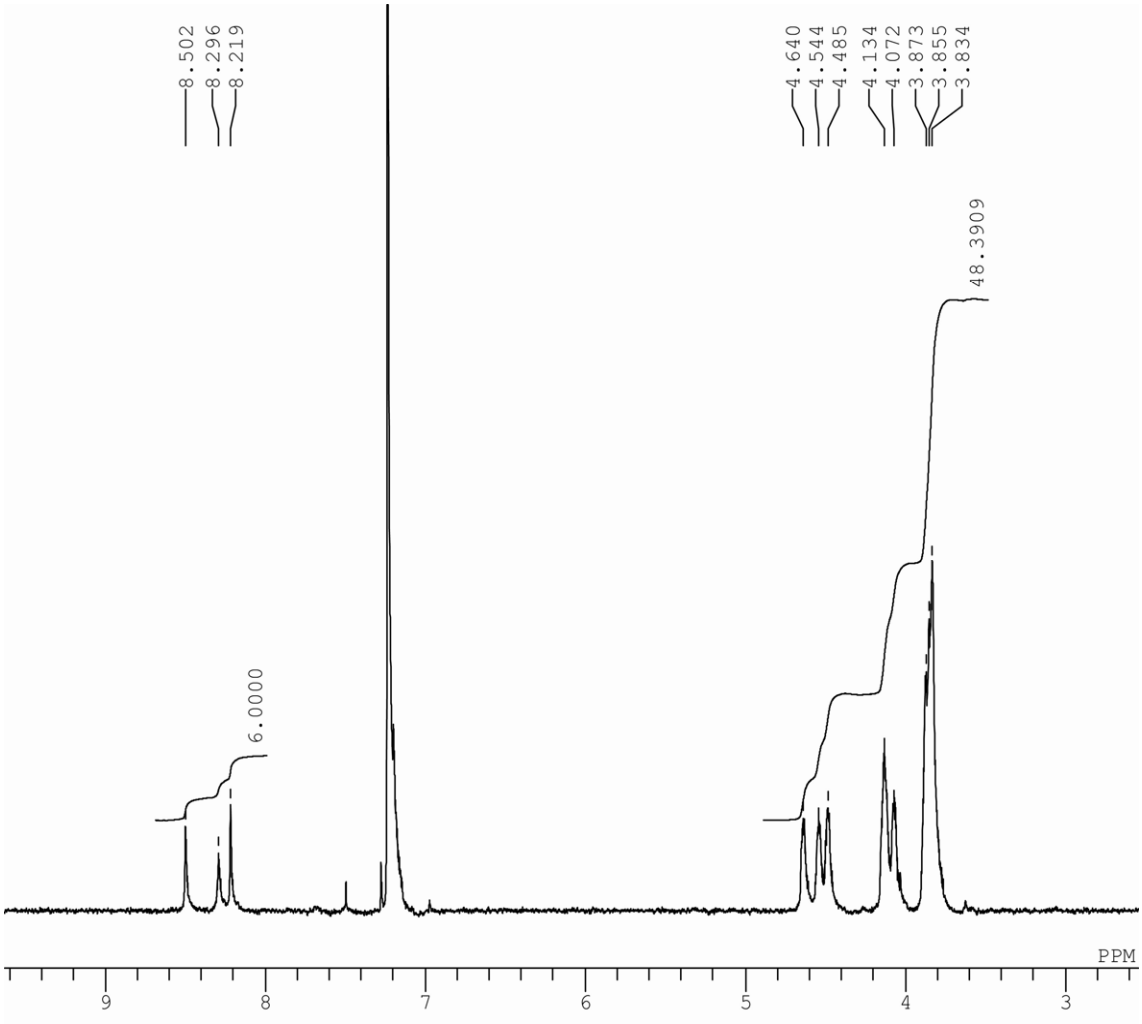
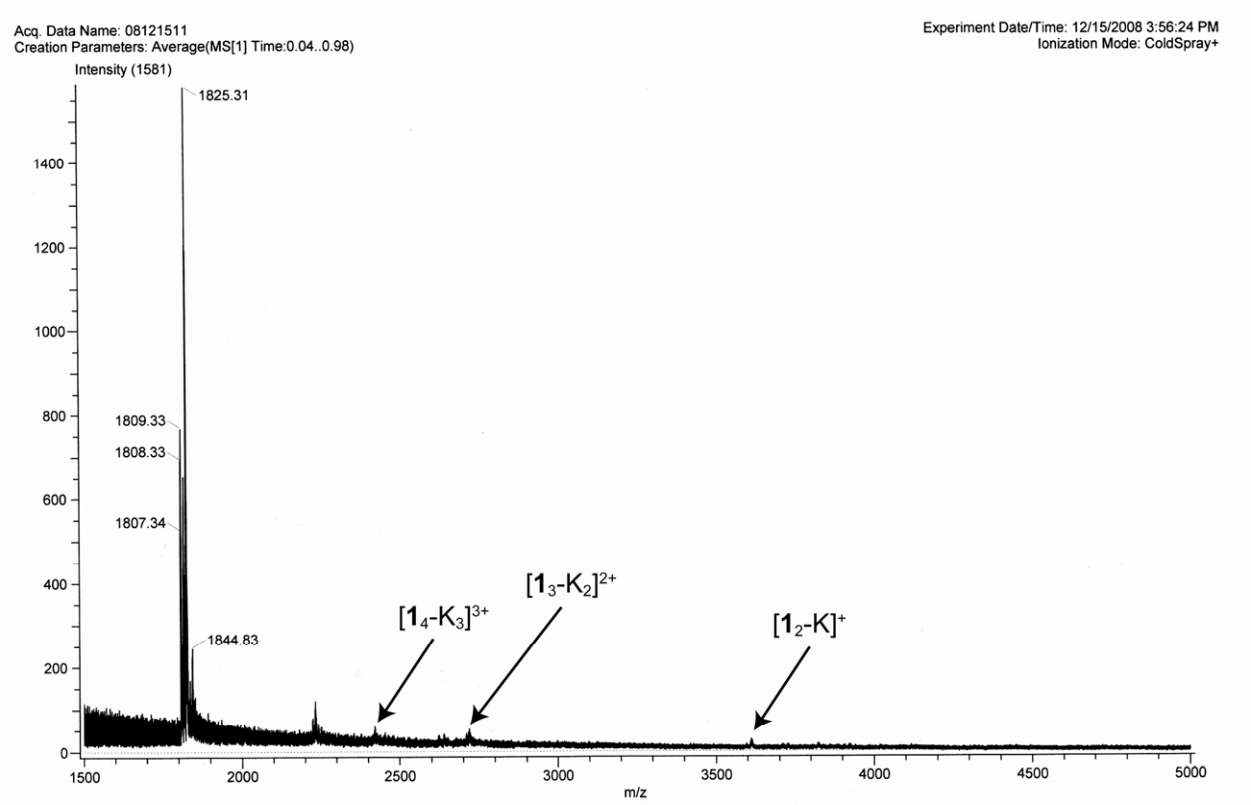
Supplementary material (ESI) for Chemical Communications

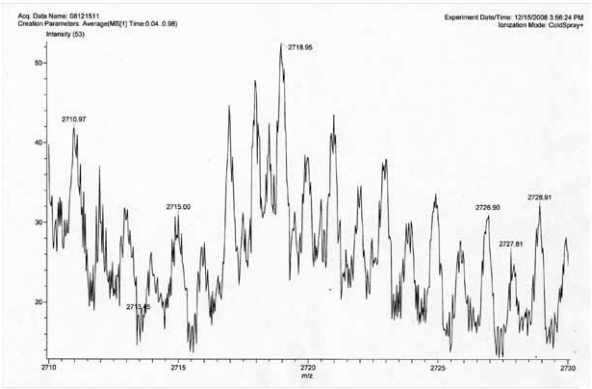
Supporting Information

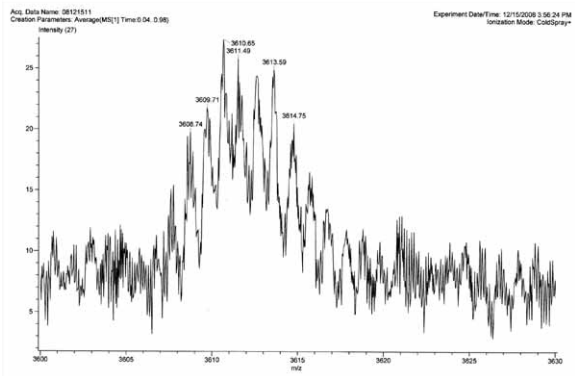
^{1}H NMR spectrum of **1**.



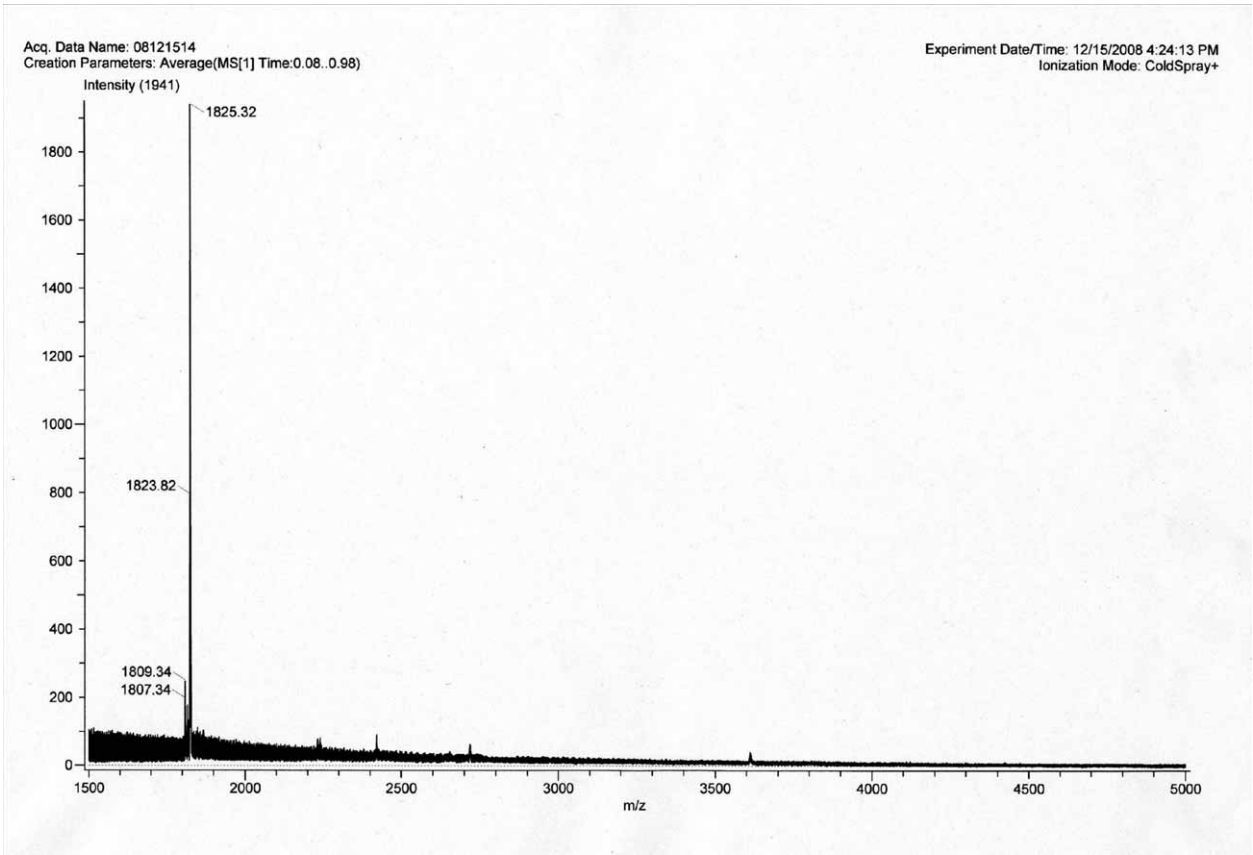
CSI-TOF mass spectra of **1** in $CHCl_3$/MeOH = 1:1 in the presence of K^+ at $[K^+]/[\mathbf{1}]$ = ca. 1.

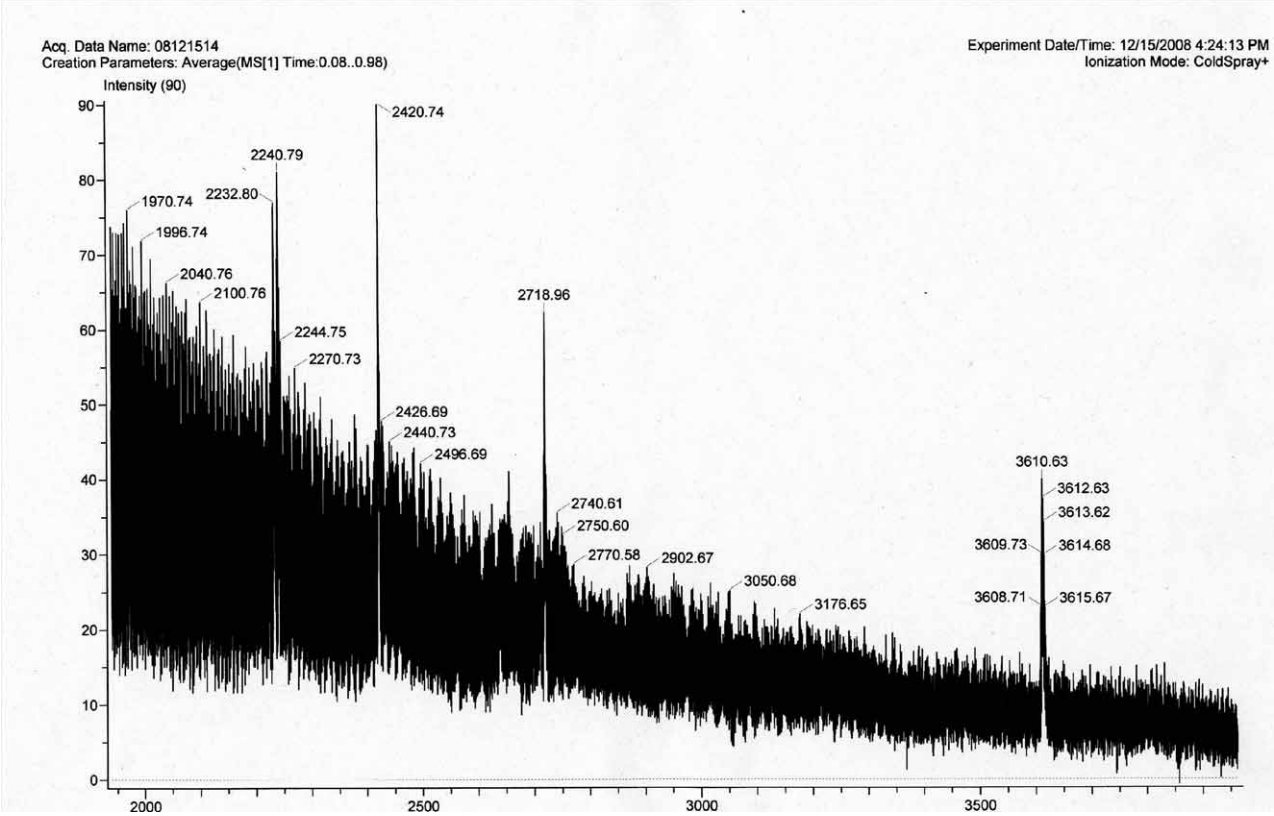






CSI-TOF mass spectra of **1** in $CHCl_3$/MeOH = 1:1 in the presence of K^+ at $[K^+]/[\mathbf{1}]$ = ca. 100.





Determination of K_1 and K_2.

Define the step complex formation constants, K_1 and K_2, as

$$\mathbf{1} + \mathrm{Na}^+ \xleftrightarrow{K_1} \mathbf{1}\mathrm{Na}$$

$$\mathbf{1}\mathrm{Na} + \mathrm{Na}^+ \xleftrightarrow{K_2} \mathbf{1}\mathrm{Na}_2,$$

$$K_1 = \frac{[\mathbf{1}\mathrm{Na}]}{[\mathbf{1}][\mathrm{Na}]}, \quad K_2 = \frac{[\mathbf{1}\mathrm{Na}_2]}{[\mathbf{1}\mathrm{Na}][\mathrm{Na}]}.$$

Therefore,

$$[\mathbf{1}\mathrm{Na}] = K_1[\mathbf{1}][\mathrm{Na}], \quad [\mathbf{1}\mathrm{Na}_2] = K_1K_2[\mathbf{1}][\mathrm{Na}]^2.$$

The initial molar concentration of **1** (or total concentration of **1**) can be defined as

$$S = [\mathbf{1}] + [\mathbf{1}\mathrm{Na}] + [\mathbf{1}\mathrm{Na}_2] = [\mathbf{1}] + K_1[\mathbf{1}][\mathrm{Na}] + K_1K_2[\mathbf{1}][\mathrm{Na}]^2$$
$$= \left(1 + K_1[\mathrm{Na}] + K_1K_2[\mathrm{Na}]^2\right)[\mathbf{1}].$$

The molar fraction of [**1**Na2] can be written as

$$f = \frac{[\mathbf{1}\mathrm{Na}_2]}{S} = \frac{K_1K_2[\mathrm{Na}]^2}{1 + K_1[\mathrm{Na}] + K_1K_2[\mathrm{Na}]^2}.$$

A curve fitting of the experimentally obtained relationship between f and [Na] (Fig. S1, square plots) by using the above formula (red curve) gave two undetermined coefficients, K_1 and K_2. Accordingly, log K_1 and log K_2 are estimated to be 5.39 and –1.00, respectively.

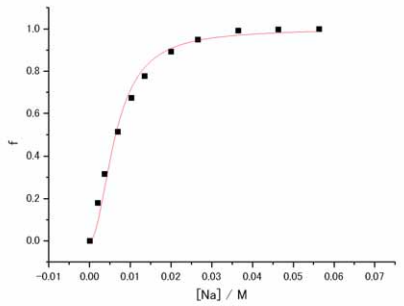


Figure S1 Plot of molar fraction of 1 against [Na]. Result of the curve fitting procedure is depicted by the red curve.