

SUPPORTING INFORMATION

Surfactant-assisted chromogenic sensing of cyanide in water

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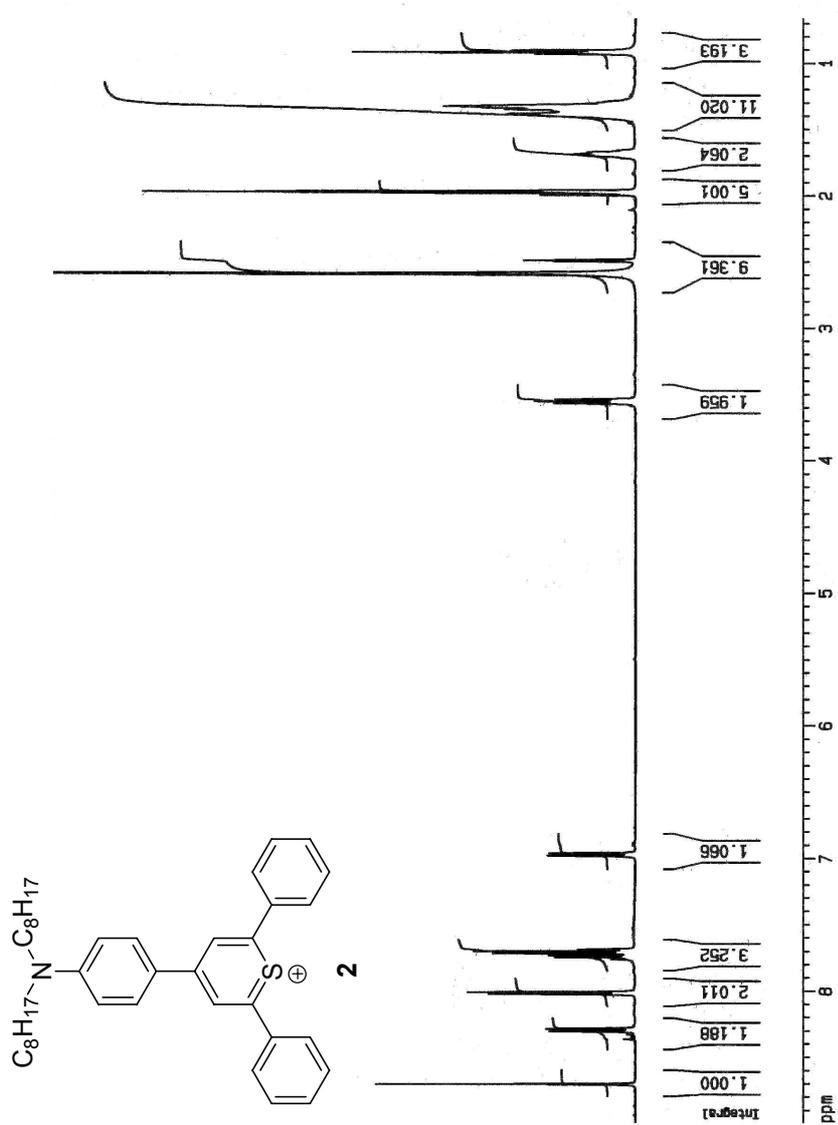


Figure SI-1. $^1\text{H-NMR}$ spectra of receptor **2** in CD_3CN .

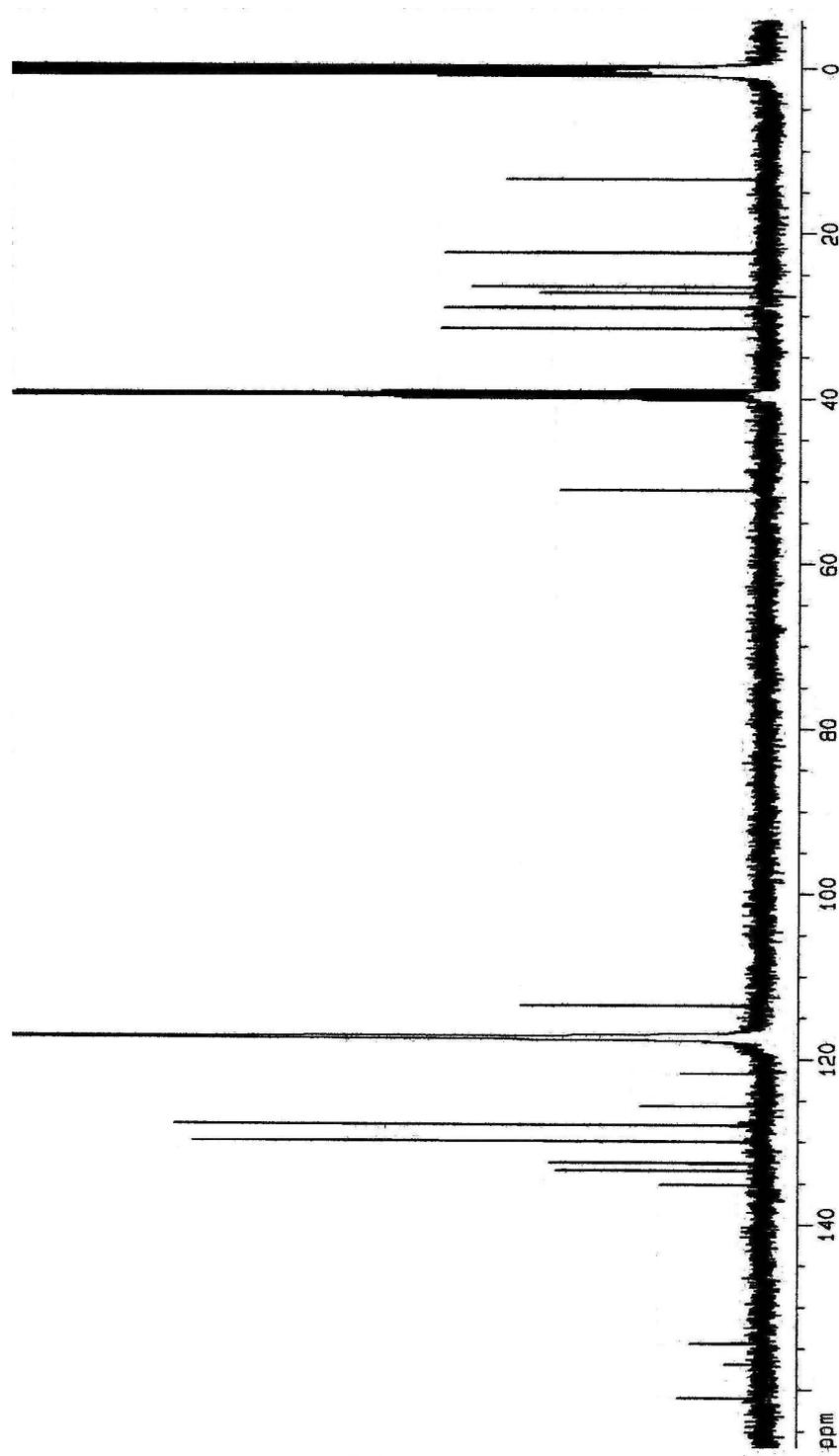


Figure SI-2. ^{13}C -NMR spectra of receptor **2** in CD_3CN .

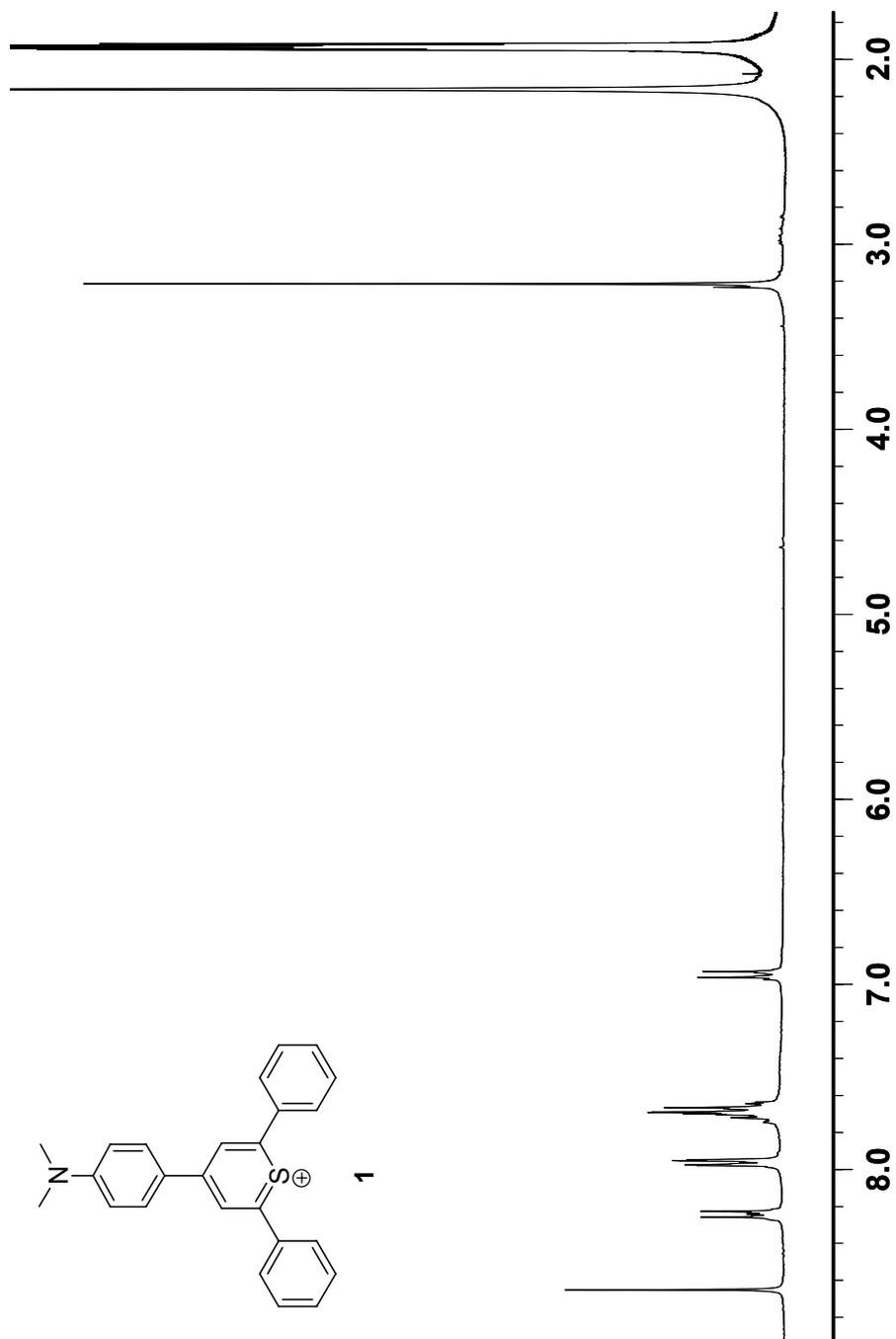


Figure SI-3. ¹H-NMR spectra of receptor **1** in CD₃CN.

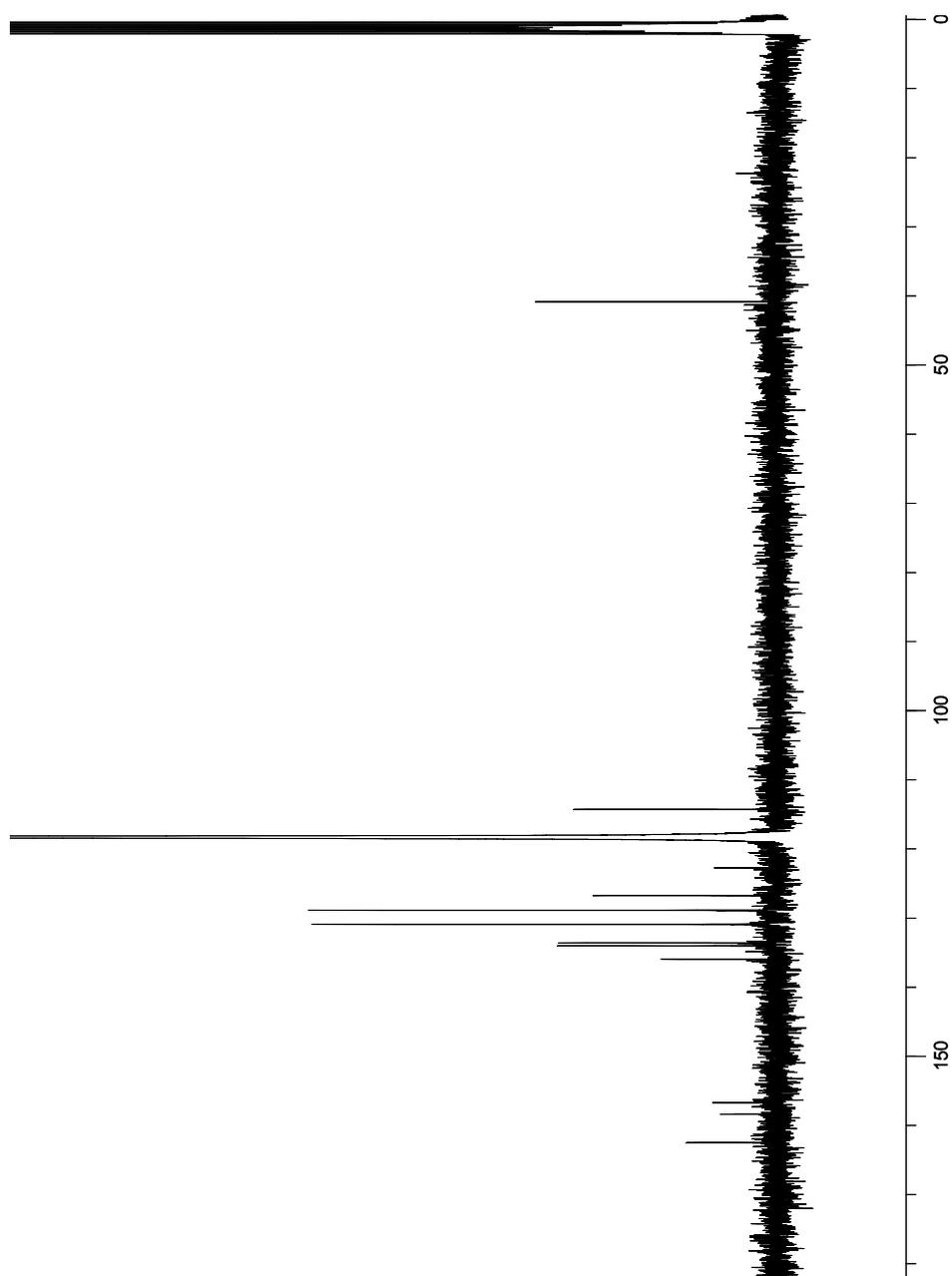


Figure SI-4. ^{13}C -NMR spectra of receptor 1 in CD_3CN .

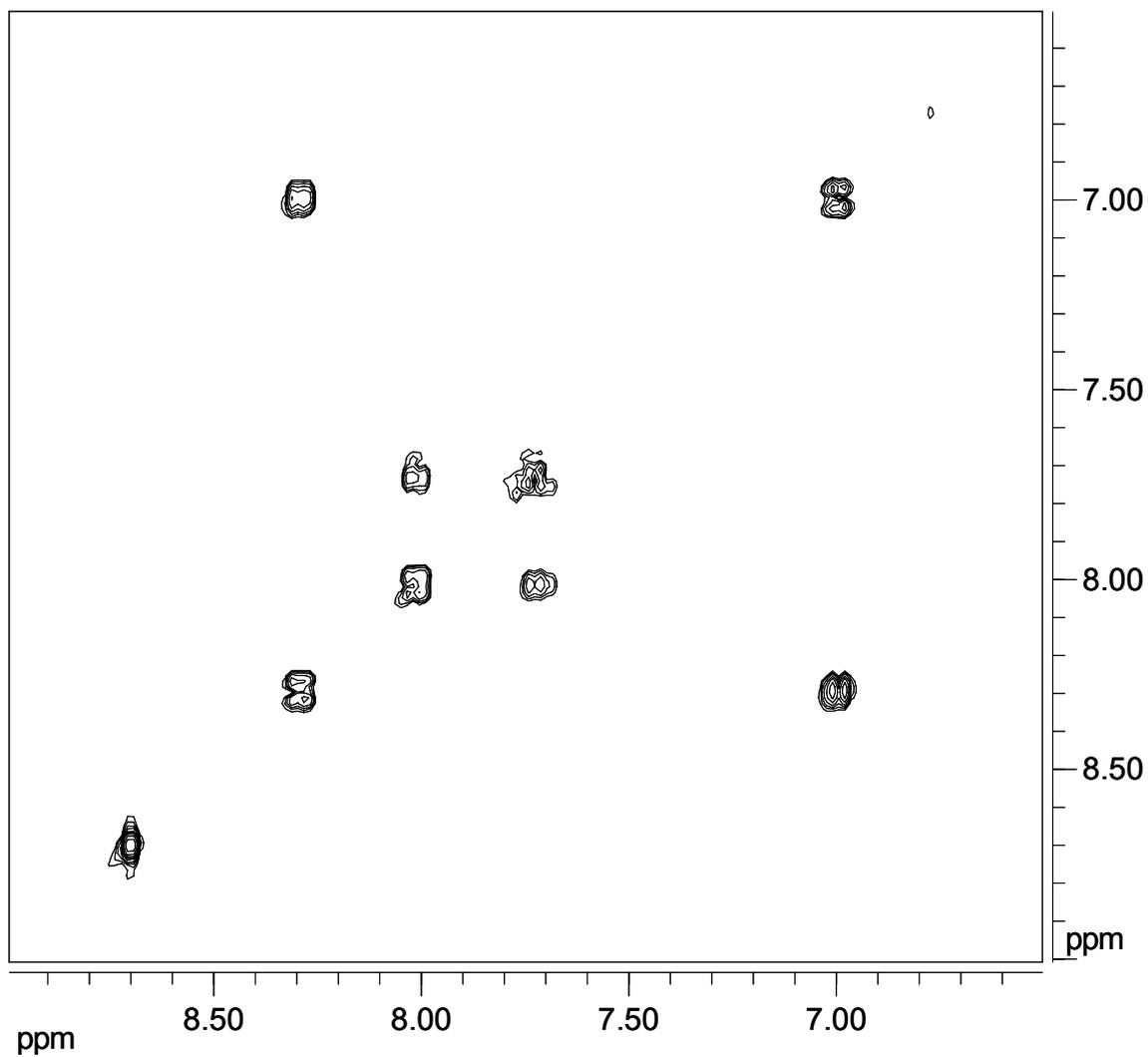


Figure SI-5. Proton-proton 2D NMR spectra of receptor **1** in CD₃CN.

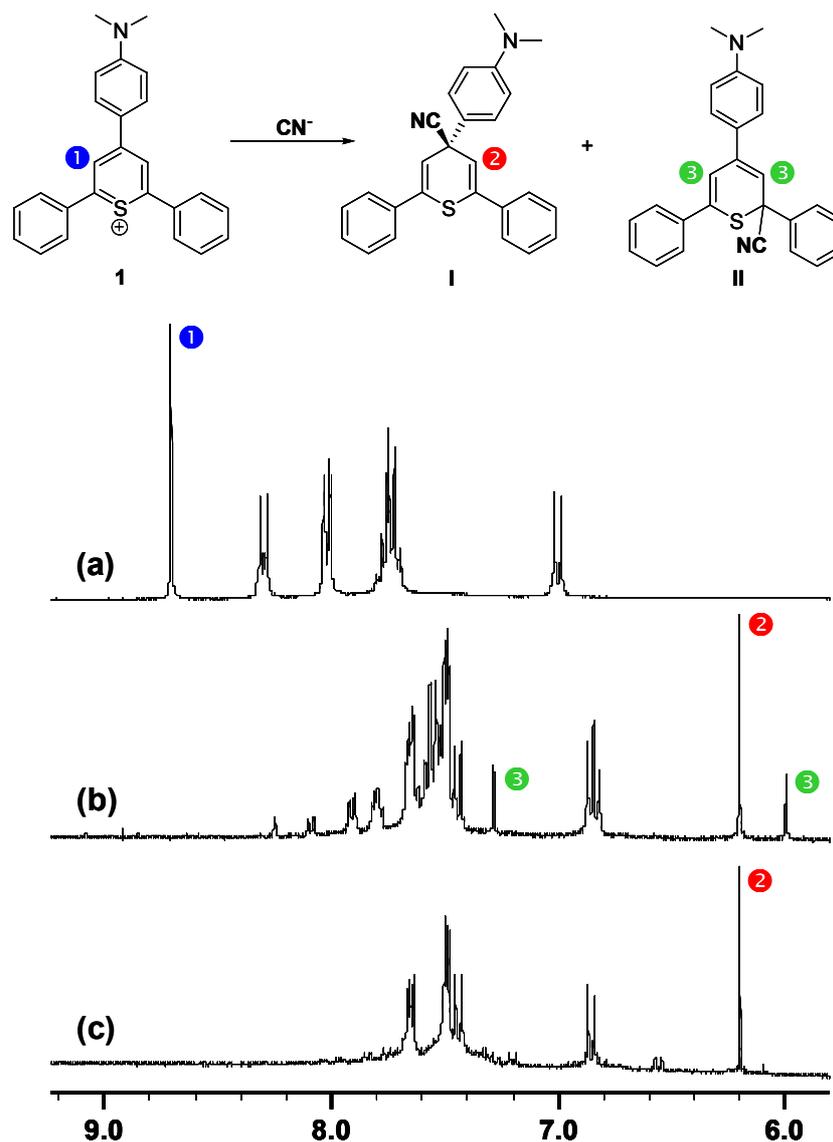


Figure SI-6. (a) $^1\text{H-NMR}$ spectra of receptor **1** in CD_3CN showing the aromatic protons, (b) $^1\text{H-NMR}$ spectra of receptor **1** in CD_3CN in the presence of 1 equivalent of cyanide anion and (c) $^1\text{H-NMR}$ spectra of receptor **1** in CD_3CN in the presence of 10 equivalents of cyanide anion.

Figure S1-6 shows the aromatic signals of the $^1\text{H-NMR}$ spectra of (a) receptor **1** alone, (b) receptor **1** in the presence of 1 equivalent of cyanide anion and (c) receptor **1** in the presence of 10 equivalents of cyanide anion. As could be seen in spectra (a) the thiopyrylium proton appears as a narrow singlet centred at 8.63 ppm. Upon addition of one equivalent of cyanide anion this singlet split into three new singlets centred at 5.96, 6.17 and 7.26 ppm (see spectra b). The singlet centred at 6.17 ppm was assigned to the product obtained from nucleophilic attack of cyanide over C4 on the thiopyrylium ring (structure **I**), whereas the other two signals were attributed to the product formed by cyanide addition over C2 (structure **II**). From the areas of the three singlets, a ratio of 75:25 for structures **I:II** was determined. However, upon addition of 10 equivalents of cyanide only the product of nucleophilic attack over C4 carbon was formed because the only singlet observed is centred at 6.17 ppm (see spectra c).

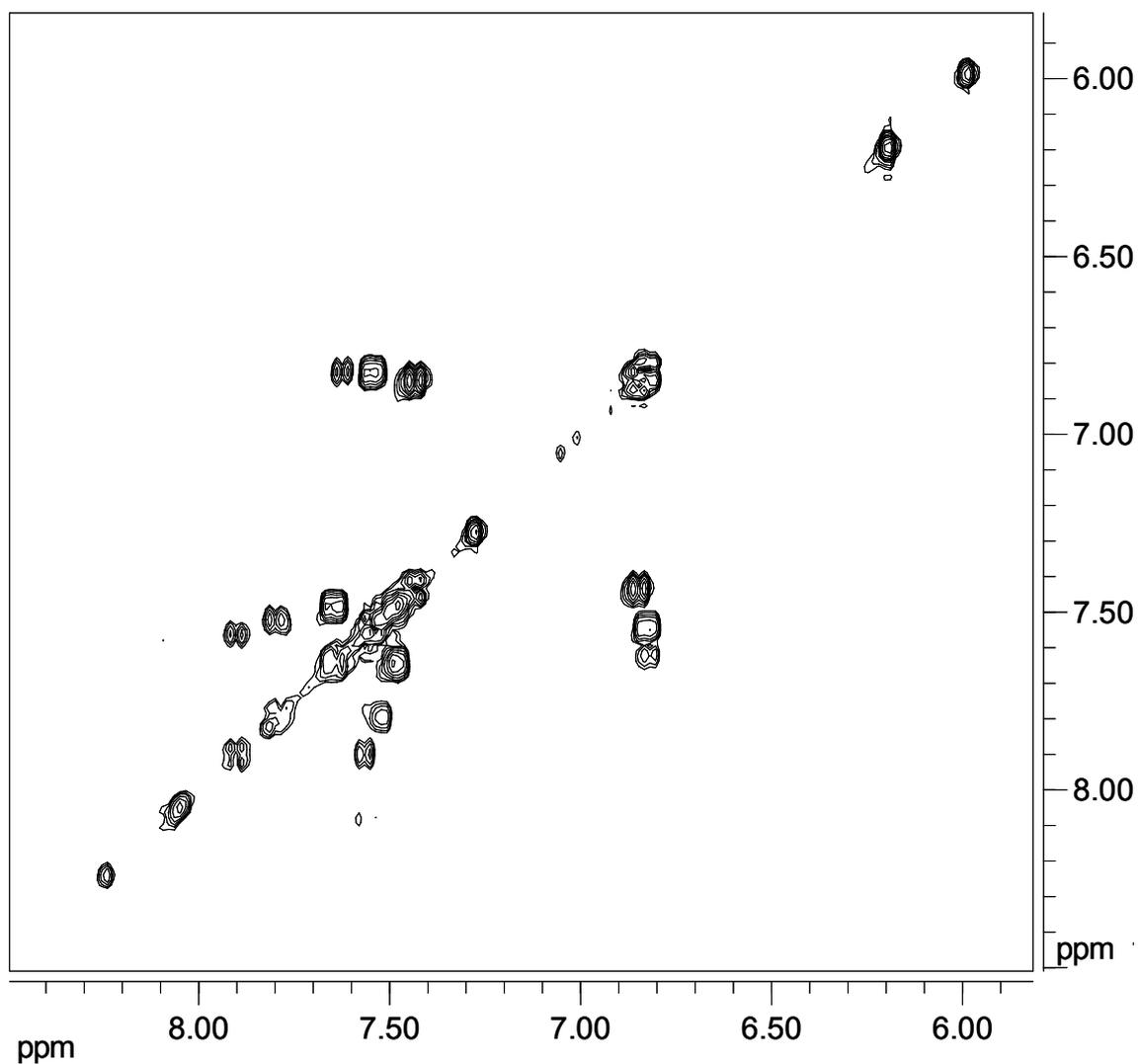


Figure SI-7. Proton-proton 2D NMR spectra of receptor **1** in the presence of one equivalent of cyanide anion in CD_3CN .