

Supplementary Material

Covalently immobilizable tris(pyridino)-crown ether for separation of amines based on their degree of substitution

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Contents

1. ¹H-NMR and ¹³C-NMR spectra of the new compounds
 2. ¹H-NMR and ¹³C-NMR spectra of the previously reported partially characterized compound
- 10**
3. Spectrophotometric investigation of the new crown ether (**1**)

1. ^1H -NMR and ^{13}C -NMR spectra of the new compounds

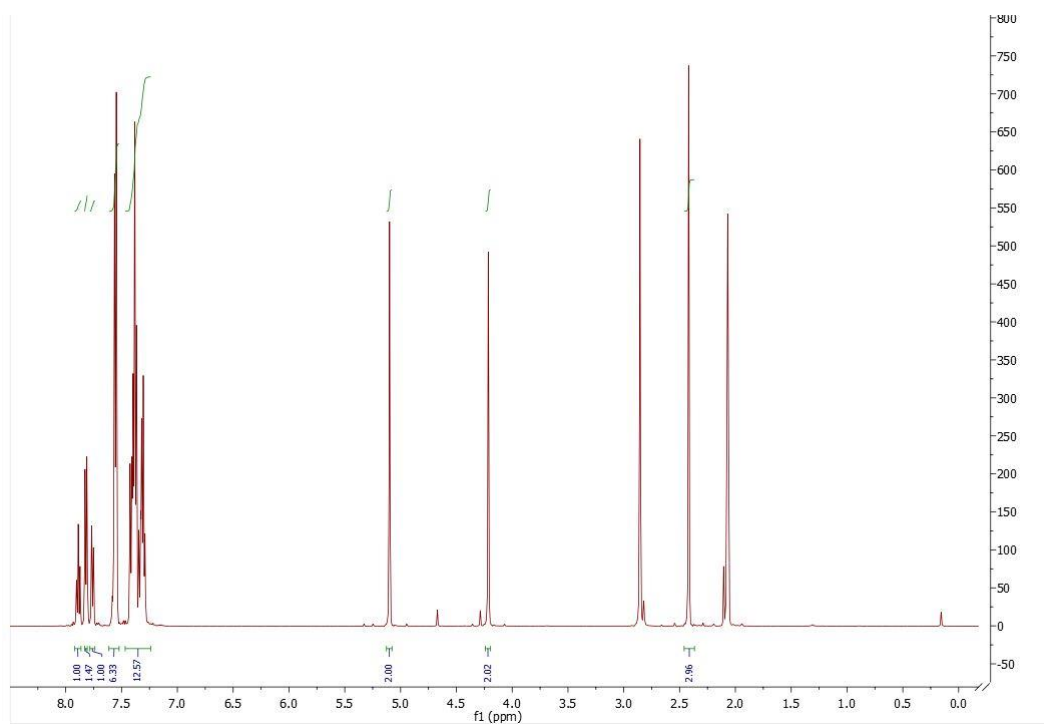


Figure S1. ^1H -NMR spectrum of **5** (acetone- d_6)

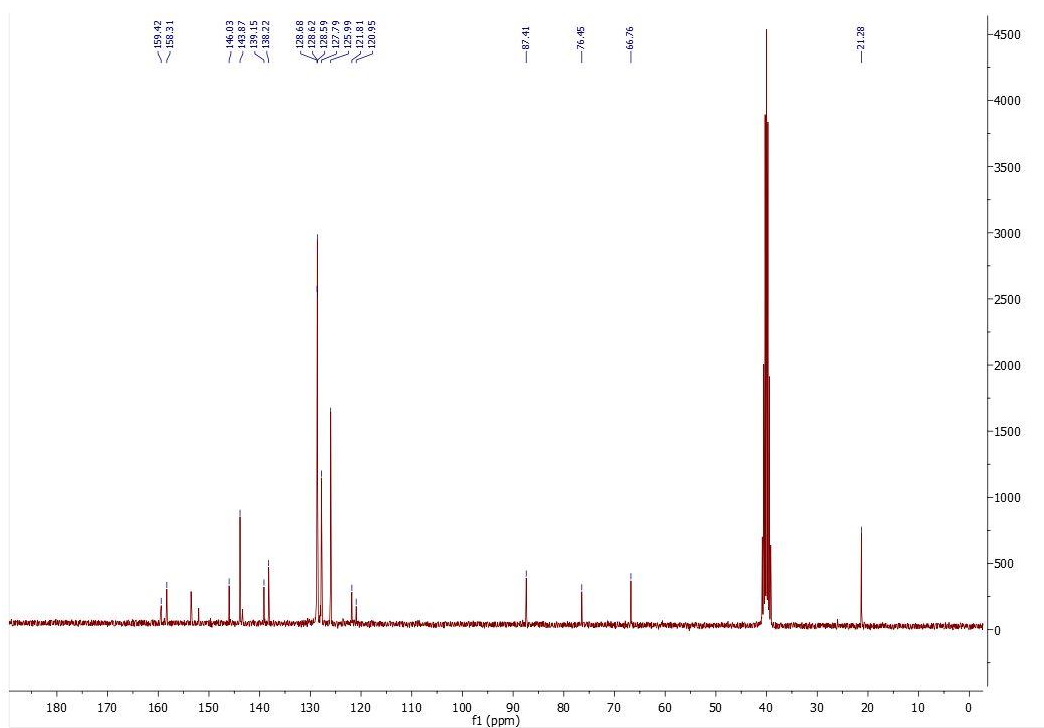


Figure S2. ^{13}C -NMR spectrum of **5** (CDCl_3)

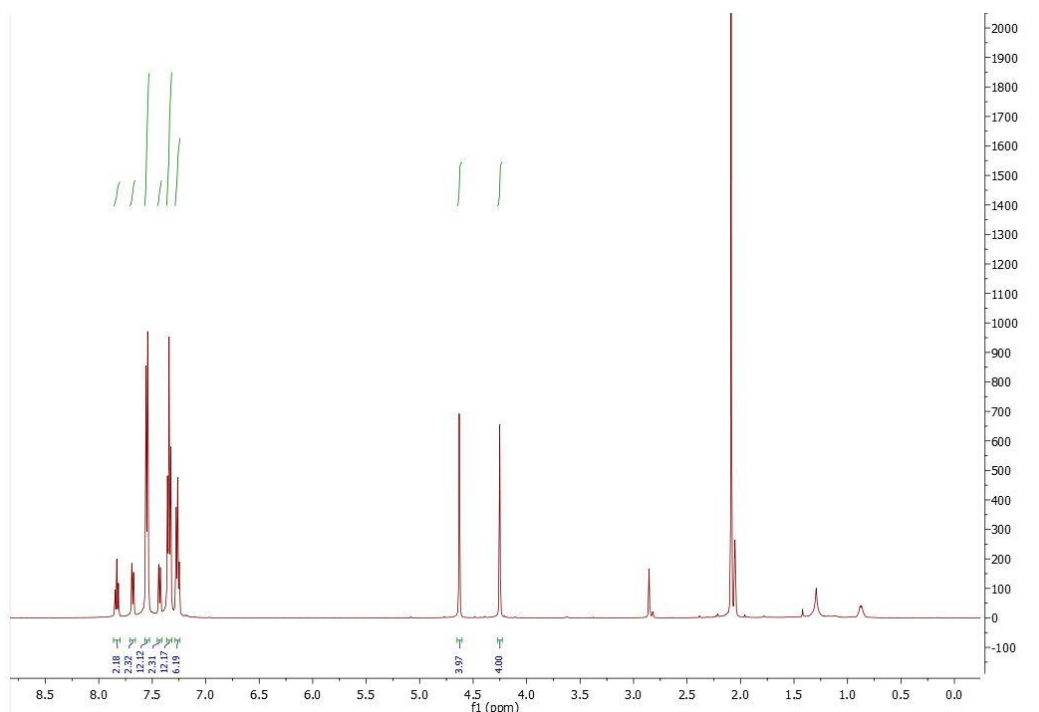


Figure S3. ¹H-NMR spectrum of **7** (acetone-*d*₆)

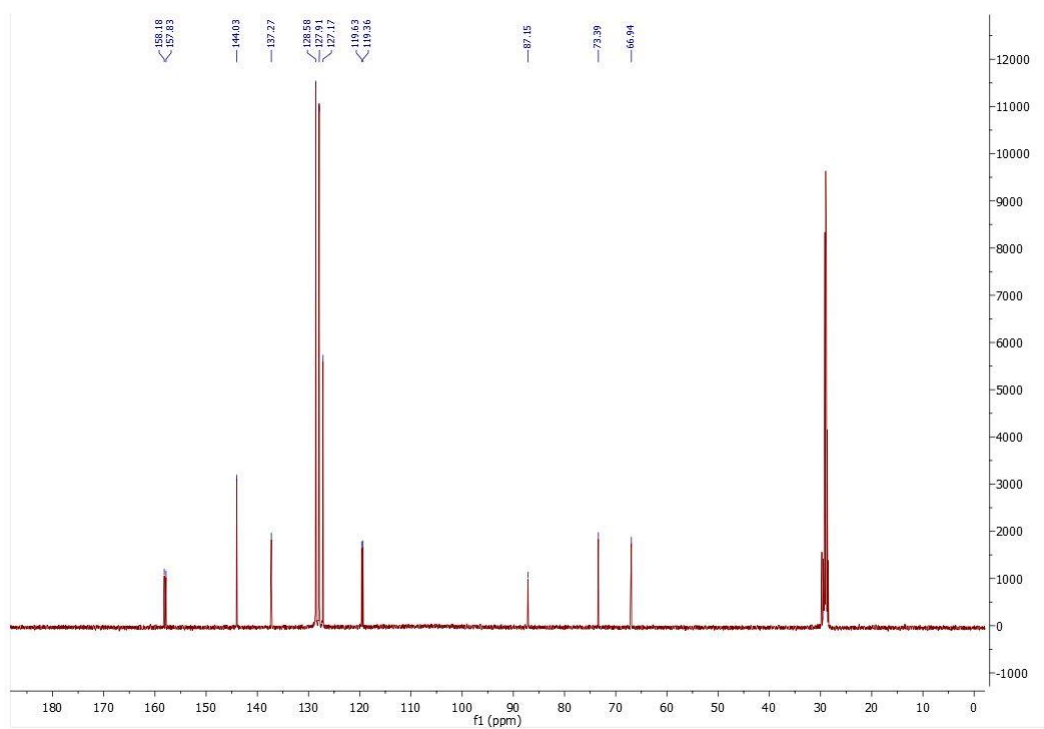


Figure S4. ¹³C-NMR spectrum of **7** (acetone-*d*₆)

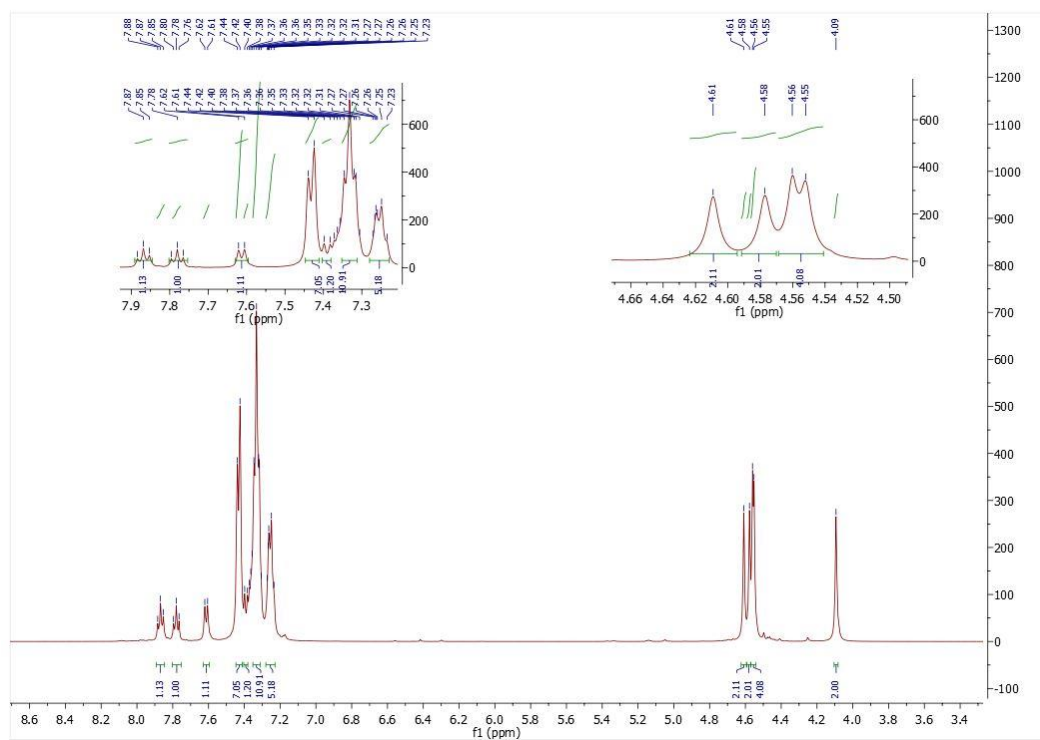


Figure S5. ¹H-NMR spectrum of **8** (DMSO-*d*₆)

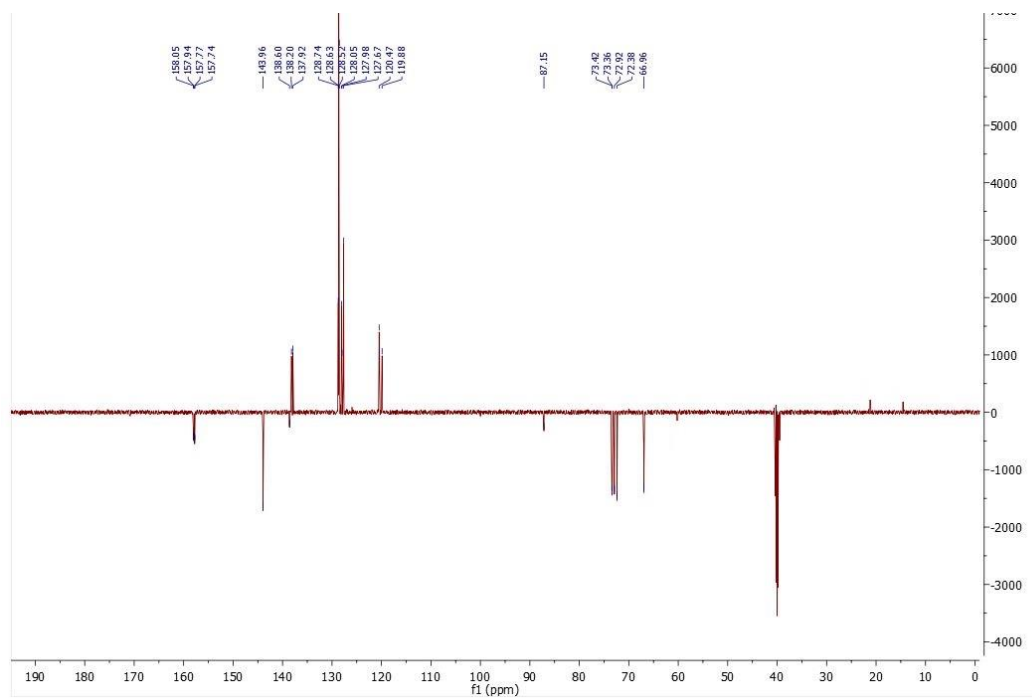


Figure S6. ¹³C-NMR spectrum of **8** (DMSO-*d*₆)

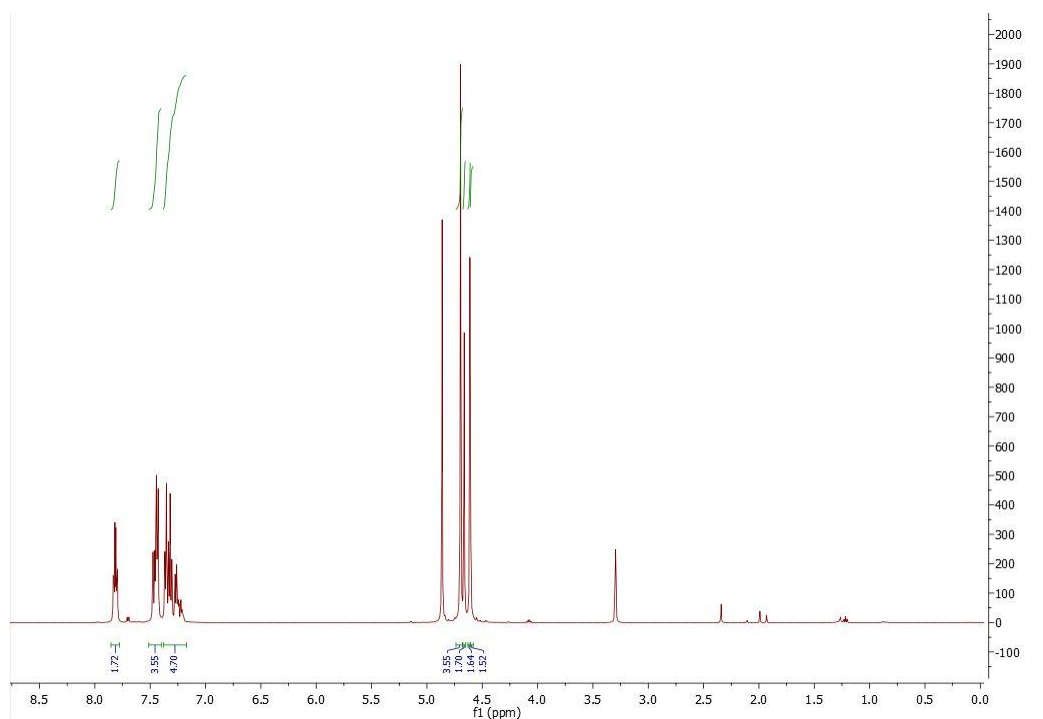


Figure S7. ¹H-NMR spectrum of **9** (methanol-*d*₄)

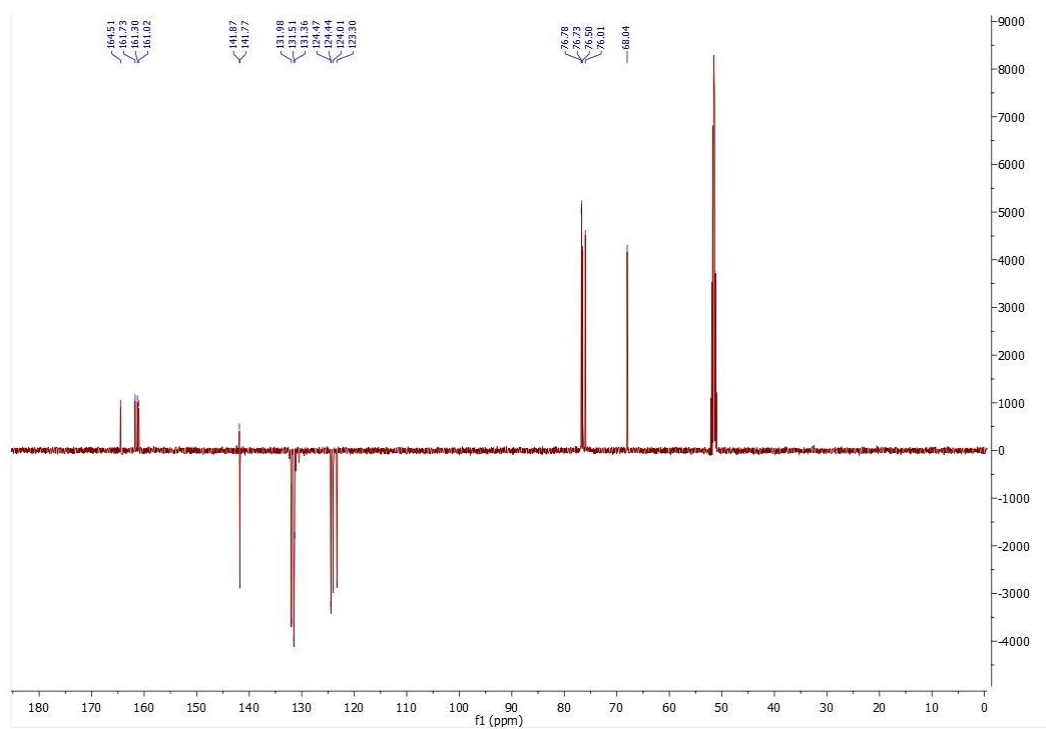


Figure S8. ¹³C-NMR spectrum of **9** (CDCl₃)

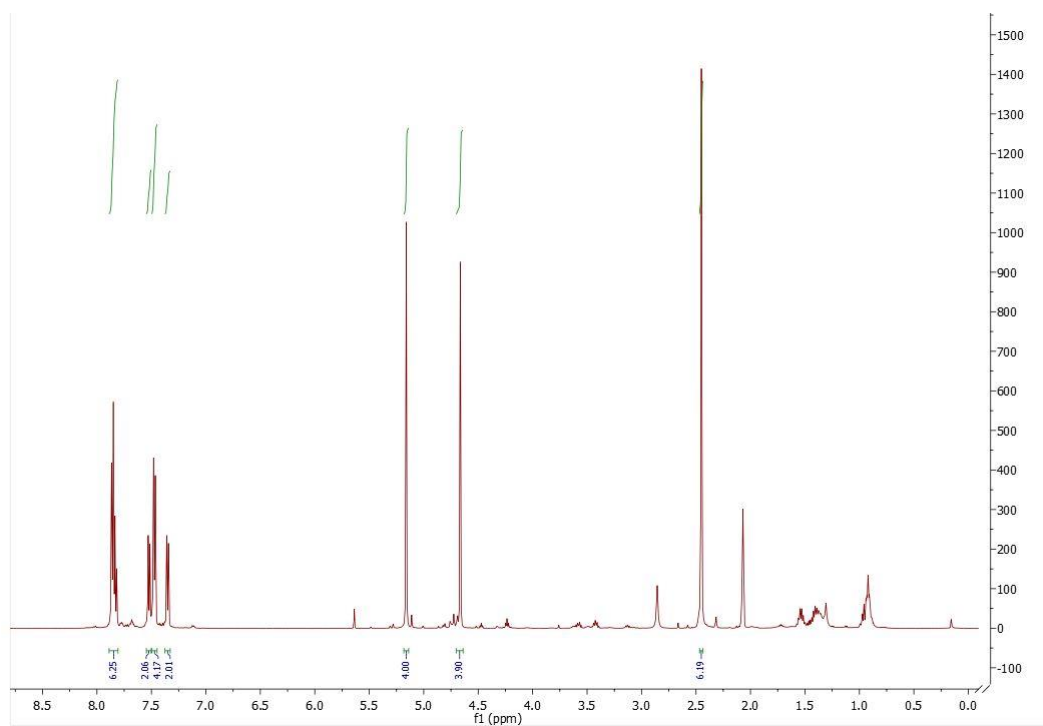


Figure S9. ¹H-NMR spectrum of **11** (acetone-*d*₆)

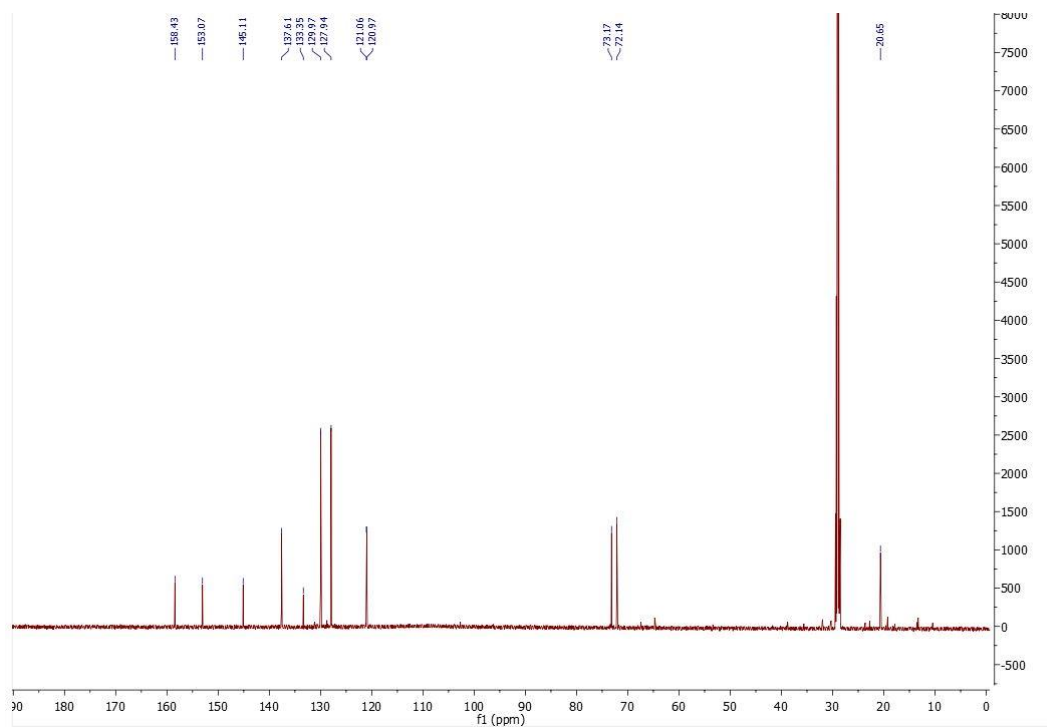


Figure S10. ¹³C-NMR spectrum of **11** (acetone-*d*₆)

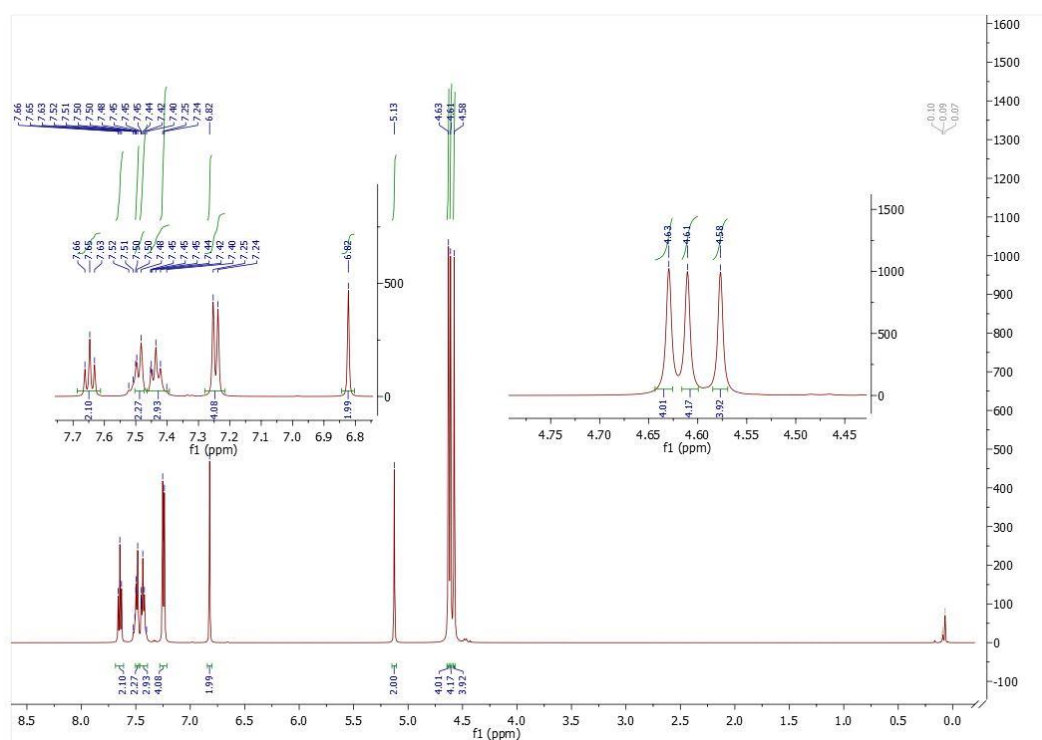


Figure S11. ^1H -NMR spectrum of **1** (acetone- d_6)

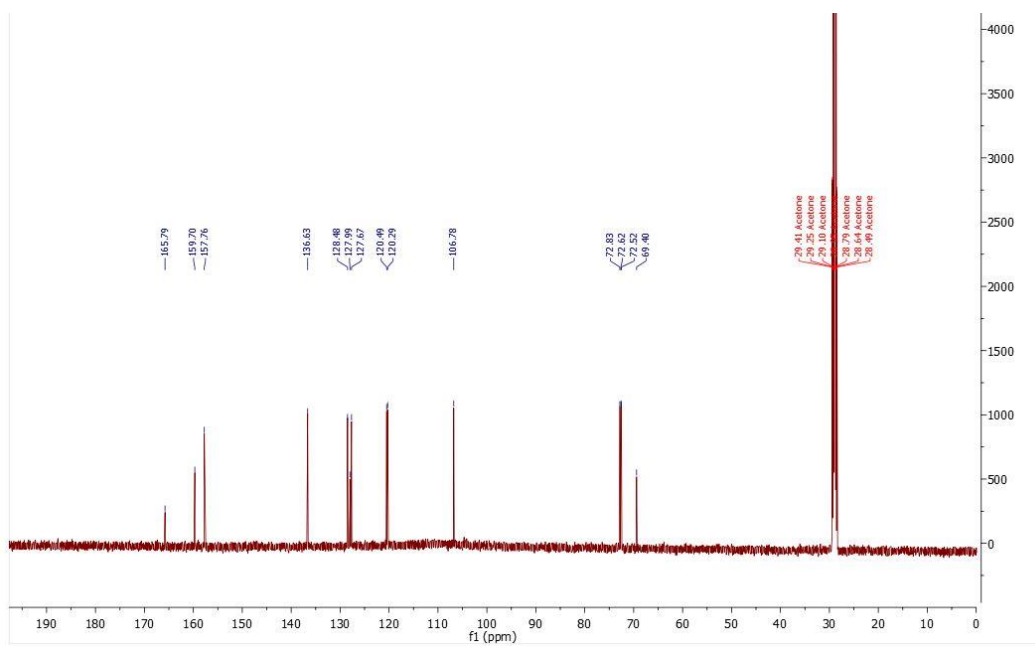


Figure S12. ^{13}C -NMR spectrum of **1** (acetone- d_6)

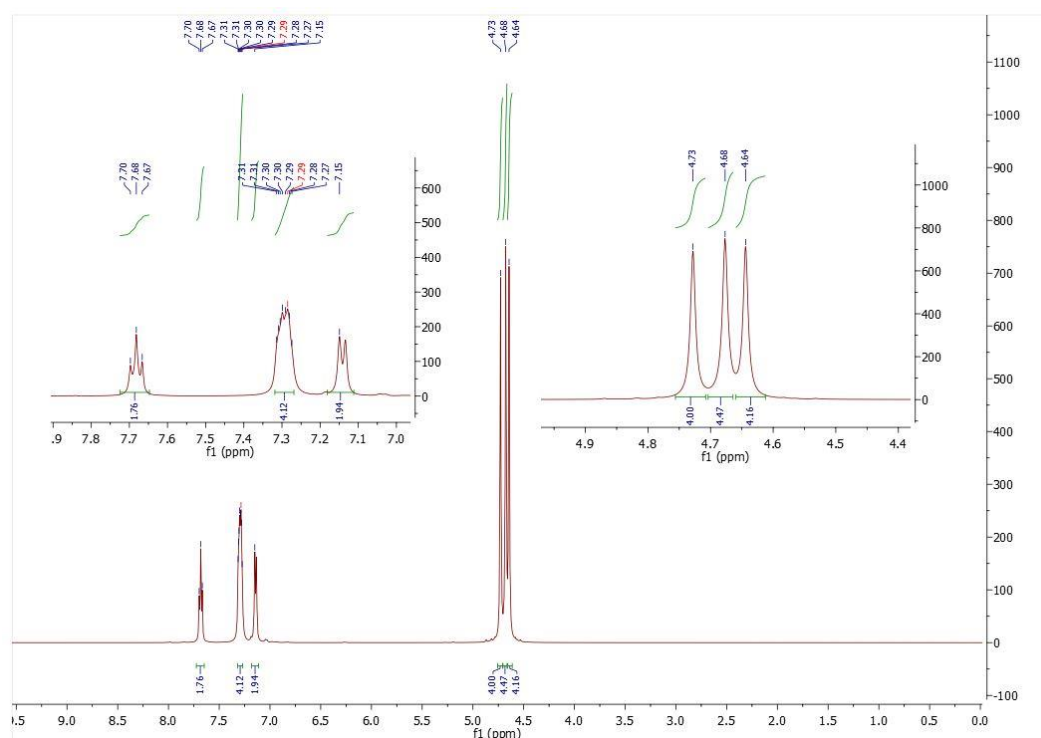


Figure S13. ^1H -NMR spectrum of **14** (CDCl_3)

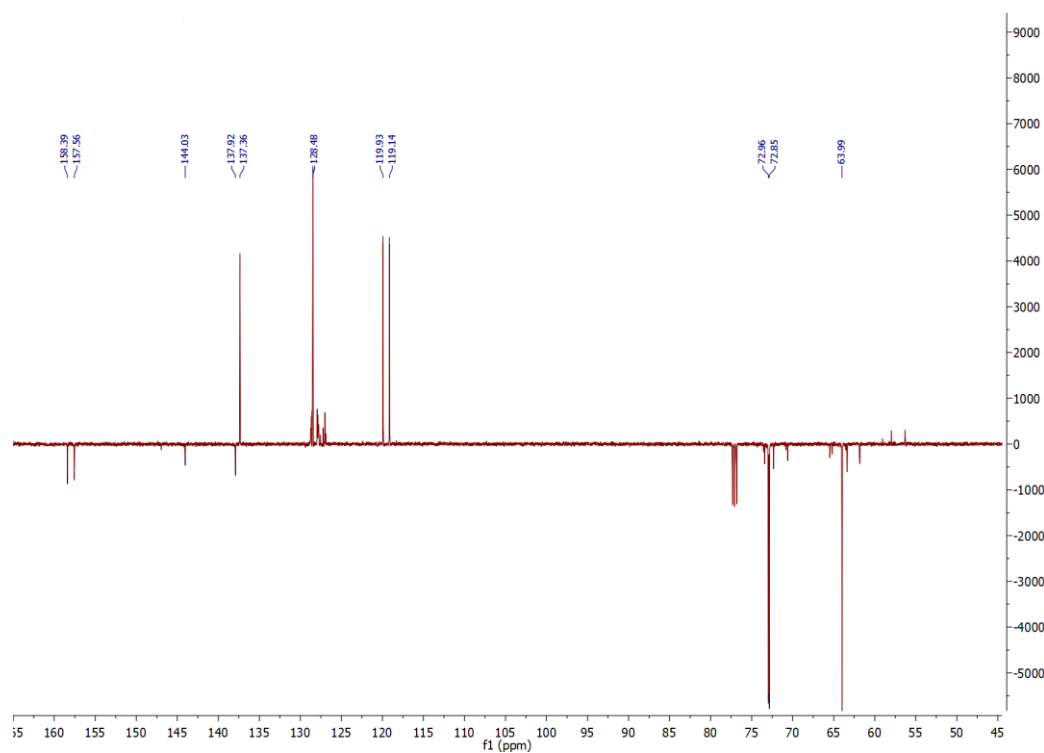


Figure S14. ^{13}C -NMR spectrum of **14** (CDCl_3)

2. ¹H-NMR and ¹³C-NMR spectra of the previously reported partially characterized compound 10

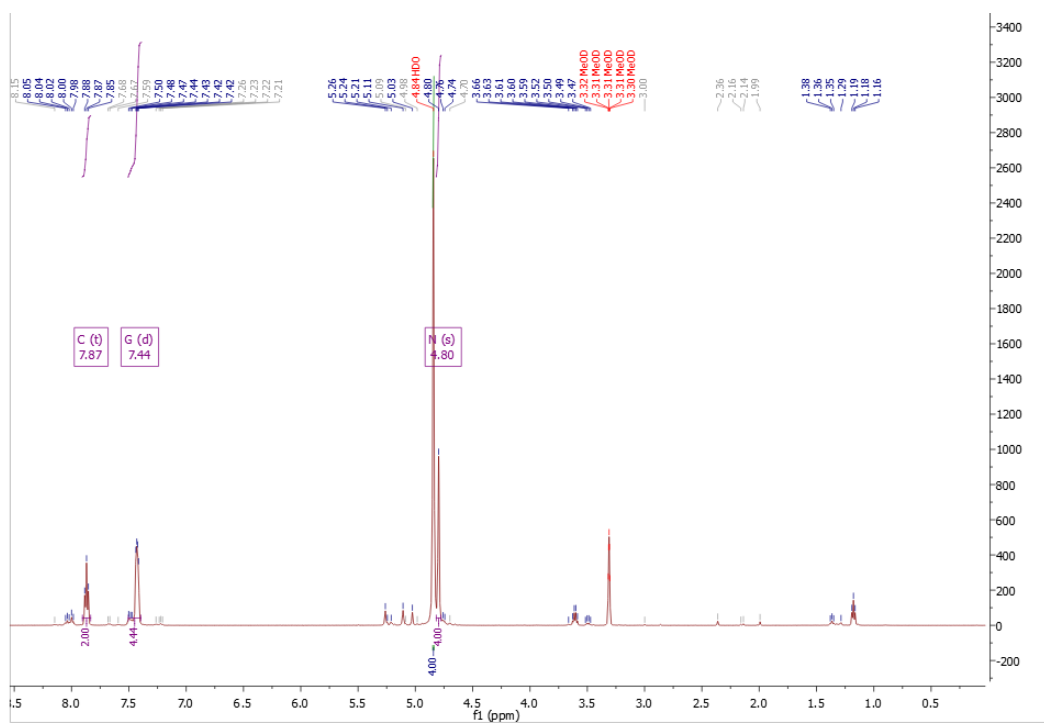


Figure S15. ^1H -NMR spectrum of **10** (methanol- d_4)

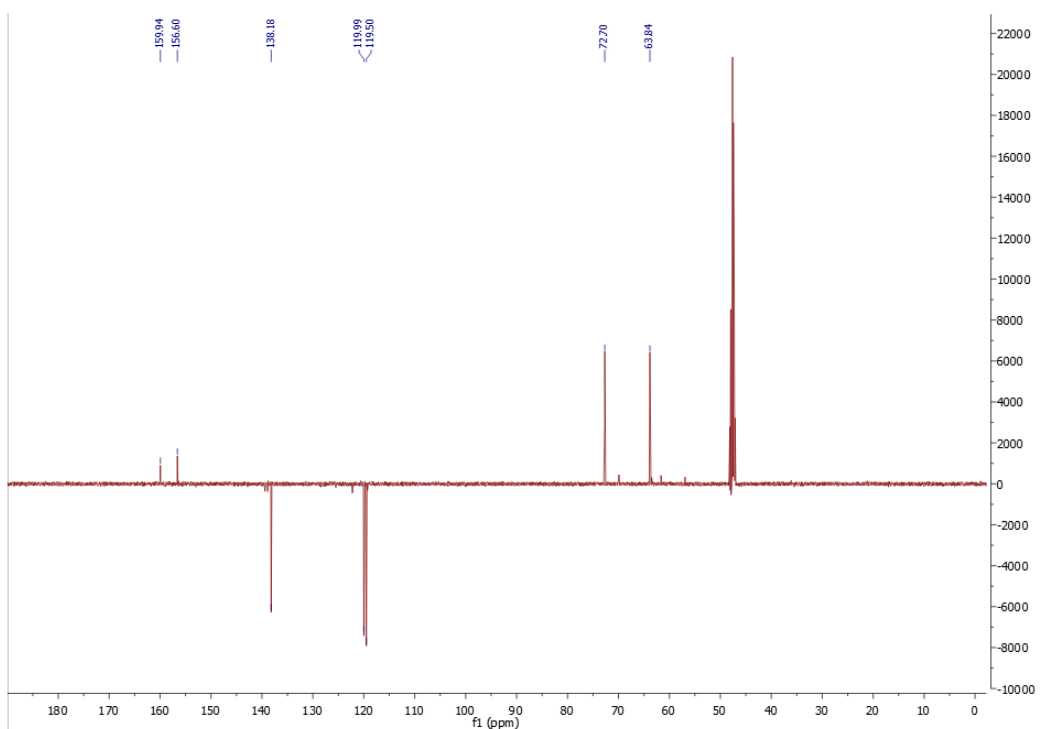


Figure S16. ^{13}C -NMR spectrum of **10** (methanol- d_4)

3. Spectrophotometric investigation of the new crown ether (**1**)

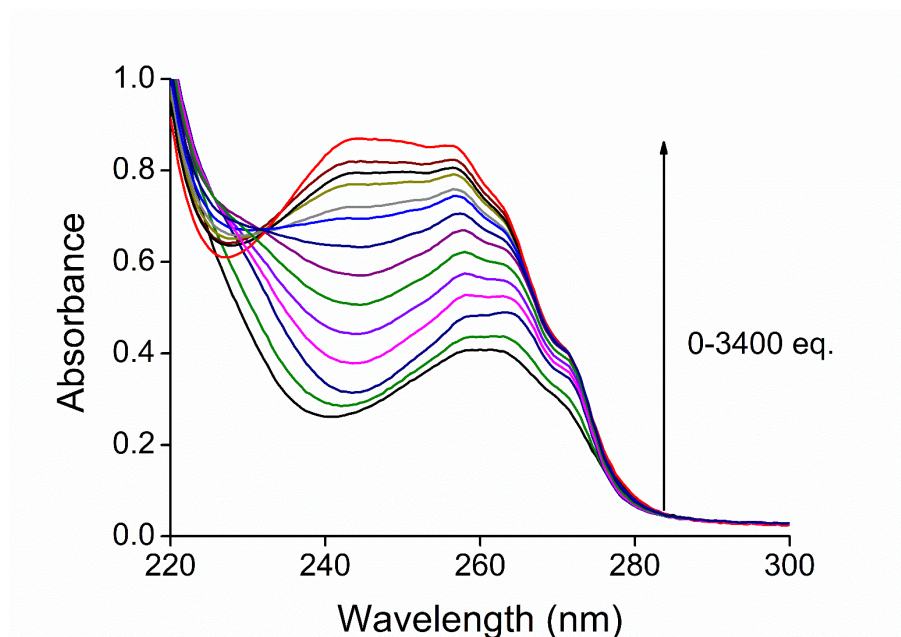


Figure S17. Series of absorption spectra for titrating macrocycle **1** with protonated amine **15** in acetonitrile ($c_{\text{macrocycle}}=5 \cdot 10^{-7} \text{ mol} \cdot \text{L}^{-1}$)

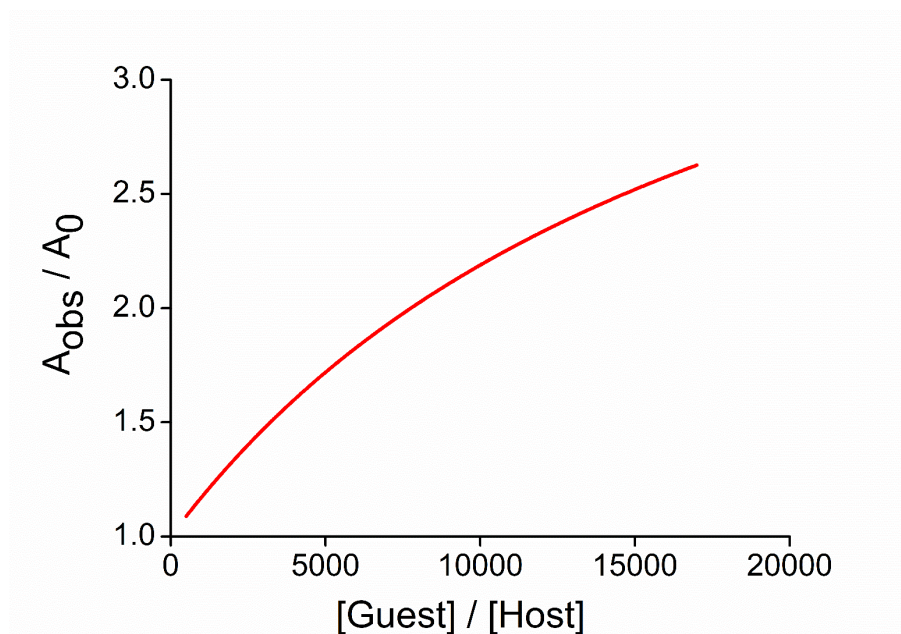


Figure S18. The globally fitted nonlinear regression curve for determining $\log K$ value based on titrating macrocycle **1** with protonated amine **15** in acetonitrile ($c_{\text{macrocycle}}=5 \cdot 10^{-7} \text{ mol} \cdot \text{L}^{-1}$)

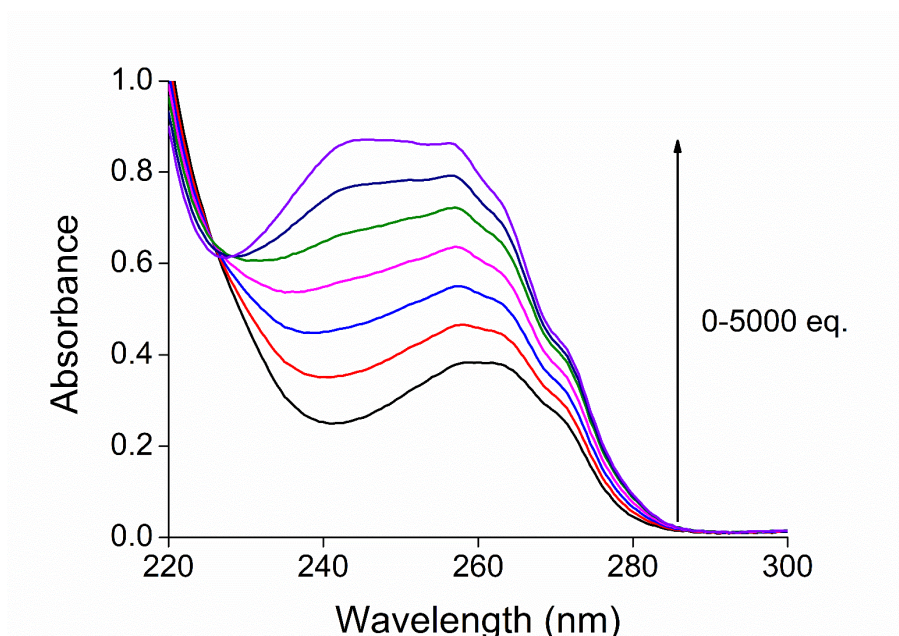


Figure S19. Series of absorption spectra for titrating macrocycle **1** with protonated amine **16** in acetonitrile ($c_{\text{macrocycle}}=5 \cdot 10^{-7} \text{ mol} \cdot \text{L}^{-1}$)

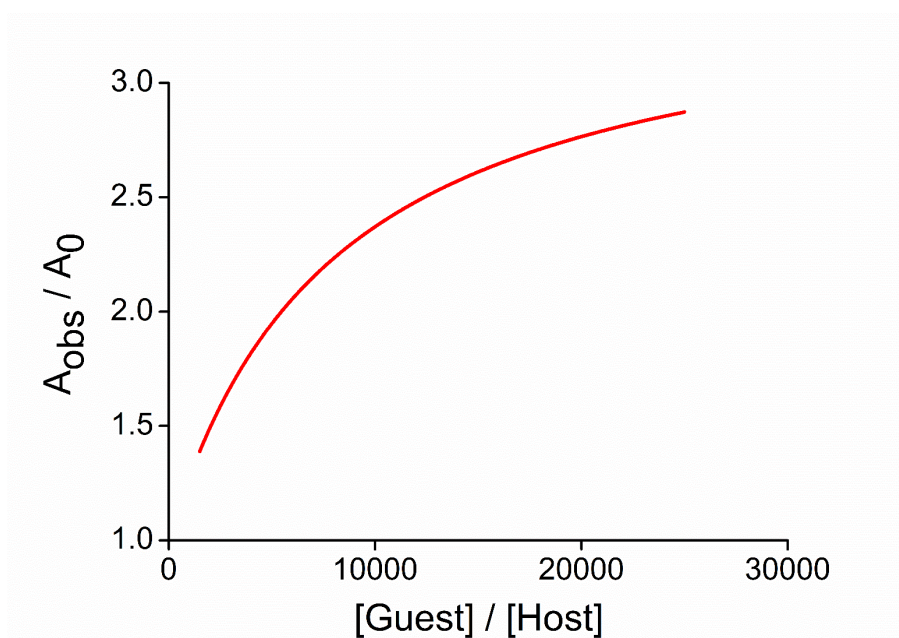


Figure S20. The globally fitted nonlinear regression curve for determining $\log K$ value based on titrating macrocycle **1** with protonated amine **16** in acetonitrile ($c_{\text{macrocycle}}=5 \cdot 10^{-7} \text{ mol} \cdot \text{L}^{-1}$)

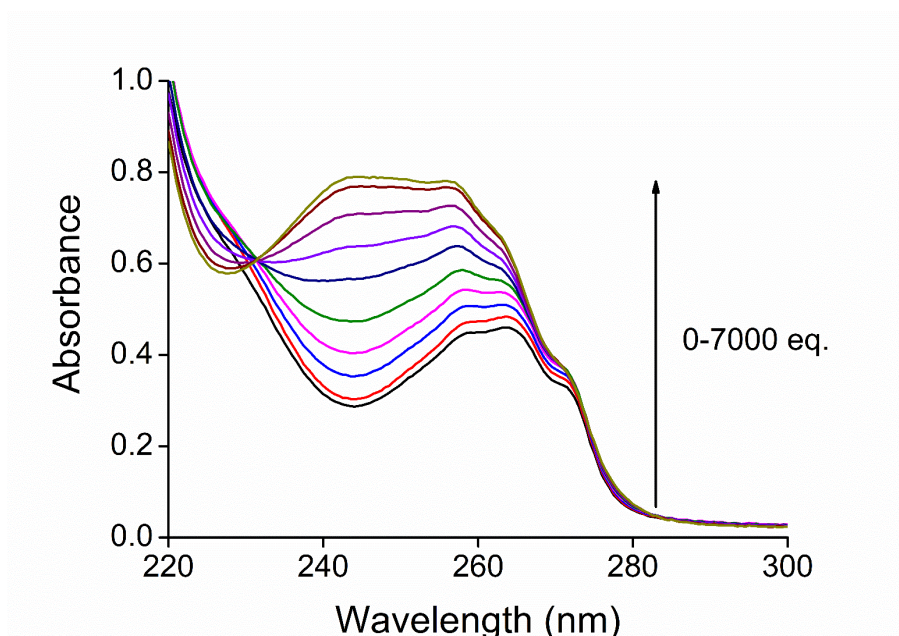


Figure S21. Series of absorption spectra for titrating macrocycle **1** with protonated amine **17** in acetonitrile ($c_{\text{macrocycle}}=5 \cdot 10^{-7} \text{ mol} \cdot \text{L}^{-1}$)

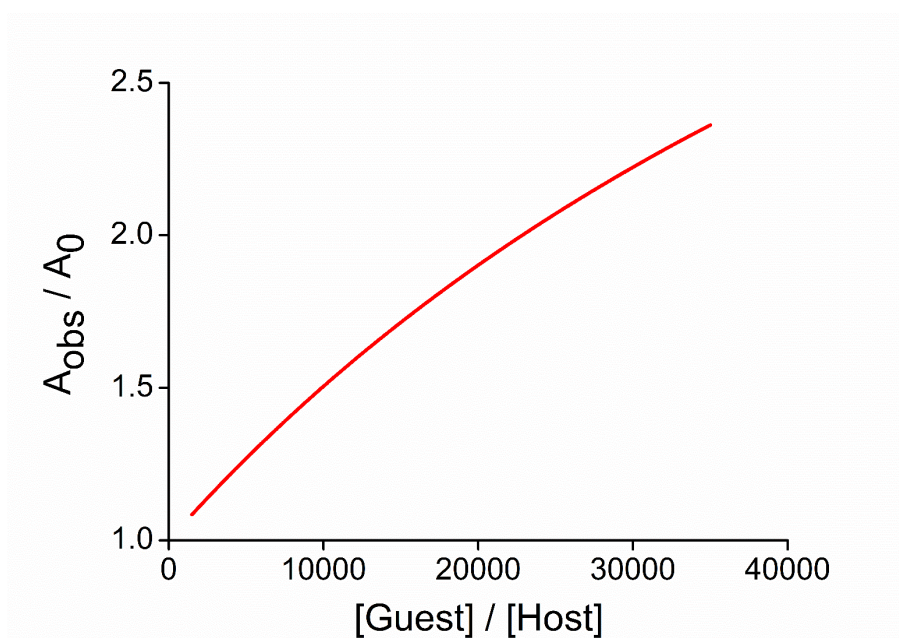


Figure S22. The globally fitted nonlinear regression curve for determining $\log K$ value based on titrating macrocycle **1** with protonated amine **17** in acetonitrile ($c_{\text{macrocycle}}=5 \cdot 10^{-7} \text{ mol} \cdot \text{L}^{-1}$)

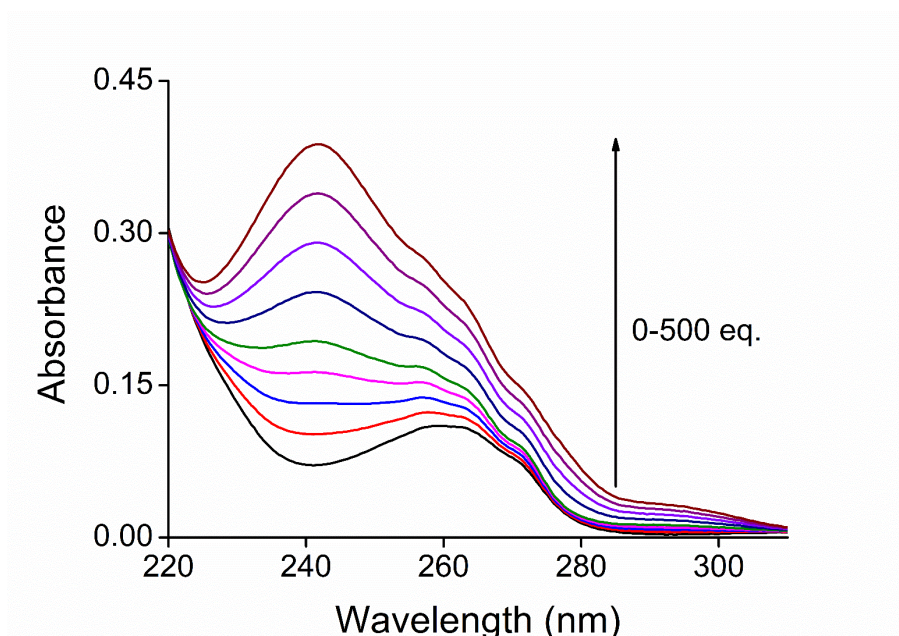


Figure S23. Series of absorption spectra for titrating macrocycle **1** with protonated amine **18** in acetonitrile ($c_{\text{macrocycle}}=5 \cdot 10^{-8} \text{ mol} \cdot \text{L}^{-1}$)

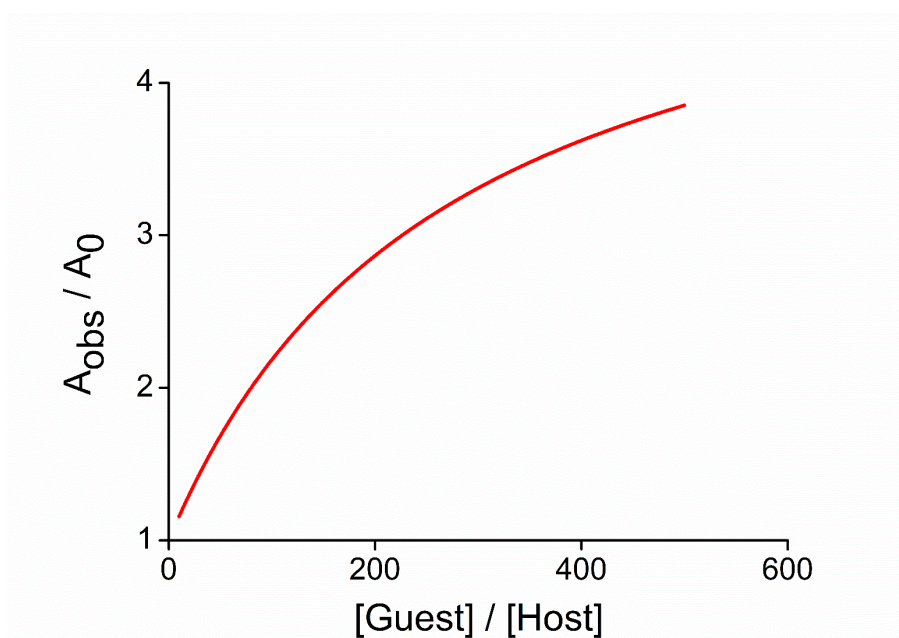


Figure S24. The globally fitted nonlinear regression curve for determining $\log K$ value based on titrating macrocycle **1** with protonated amine **18** in acetonitrile ($c_{\text{macrocycle}}=5 \cdot 10^{-8} \text{ mol} \cdot \text{L}^{-1}$)

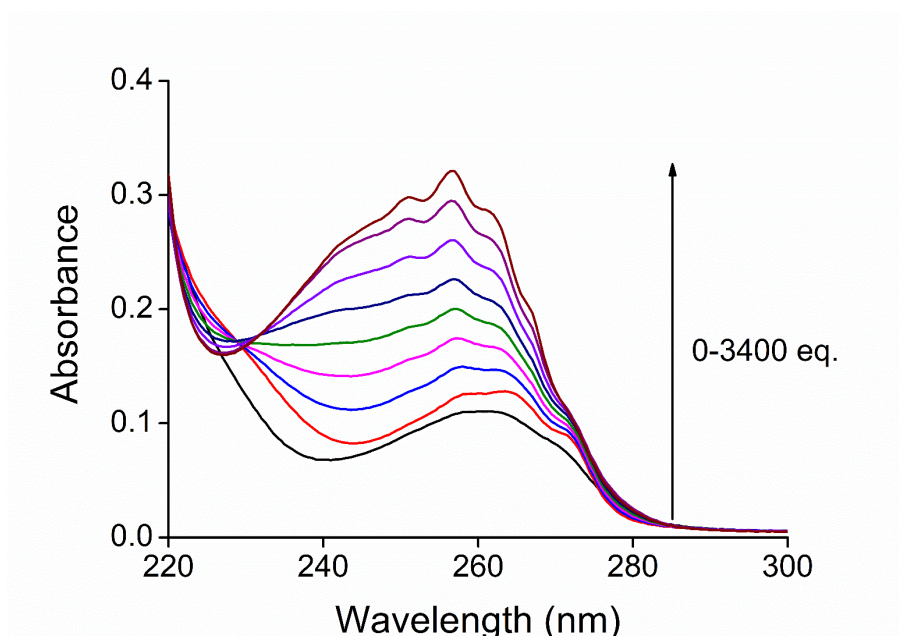


Figure S25. Series of absorption spectra for titrating macrocycle **1** with protonated amine **21** in acetonitrile ($c_{\text{macrocycle}}=5 \cdot 10^{-8} \text{ mol} \cdot \text{L}^{-1}$)

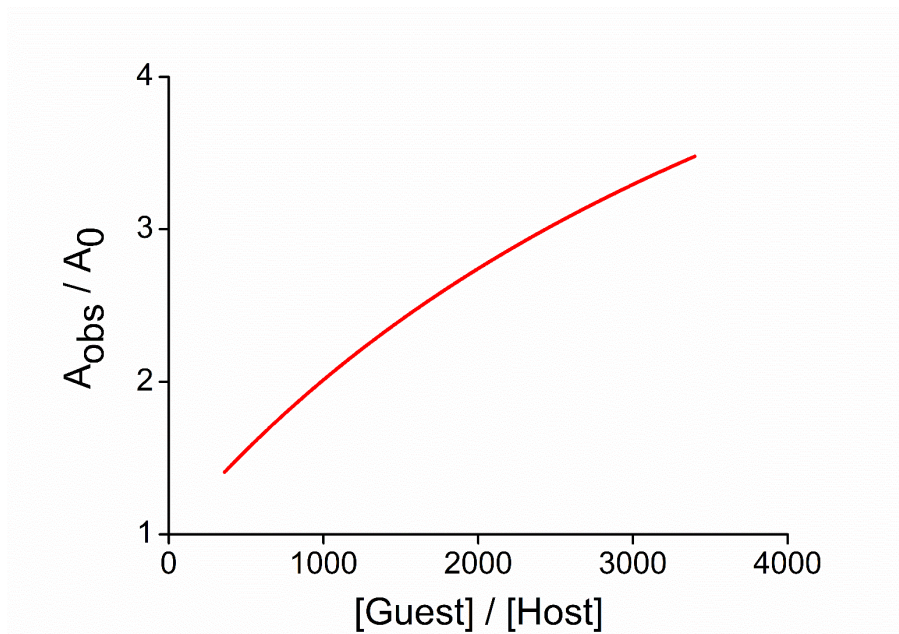


Figure S26. The globally fitted nonlinear regression curve for determining $\log K$ value based on titrating macrocycle **1** with protonated amine **21** in acetonitrile ($c_{\text{macrocycle}}=5 \cdot 10^{-8} \text{ mol} \cdot \text{L}^{-1}$)

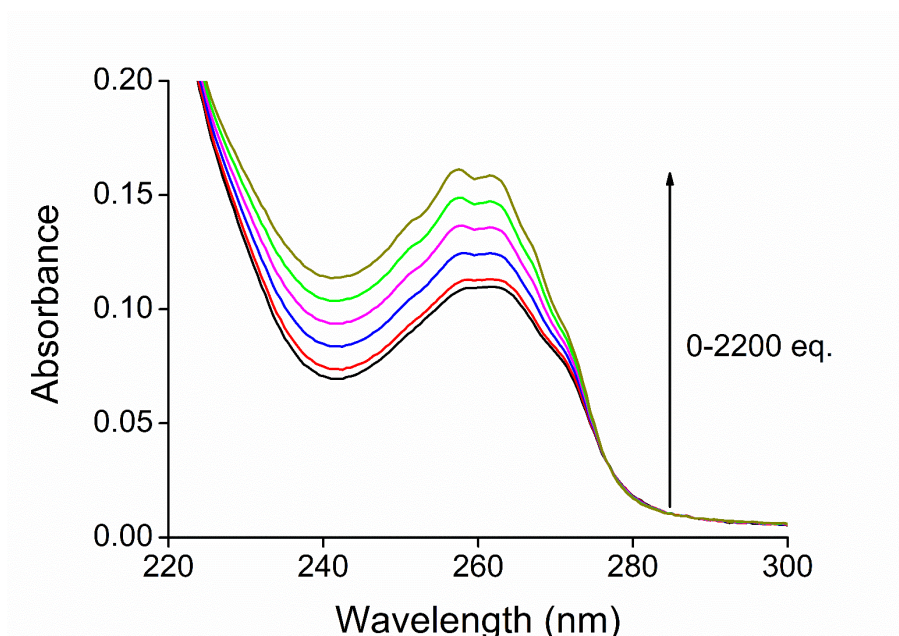


Figure S27. Series of absorption spectra for titrating macrocycle **1** with protonated amine **22** in acetonitrile ($c_{\text{macrocycle}}=5 \cdot 10^{-8} \text{ mol} \cdot \text{L}^{-1}$)

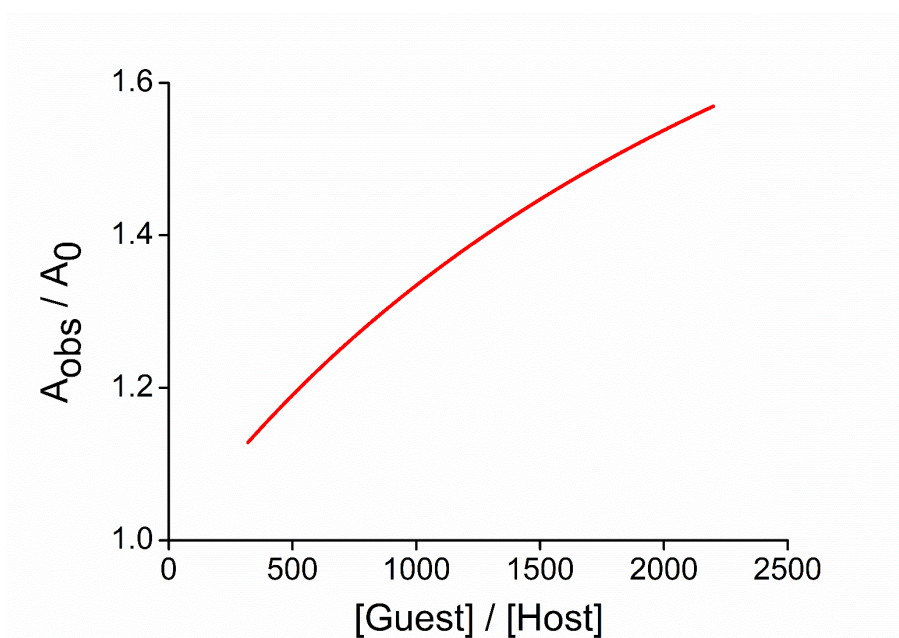


Figure S28. The globally fitted nonlinear regression curve for determining $\log K$ value based on titrating macrocycle **1** with protonated amine **22** in acetonitrile ($c_{\text{macrocycle}}=5 \cdot 10^{-8} \text{ mol} \cdot \text{L}^{-1}$)

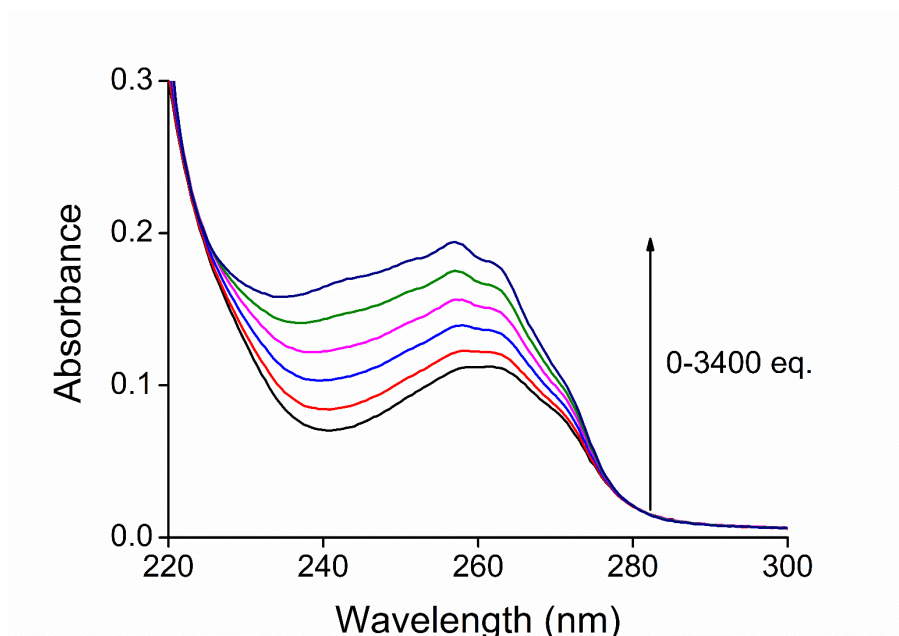


Figure S29. Series of absorption spectra for titrating macrocycle **1** with protonated amine **23** in acetonitrile ($c_{\text{macrocycle}}=5 \cdot 10^{-8} \text{ mol} \cdot \text{L}^{-1}$)

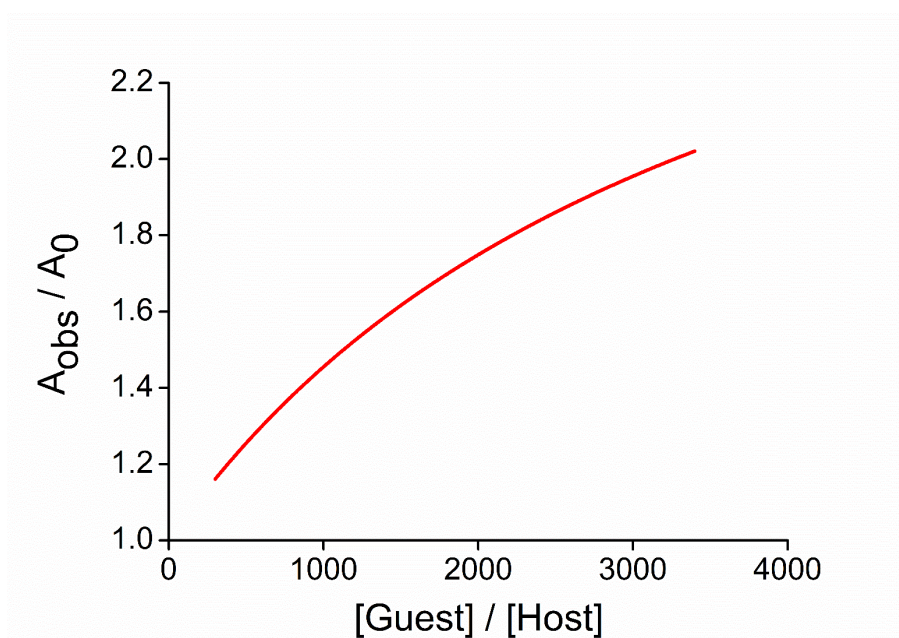


Figure S30. The globally fitted nonlinear regression curve for determining $\log K$ value based on titrating macrocycle **1** with protonated amine **23** in acetonitrile ($c_{\text{macrocycle}}=5 \cdot 10^{-8} \text{ mol} \cdot \text{L}^{-1}$)

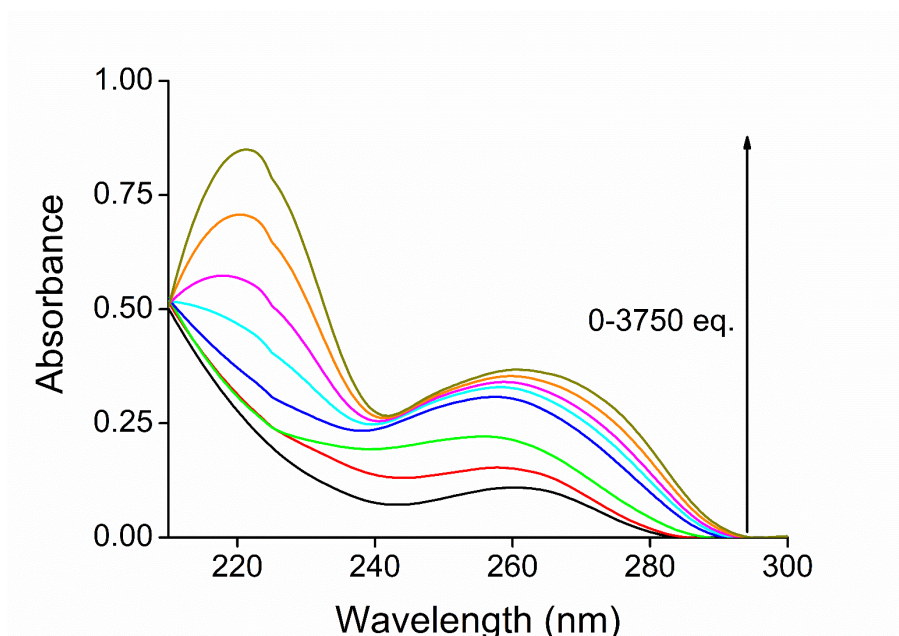


Figure S31. Series of absorption spectra for titrating macrocycle **1** with protonated amine **24** in acetonitrile ($c_{\text{macrocycle}}=5 \cdot 10^{-8} \text{ mol} \cdot \text{L}^{-1}$)

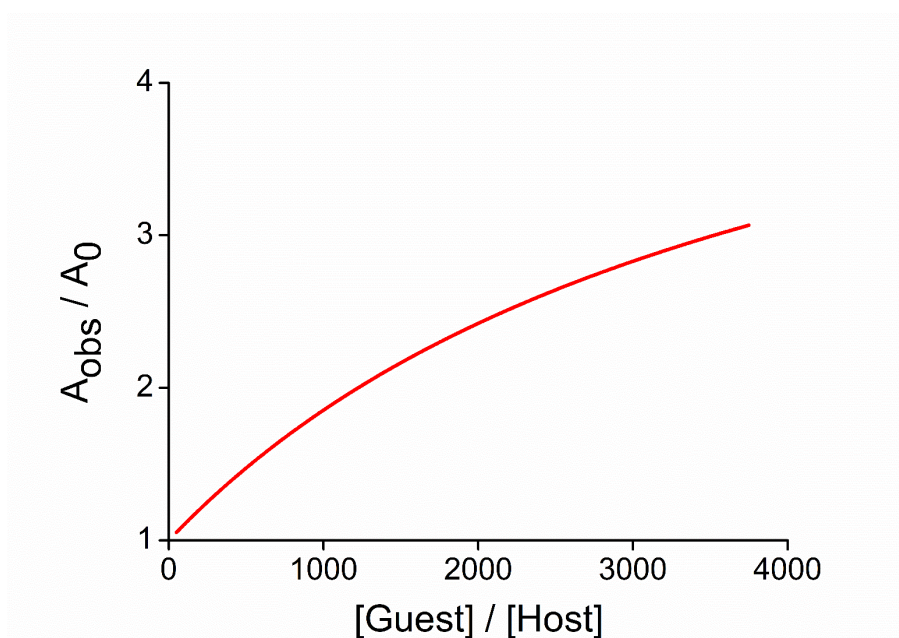


Figure S32. The globally fitted nonlinear regression curve for determining $\log K$ value based on titrating macrocycle **1** with protonated amine **24** in acetonitrile ($c_{\text{macrocycle}}=5 \cdot 10^{-8} \text{ mol} \cdot \text{L}^{-1}$)

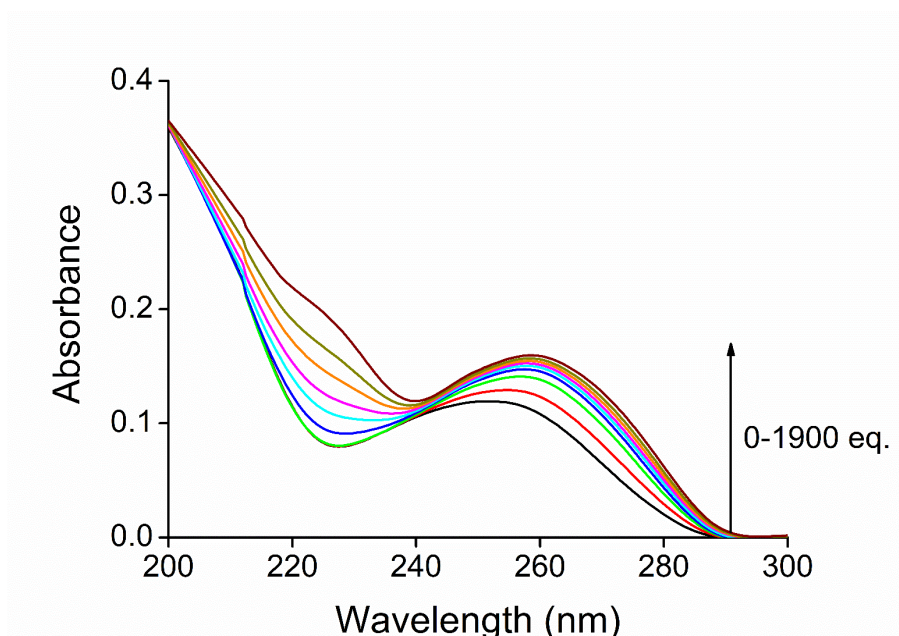


Figure S33. Series of absorption spectra for titrating macrocycle **1** with protonated amine **25** in acetonitrile ($c_{\text{macrocycle}}=5 \cdot 10^{-8} \text{ mol} \cdot \text{L}^{-1}$)

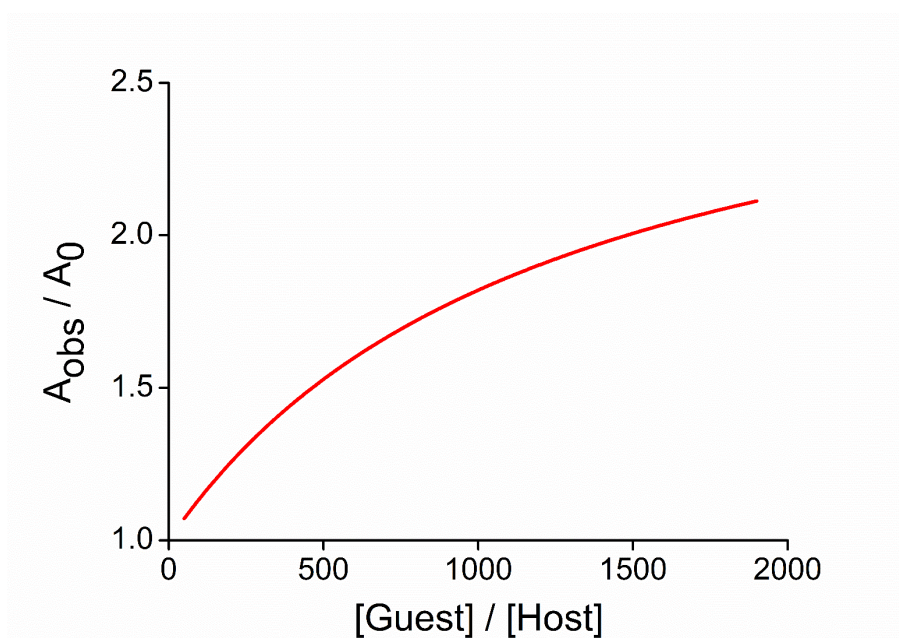


Figure S34. The globally fitted nonlinear regression curve for determining $\log K$ value based on titrating macrocycle **1** with protonated amine **25** in acetonitrile ($c_{\text{macrocycle}}=5 \cdot 10^{-8} \text{ mol} \cdot \text{L}^{-1}$)

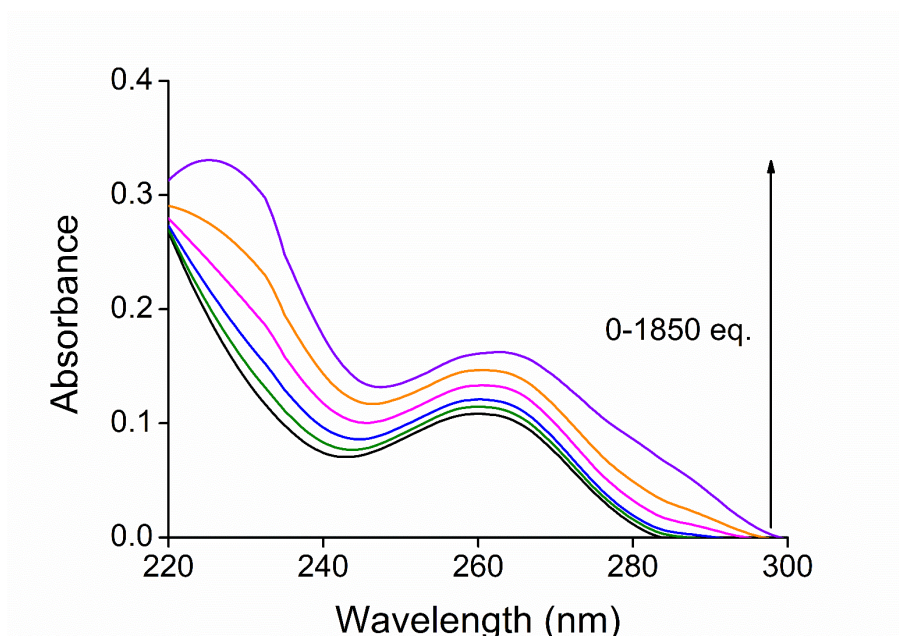


Figure S35. Series of absorption spectra for titrating macrocycle **1** with protonated amine **26** in acetonitrile ($c_{\text{macrocycle}}=5 \cdot 10^{-8} \text{ mol} \cdot \text{L}^{-1}$)

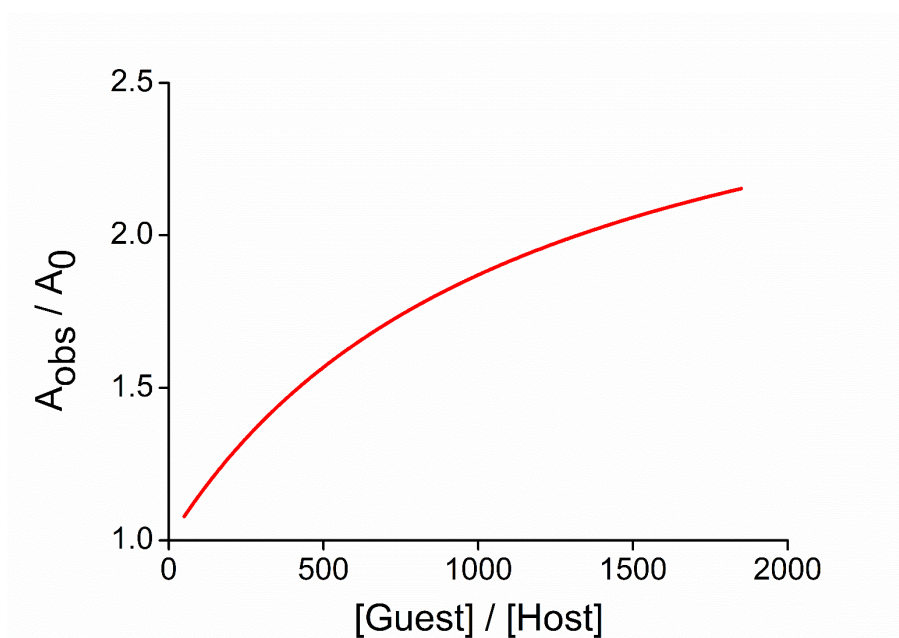


Figure S36. The globally fitted nonlinear regression curve for determining $\log K$ value based on titrating macrocycle **1** with protonated amine **26** in acetonitrile ($c_{\text{macrocycle}}=5 \cdot 10^{-8} \text{ mol} \cdot \text{L}^{-1}$)

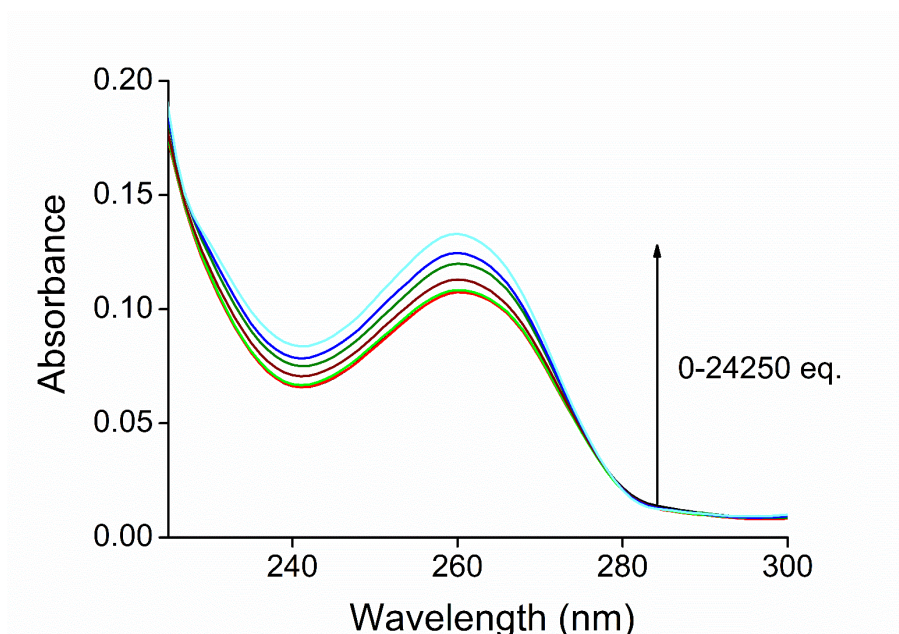


Figure S37. Series of absorption spectra for titrating macrocycle **1** with protonated amine **27** in acetonitrile ($c_{\text{macrocycle}}=5 \cdot 10^{-8} \text{ mol} \cdot \text{L}^{-1}$)

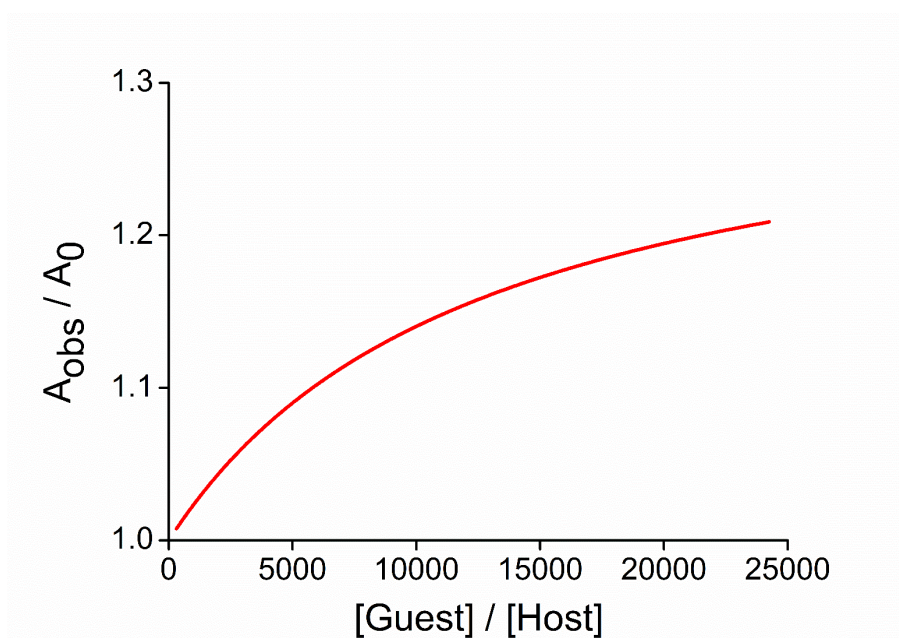


Figure S38. The globally fitted nonlinear regression curve for determining $\log K$ value based on titrating macrocycle **1** with protonated amine **27** in acetonitrile ($c_{\text{macrocycle}}=5 \cdot 10^{-8} \text{ mol} \cdot \text{L}^{-1}$)