR spectral changes of **4c** upon addition of $TBA^{+}Cl^{-}$ (top), and titration curves (bottom) plots for NH (left) and OH (right): the experimental data (dots) are fitted to theoretical ones (lines) with the association constant, $K_a = (8.0 \pm 0.1) \times 10^3\ M^{-1}$.

4d + TBA^+Cl^-

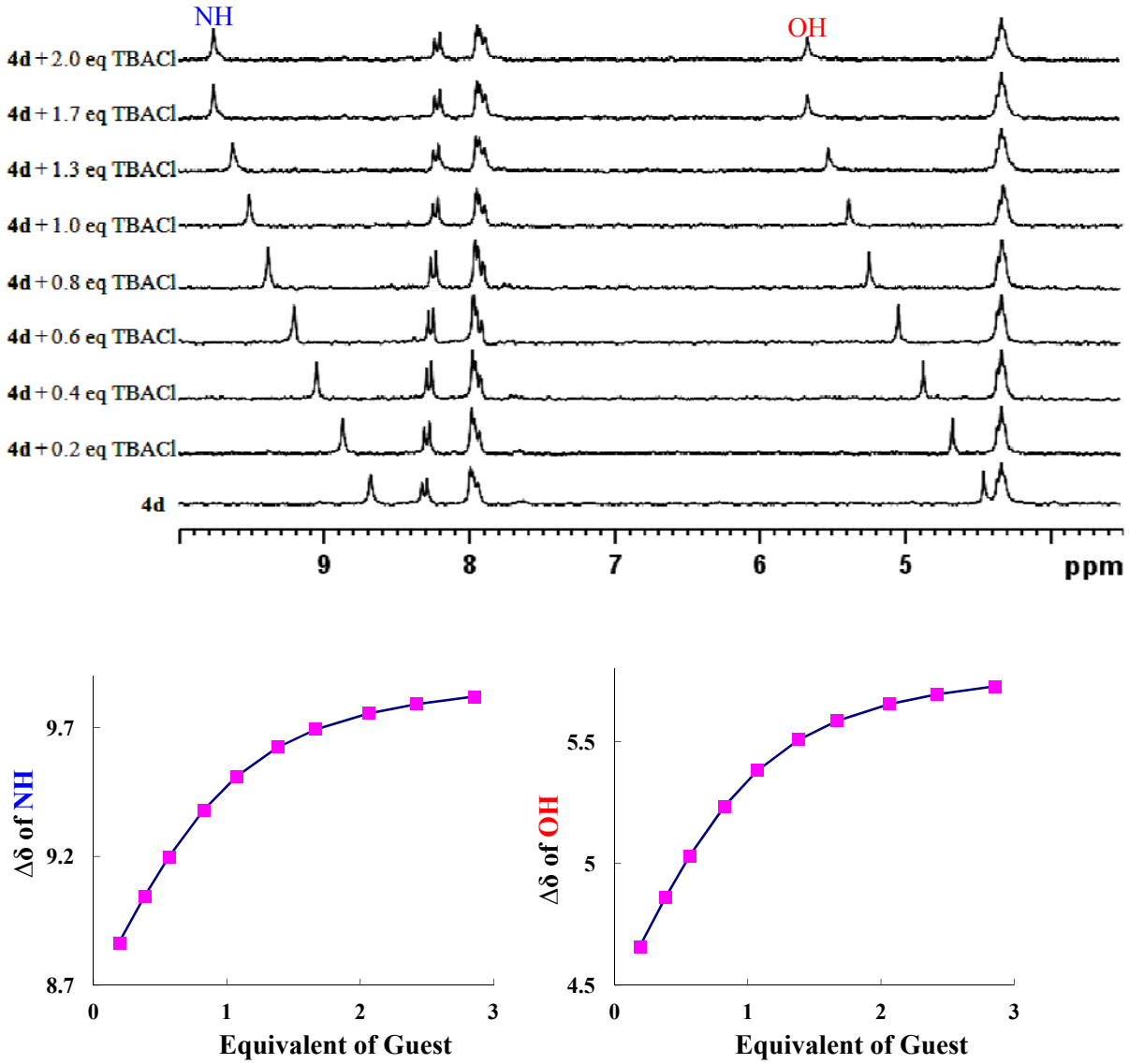


Figure S5. ^{1}H NMR spectral changes of **4d** upon addition of TBA^+Cl^- (top), and titration curves (bottom) plots for NH (left) and OH (right): the experimental data (dots) are fitted to theoretical ones (lines) with the association constant, $K_a = (9.2 \pm 0.1) \times 10^3\ M^{-1}$.

4e + TBA^+Cl^-

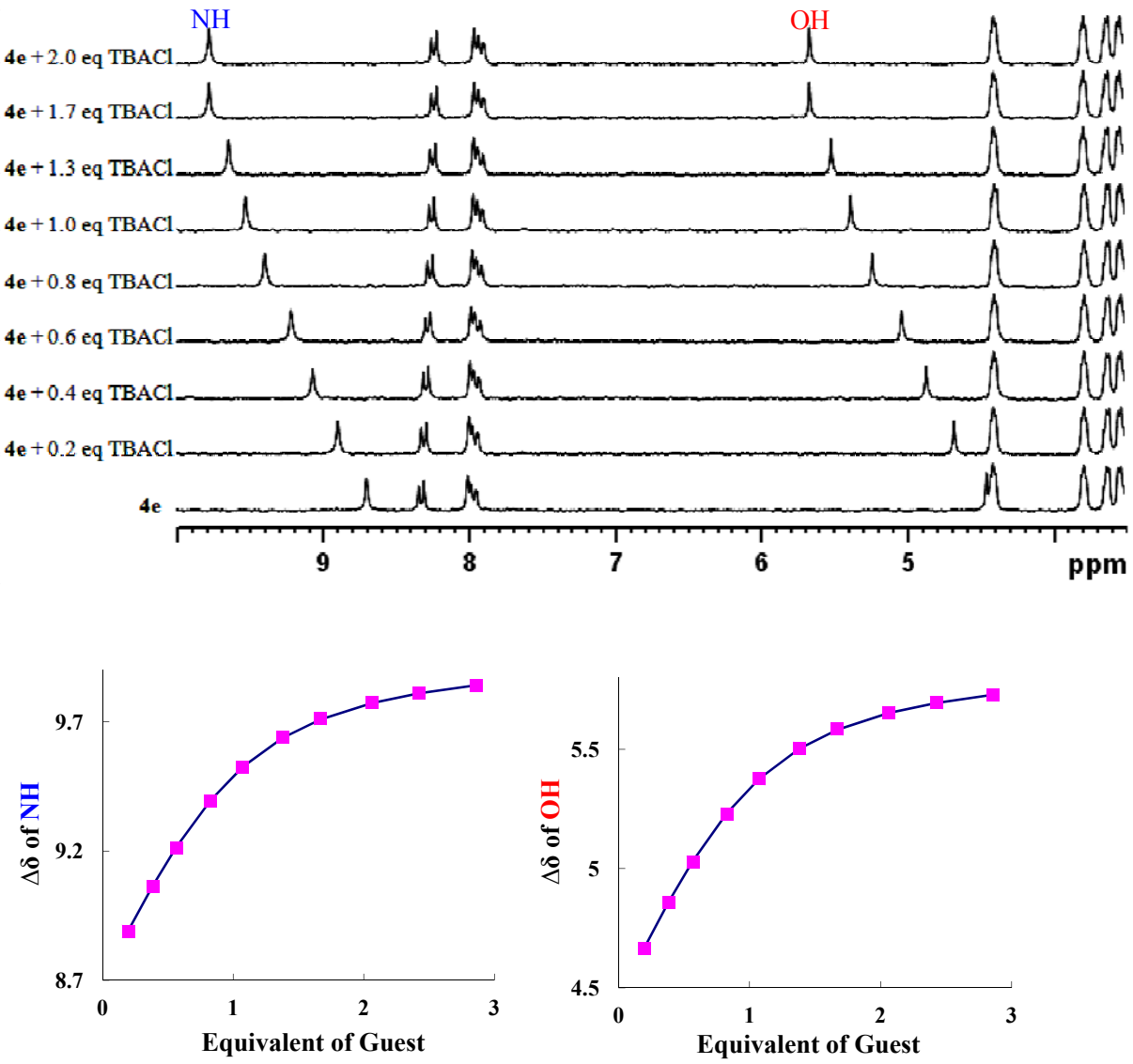


Figure S6. ^1H NMR spectral changes of **4e** upon addition of TBA^+Cl^- (top), and titration curves (bottom) plots for NH (left) and OH (right): the experimental data (dots) are fitted to theoretical ones (lines) with the association constant, $K_a = (8.7 \pm 0.2) \times 10^3\ M^{-1}$.

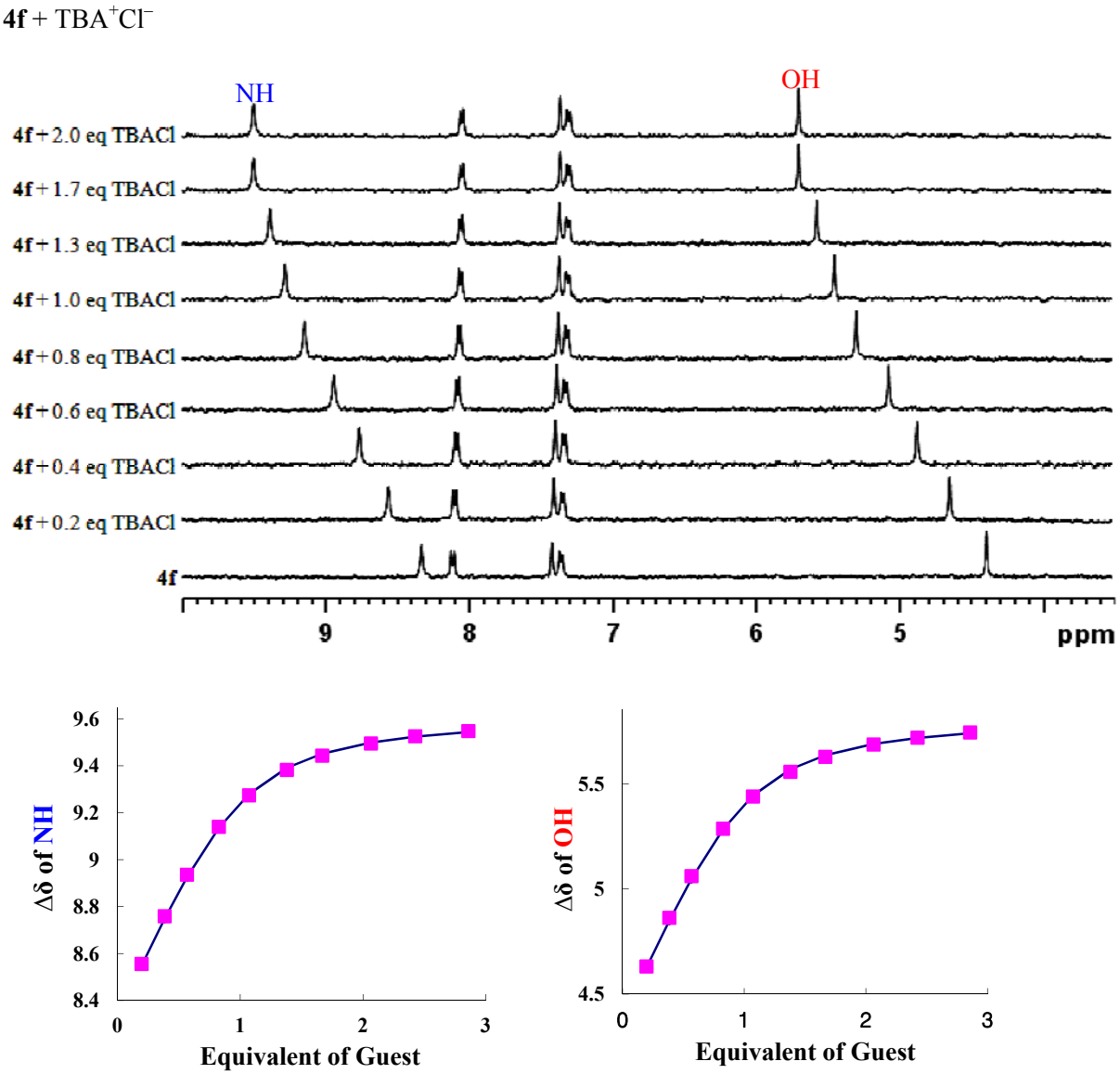


Figure S7. ^{1}H NMR spectral changes of **4f** upon addition of $TBA^{+}Cl^{-}$ (top), and titration curves (bottom) plots for NH (left) and OH (right): the experimental data (dots) are fitted to theoretical ones (lines) with the association constant, $K_a = (1.7 \pm 0.1) \times 10^4\ M^{-1}$.

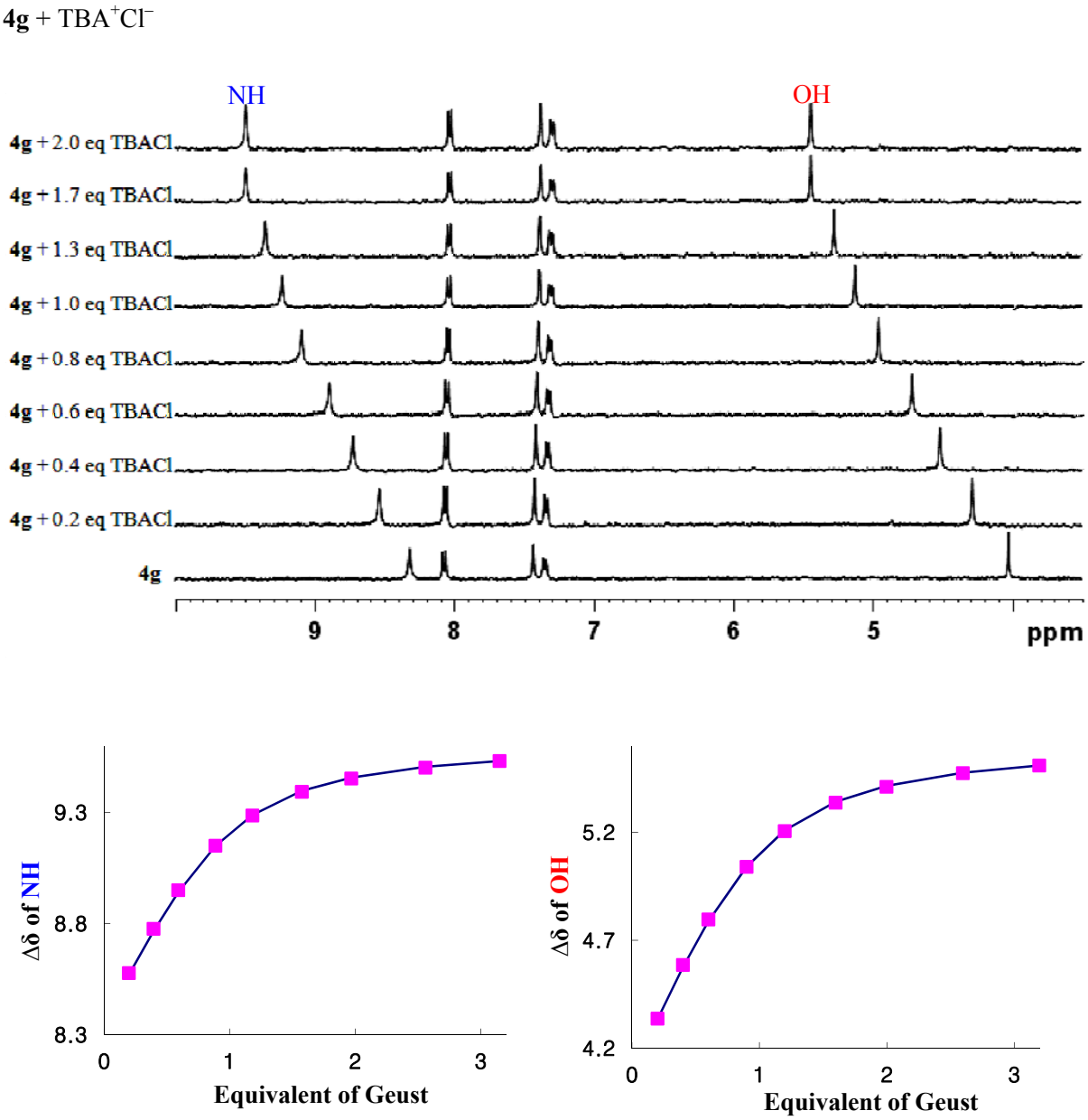


Figure S8. ^{1}H NMR spectral changes of **4g** upon addition of $TBA^{+}Cl^{-}$ (top), and titration curves (bottom) plots for NH (left) and OH (right): the experimental data (dots) are fitted to theoretical ones (lines) with the association constant, $K_a = (1.3 \pm 0.1) \times 10^4\ M^{-1}$.

4h + TBA^+Cl^-

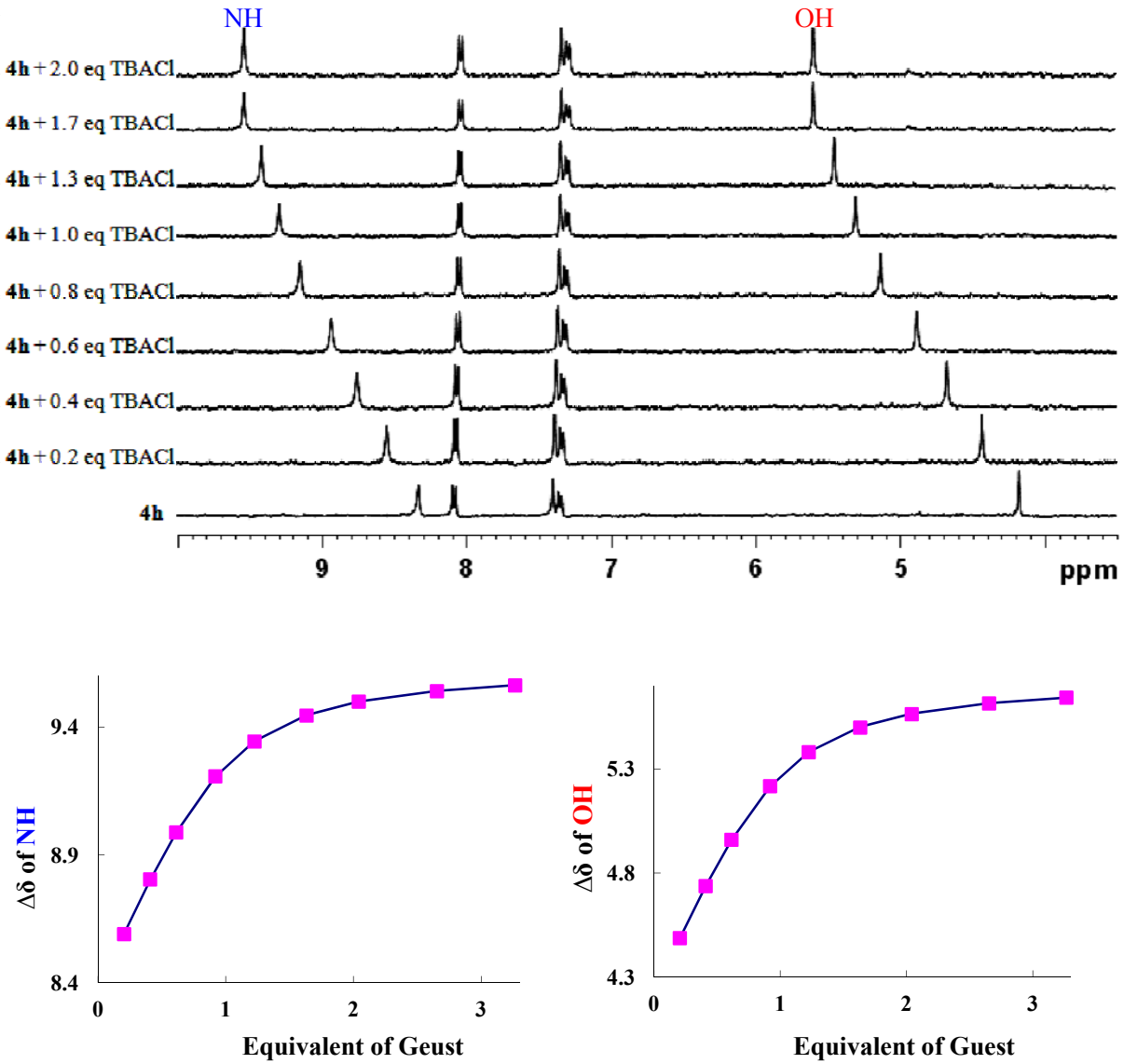
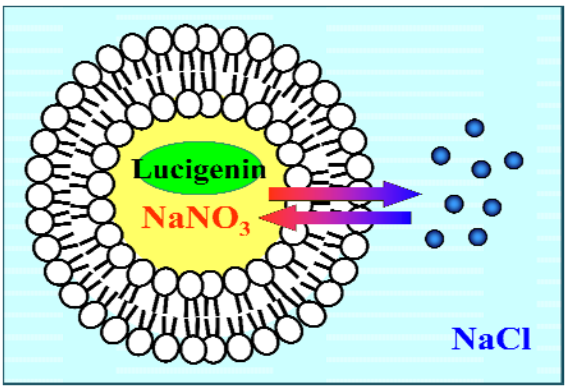


Figure S9. ^{1}H NMR spectral changes of **4h** upon addition of TBA^+Cl^- (top), and titration curves (bottom) plots for NH (left) and OH (right): the experimental data (dots) are fitted to theoretical ones (lines) with the association constant, $K_a = (1.7 \pm 0.1) \times 10^4\ M^{-1}$.

4. Transport experiments



1) Preparation of POPC vesicles

The solution of 1-palmitoyl-2-oleoyl-*sn*-glycero-3-phosphocholine (POPC) (Avanti) in chloroform was evacuated and dried under vacuum for 6 h to form a lipid thin film. The film was rehydrated by vortexing for 5 min with the internal solution (200 mM $NaNO_3$ and 1mM lucigenin and 10 mM phosphate buffer, pH 7.2). Then, the lipid suspension was to complete eight freeze–thaw cycles and allowed to age for 1 h at room temperature followed by extruding 27 times through a 200 nm polycarbonate membrane (Avanti, The Mini-Extruder set). The resulting vesicles were separated from unencapsulated lucigenin by the Sephadex G-50 column (eluent 200 mM $NaNO_3$ and 10 mM phosphate buffer, pH 7.2).

2) Transport Experiments

Unilamellar POPC vesicles, prepared as described above, were diluted in an external solution (200 mM $NaNO_3$ and 10 mM phosphate buffer, pH 7.2) to the lipid concentration was 1 mM. 2 mL of POPC stock solution was transferred to the cuvette and 30 μL of 2 M NaCl and DMSO solution of receptor were added to start the experiment. The chloride influx to the lipid bilayer was detected by fluorescence spectrophotometer. After 400 s, 10% Triton X-100 was added to lipid solution to lyse the vesicles.

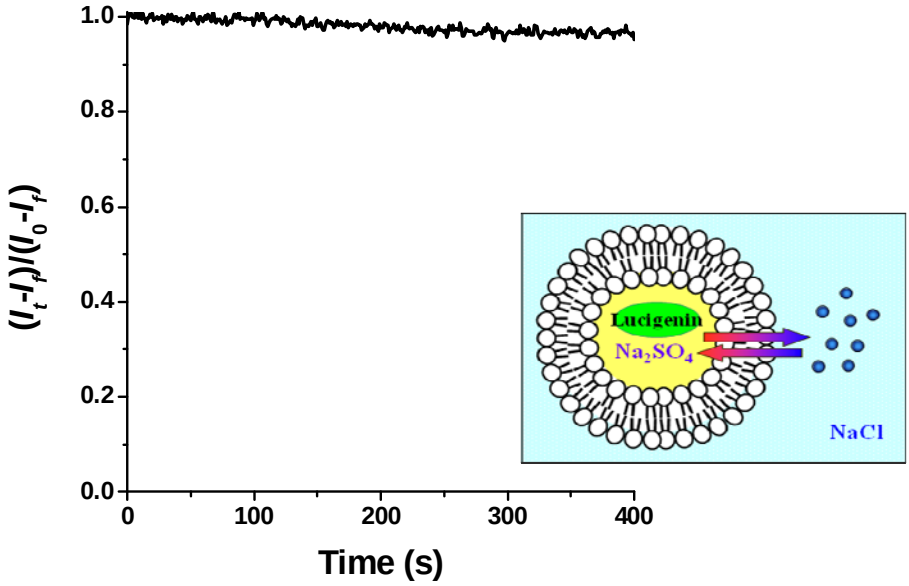


Figure S10. Transport experiments with vesicles containing 100 mM Na_2SO_4, 1 mM lucigenin and 10 mM phosphate buffer pH 7.2, and suspended in phosphate buffer solution (pH = 7.2) containing 200 mM $NaNO_3$ and 30 mM NaCl. The DMSO solution of receptor **4h** (1 mol% relative to POPC) was injected at 0 s. Sulfate is a highly polar anion and challenging to pass through the lipid membrane.

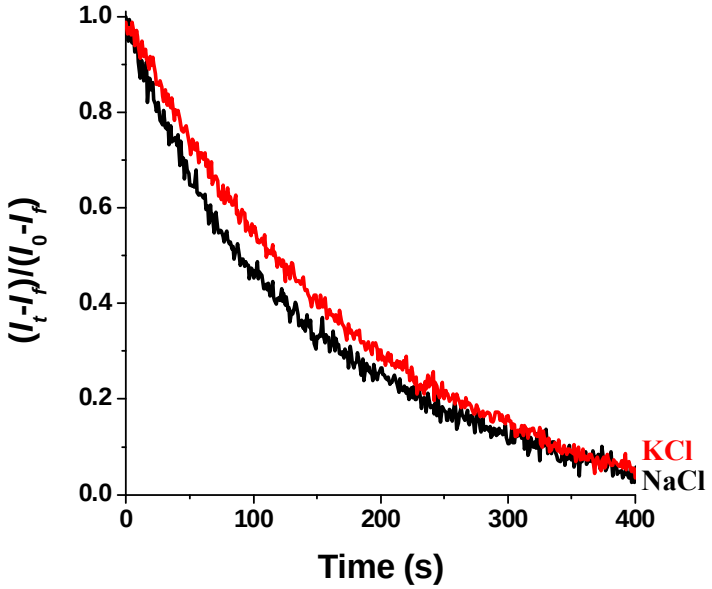


Figure S11. Transport experiments with vesicles containing 200 mM $NaNO_3$, 1 mM lucigenin and 10 mM phosphate buffer pH 7.2, and suspended in phosphate buffer solution (pH = 7.2) containing 200 mM $NaNO_3$ and 30 mM NaCl or KCl. The DMSO solution of receptor **4h** (1 mol% relative to POPC) was injected at 0 s.

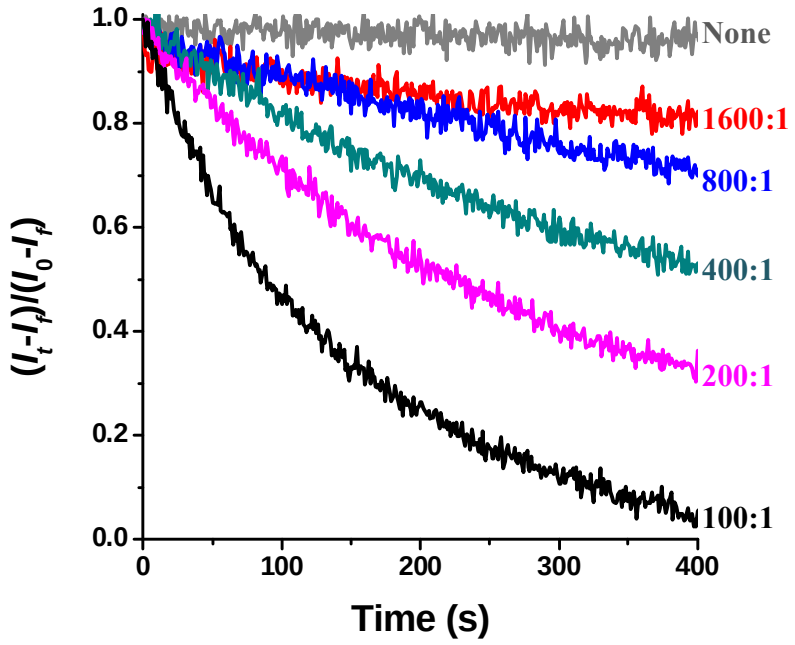


Figure S12. Transport experiments with the different amounts of **4h** (POPC/**4h** 100:1 to 1600:1) in the vesicles containing 200 mM $NaNO_3$, 1 mM lucigenin and 10 mM phosphate buffer pH 7.2, and suspended in phosphate buffer solution (pH = 7.2) containing 200 mM $NaNO_3$ and 30 mM NaCl.

At each receptor concentration, the reaction rate was calculated by first order integrated rate expression.

$$(I_0\text{-}I_t)/(I_0\text{-}I_f) = 1\text{-}e^{-k_{abs}t}$$

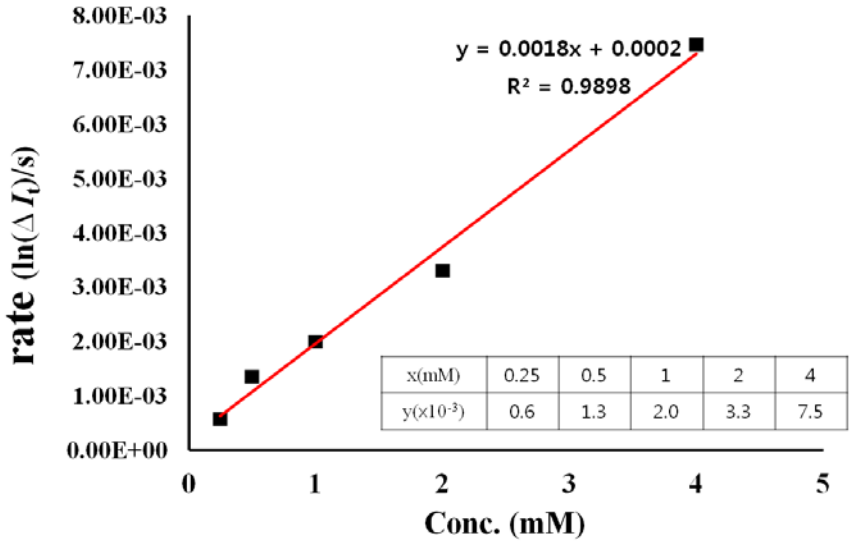


Figure S13. A Plot of transport rates versus concentrations of **4h**.