

Ion pair cooperative binding by an L-tyrosine based polymerizable molecular receptor
by
*Szymon Zdanowski and Jan Romański**

Department of Chemistry, University of Warsaw, Pasteura 1, 02-093 Warsaw, Poland

CONTENTS

1. General	1
2. NMR spectra	2
3. UV-Vis measurements (Job Plots, Dilution curves, Binding isotherms)	6

GENERAL INFORMATION

Unless specifically indicated, all other chemicals and reagents used in this study were purchased from commercial sources and used as received. Purification of products was performed using column chromatography on silica gel (Merck Kieselgel 60, 230-400 mesh) with mixtures of chloroform/methanol. Thin-layer chromatography (TLC) was performed on silica gel plates (Merck Kieselgel 60 F254).

¹H and ¹³C NMR spectra were recorded on a Bruker 300 MHz or Varian Unity Plus 200 MHz spectrometer. ¹H NMR chemical shifts δ are reported in ppm referenced to residual solvent signal (DMSO-d₆ or CDCl₃). UV-Vis titrations were performed in acetonitrile using a Thermo Spectronic Unicam UV500 Spectrophotometer. High resolution mass spectra (HRMS) were measured on a Quattro LC Micromass unit using ESI technique.

Fig. S1 and S2: ^1H and ^{13}C NMR of receptor 1.

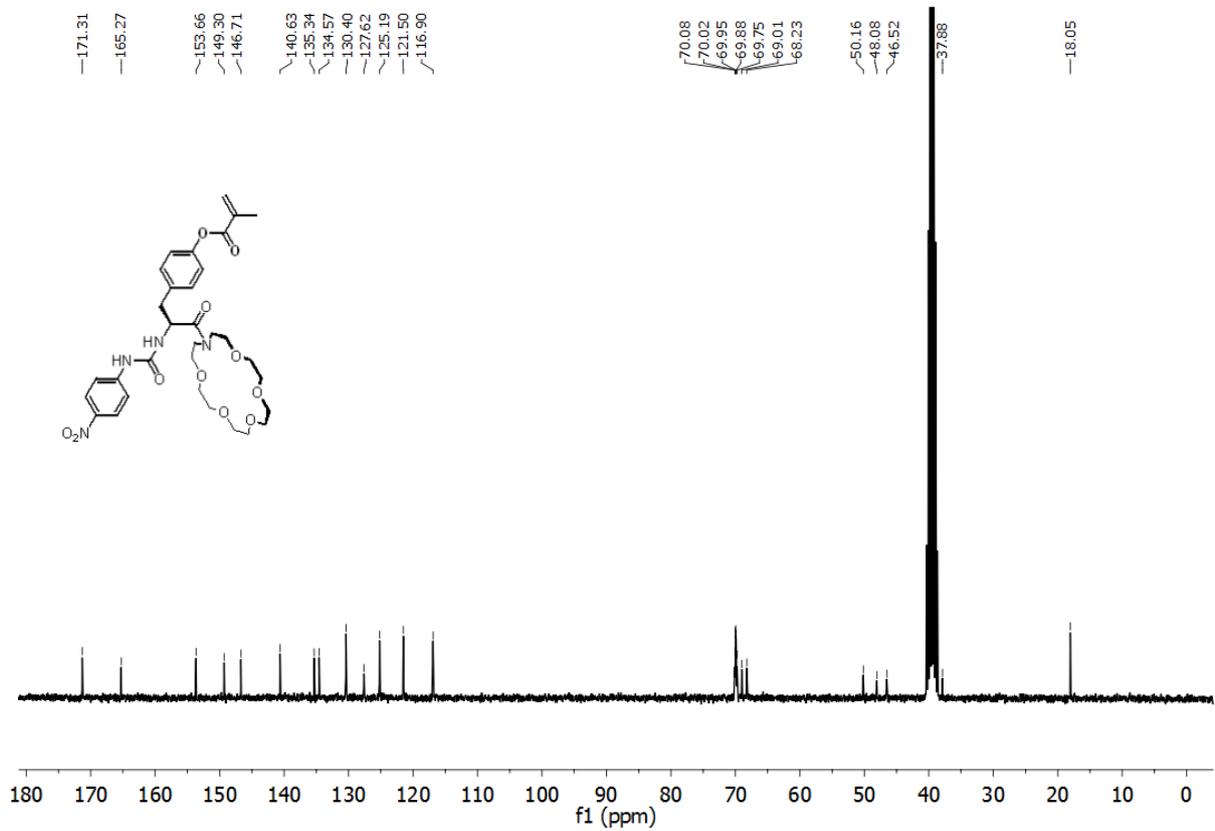
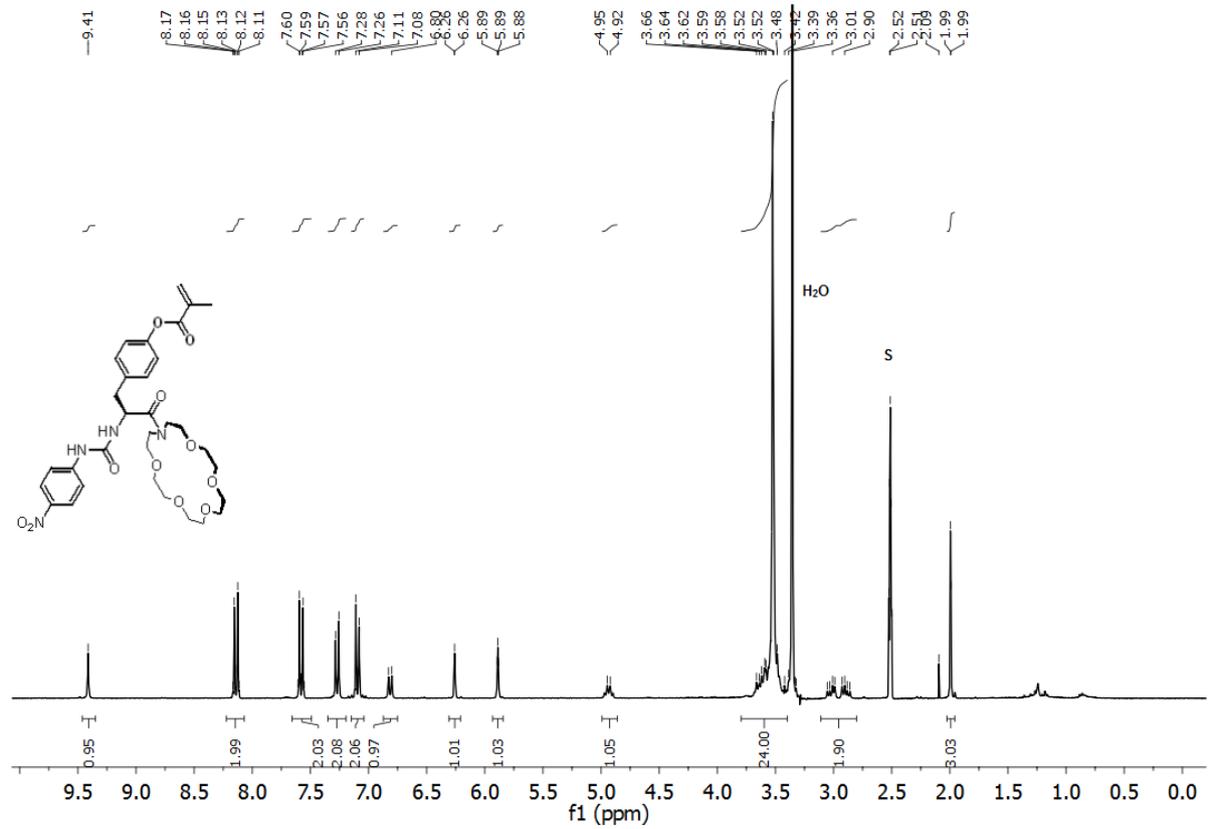


Fig. S3 and S4: ^1H and ^{13}C NMR of receptor 2.

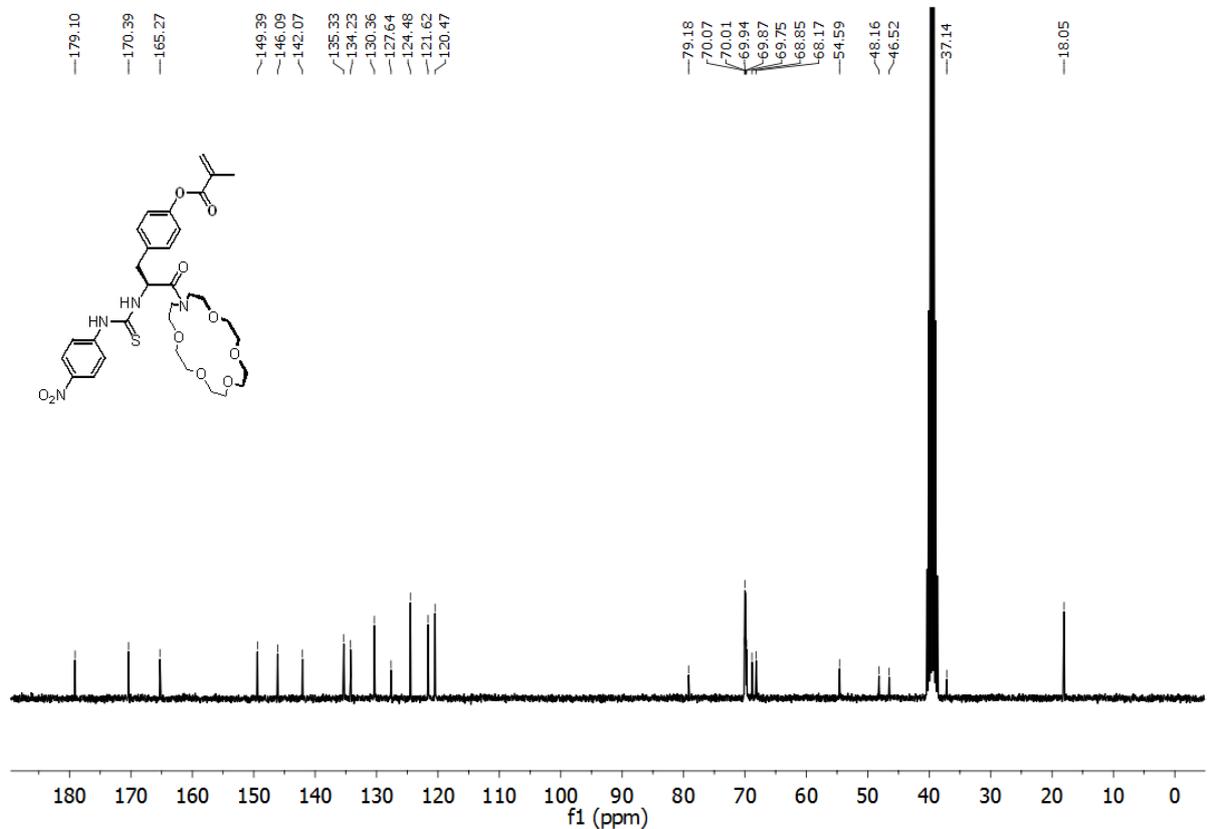
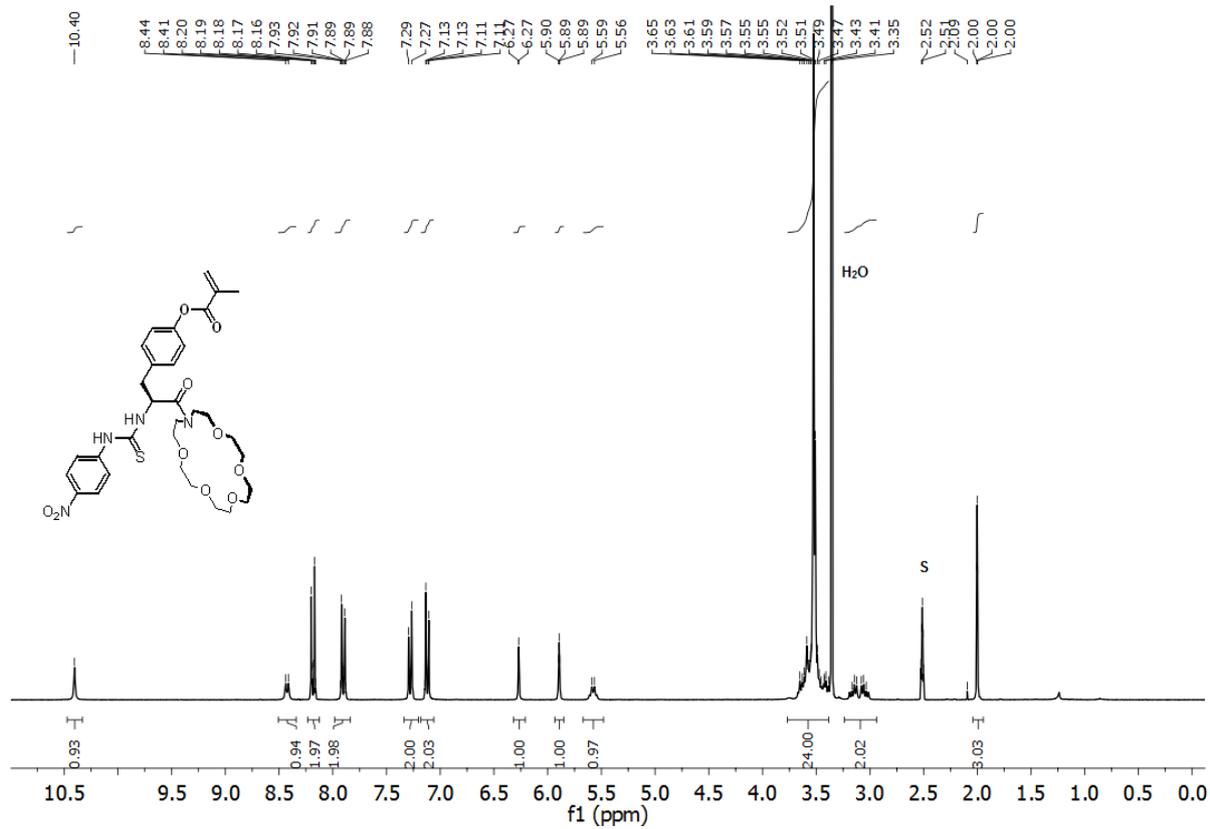


Fig. S5 and S6: ^1H and ^{13}C NMR of receptor 3.

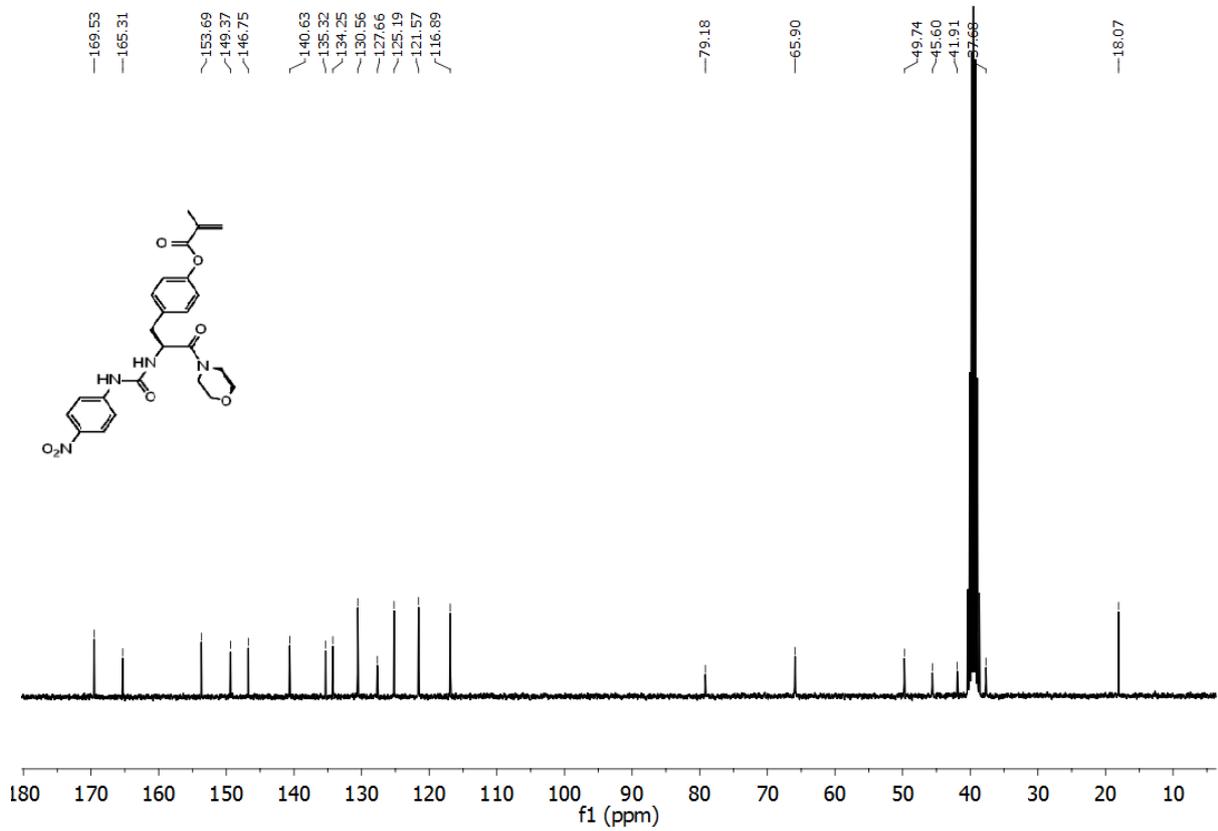
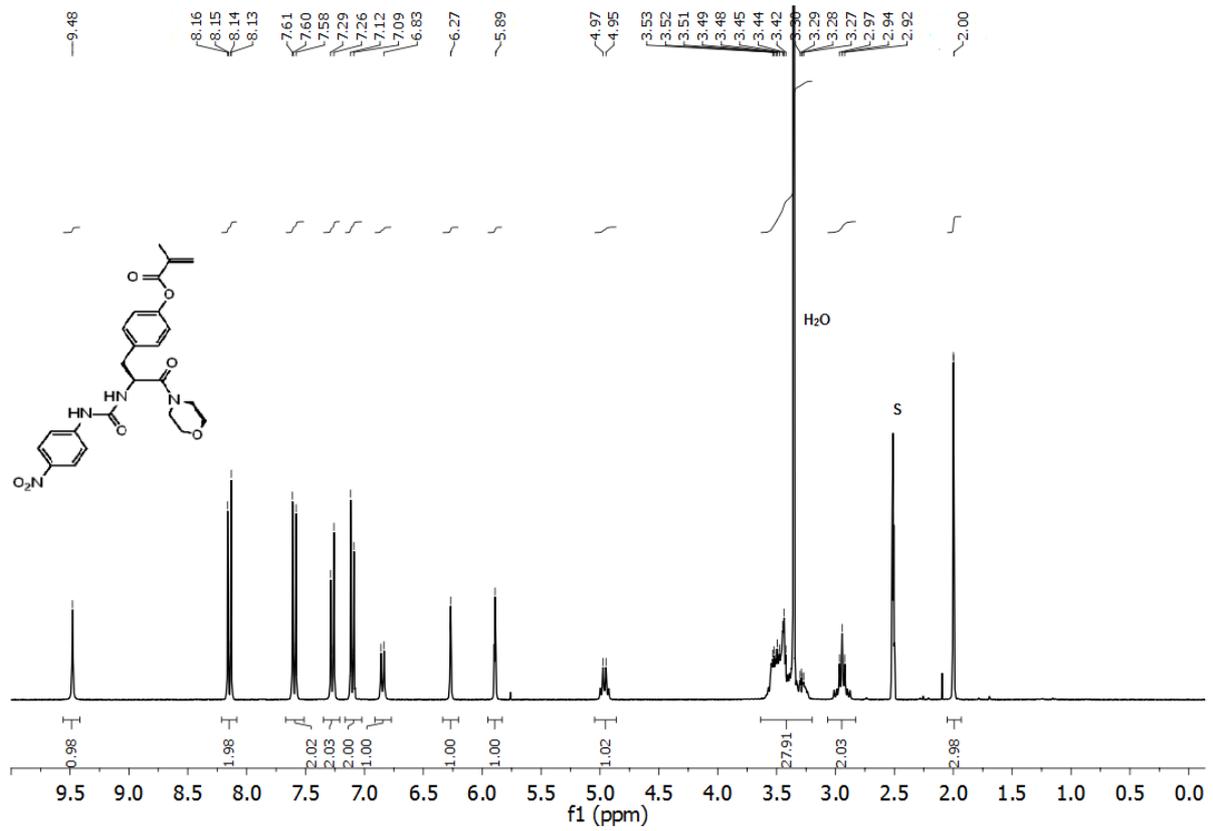


Fig. S7 ^1H and of copolymer 6.

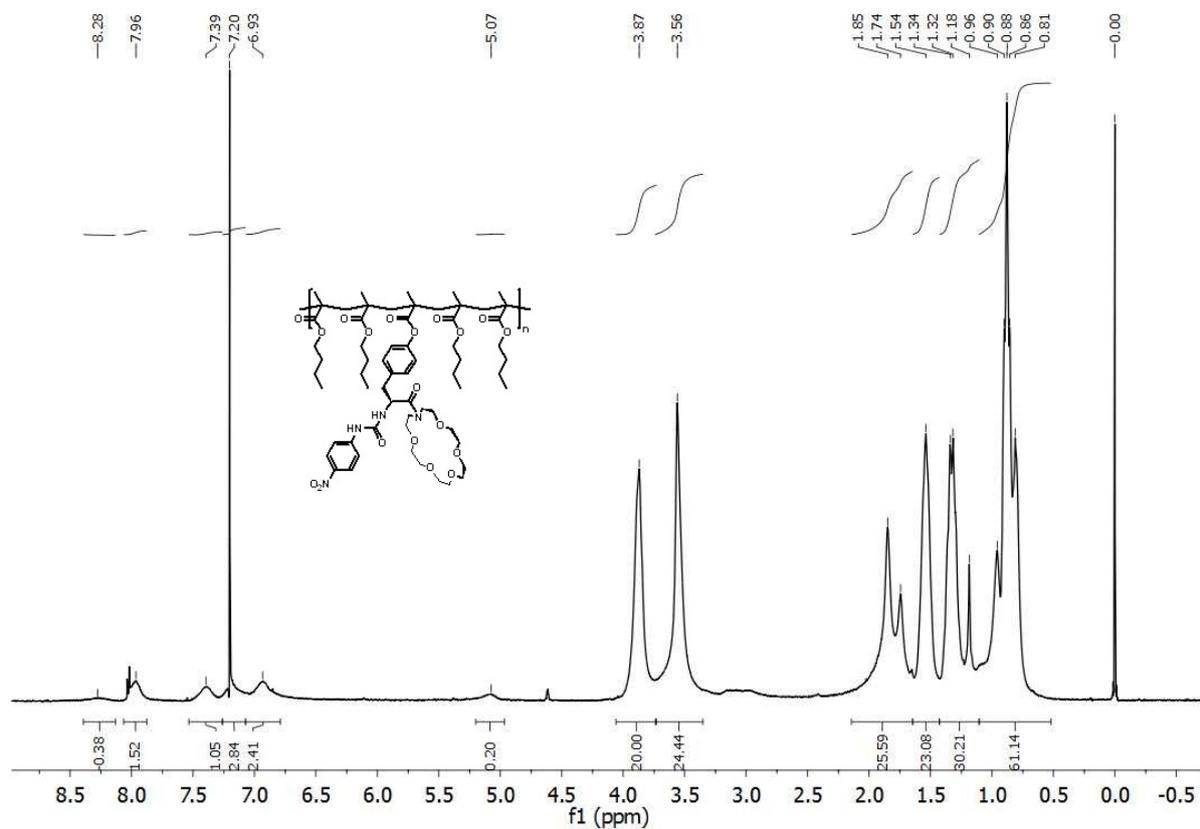
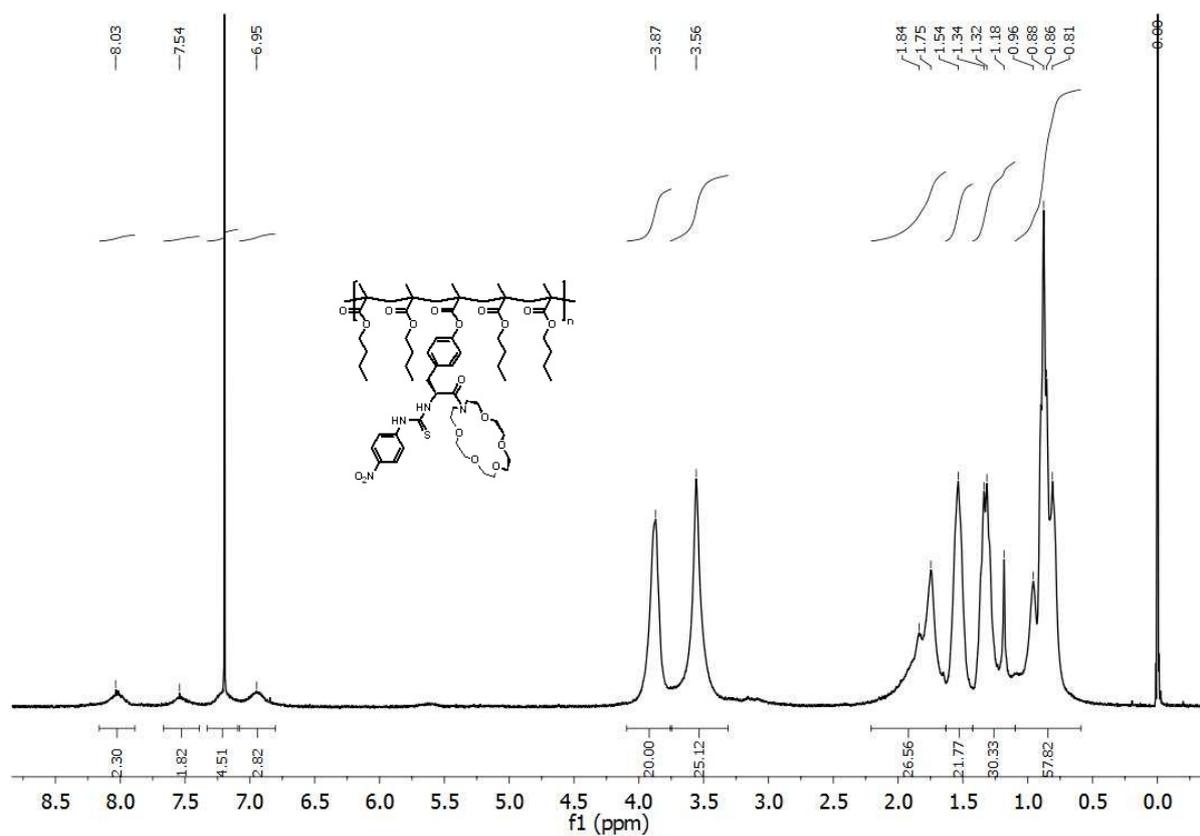
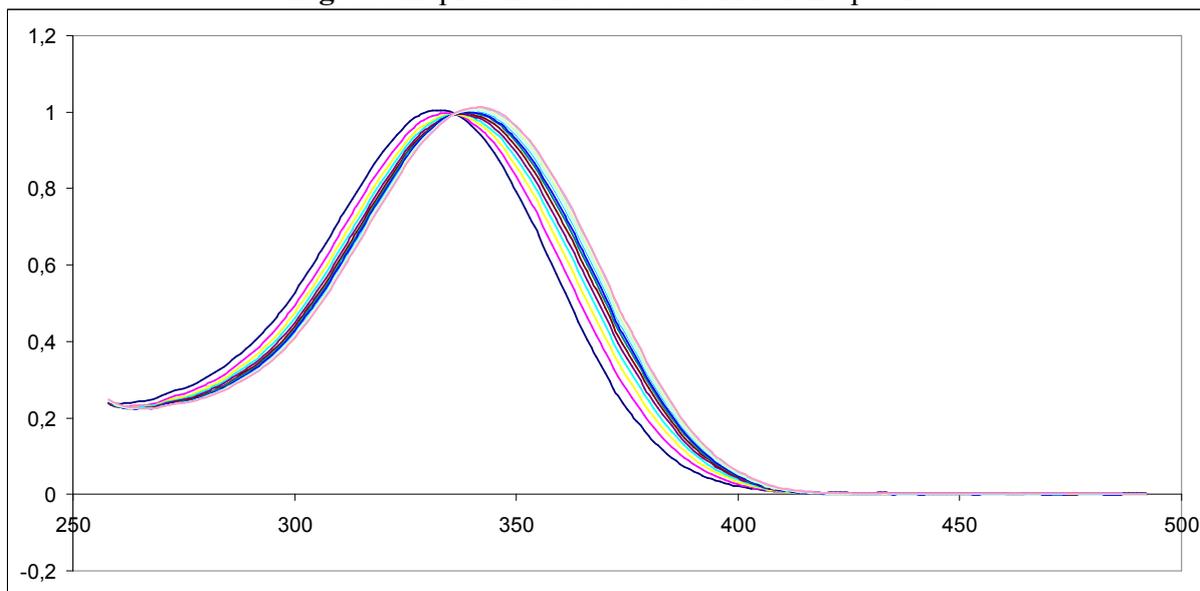


Fig. S8 ^1H and of copolymer 7.



UV-VIS EXPERIMENTS

Fig. S9: Representative UV-Vis Titration Spectra



DILUTION AND JOB PLOTS.

Fig. S10: Dilution curve of receptor 1.

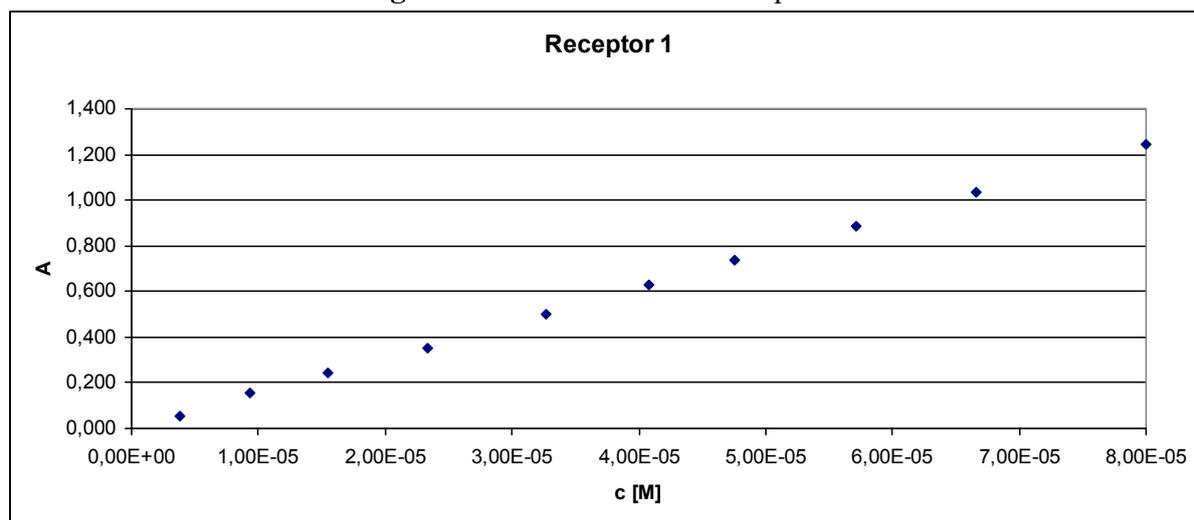


Fig. S11: Job plot (Host: Receptor 1, guest: Cl⁻)

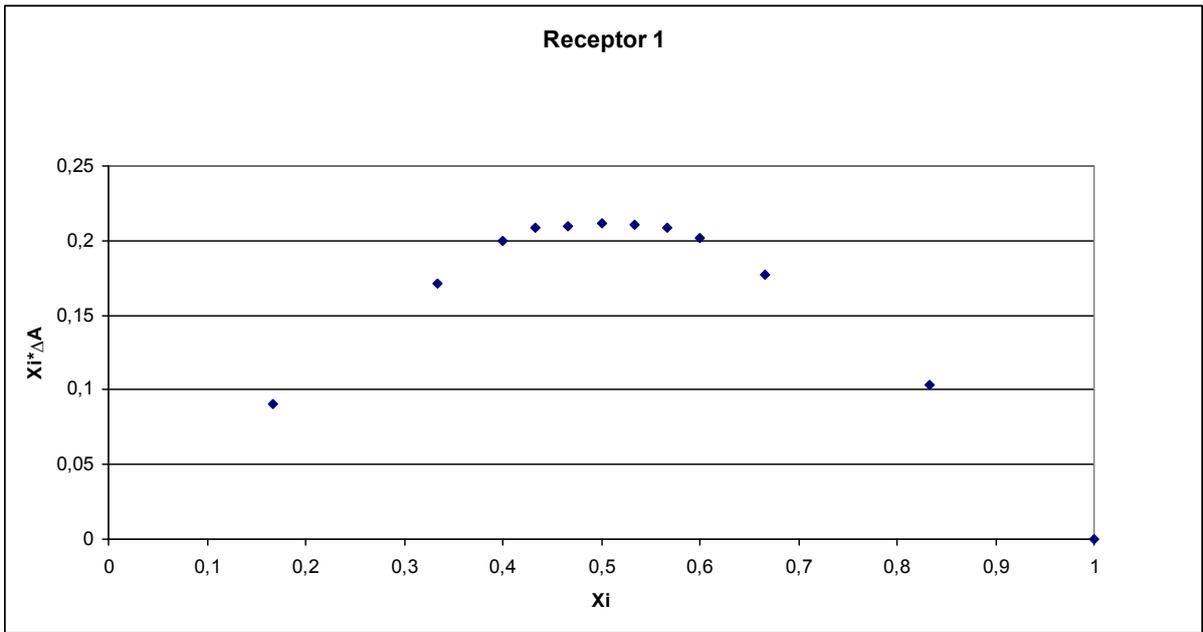


Fig. S12: Dilution curve of receptor 2.

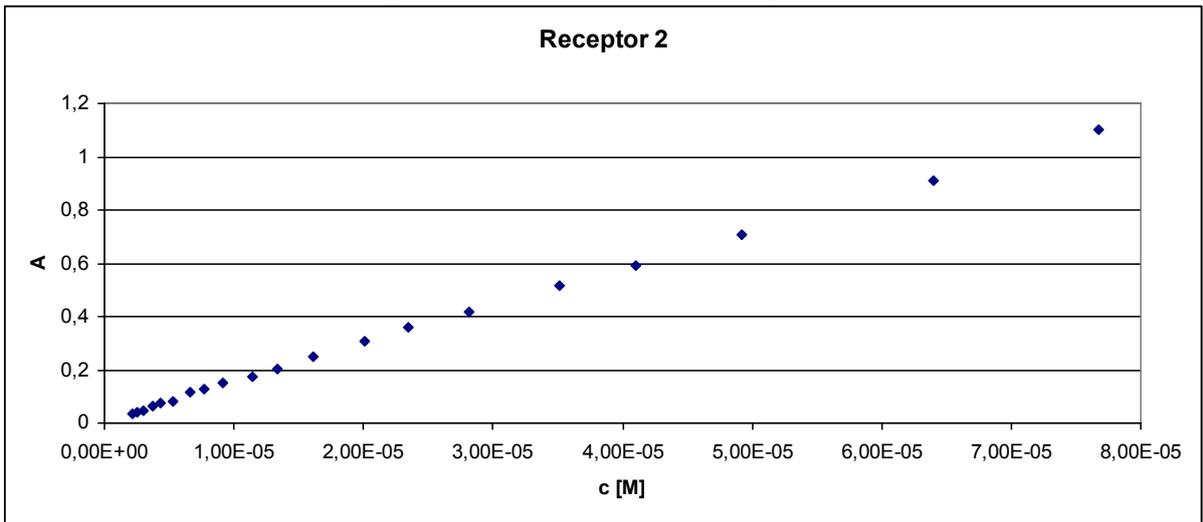


Fig. S13: Job plot (Host: Receptor 1, guest: Cl^-)

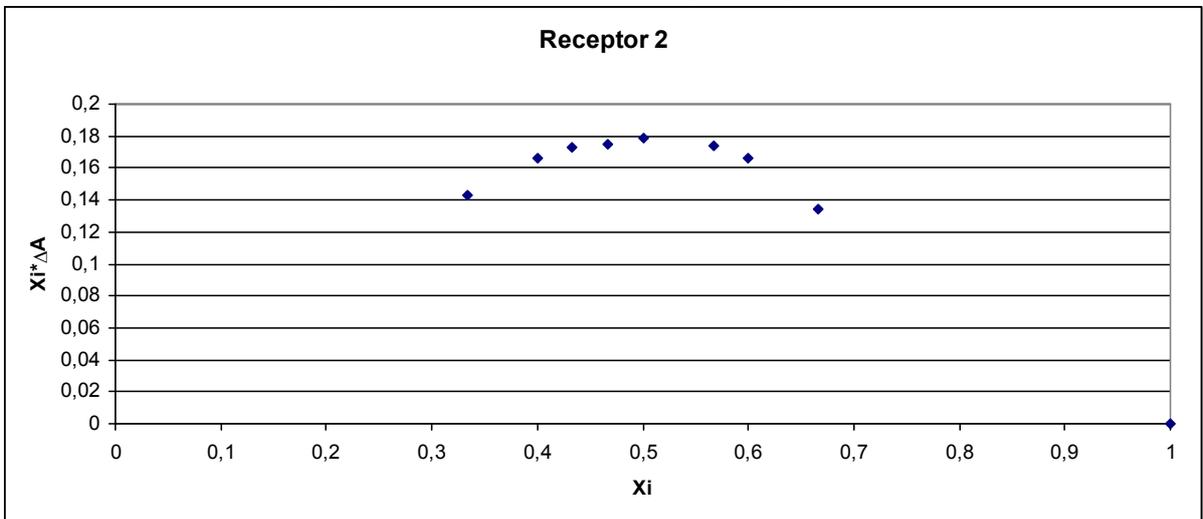


Fig. S14: UV-Vis titration binding isotherms of receptor **1** with TBACl and TBACl in the presence of 1 equivalent of NaPF₆, KPF₆, NH₄PF₆ and binding isotherm of receptor **1** with NaPF₆.

