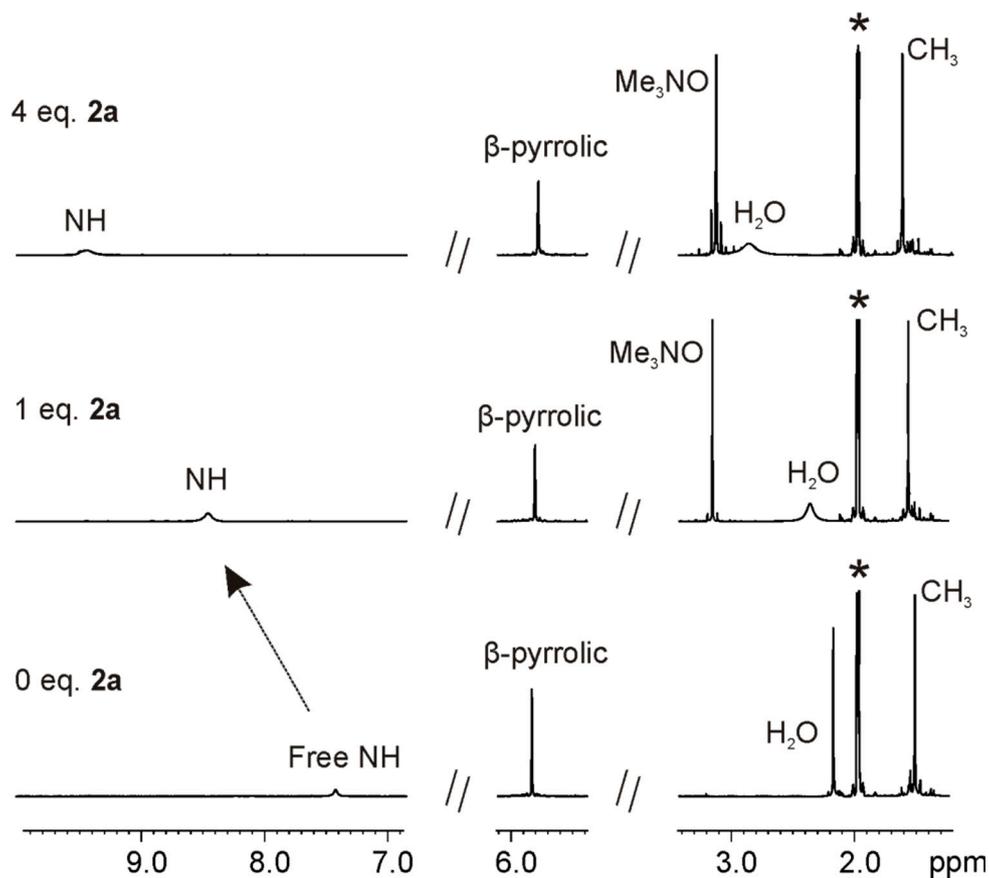
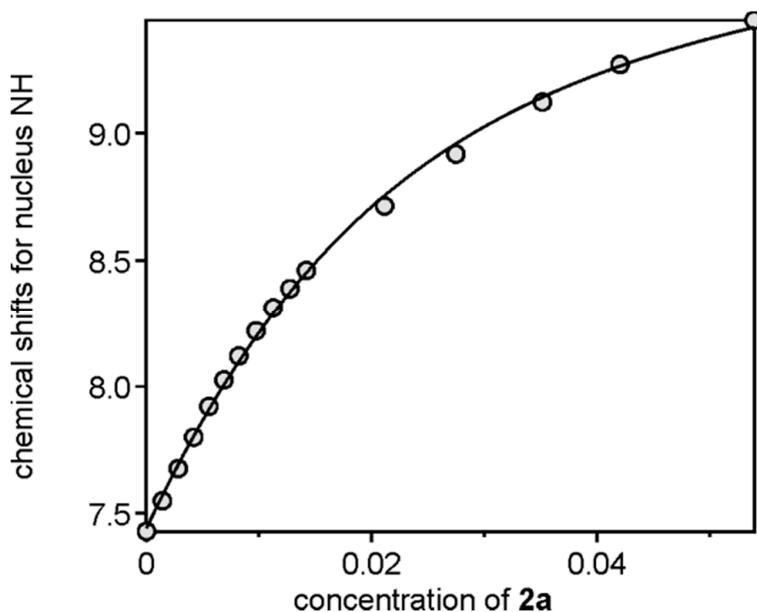


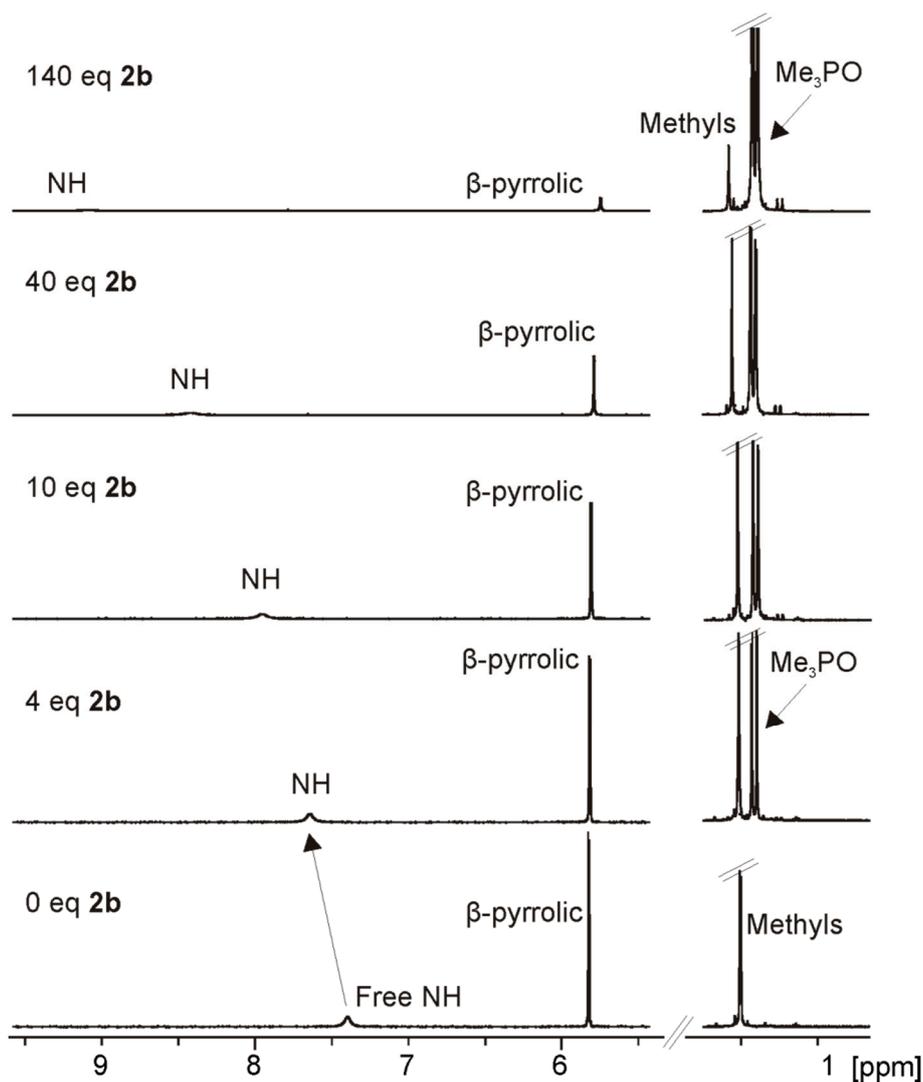
## Supporting Information



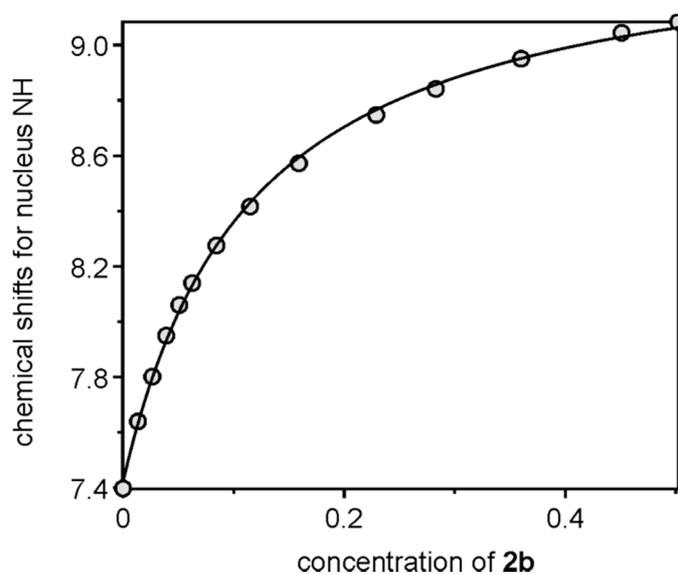
**Figure S1.** Changes in the  $^1\text{H}$ -NMR spectra during the titration of **1a** with **2a** in  $\text{CD}_3\text{CN}$ . \* signal for the proton in partially deuterated solvent  $\text{CHD}_2\text{CN}$ .



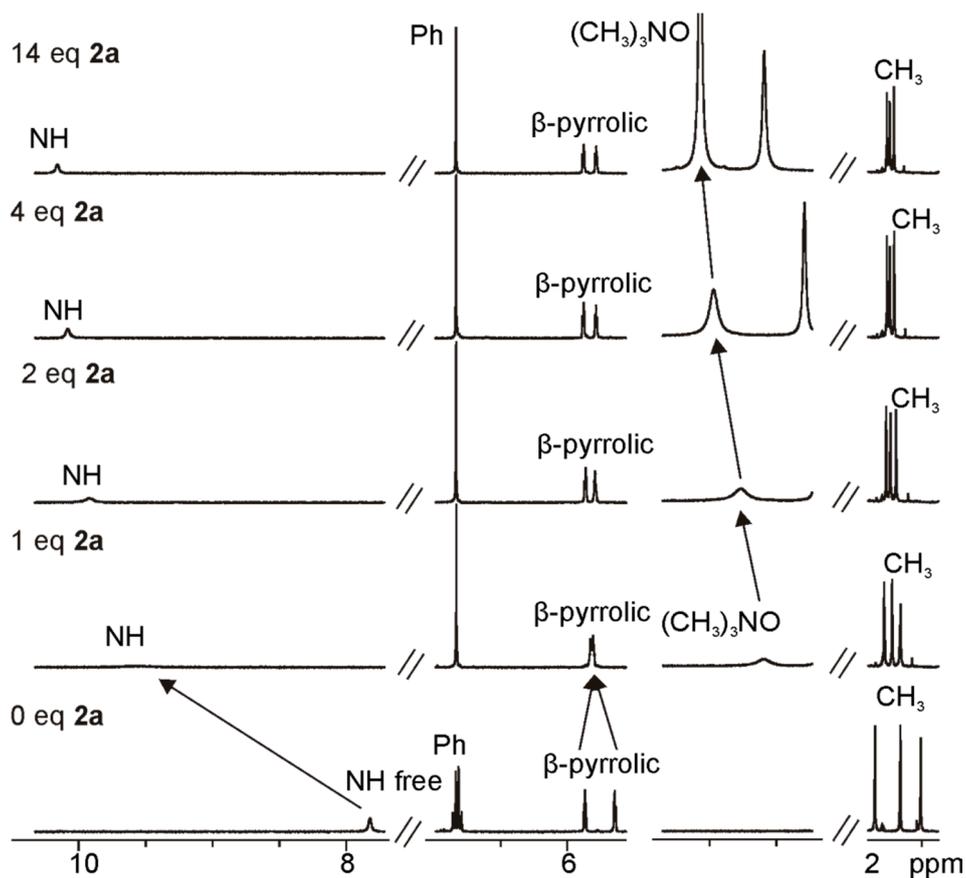
**Figure S2.** Fit of the chemical shift changes, experienced by NH protons of **1a** during the titration with **2a**, using a 1:1 binding model (line) implemented in the HypNMR2008 software.



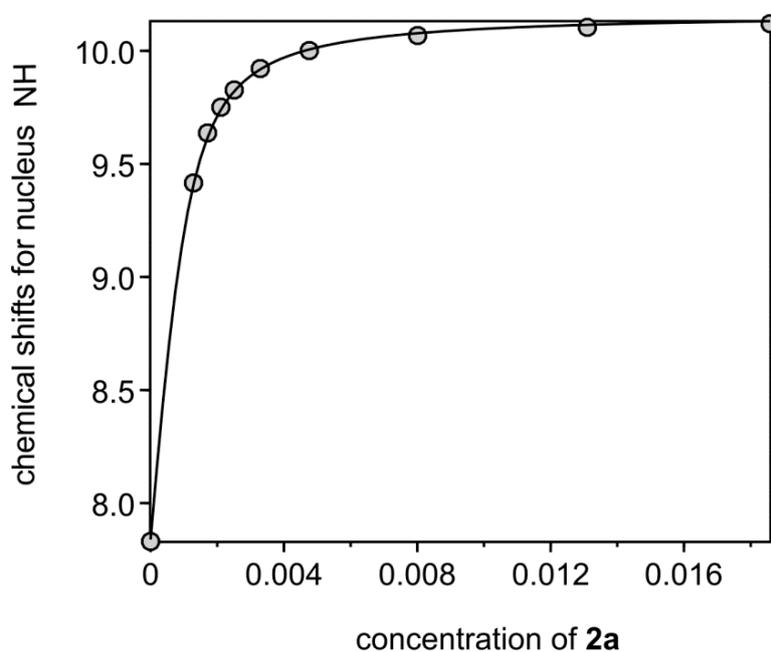
**Figure S3.** Changes in the  $^1\text{H}$ -NMR spectra during the titration of **1a** with **2b** in  $\text{CD}_3\text{CN}$ .



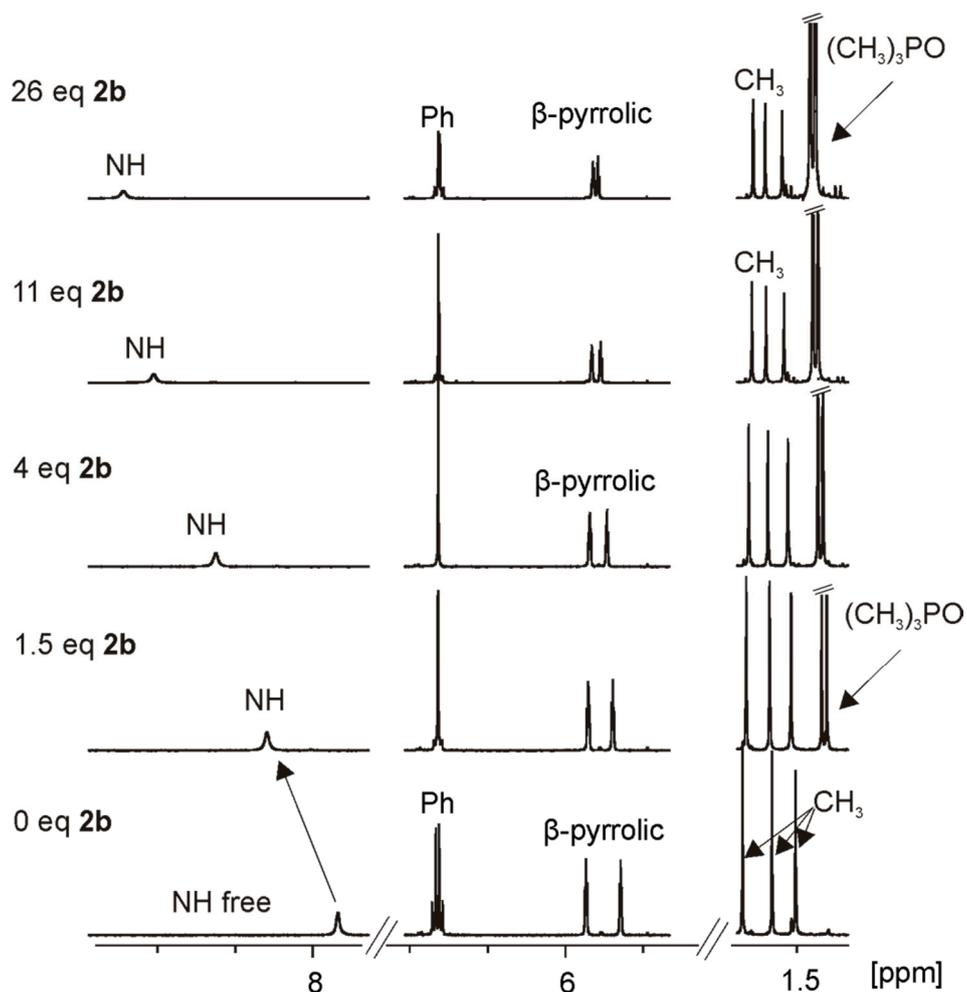
**Figure S4.** Fit of the chemical shift changes, experienced by NH protons of **1a** during the titration with **2b**, using a 1:1 binding model (line) implemented in the HypNMR2008 software.



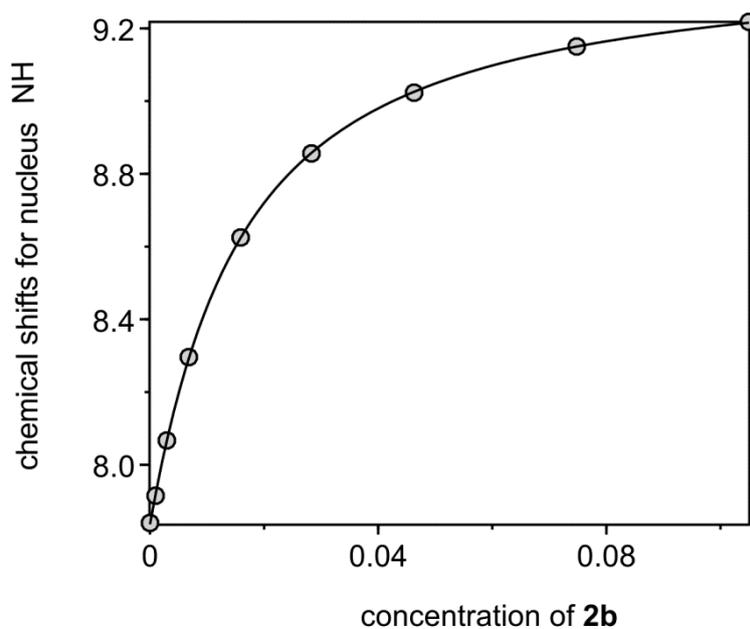
**Figure S5.** Changes in the  $^1\text{H}$ -NMR spectra during the titration of **1b** with **2a** in  $\text{CD}_3\text{CN}$ .



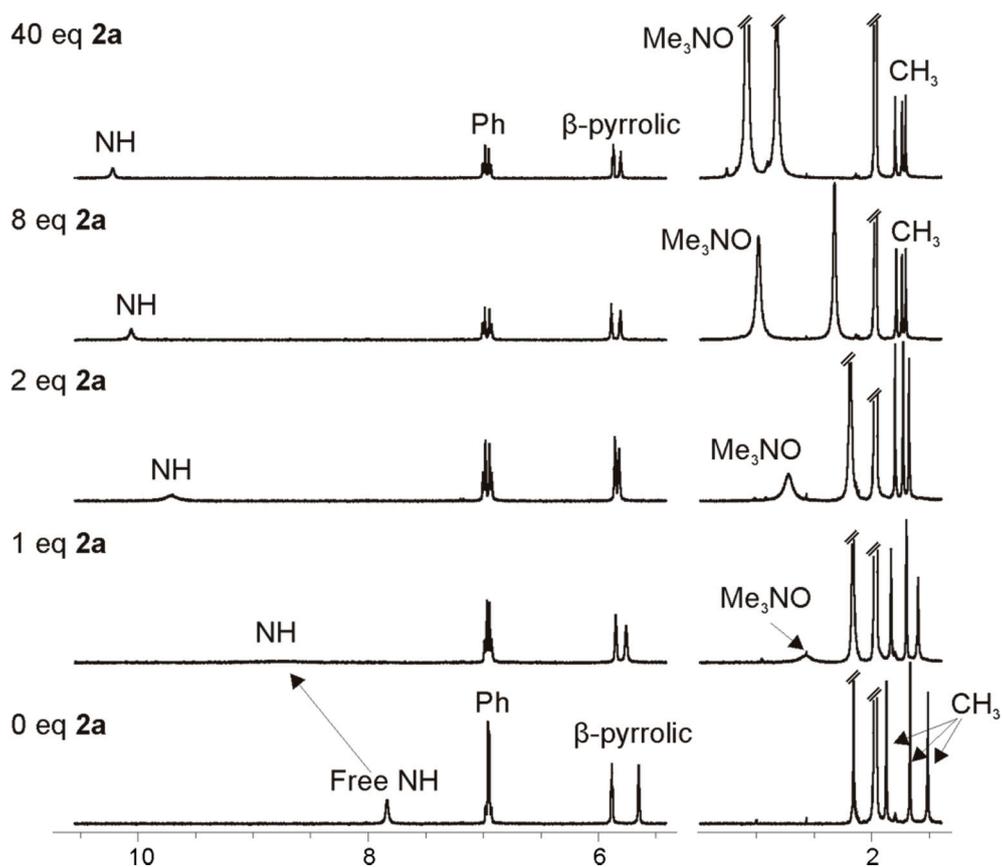
**Figure S6.** Fit of the chemical shift changes, experienced by NH protons of **1b** during the titration with **2a**, using a 1:1 binding model (line) implemented in the HypNMR2008 software.



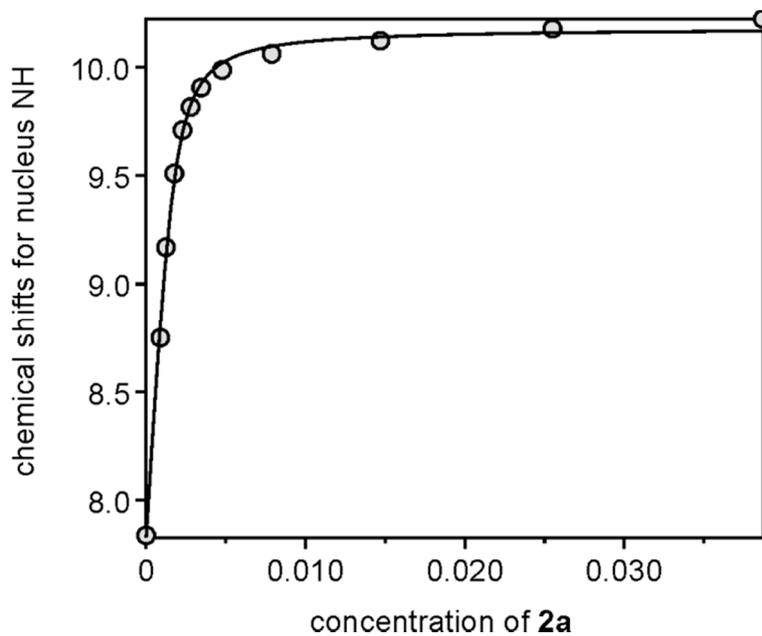
**Figure S7.** Changes in the  $^1\text{H}$ -NMR spectra during the titration of **1b** with **2b** in  $\text{CD}_3\text{CN}$ .



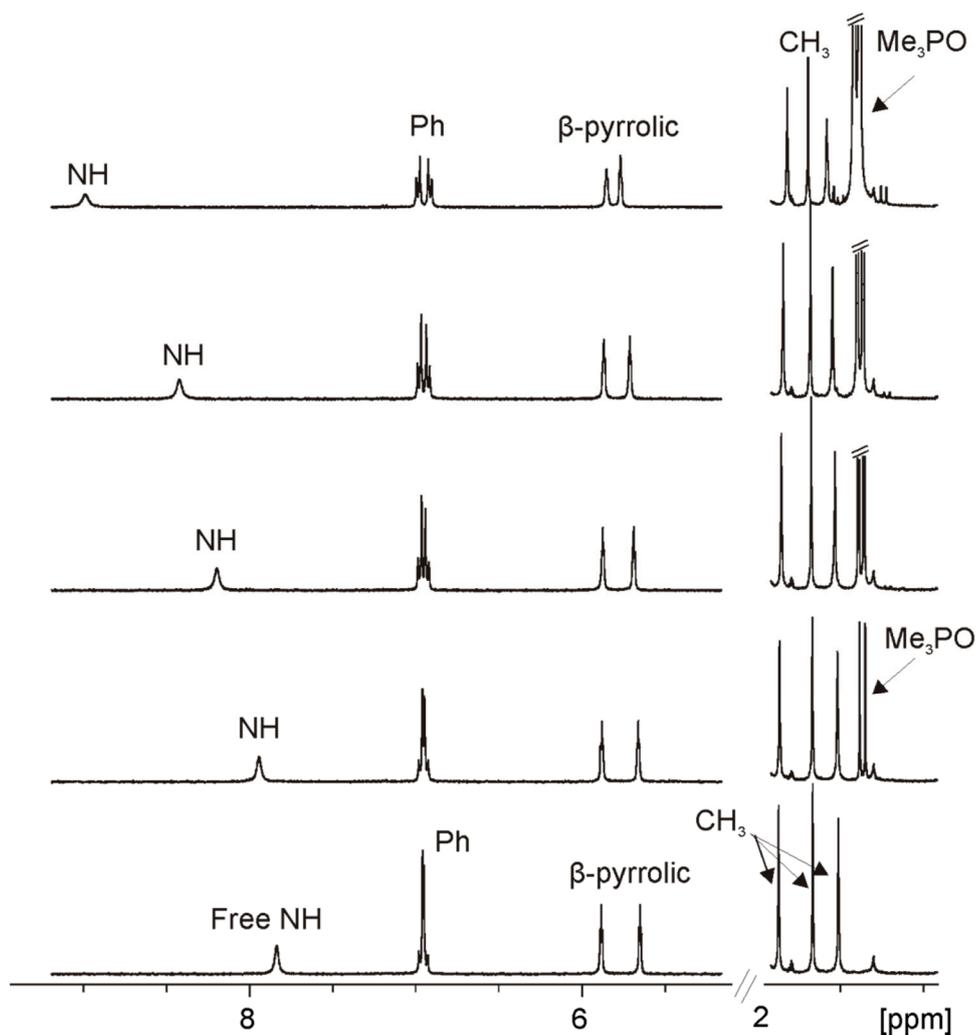
**Figure S8.** Fit of the chemical shift changes, experienced by NH protons of **1b** during the titration with **2b**, using a 1:1 binding model (line) implemented in the HypNMR2008 software.



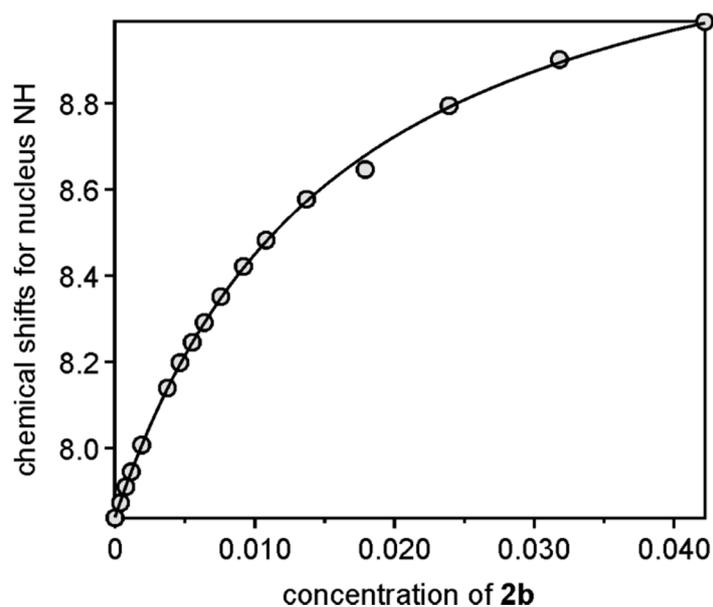
**Figure S9.** Changes in the  $^1\text{H}$ -NMR during the titration of **1c** with **2a** in  $\text{CD}_3\text{CN}$ .



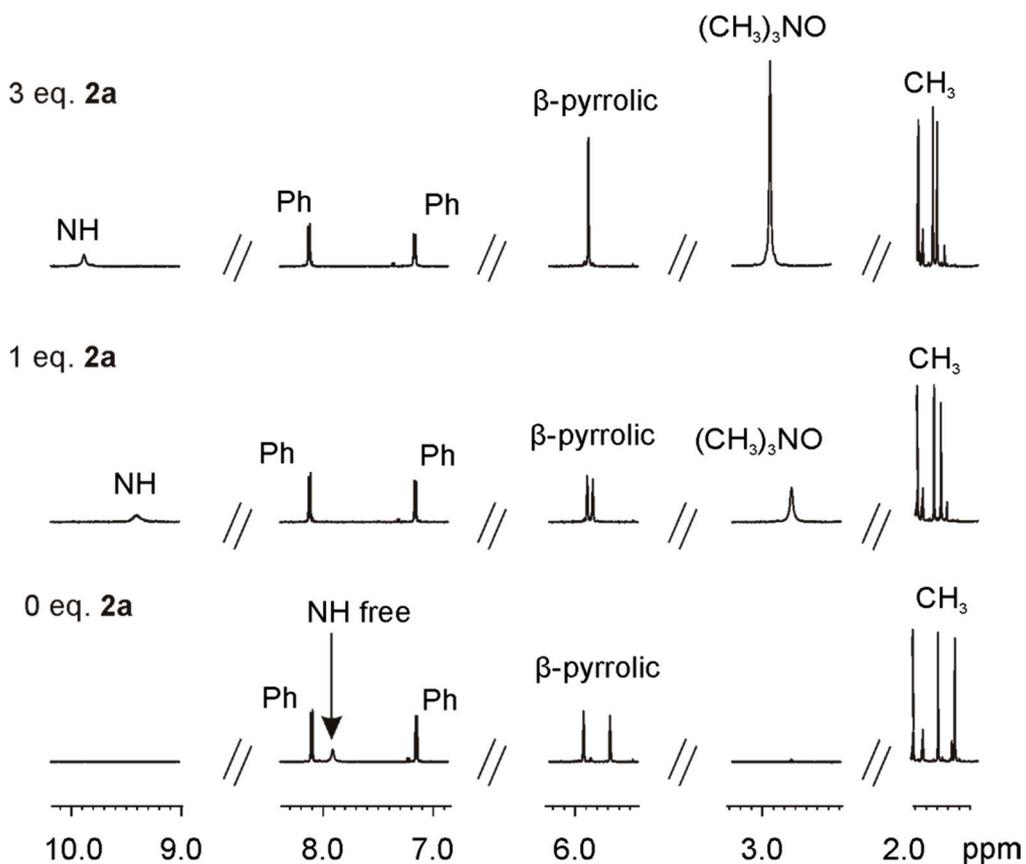
**Figure S10.** Fit of the chemical shift changes, experienced by NH protons of **1c** during the titration with **2a**, using a 1:1 binding model (line) implemented in the HypNMR2008 software.



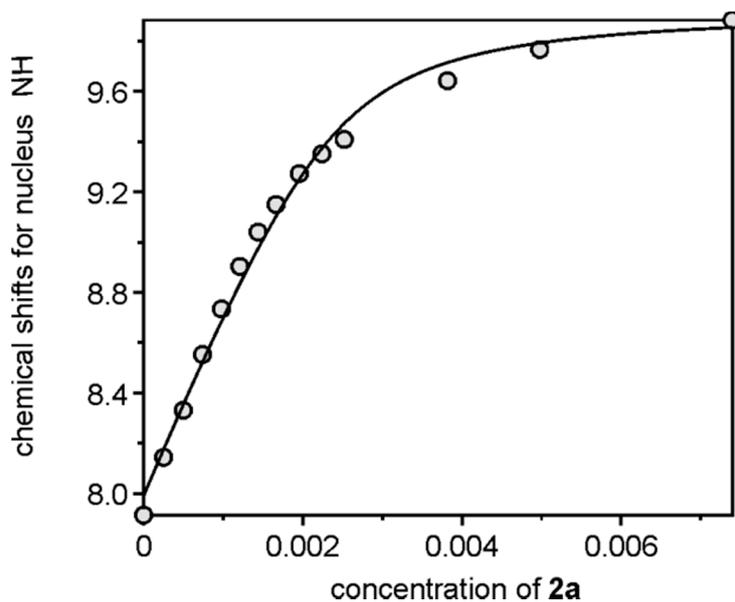
**Figure S11.** Changes in the  $^1\text{H-NMR}$  during the titration of **1c** with **2b** in  $\text{CD}_3\text{CN}$ .



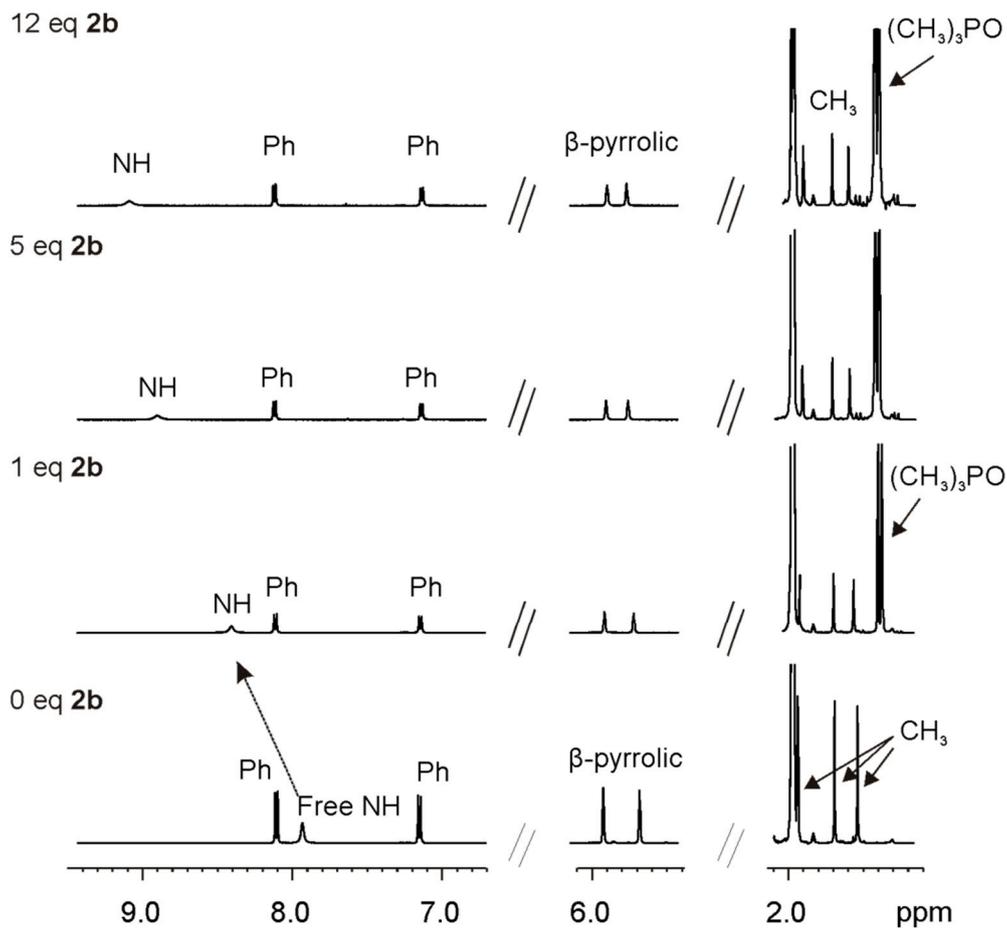
**Figure S12.** Fit of the chemical shift changes, experienced by NH protons of **1c** during the titration with **2b**, using a 1:1 binding model (line) implemented in the HypNMR2008 software.



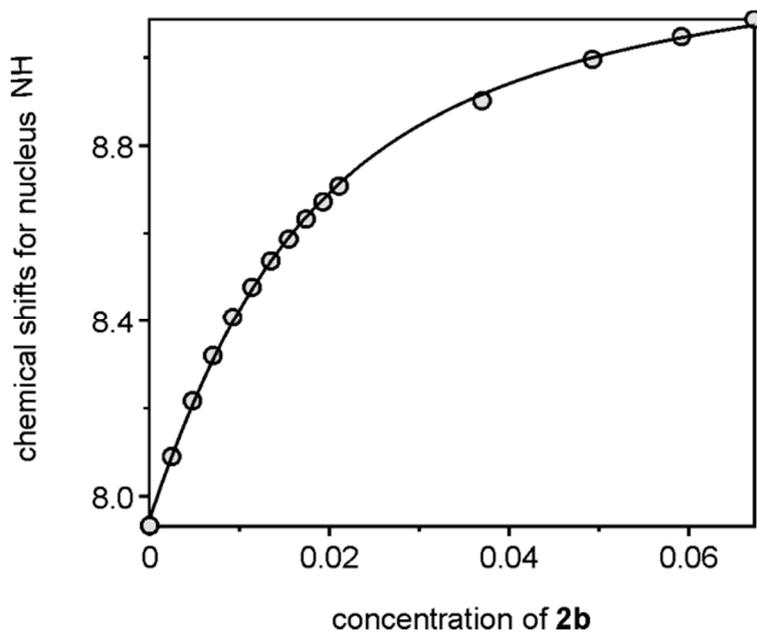
**Figure S13.** Changes in the  $^1\text{H-NMR}$  spectra during the titration of **1d** with **2a** in  $\text{CD}_3\text{CN}$ .



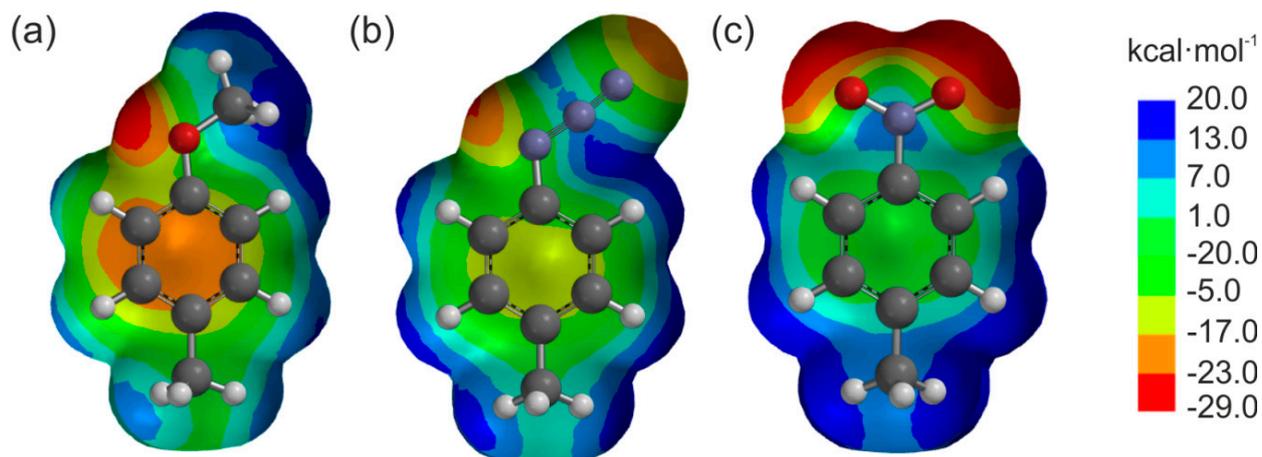
**Figure S14.** Fit of the chemical shift changes, experienced by NH protons of **1d** during the titration with **2a**, using a 1:1 binding model (line) implemented in the HypNMR2008 software.



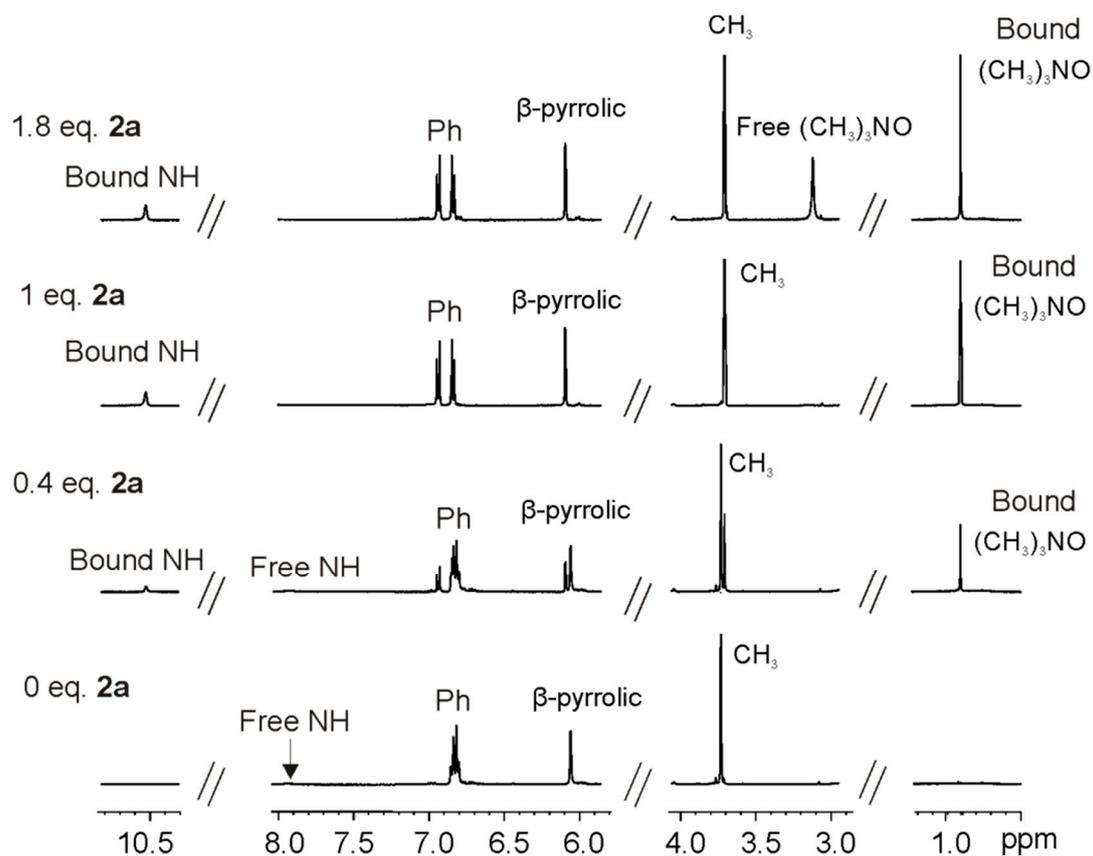
**Figure S15.** Changes in the  $^1\text{H-NMR}$  spectra during the titration of **1d** with **2b** in  $\text{CD}_3\text{CN}$ .



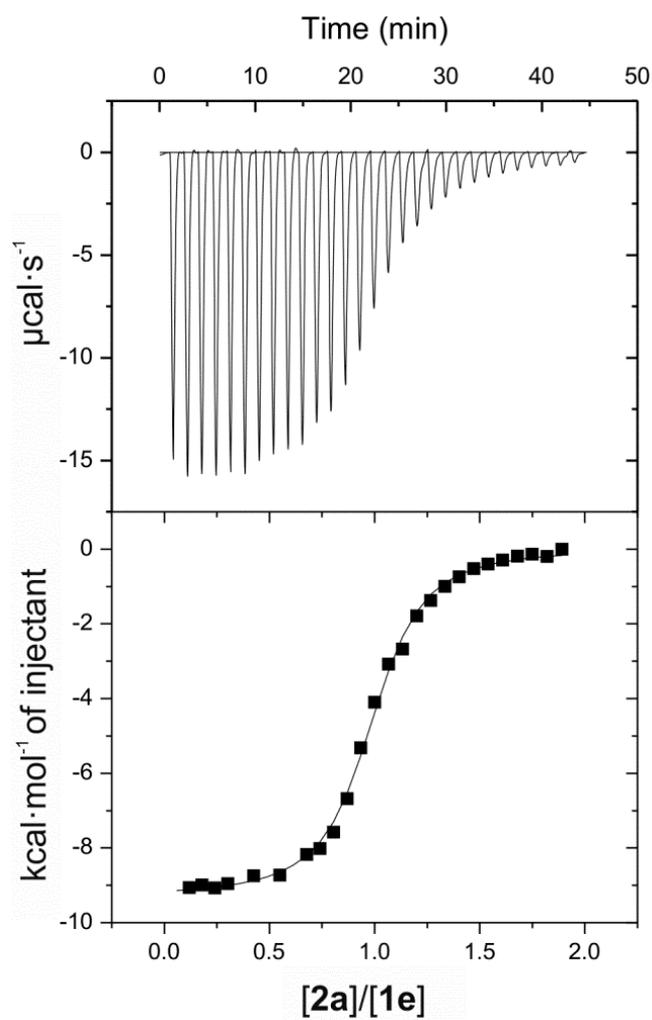
**Figure S16.** Fit of the chemical shift changes, experienced by NH protons of **1d** during the titration with **2b**, using a 1:1 binding model (line) implemented in the HypNMR2008 software.



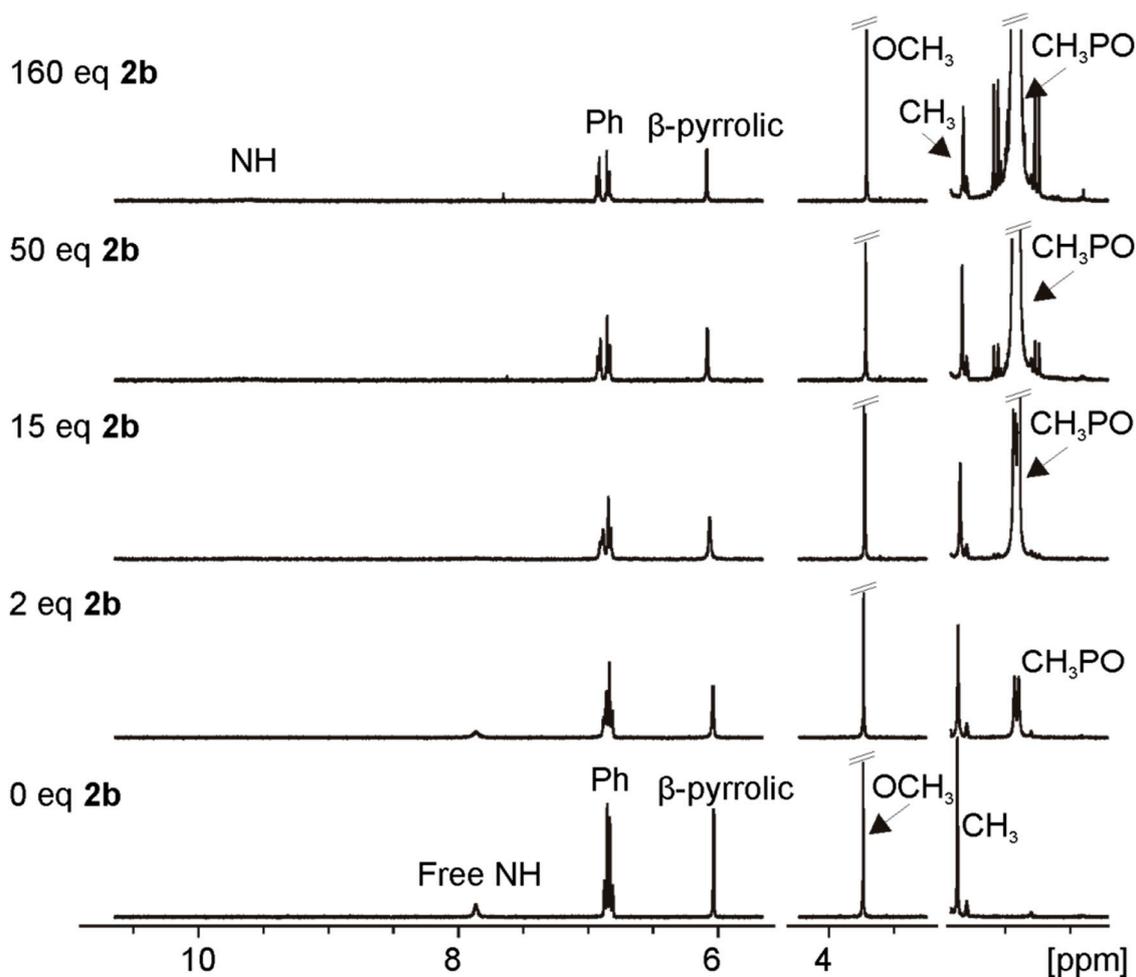
**Figure S17.** Representation of the electrostatic potential on the Van der Waals surface corresponding to the aromatic walls of **1b** (a) **1c** (b) and **1d** (c). The surface was calculated by using B3LYP 6-31G\* in vacuum.



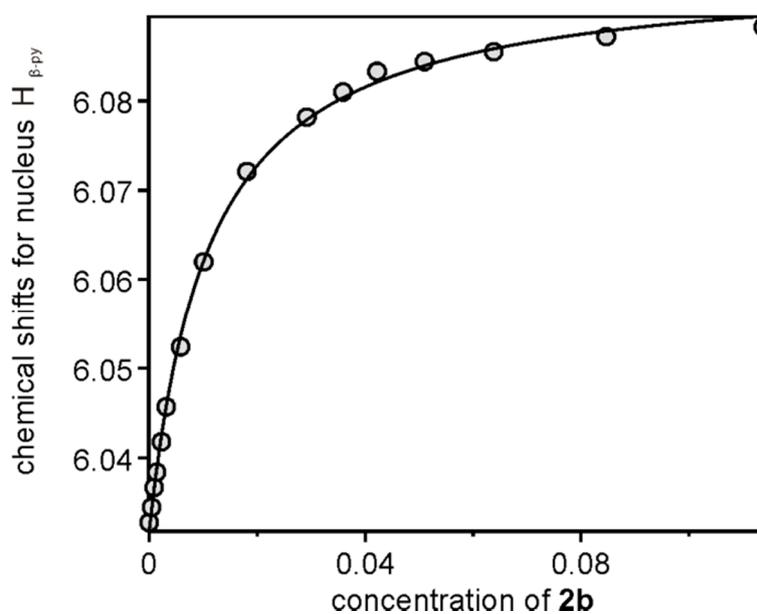
**Figure S18.** Changes in the  $^1\text{H-NMR}$  spectra during the titration of **1e** with **2a** in  $\text{CD}_3\text{CN}$ .



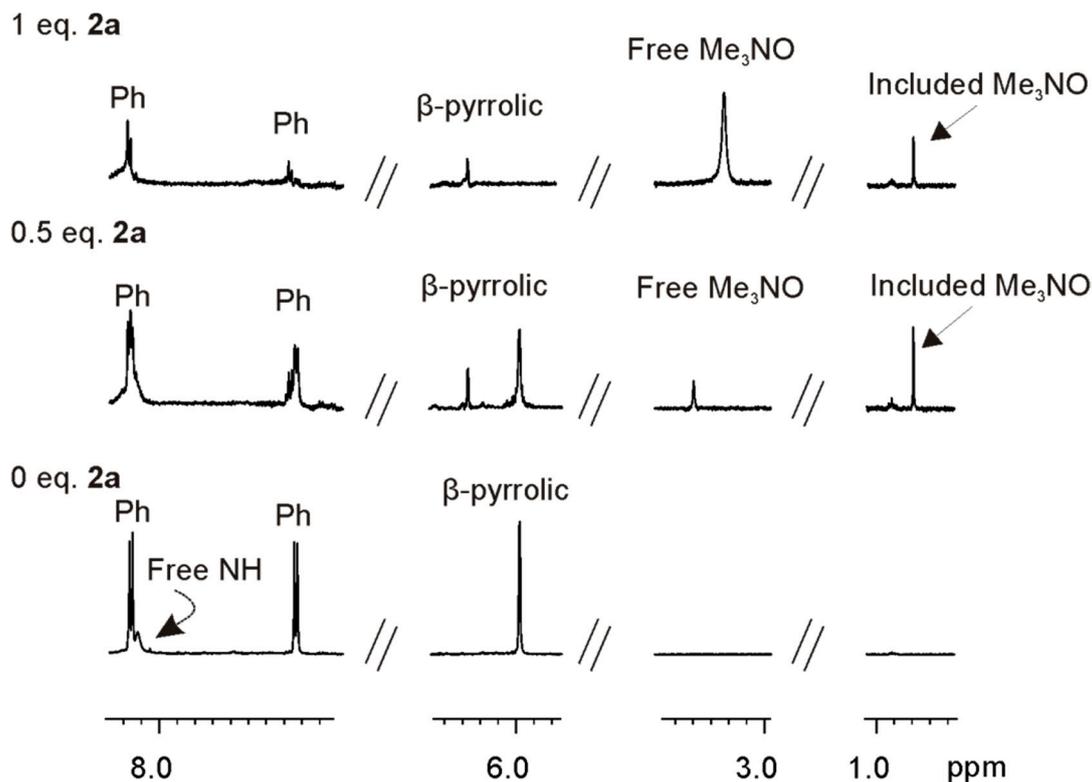
**Figure S19.** ITC titration experiment of the formation of the  $\mathbf{2a} \subset \mathbf{1e}$  complex. **Top:** rawdata; **Bottom:** normalized integration data of the evolved heat per injection in terms of  $\text{kcal}\cdot\text{mol}^{-1}$  of injectant ( $\mathbf{2a}$ ) plotted against the molar ratio  $\mathbf{2a-1e}$ . To determine the values of the thermodynamic variables the ITC data have been fitted to a 1:1 binding model (black line).



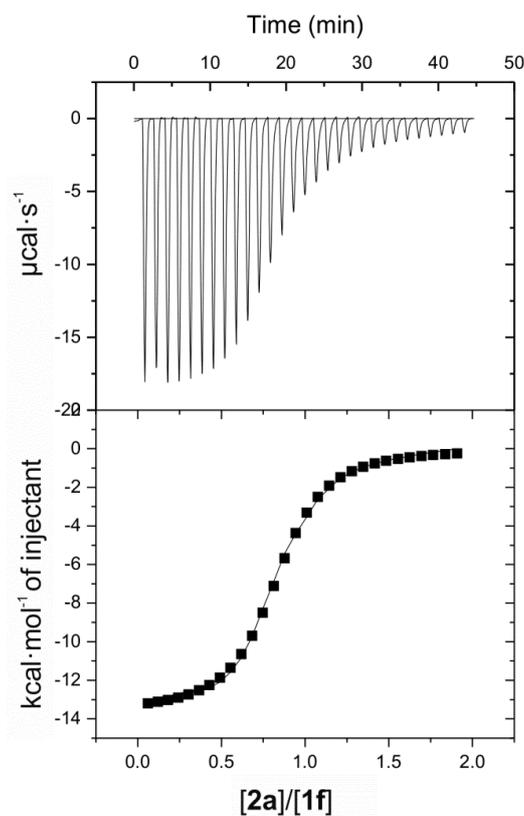
**Figure S20.** Changes in the  $^1\text{H}$ -NMR spectra during the titration of **1e** with **2b** in  $\text{CD}_3\text{CN}$ .



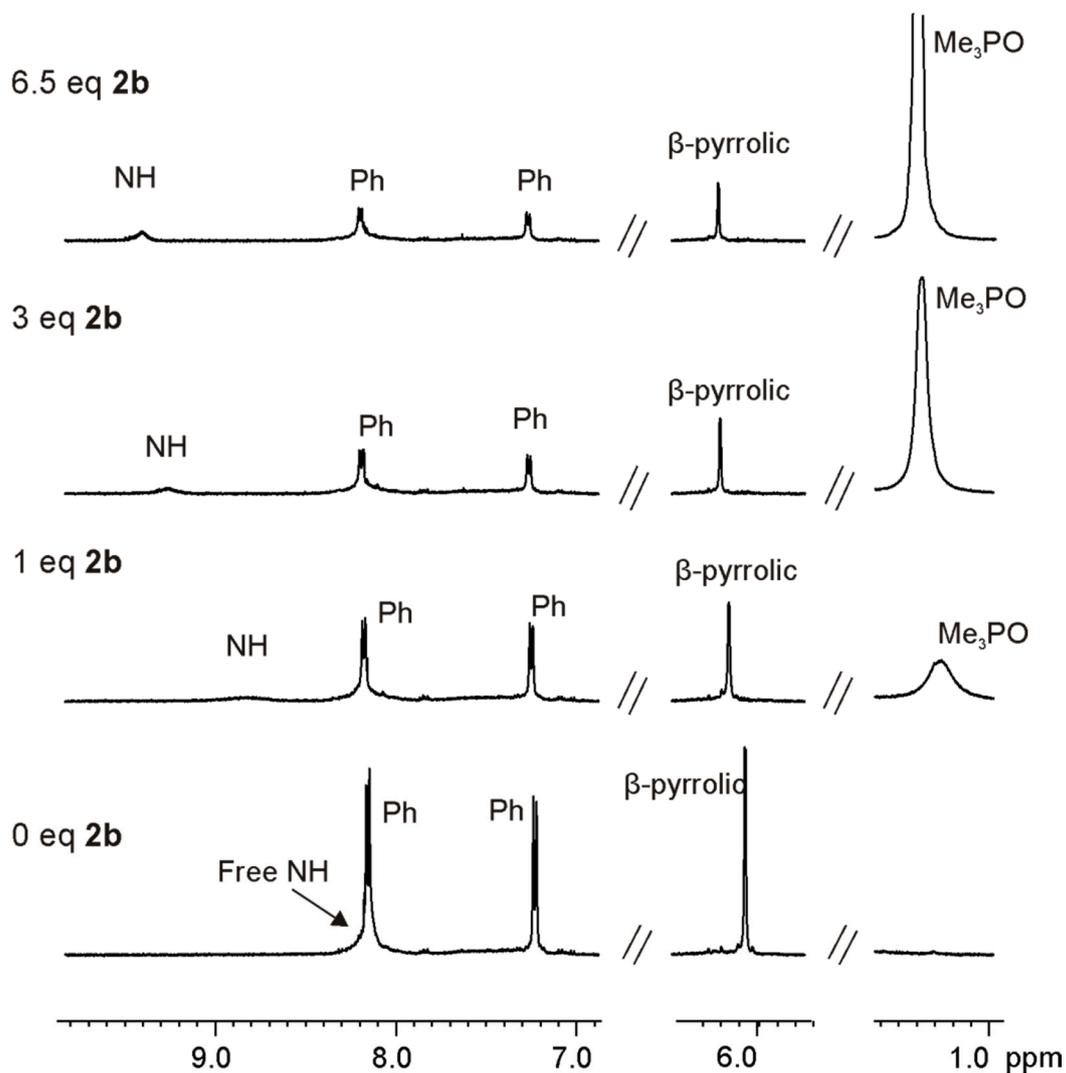
**Figure S21.** Fit of the chemical shift changes, experienced by NH protons of **1e** during the titration with **2b**, using a 1:1 binding model (line) implemented in the HypNMR2008 software.



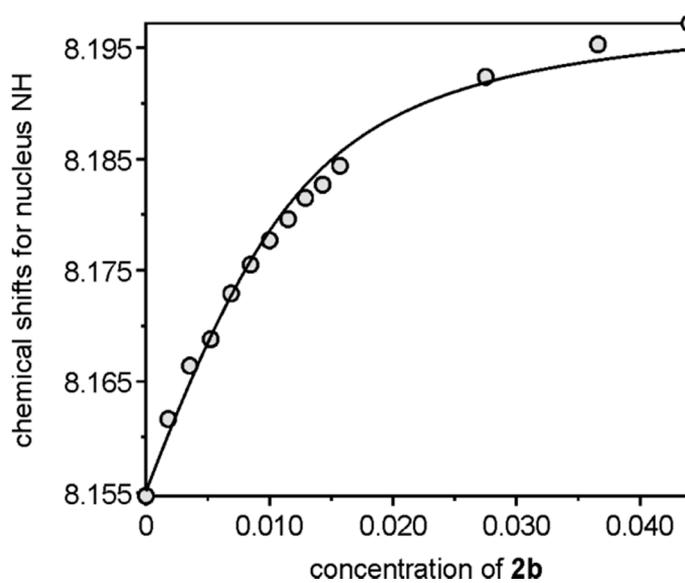
**Figure S22.** Changes in the  $^1\text{H-NMR}$  spectra during the titration of **1f** with **2a** in  $\text{CD}_3\text{CN}$ .



**Figure S23.** ITC titration experiment of the formation of the **2a**  $\subset$  **1f** complex. Top: rawdata. Bottom: normalized integration data of the evolved heat per injection in terms of  $\text{kcal}\cdot\text{mol}^{-1}$  of injectant (**2a**) plotted against the molar ratio **2a**–**1f**. To determine the values of the thermodynamic variables the ITC data have been fitted to a 1:1 binding model (black line).



**Figure S24.** Changes in the  $^1\text{H}$ -NMR spectra during the titration of **1f** with **2b** in  $\text{CD}_3\text{CN}$ .



**Figure S25.** Fit of the chemical shift changes, experienced by NH protons of **1f** during the titration with **2b**, using a 1:1 binding model (line) implemented in the HypNMR2008 software.