

Supporting information
for the article

**Polyoxa- and Polyazamacrocycles Incorporating 6,7-
diaminoquinoxaline Moiety: Synthesis and Application as
Tunable Optical pH-Indicators in Aqueous Solution**

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1.Spectroscopic Studies of 3, 5c and 5e in Organic Solvents.

Table S1. Photophysical data for compounds 3, 5c and 5e in various solvents

Compound	Solvent	$\lambda_{\text{abs}}, \text{nm}$ ($\log \epsilon$) ^a	$\lambda_{\text{em}}, \text{nm}$	$\Phi, \%$ ^b	Brightness, B, $\text{M}^{-1} \text{cm}^{-1} \text{c}$
3	toluene	400 (4.35)	453	34	7597
	dioxane	258 (4.49)	450	53	12261
		281 (4.47)			
		404 (4.36)			
	CH ₂ Cl ₂	402 (4.25)	465	52	9296
	MeCN	261 (4.51)	465	59	13494
		279 (4.50)			
		404 (4.36)			
	MeOH	261 (4.62)	482	48	10978
		279 (4.53)			
		416 (4.36)			
	H ₂ O (pH = 6) ^c	256 (4.22)	507	27	3132
		277 (4.18)			
		412 (4.06)			
5c	toluene	408 (4.29)	450	50	12492
	dioxane	261 (4.24)	451	70	12125
		283 (4.22)			
		408 (4.14)			
	CH ₂ Cl ₂	410 (4.14)	462	59	10220
	MeCN	262 (4.38)	465	44	9674
		282 (4.35)			
		409 (4.24)			
	MeOH	261 (4.45)	486	64	11726
		279 (4.39)			
		420 (4.16)			
	H ₂ O (pH = 6) ^c	256 (4.19)	510	34	3944
		277 (4.14)			
		418 (4.06)			
5e	toluene	416 (4.30)	452	42	8355
	dioxane	262 (4.31)	456	33	4837
		283 (4.30)			
		411 (4.17)			
	CH ₂ Cl ₂	405 (3.94)	476	42	3628
	MeCN	257 (4.39)	480	44	6795
		278 (4.36)			
		400 (4.19)			
	MeOH	256 (4.39)	498	60	9423
		279 (4.34)			

	412 (4.20)			
H ₂ O (pH = 6) ^c	256 (4.38)	526	36	5148
	277 (4.33)			
	407 (4.15)			

^aMolar extinction coefficient (ϵ) is expressed in M⁻¹ cm⁻¹. ^b Quantum yields were determined using quinine sulfate in 0.05M H₂SO₄ (Φ = 53%) as a standard. ^c $B = \Phi(\lambda) \times \epsilon(\lambda_{ex})$. [1], the lowest absorption band (ICT) was used for the calculation. ^c 1 vol% MeOH in H₂O.

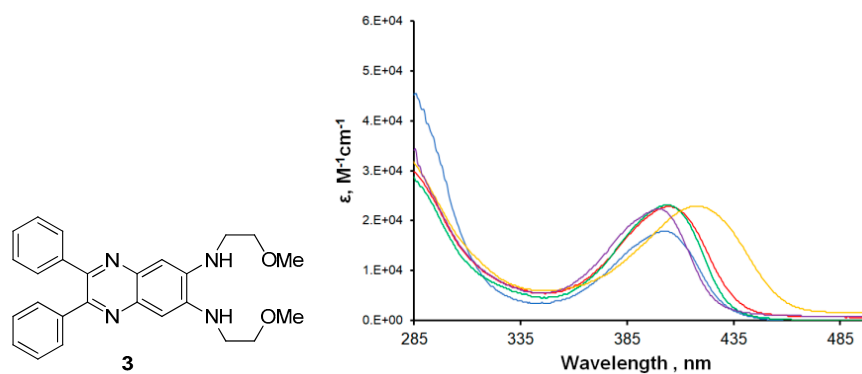


Figure S1. UV-vis spectra of **3** in toluene (violet), dioxane (green), CH₂Cl₂ (blue), MeCN (red) and MeOH (yellow).

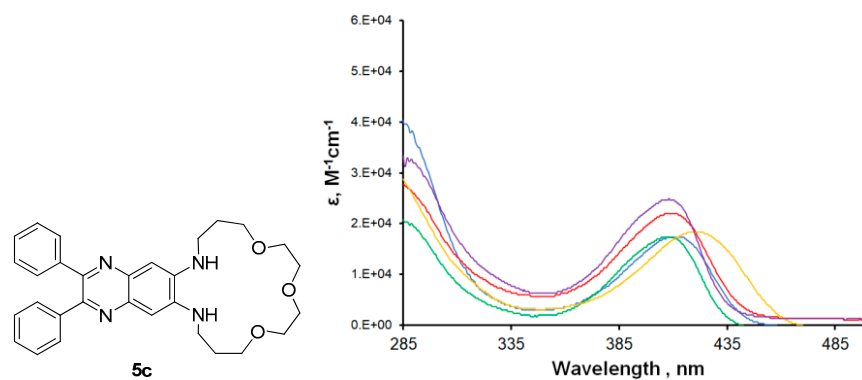


Figure S2. UV-vis spectra of **5c** in toluene (violet), dioxane (green), CH₂Cl₂ (blue), MeCN (red) and MeOH (yellow).

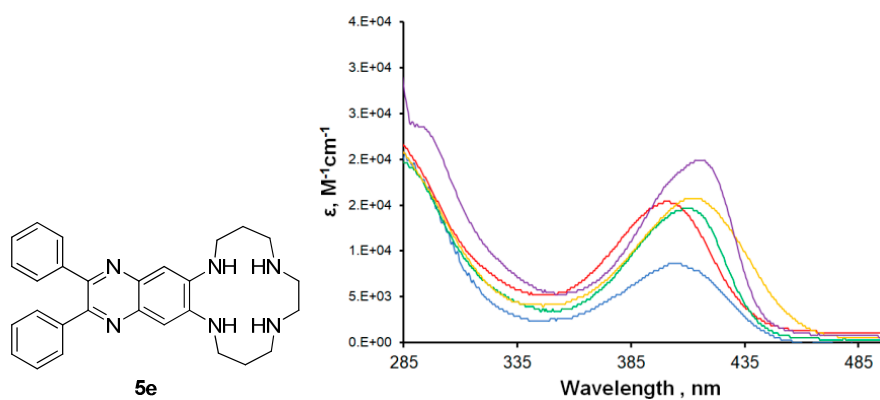


Figure S3. UV-vis spectra of **5e** in toluene (violet), dioxane (green), CH₂Cl₂ (blue), MeCN (red) and MeOH (yellow).

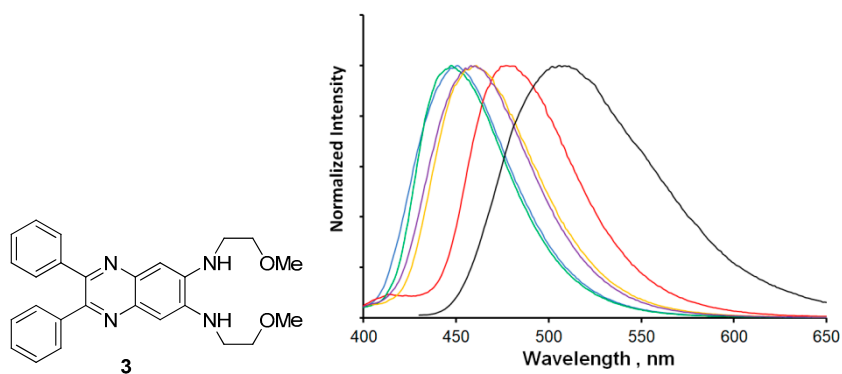


Figure S4. Normalized fluorescence spectra of **3** ($\lambda_{\text{ex}} = 420$ nm) in toluene (blue), dioxane (green), CH_2Cl_2 (violet), MeCN (yellow), MeOH (red), water (1 vol% MeOH, pH = 6, black).

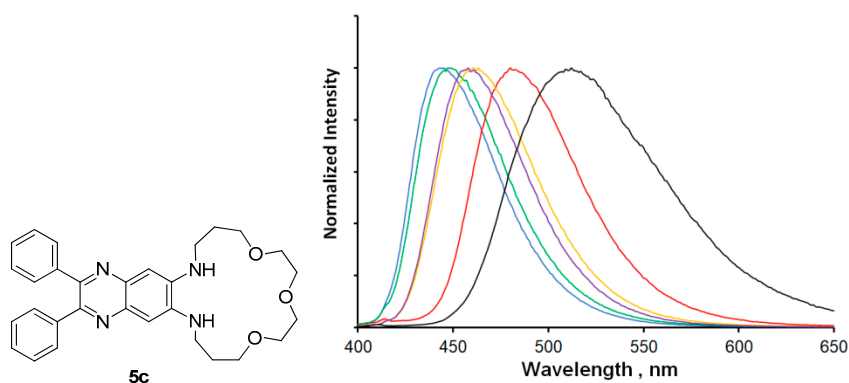


Figure S5. Normalized fluorescence spectra of **5c** ($\lambda_{\text{ex}} = 420$ nm) in toluene (blue), dioxane (green), CH_2Cl_2 (violet), MeCN (yellow), MeOH (red), water (1 vol% MeOH, pH = 6, black).

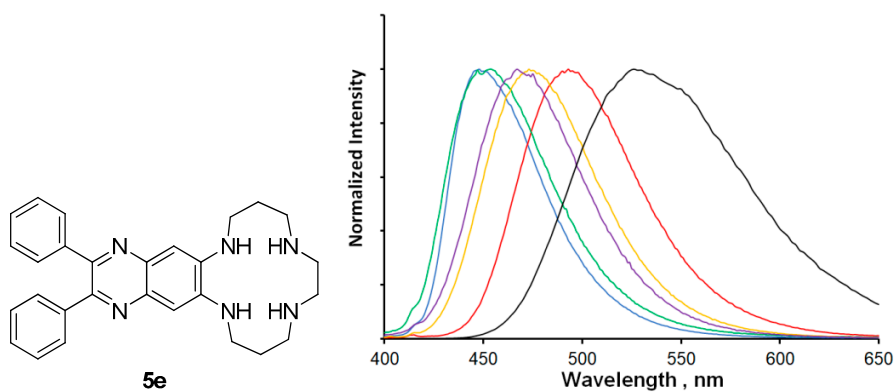
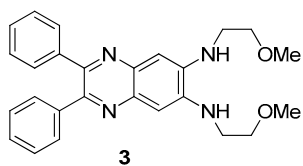


Figure S6. Normalized fluorescence spectra of **5c** ($\lambda_{\text{ex}} = 420$ nm) in toluene (blue), dioxane (green), CH_2Cl_2 (violet), MeCN (yellow), MeOH (red), water (pH = 6, black). The spectrum in water corresponds $[\mathbf{5eH}]^+$.

2. Spectroscopic studies of **3**, **5c** and **5e** in aqueous solutions



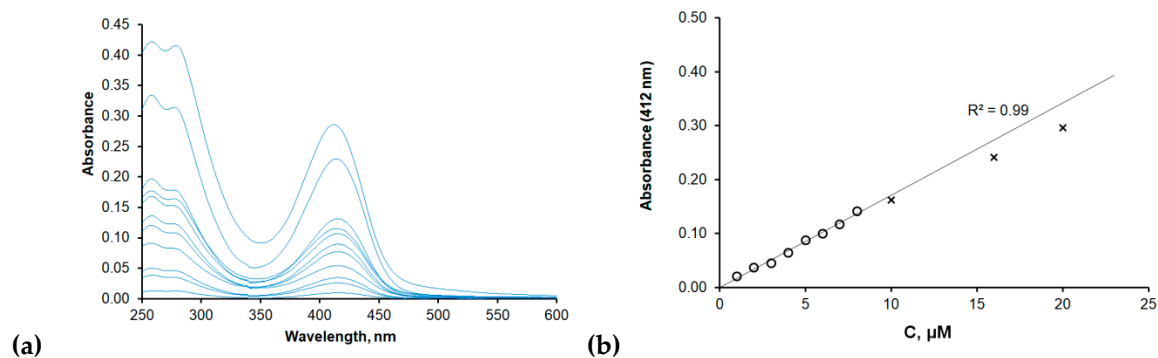


Figure S7. (a) UV-vis spectra of **3** in aqueous solutions (1% MeOH, pH = 6). (b) Dependence of the absorbance intensity on **3** concentration in aqueous solutions (1 vol% MeOH, pH = 6).

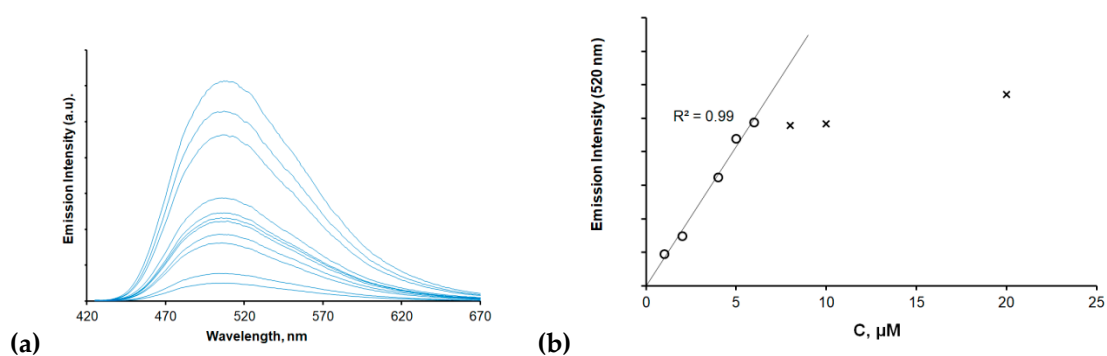


Figure S8. (a) Fluorescence spectra of **3** in aqueous solutions (1 vol % MeOH, pH = 6, $\lambda_{\text{ex}} = 415$ nm). (b) Dependence of the emission intensity on **3** concentration in aqueous solutions (1 vol % MeOH, pH = 6, $\lambda_{\text{ex}} = 415$ nm).

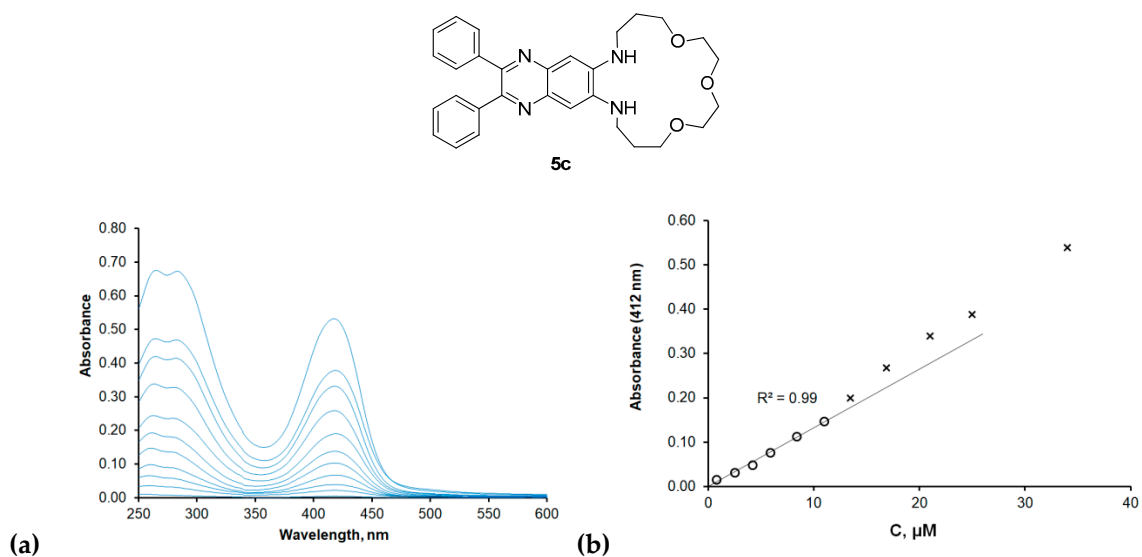


Figure S9. (a) UV-vis spectra of **5c** in aqueous solutions (1 vol % MeOH, pH = 6). (b) Dependence of the absorbance intensity on **5c** concentration in aqueous solutions (1 vol % MeOH, pH = 6).

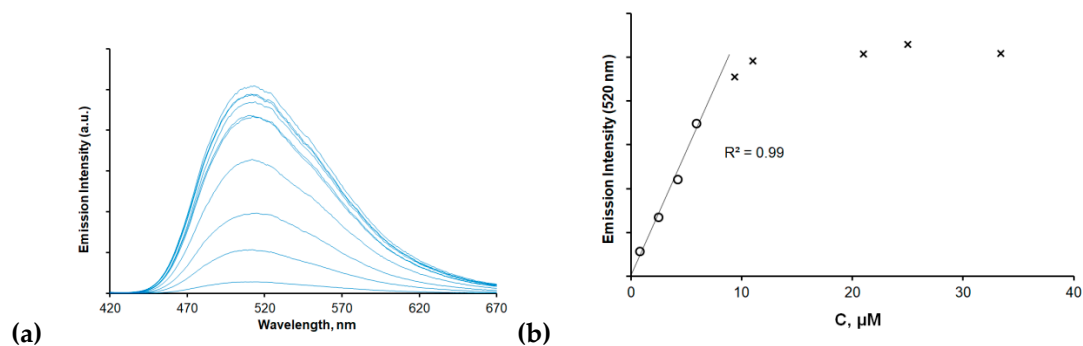


Figure S10. (a) Fluorescence spectra of **5c** in aqueous solutions (1 vol% MeOH, pH = 6, $\lambda_{\text{ex}} = 415 \text{ nm}$). (b) Dependence of the emission intensity on **5c** concentration in aqueous solutions (1 vol% MeOH, pH = 6, $\lambda_{\text{ex}} = 415 \text{ nm}$).

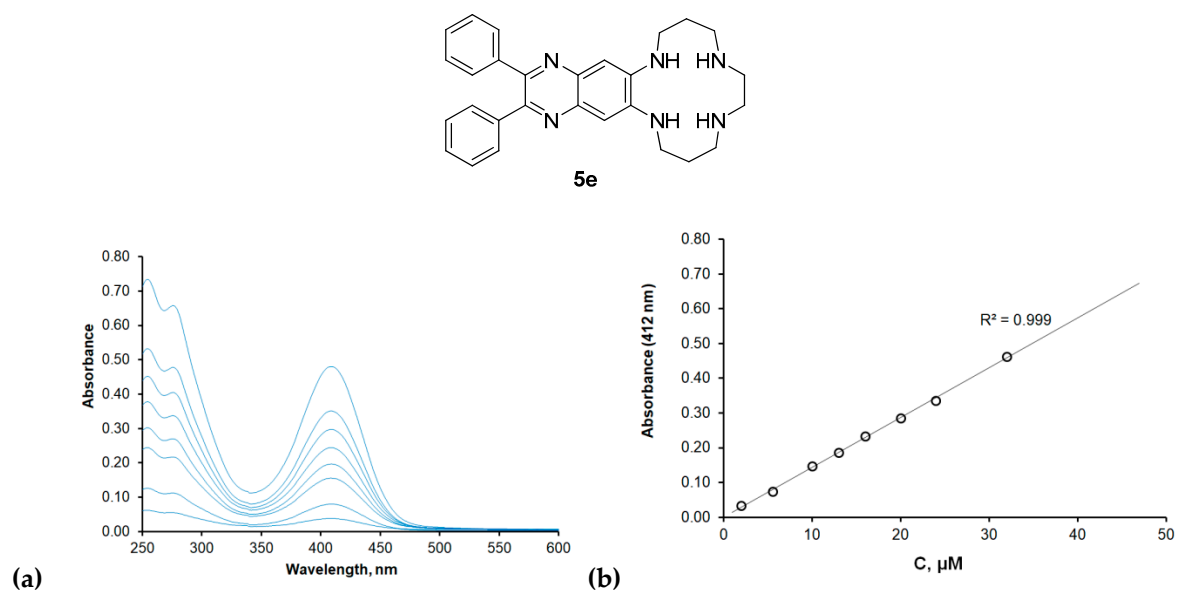


Figure S11. (a) UV-vis spectra of **5e** in aqueous solutions (pH = 6). (b) Dependence of the absorbance intensity on **5e** concentration in aqueous solutions (pH = 6).

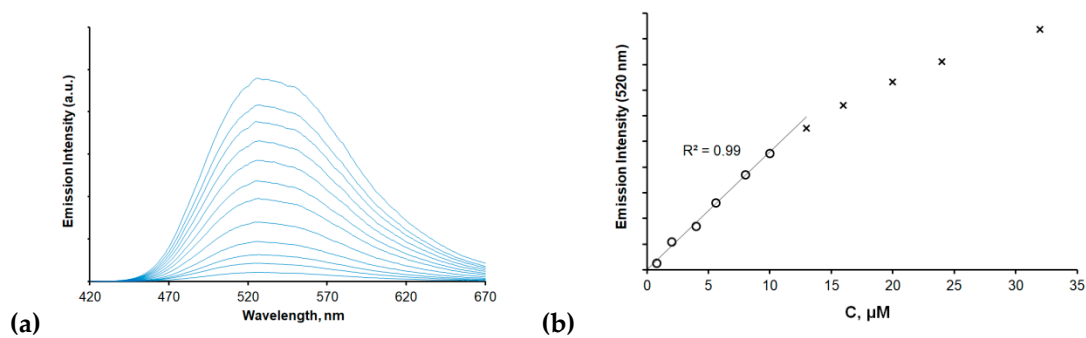


Figure S12. (a) Fluorescence spectra of **5e** in aqueous solutions (pH = 6, $\lambda_{\text{ex}} = 415$ nm). (b) Dependence of the emission intensity on **5e** concentration in aqueous solutions (pH = 6, $\lambda_{\text{ex}} = 415$ nm).

3. Studies of **3** and **5a-d** for Metal Cations Binding in Acetonitrile.

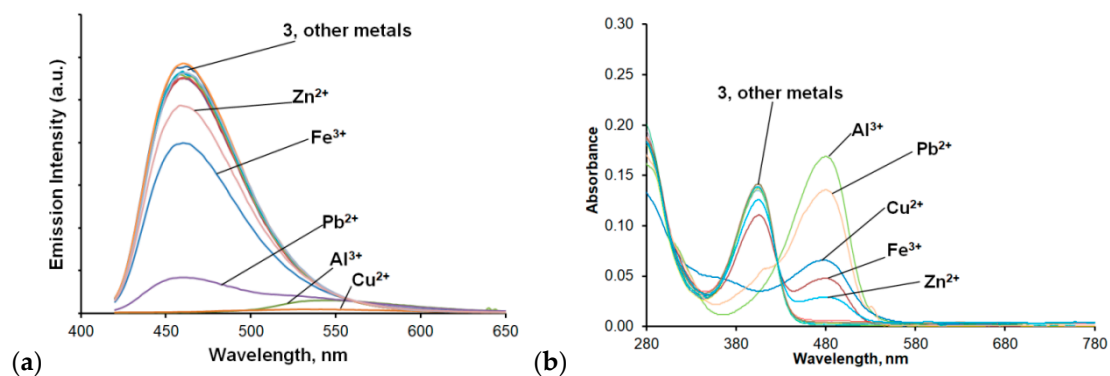
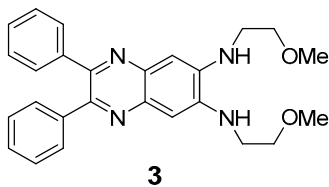


Figure S13. Luminescence (a) and absorption (b) spectra of **3** in acetonitrile ($[\mathbf{3}] = 6.0 \mu\text{M}$, $\lambda_{\text{ex}} = 405 \text{ nm}$) before and after addition of 5 equiv. of metal perchlorate salts.

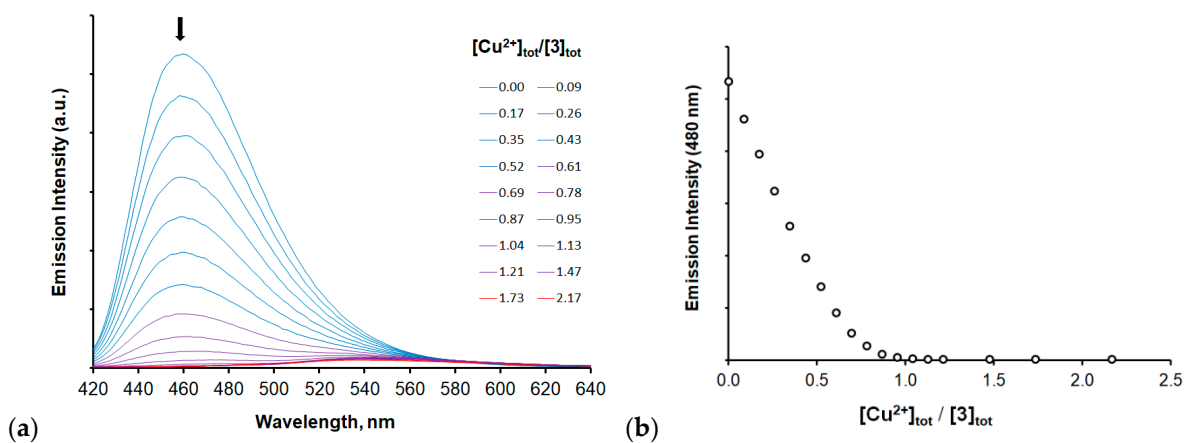


Figure S14. (a) Evolution of the emission spectrum of **3** in acetonitrile ($[\mathbf{3}]_{\text{tot}} = 6.0 \mu\text{M}$, $\lambda_{\text{ex}} = 405 \text{ nm}$) upon addition of $\text{Cu}(\text{ClO}_4)_2$ (0–2.1 equiv.). (b) Changes of the emission intensity as a function of the $[\text{Cu}^{2+}]_{\text{tot}}/[\mathbf{3}]_{\text{tot}}$ ratio at $\lambda_{\text{em}} = 480 \text{ nm}$.

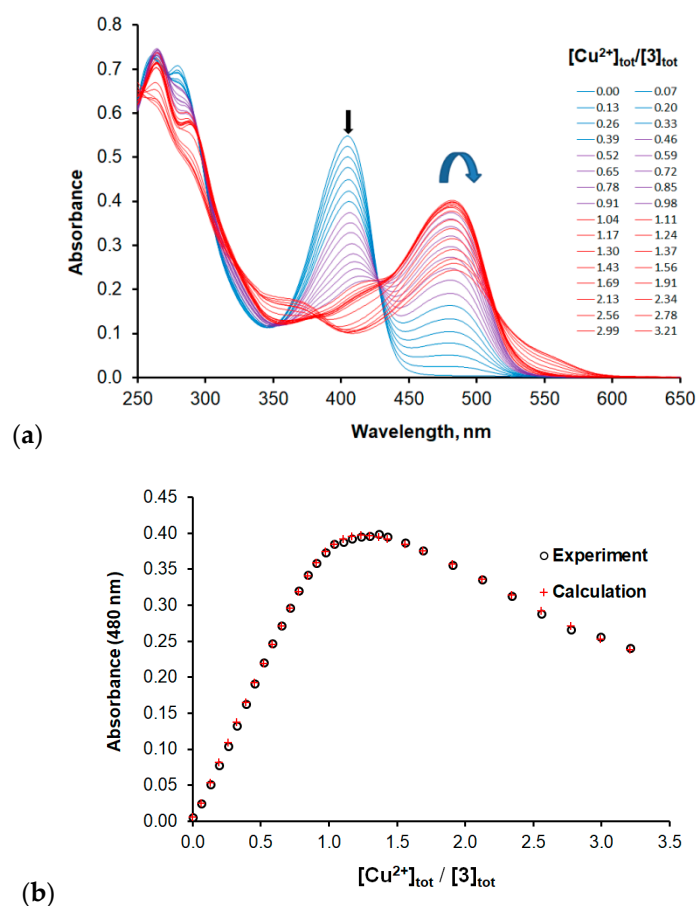


Figure S15. Evolution of the UV-vis absorption spectrum of **3** in acetonitrile ($[3] = 23.9 \mu\text{M}$) upon addition of $\text{Cu}(\text{ClO}_4)_2$ (0–3.2 equiv.). Changes of the absorbance as a function of the $[\text{Cu}^{2+}]_{\text{tot}}/[\text{3}]_{\text{tot}}$ ratio at $\lambda = 480 \text{ nm}$.

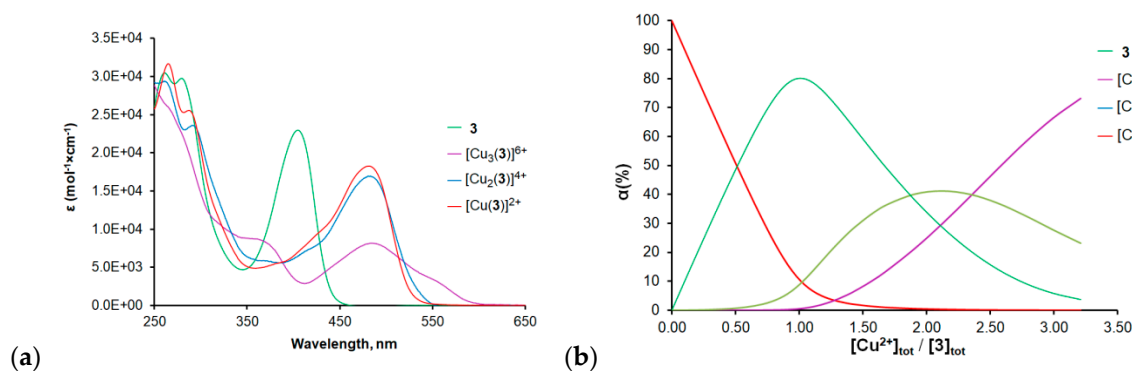
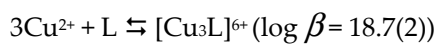
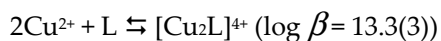
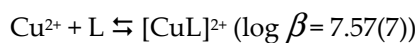


Figure S16. UV-vis spectra of **3**, $[\text{Cu}(\text{3})]^{2+}$, $[\text{Cu}_2(\text{3})]^{4+}$ and $[\text{Cu}_3(\text{3})]^{6+}$ in acetonitrile calculated using HypSpec program.[2] (b) Species distribution diagram for the **3**/ Cu^{2+} system in acetonitrile calculated using HypSpec program.[2] Data were fit with HypSpec using the following model:



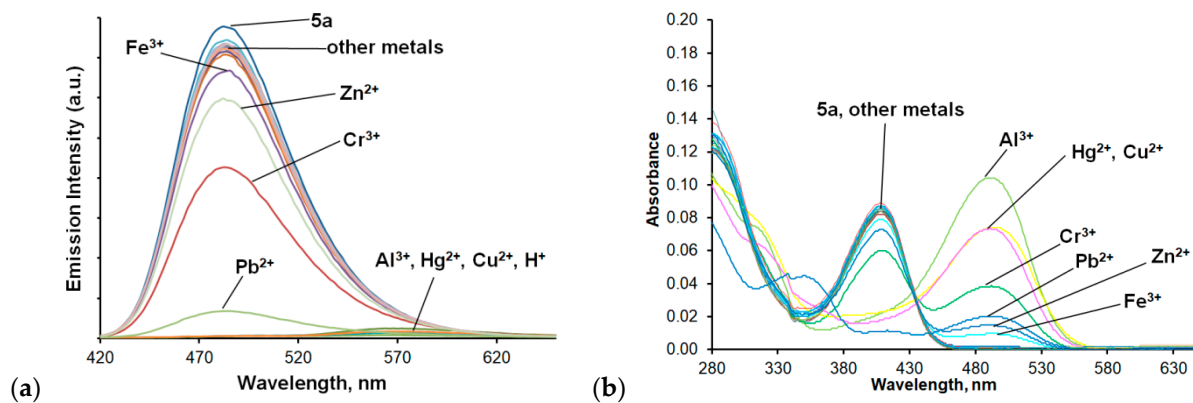
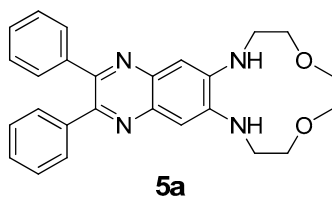


Figure S17. Luminescence (a) and absorption (b) spectra of **5a** in acetonitrile ($[\mathbf{5a}] = 5.2 \mu\text{M}$, $\lambda_{\text{ex}} = 408 \text{ nm}$) before and after addition of 5 equiv. of metal perchlorate salts.

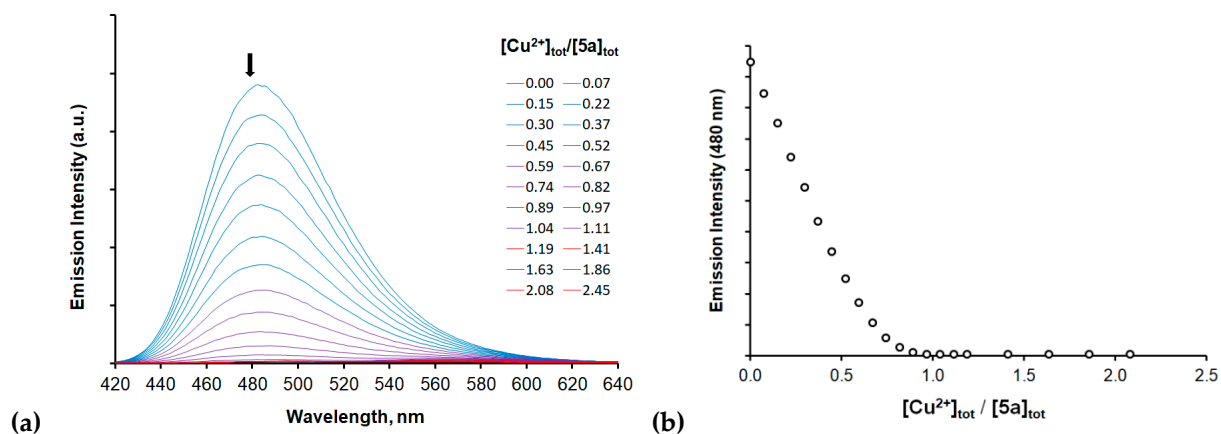


Figure S18. (a) Evolution of the emission spectrum of **5a** in acetonitrile ($[\mathbf{5a}]_{\text{tot}} = 5.2 \mu\text{M}$, $\lambda_{\text{ex}} = 408 \text{ nm}$) upon addition of $\text{Cu}(\text{ClO}_4)_2$ (0–2.4 equiv.). (b) Changes of the emission intensity as a function of the $[\text{Cu}^{2+}]_{\text{tot}}/[\mathbf{5a}]_{\text{tot}}$ ratio at $\lambda_{\text{em}} = 480 \text{ nm}$.

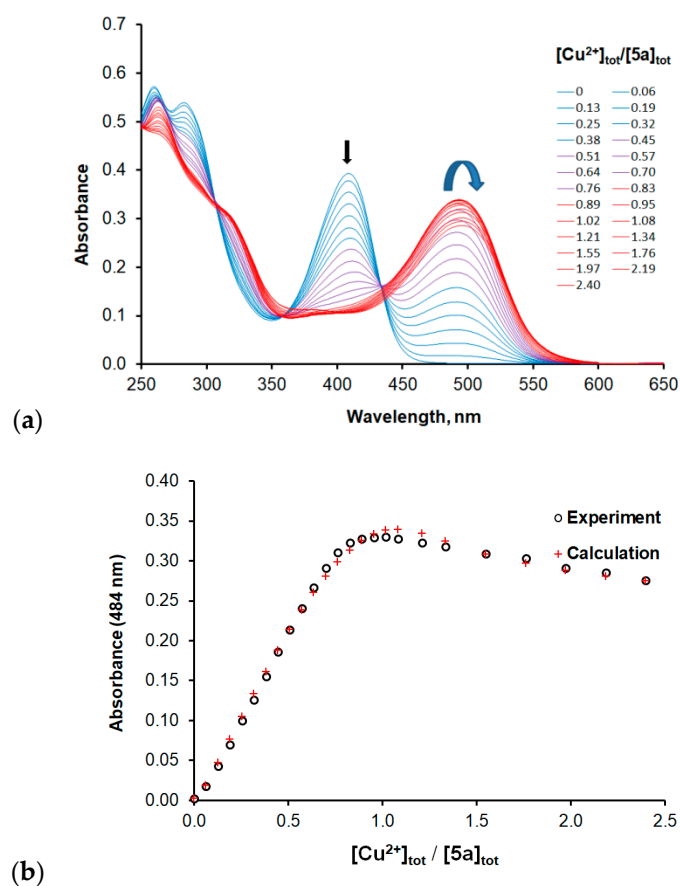


Figure S19. (a) Evolution of the UV-vis absorption spectrum of **5a** in acetonitrile ($[5a] = 24.4 \mu\text{M}$) upon addition of $\text{Cu}(\text{ClO}_4)_2$ (0–2.4 equiv.). (b) Changes of the absorbance as a function of the $[\text{Cu}^{2+}]_{\text{tot}}/[\text{5a}]_{\text{tot}}$ ratio at $\lambda = 484 \text{ nm}$.

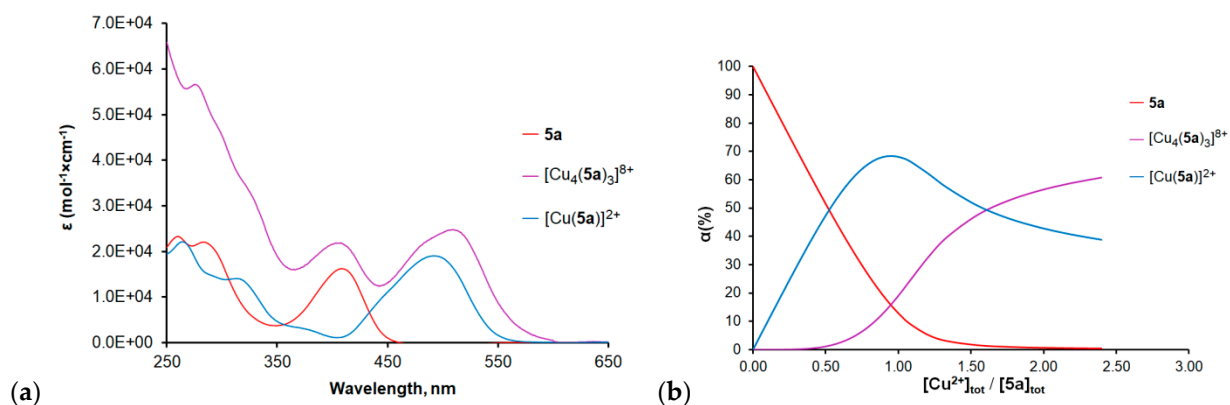
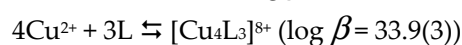
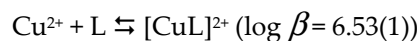
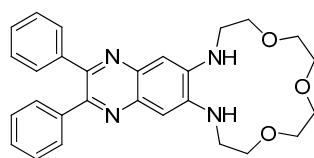


Figure S20. (a) UV-vis spectra of **5a**, $[\text{Cu}(\text{5a})]^{2+}$ and $[\text{Cu}_4(\text{5a})_3]^{8+}$ in acetonitrile calculated using HypSpec program.[2] (b) Species distribution diagram for the **5a**/ Cu^{2+} system in acetonitrile calculated using HypSpec program.[2] Data were fit with HypSpec using the following model:





5b

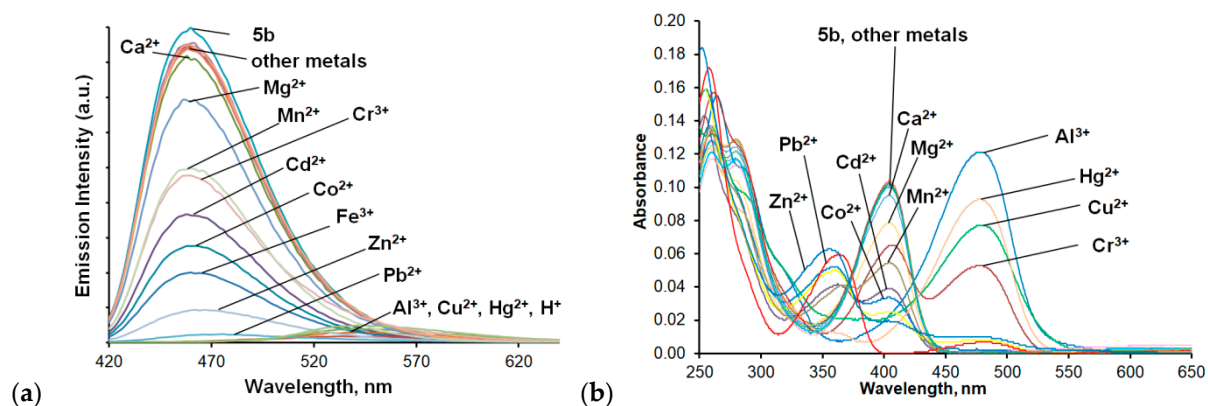


Figure S21. Luminescence (a) and absorption (b) spectra of **5b** in acetonitrile ($[\mathbf{5b}] = 4.8 \mu\text{M}$, $\lambda_{\text{ex}} = 404 \text{ nm}$) before and after addition of 5 equiv. of metal perchlorate salts.

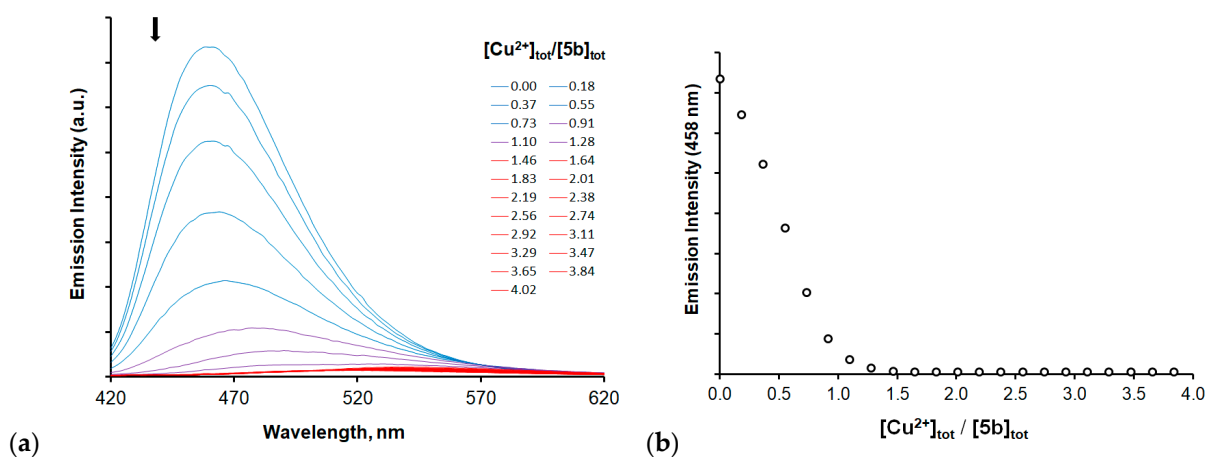


Figure S22. (a) Evolution of the emission spectrum of **5b** in acetonitrile ($[\mathbf{5b}]_{\text{tot}} = 4.8 \mu\text{M}$, $\lambda_{\text{ex}} = 404 \text{ nm}$) upon addition of $\text{Cu}(\text{ClO}_4)_2$ (0–4 equiv.). (b) Changes of the emission intensity as a function of the $[\text{Cu}^{2+}]_{\text{tot}}/[\mathbf{5b}]_{\text{tot}}$ ratio at $\lambda_{\text{em}} = 458 \text{ nm}$.

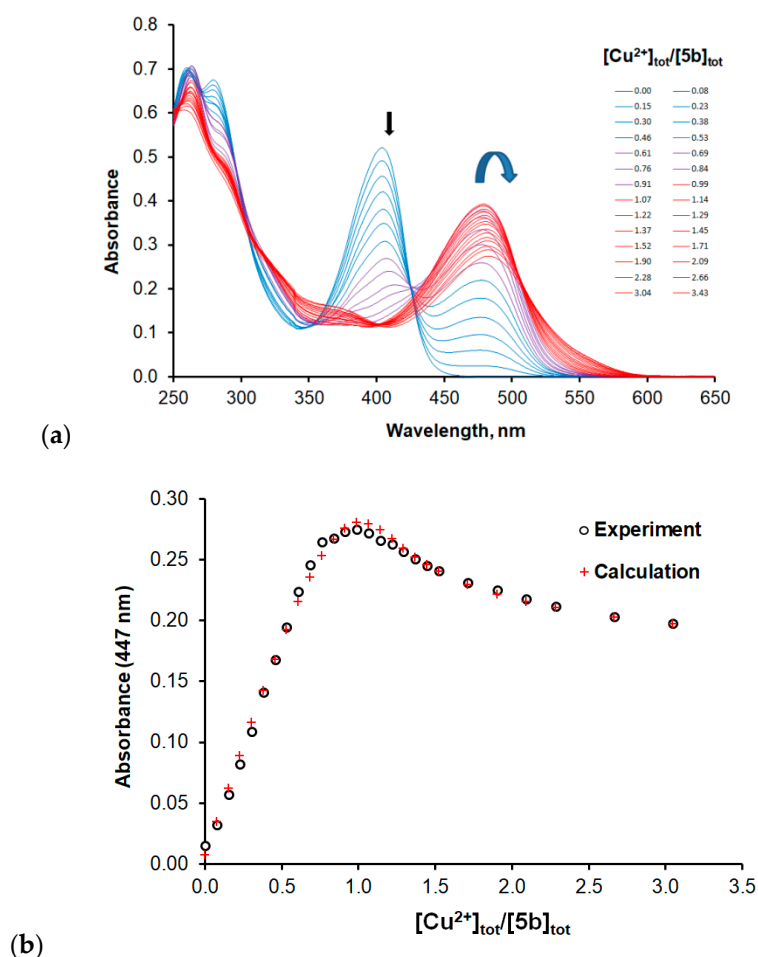


Figure S23. (a) Evolution of the UV-vis absorption spectrum of **5b** in acetonitrile ($[5b] = 23.3 \mu M$) upon addition of $Cu(ClO_4)_2$ (0–3 equiv.). (b) Changes of the absorbance as a function of the $[Cu^{2+}]_{tot}/[5b]_{tot}$ ratio at $\lambda = 447 \text{ nm}$.

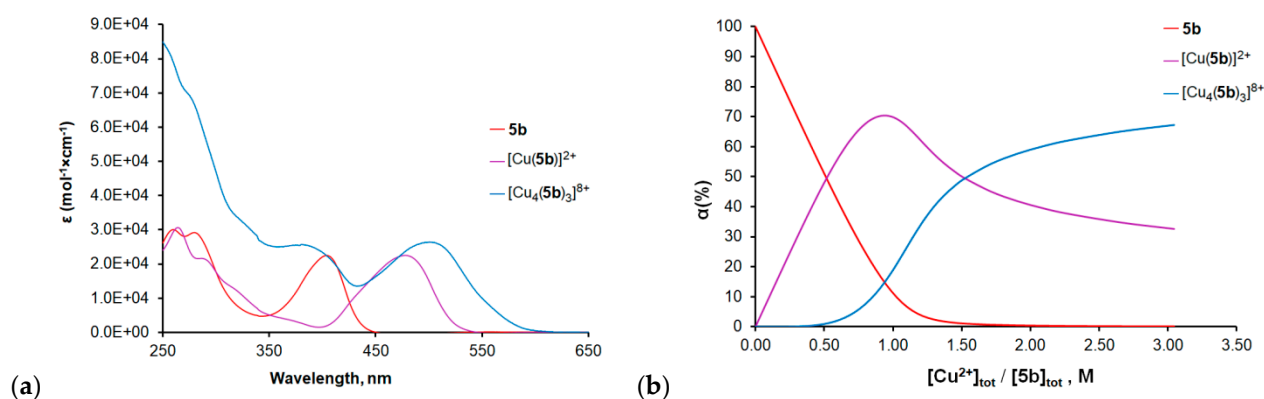
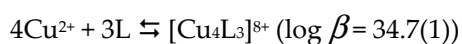
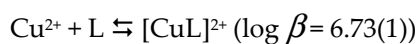
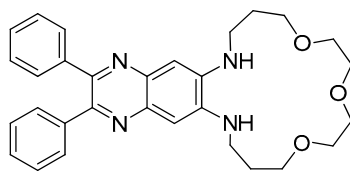


Figure S24. (a) UV-vis spectra of **5b**, $[Cu(5b)]^{2+}$ and $[Cu_4(5b)_3]^{8+}$ in acetonitrile calculated using HypSpec program.[2] (b) Species distribution diagram for the **5b**/ Cu^{2+} system in acetonitrile calculated using HypSpec program.[2] Data were fit with HypSpec using the following model:





5c

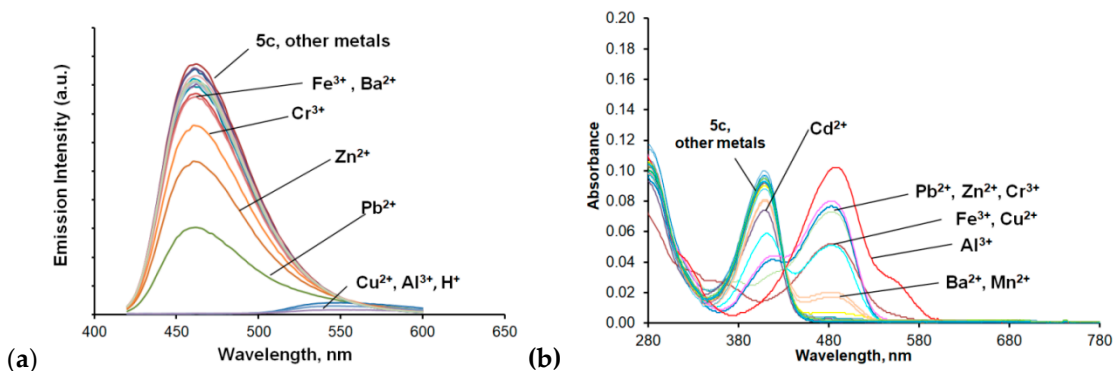


Figure S25. Luminescence (a) and absorption (b) spectra of **5c** in acetonitrile ($[5c] = 4.2 \mu\text{M}$, $\lambda_{\text{ex}} = 409 \text{ nm}$) before and after addition of 5 equiv. of metal perchlorate salts.

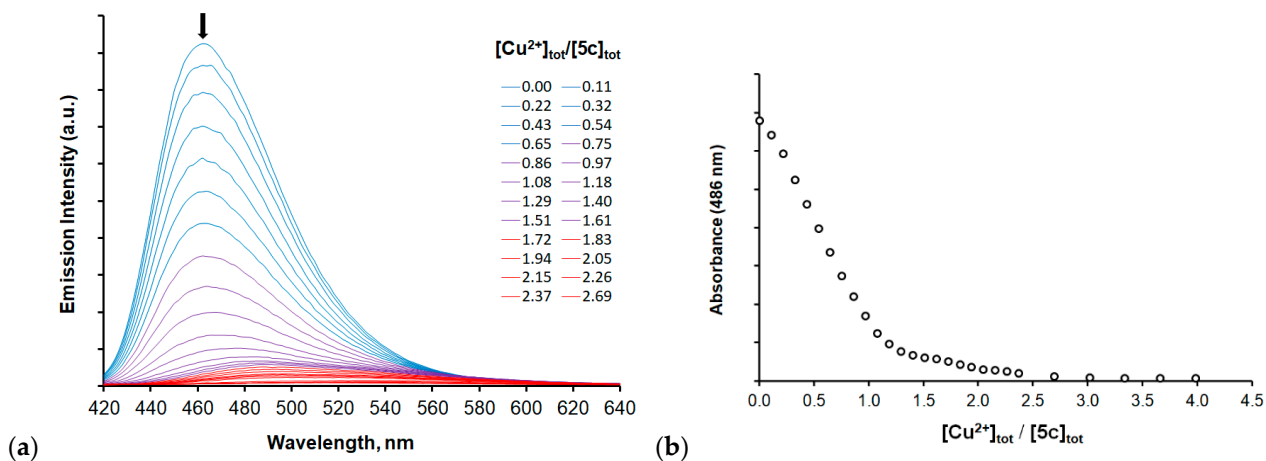
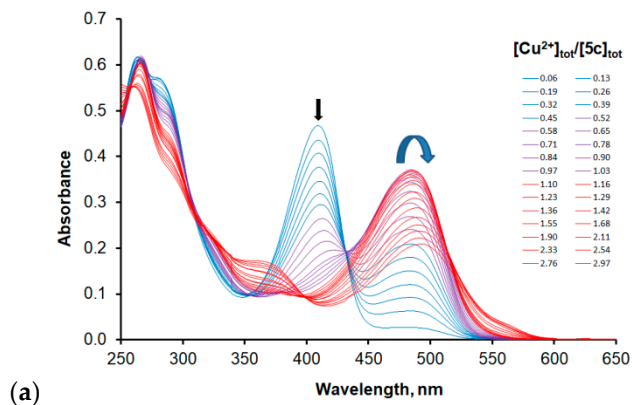


Figure S26. (a) Evolution of the emission spectrum of **5c** in acetonitrile ($[5c]_{\text{tot}} = 4.2 \mu\text{M}$, $\lambda_{\text{ex}} = 409 \text{ nm}$) upon addition of $\text{Cu}(\text{ClO}_4)_2$ (0–4 equiv.). (b) Changes of the emission intensity as a function of the $[\text{Cu}^{2+}]_{\text{tot}}/[\text{5c}]_{\text{tot}}$ ratio at $\lambda_{\text{em}} = 486 \text{ nm}$.



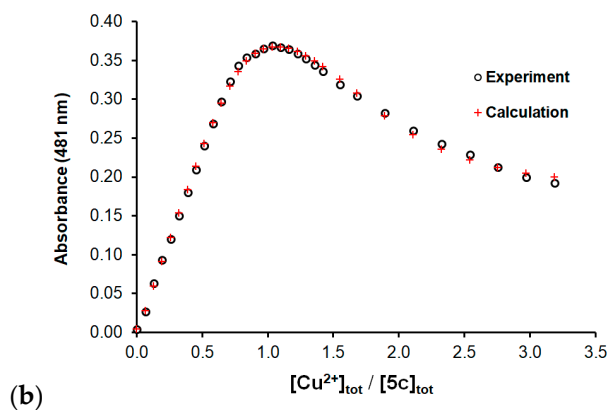


Figure S27. (a) Evolution of the UV–vis absorption spectrum of **5c** in acetonitrile ($[5c] = 24.4 \mu\text{M}$) upon addition of $\text{Cu}(\text{ClO}_4)_2$ (0–3 equiv.). (b) Changes of the absorbance as a function of the $[\text{Cu}^{2+}]_{\text{tot}}/[\mathbf{5c}]_{\text{tot}}$ ratio at $\lambda = 481 \text{ nm}$.

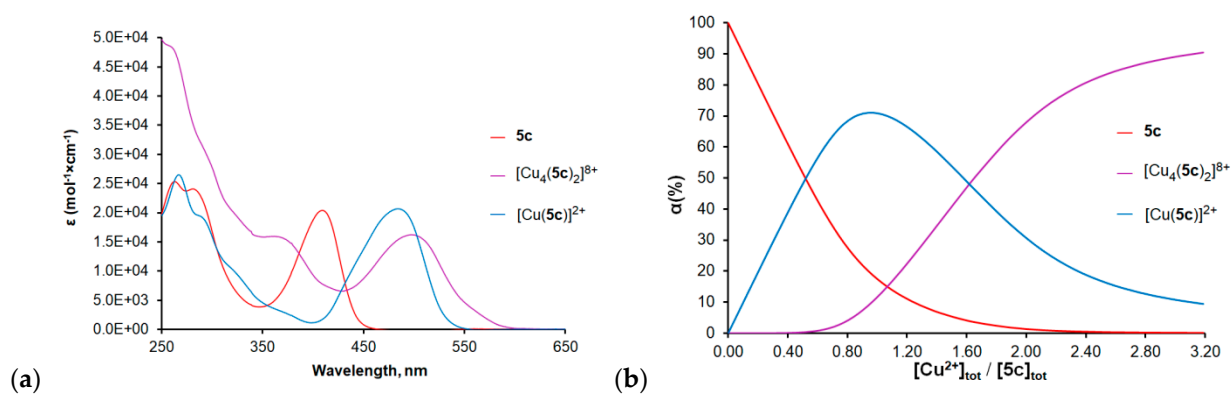
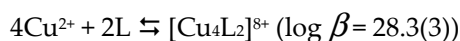
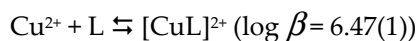


Figure S28. (a) UV–vis spectra of **5c**, $[\text{Cu}(\mathbf{5c})]^{2+}$ and $[\text{Cu}_4(\mathbf{5c})_2]^{8+}$ in acetonitrile calculated using HypSpec program.[2] (b) Species distribution diagram for the **5c**/ Cu^{2+} system in acetonitrile calculated using HypSpec program.[2] Data were fit with HypSpec using the following model:



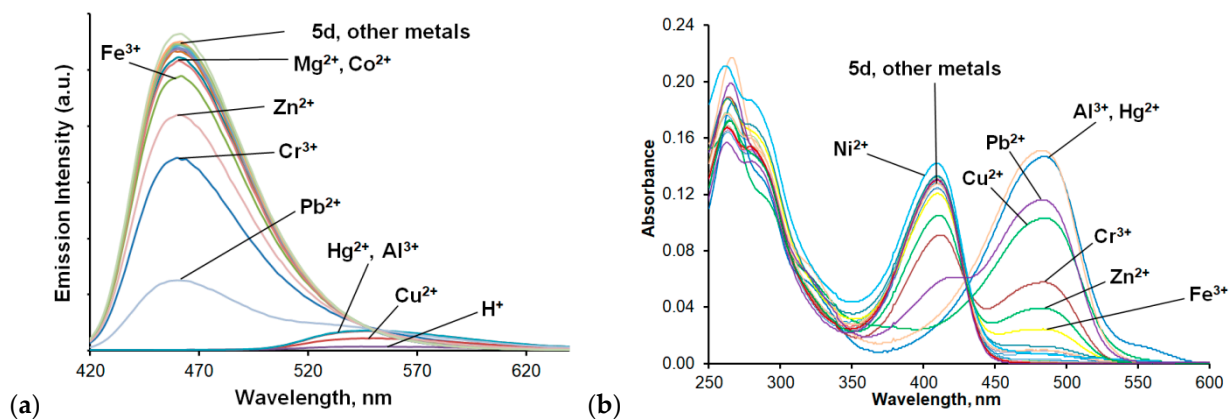
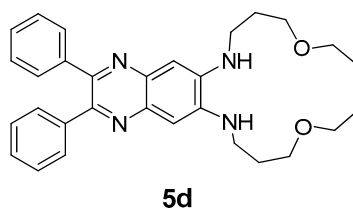


Figure S29. Luminescence (a) and absorption (b) spectra of **5d** in acetonitrile ([**5d**] = 4.8 μ M, λ_{ex} = 410 nm) before and after addition of 5 equiv. of metal perchlorate salts.

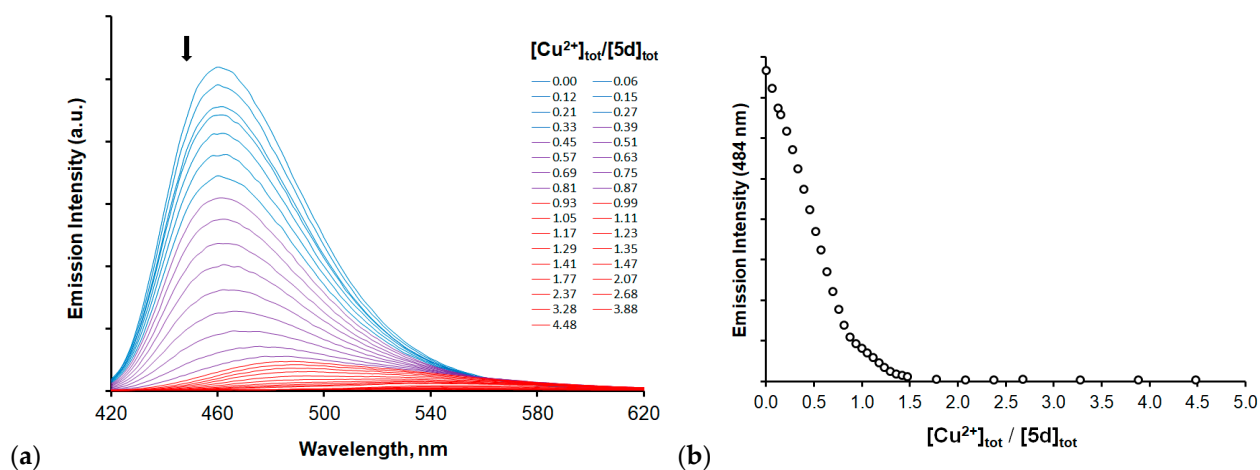


Figure S30. (a) Evolution of the emission spectrum of **5d** in acetonitrile ([**5d**]_{tot} = 4.8 μ M, λ_{ex} = 410 nm) upon addition of $\text{Cu}(\text{ClO}_4)_2$ (0–4.5 equiv.). (b) Changes of the emission intensity as a function of the $[\text{Cu}^{2+}]_{\text{tot}}/[\text{5d}]_{\text{tot}}$ ratio at λ_{em} = 486 nm.

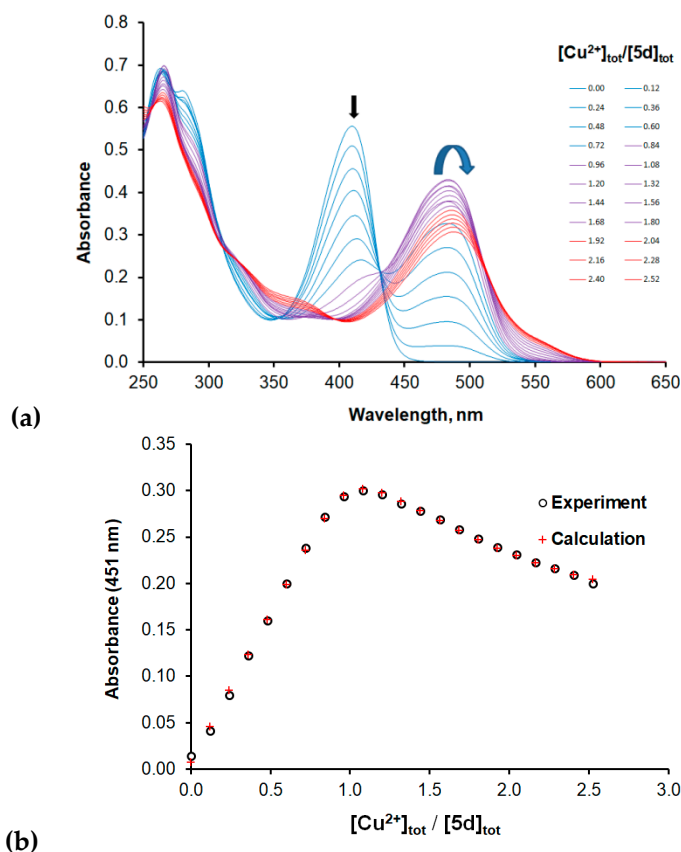


Figure S31. (a) Evolution of the UV-vis absorption spectrum of **5d** in acetonitrile ($[5d] = 21.5 \mu\text{M}$) upon addition of $\text{Cu}(\text{ClO}_4)_2$ (0–2.5 equiv.). (b) Changes of the absorbance as a function of the $[\text{Cu}^{2+}]_{\text{tot}}/[\text{5d}]_{\text{tot}}$ ratio at $\lambda = 451 \text{ nm}$.

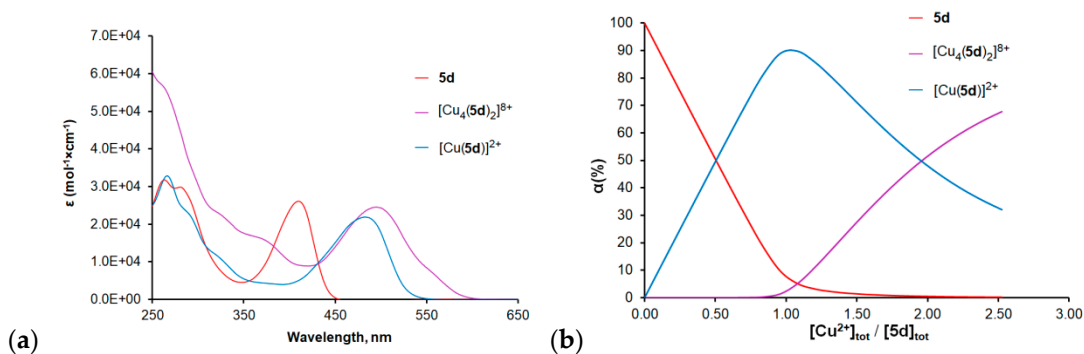
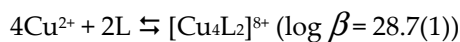
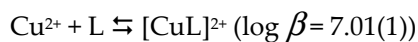


Figure S32. (a) UV-vis spectra of **5d**, $[\text{Cu}(\text{5d})]^{2+}$ and $[\text{Cu}_4(\text{5d})_2]^{8+}$ in acetonitrile calculated using HypSpec program.[2] (b) Species distribution diagram for the **5d**/ Cu^{2+} system in acetonitrile calculated using HypSpec program.[2] Data were fit with HypSpec using the following model:



4. Protonation Studies of 5c and 5e

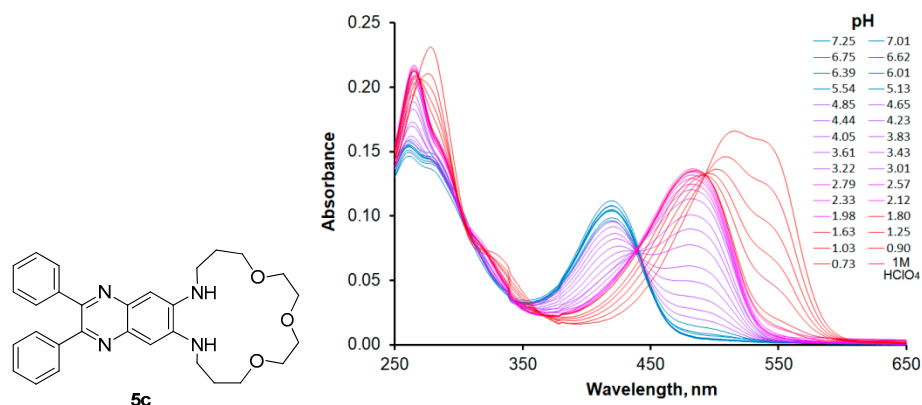


Figure S33. Spectrophotometric titration of 5c as a function of pH ($[5c]_{\text{tot}} = 8.4 \mu\text{M}$, 1 vol% MeOH, $I = 0.1 \text{ M}$ NaClO₄, pH = 0 – 7.3).

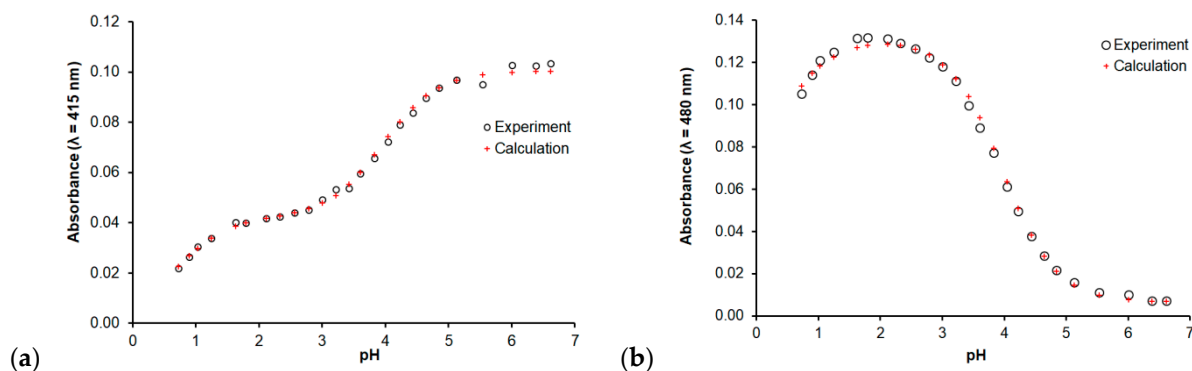


Figure S34. Absorbance changes with pH at $\lambda = 415 \text{ nm}$ (a) and $\lambda = 480 \text{ nm}$ (b) for 5c.

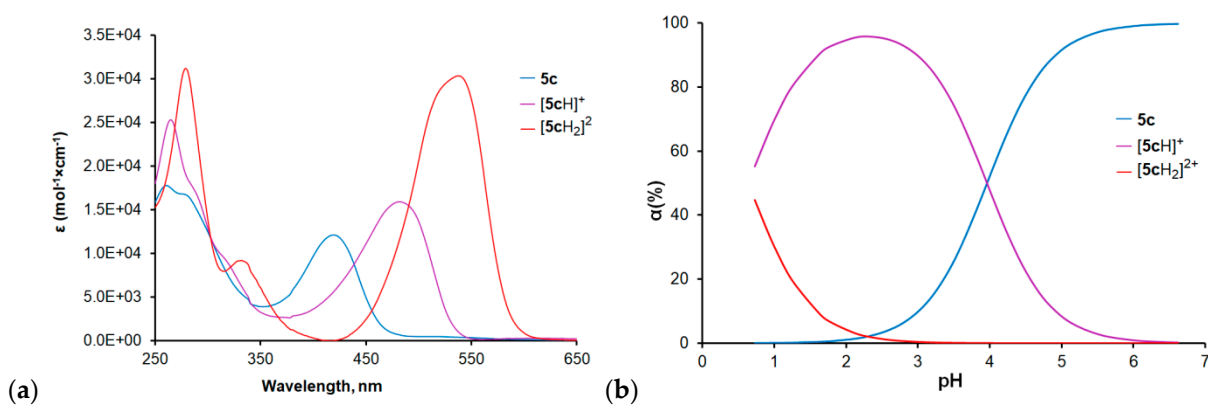


Figure S35. (a) UV-vis spectra of 5c, [5cH]⁺ and [5cH₂]²⁺ in water calculated using HypSpec program.[2] (b) Species distribution diagram for the 5c \rightleftharpoons [5cH]⁺ \rightleftharpoons [5cH₂]²⁺ system in water calculated using HypSpec program.[2]

$\text{pK}_1 = 4.10(5)$; $\text{pK}_2 = 0.6(1)$.

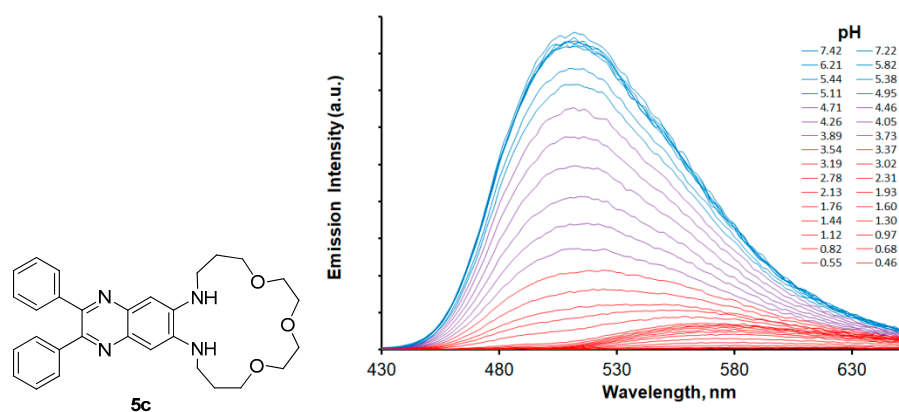


Figure S36. Fluorimetric titration of **5c** as a function of pH ($[\mathbf{5c}]_{\text{tot}} = 4.2 \mu\text{M}$, 0.5 vol% MeOH, $I = 0.1 \text{ M NaClO}_4$, $\lambda_{\text{ex}} = 420 \text{ nm}$, pH = 0.5 – 7.4).

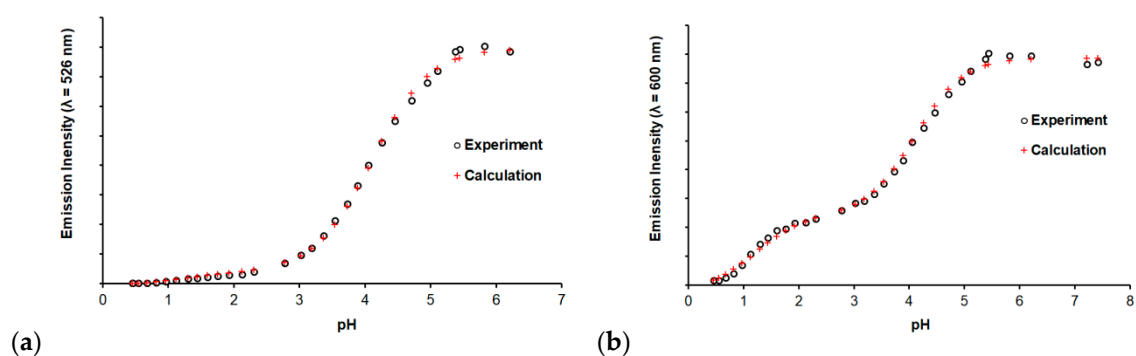


Figure S37. Emission intensity changes with pH at $\lambda = 526 \text{ nm}$ (a) and $\lambda = 600 \text{ nm}$ (b) for **5c**.

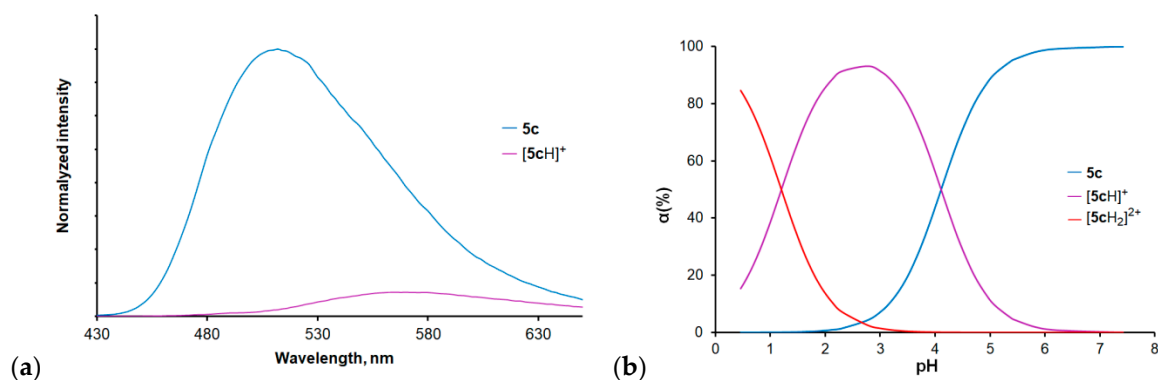


Figure S38. (a) Emission spectra of **5c** and $[\mathbf{5cH}]^+$ in water calculated using HypSpec program,[2] $[\mathbf{5cH}_2]^{2+}$ was considered to be non-emissive; (b) Species distribution diagram for the $\mathbf{5c} \rightleftharpoons [\mathbf{5cH}]^+ \rightleftharpoons [\mathbf{5cH}_2]^{2+}$ system in water calculated using HypSpec program.[2]

$\text{pK}_1 = 3.96(5)$; $\text{pK}_2 = 1.20(5)$.

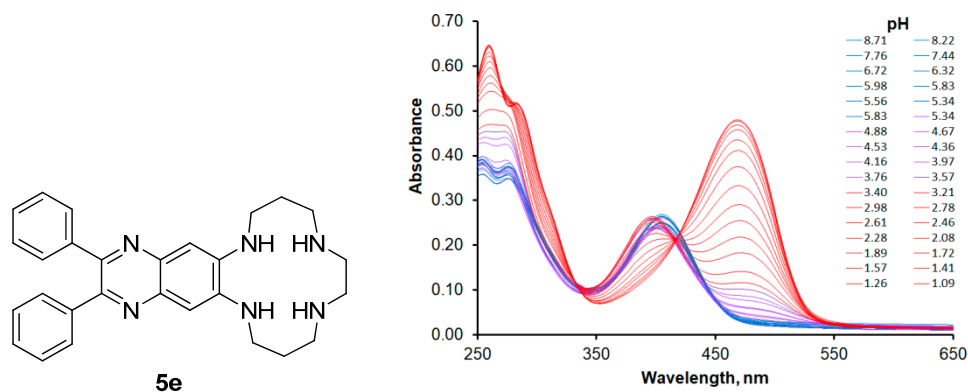


Figure S39. Spectrophotometric titration of **5e** ($[\mathbf{5e}]_{\text{tot}} = 31.1 \mu\text{M}$, $I = 0.1 \text{ M NaClO}_4$, $\text{pH} = 1.1\text{--}8.8$).

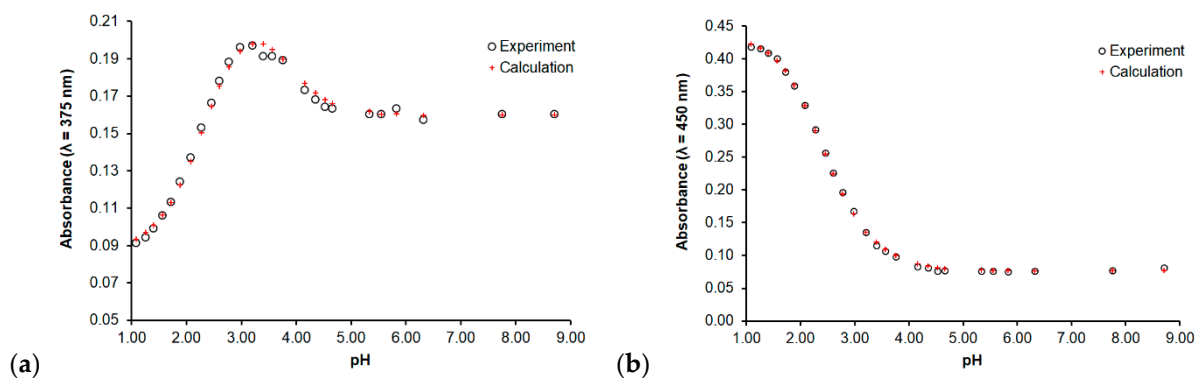


Figure S40. Absorbance changes with pH at $\lambda = 375 \text{ nm}$ (a) and $\lambda = 450 \text{ nm}$ (b) for **5e**.

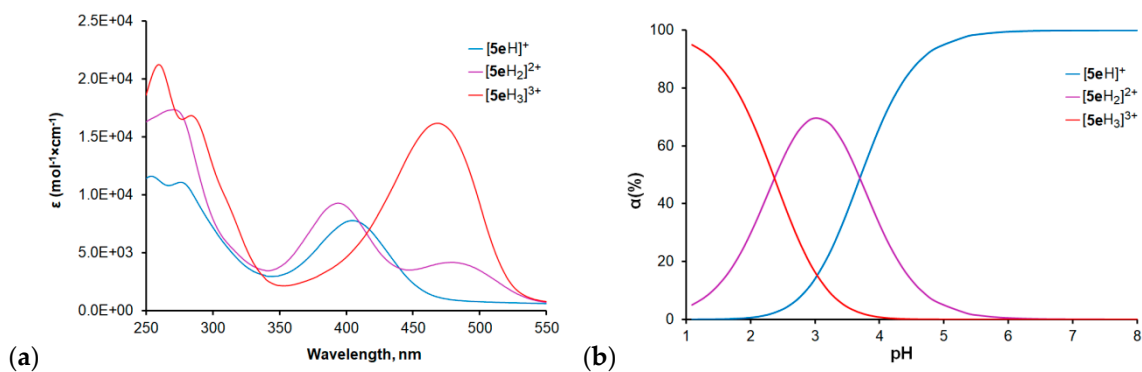


Figure S41. (a) UV-vis spectra of $[\mathbf{5eH}]^+$, $[\mathbf{5eH}_2]^{2+}$ and $[\mathbf{5eH}_3]^{3+}$ in water calculated using HypSpec program.[2] (b) Species distribution diagram for the $[\mathbf{5eH}]^+ \rightleftharpoons [\mathbf{5eH}_2]^{2+} \rightleftharpoons [\mathbf{5eH}_3]^{3+}$ system in water calculated using HypSpec program.[2]

$\text{pK}_2 = 3.69(5)$; $\text{pK}_3 = 2.36(5)$.

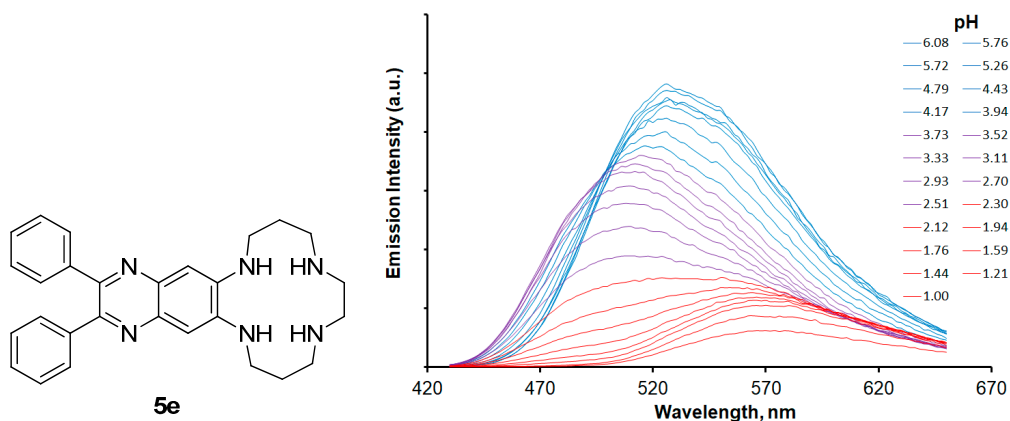


Figure S42. Fluorimetric titration of **5e** as a function of pH ($[\mathbf{5e}]_{\text{tot}} = 8.04 \mu\text{M}$, $I = 0.1 \text{ M NaClO}_4$, $\lambda_{\text{ex}} = 420 \text{ nm}$, pH = 1.0 – 6.1).

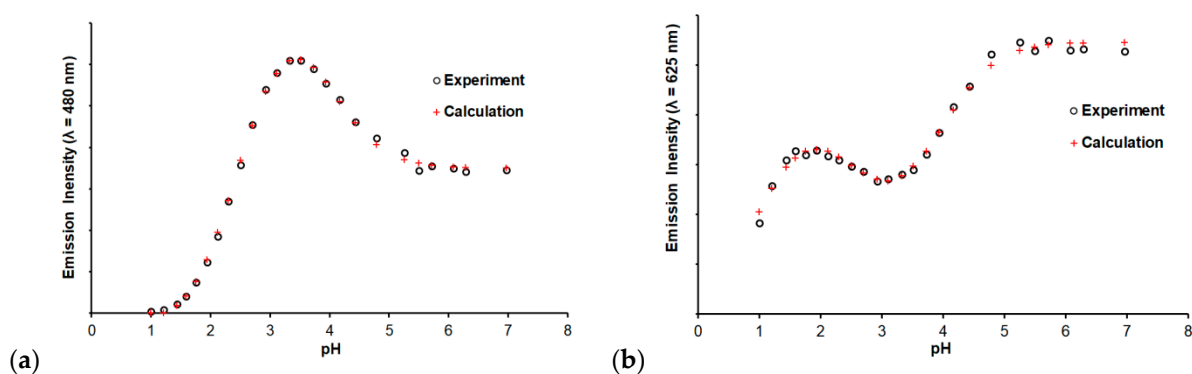


Figure S43. Emission intensity changes with pH at $\lambda = 480 \text{ nm}$ (a) and $\lambda = 625 \text{ nm}$ (b) for **5e**.

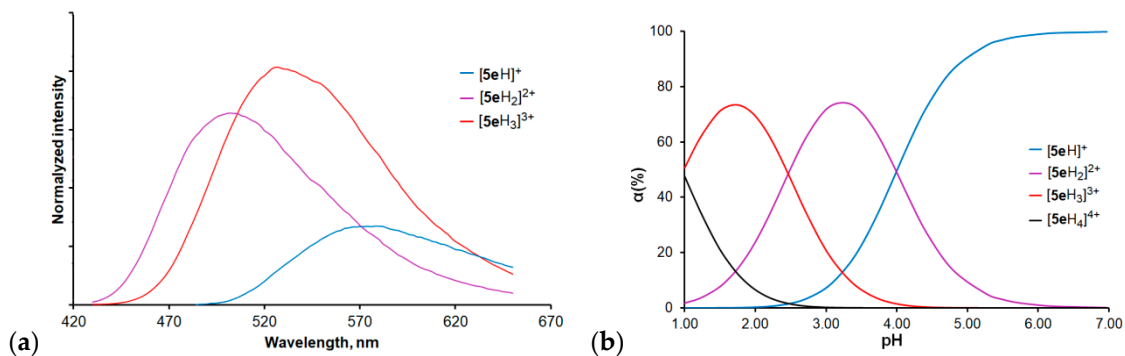
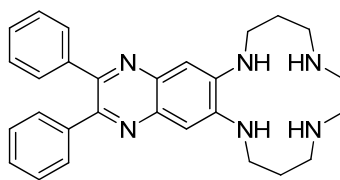


Figure S44. (a) Emission spectra of $[\mathbf{5eH}]^+$, $[\mathbf{5eH}_2]^{2+}$ and $[\mathbf{5eH}_3]^{3+}$ in water calculated using HypSpec program,[2] $[\mathbf{5eH}_4]^{4+}$ was considered to be non-emissive; (b) Species distribution diagram for the $[\mathbf{5eH}]^+ \rightleftharpoons [\mathbf{5eH}_2]^{2+} \rightleftharpoons [\mathbf{5eH}_3]^{3+} \rightleftharpoons [\mathbf{5eH}_4]^{4+}$ system in water calculated using HypSpec program.[2]

$\text{pK}_1 = 4.01(5)$; $\text{pK}_2 = 2.46(5)$; $\text{pK}_3 = 1.0(1)$.



5e

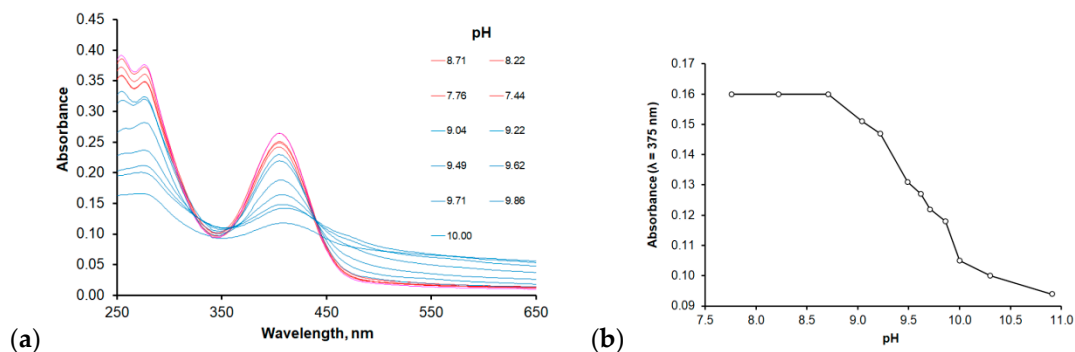


Figure S45. (a) UV-vis spectra of **5e** solution ($[\mathbf{5e}]_{\text{tot}} = 31.1 \mu\text{M}$, $I = 0.1 \text{ M NaClO}_4$, $\text{pH} = 8.7\text{--}10.0$); (b) Absorbance changes with pH at $\lambda = 375 \text{ nm}$. Formation of precipitate is observed in the cell.

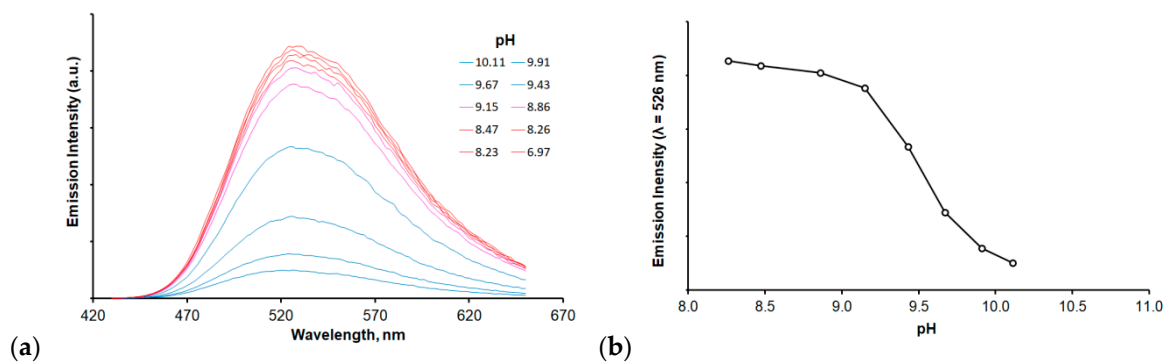


Figure S46. (a) Luminescence spectra spectra of **5e** solution ($[\mathbf{5e}]_{\text{tot}} = 8.04 \mu\text{M}$, $I = 0.1 \text{ M NaClO}_4$, $\text{pH} = 7.0\text{--}10.1$); (b) Emission intensity changes with pH at $\lambda = 526 \text{ nm}$. Formation of precipitate is observed in the cell.

5. NMR Spectra of New Compounds.

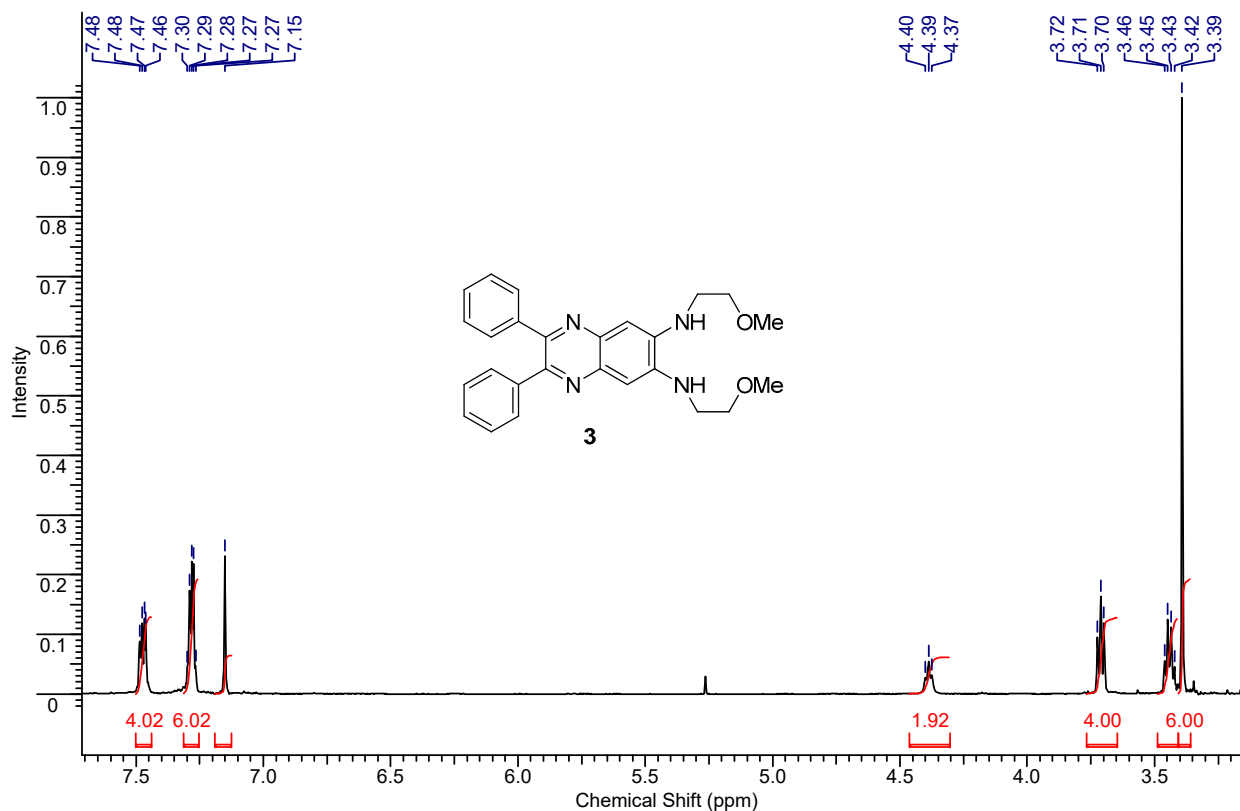


Figure S47. ¹H NMR spectrum of the compound **3** (CDCl₃, 400 MHz, 300 K).

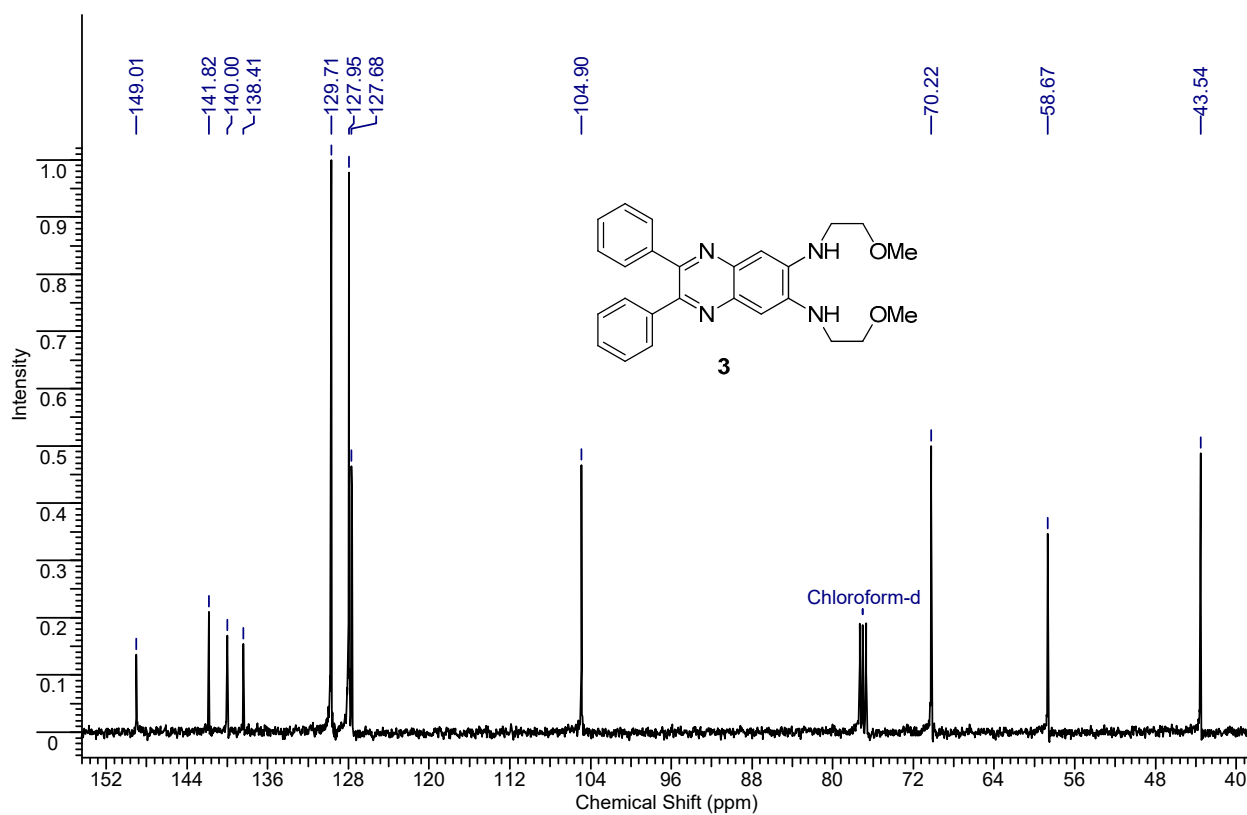


Figure S48. ¹³C NMR spectrum of the compound **3** (CDCl₃, 100.6 MHz, 300 K).

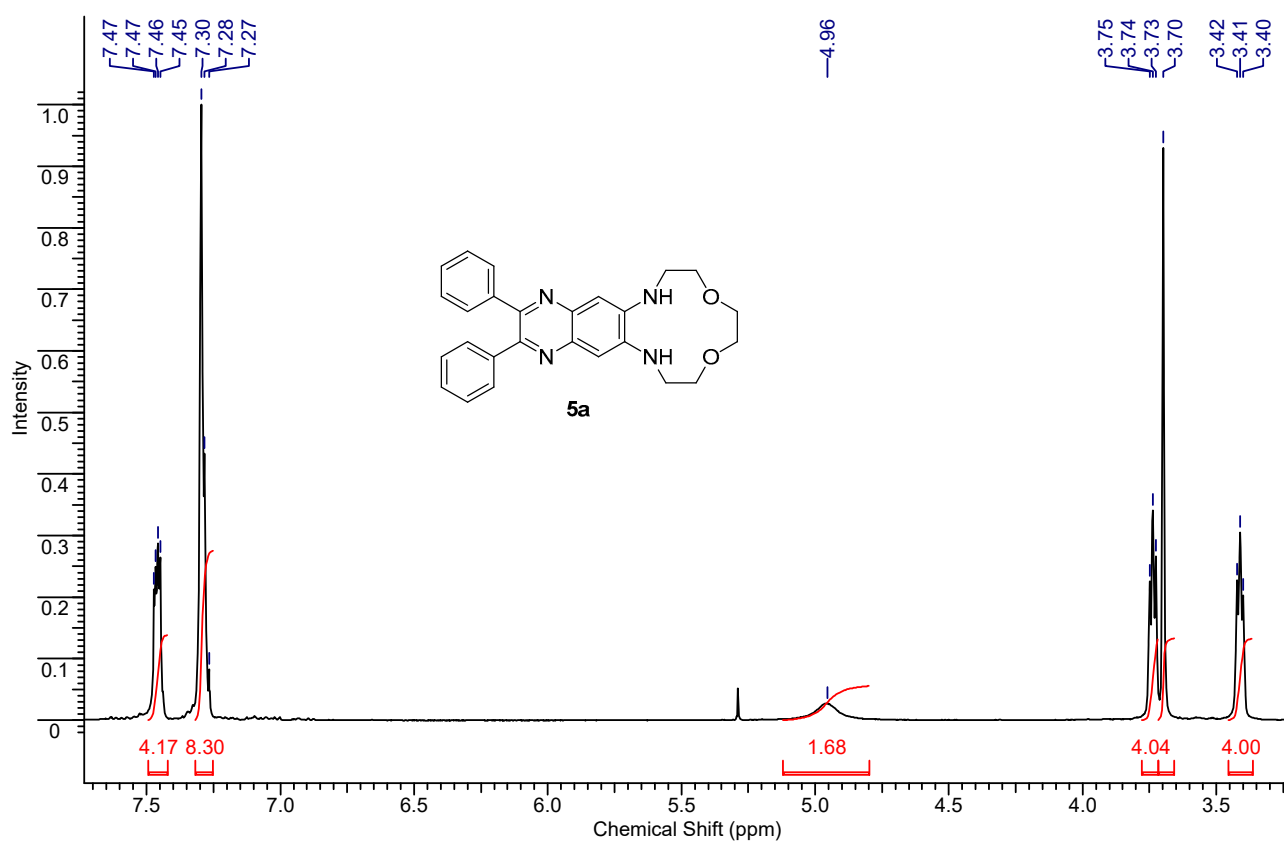


Figure S49. ¹H NMR spectrum of the compound **5a** (CDCl₃, 400 MHz, 300 K).

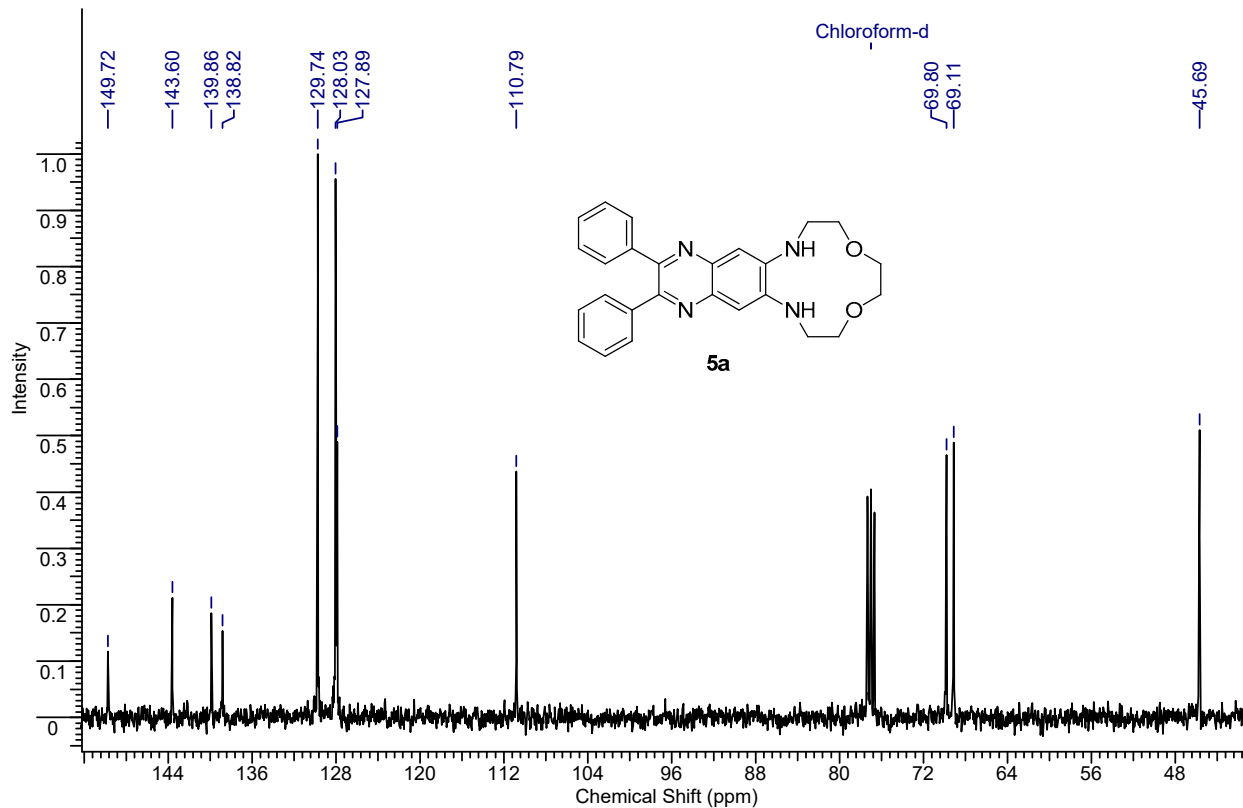


Figure S50. ¹³C NMR spectrum of the compound **5a** (CDCl₃, 100.6 MHz, 300 K).

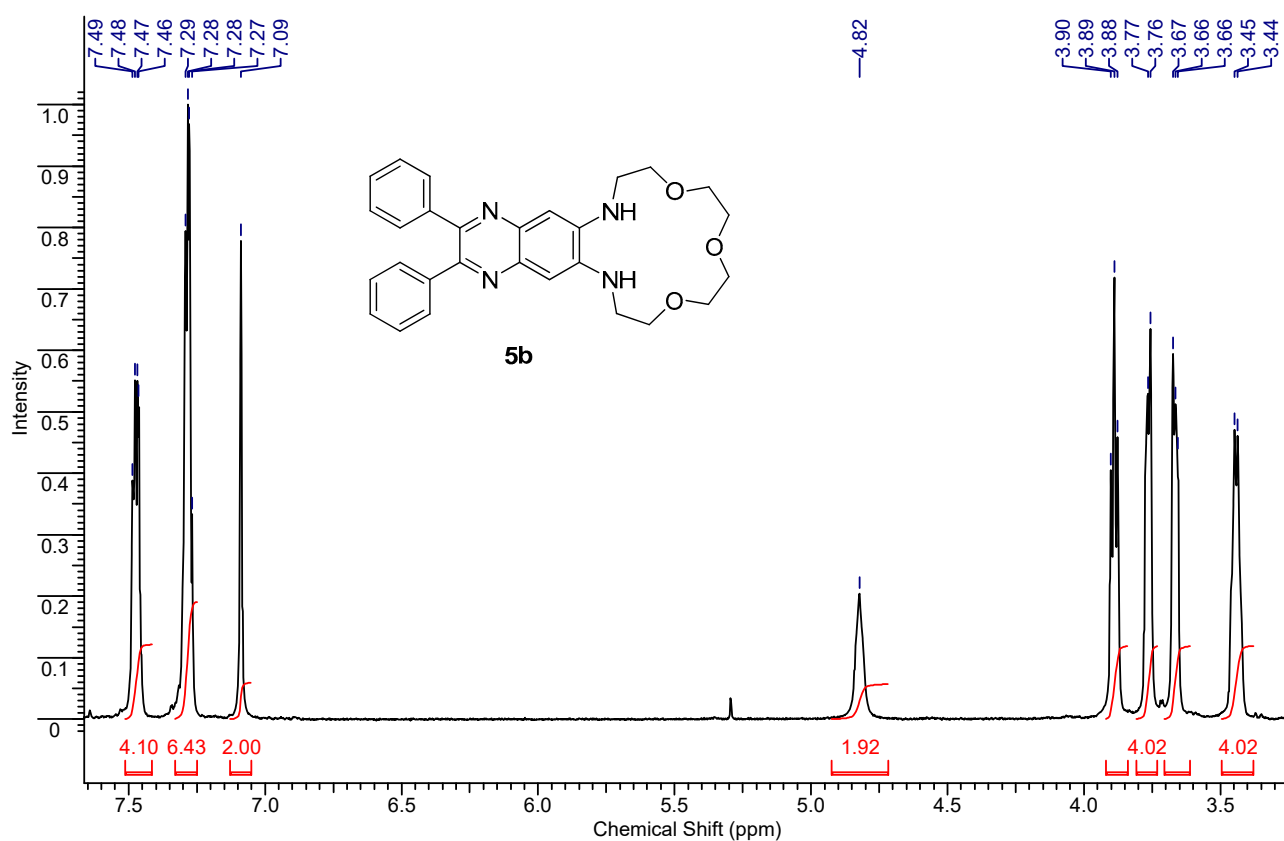


Figure S51. ¹H NMR spectrum of the compound **5b** (CDCl₃, 400 MHz, 300 K).

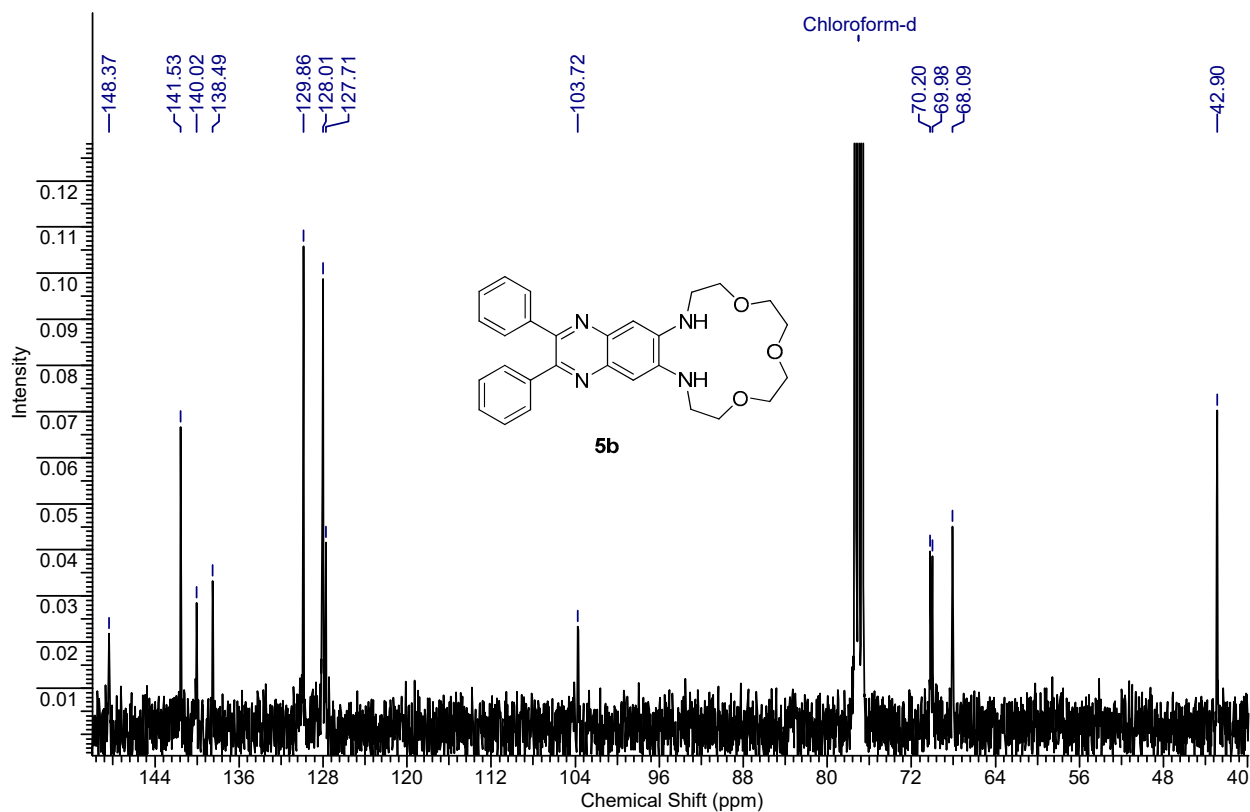


Figure S52. ¹³C NMR spectrum of the compound **5b** (CDCl₃, 100.6 MHz, 300 K).

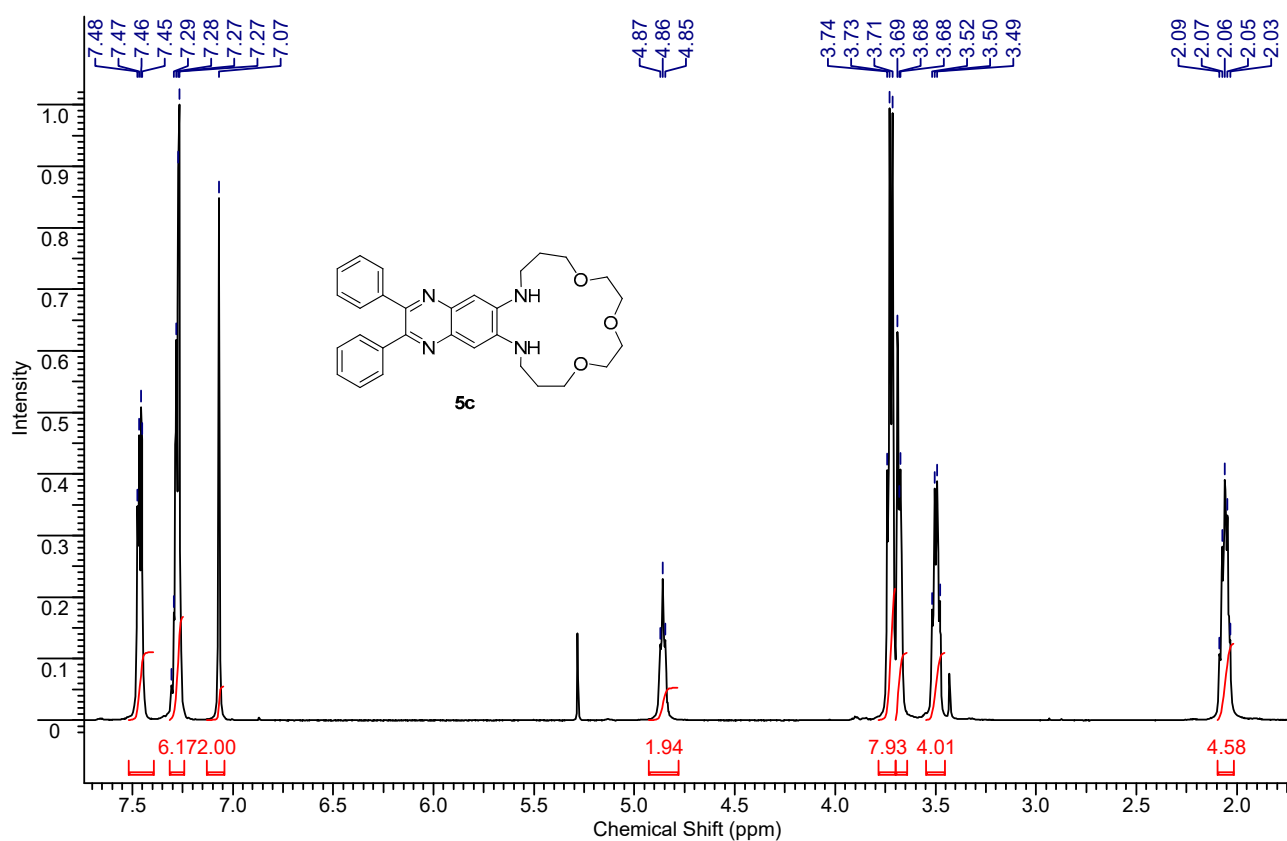


Figure S53. ¹H NMR spectrum of the compound **5c** (CDCl₃, 400 MHz, 300 K).

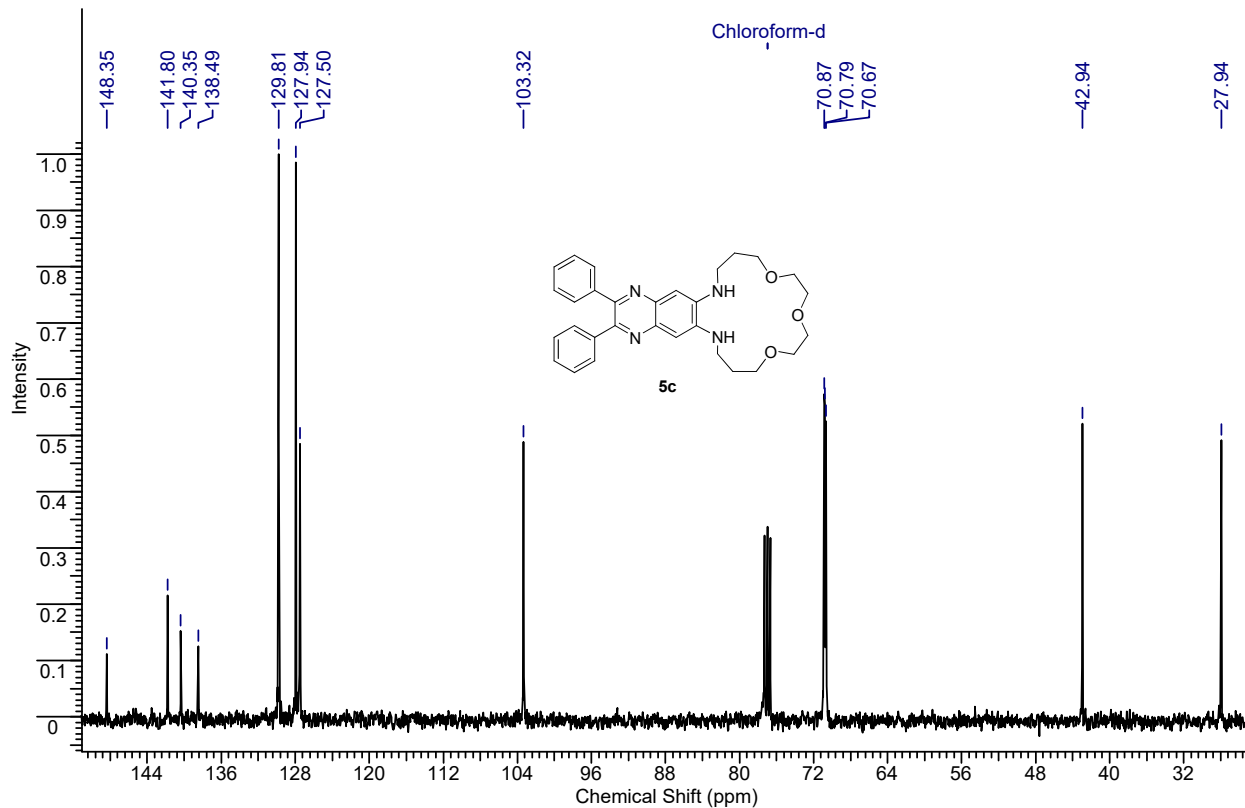


Figure S54. ¹³C NMR spectrum of the compound **5c** (CDCl₃, 100.6 MHz, 300 K).

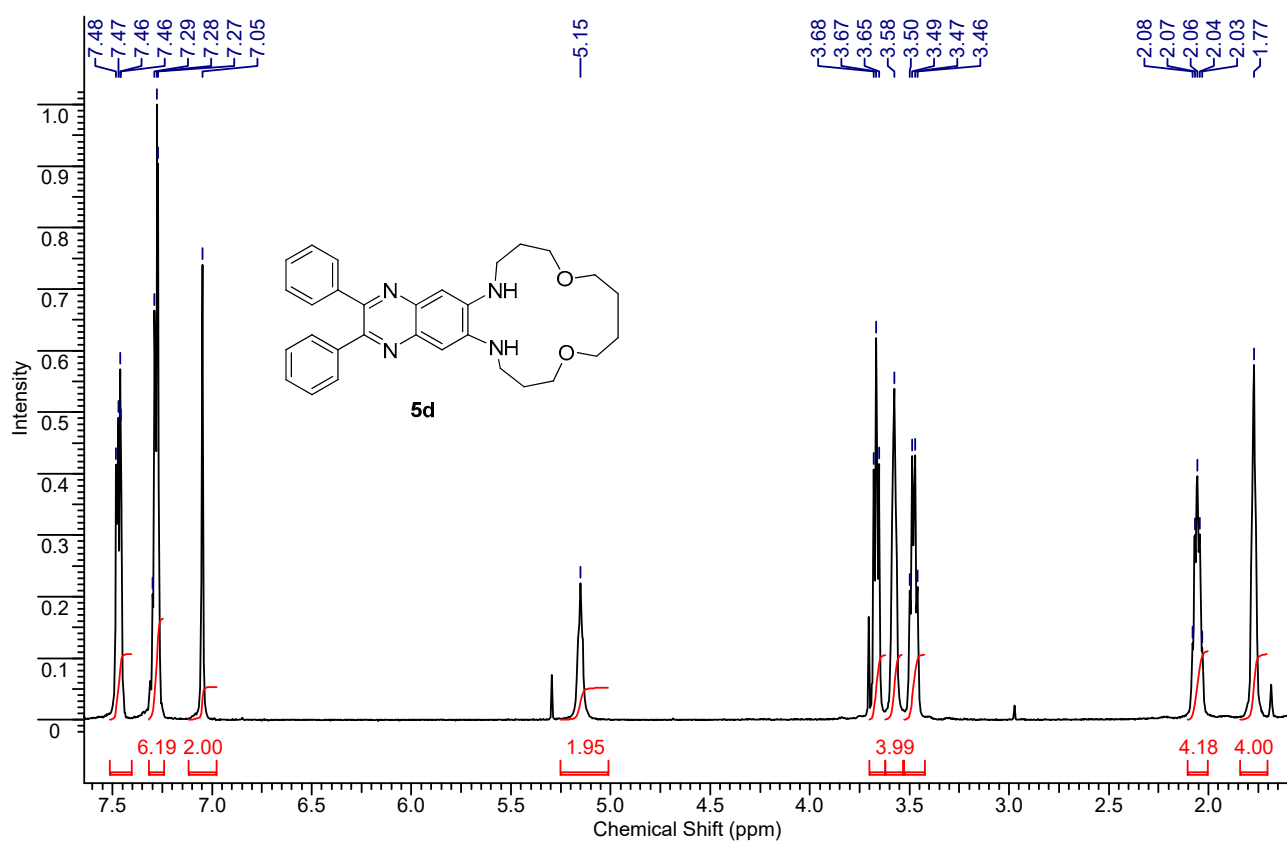


Figure S55. ¹H NMR spectrum of the compound **5d** (CDCl₃, 400 MHz, 300 K).

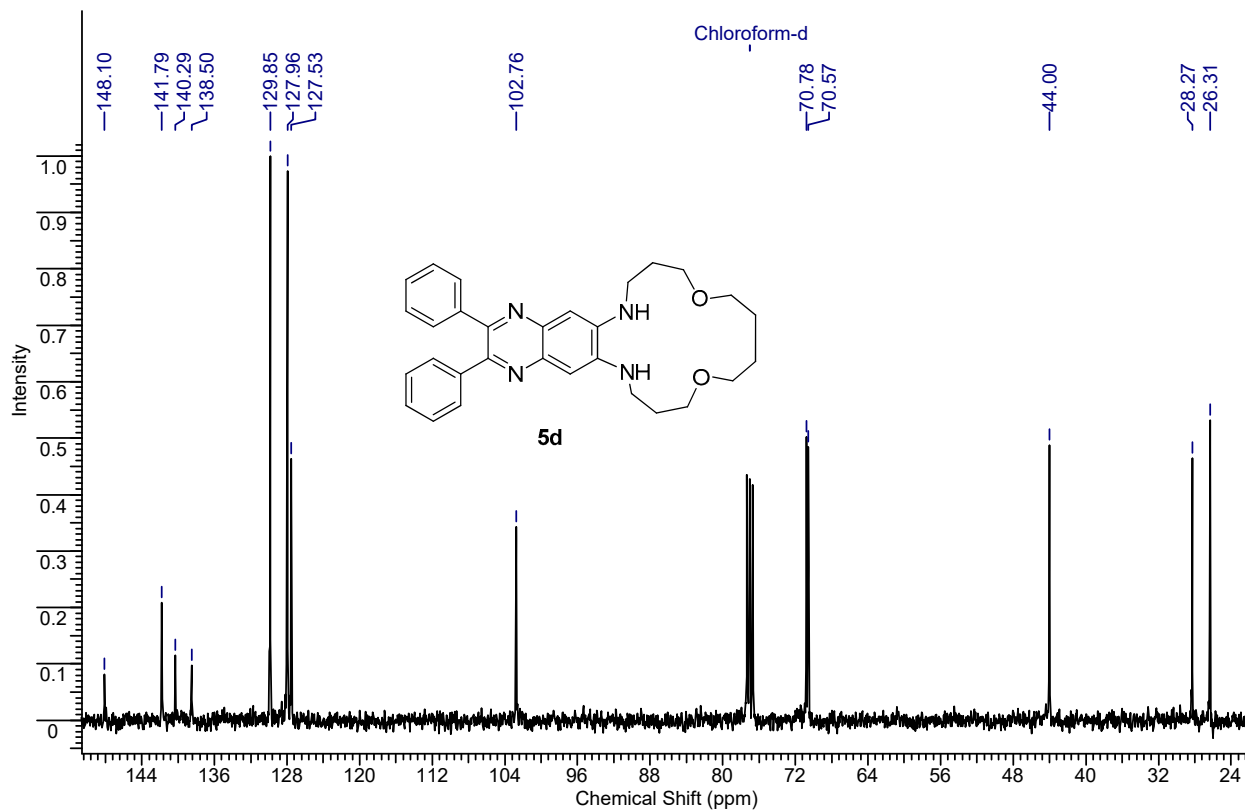


Figure S56. ¹³C NMR spectrum of the compound **5d** (CDCl₃, 100.6 MHz, 300 K).

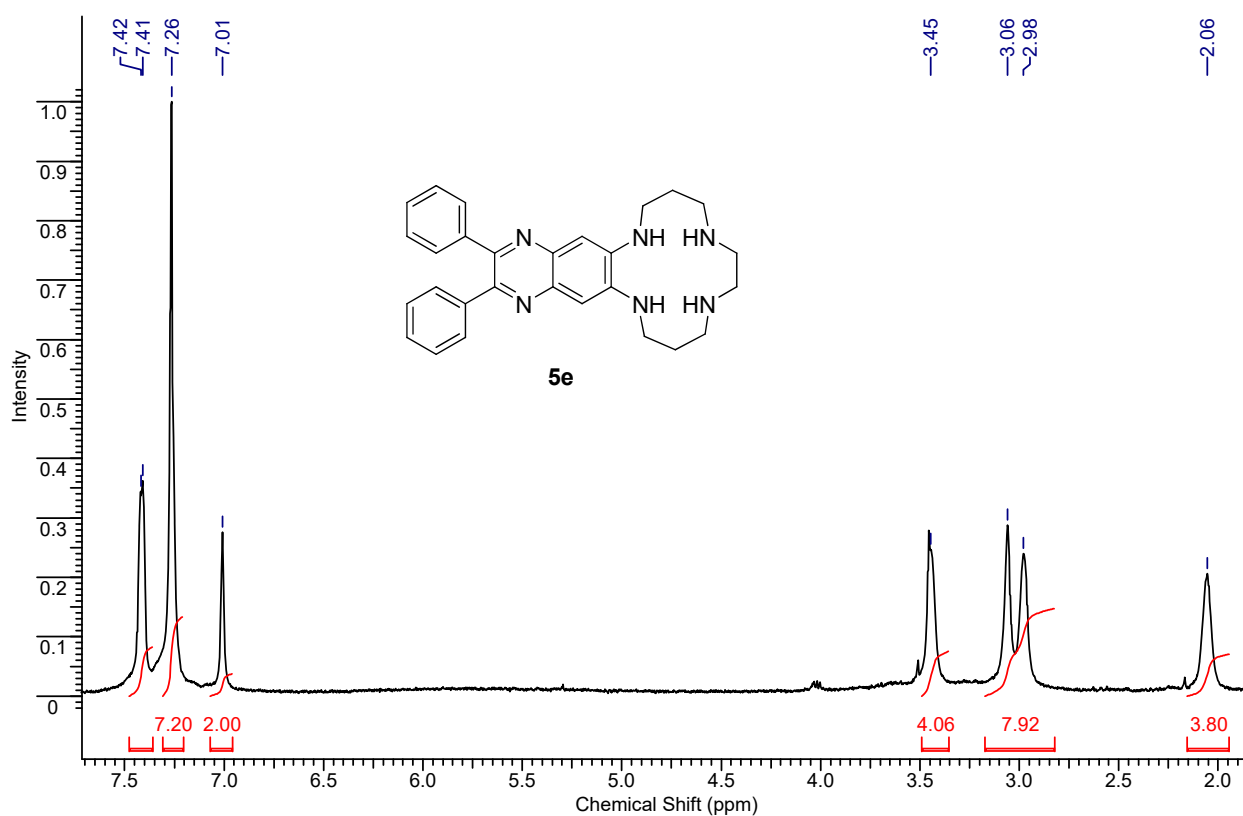


Figure S57. ^1H NMR spectrum of the compound **5e** ($\text{CDCl}_3/\text{CD}_3\text{OD}$, 5:1 v/v, 400 MHz, 300 K).

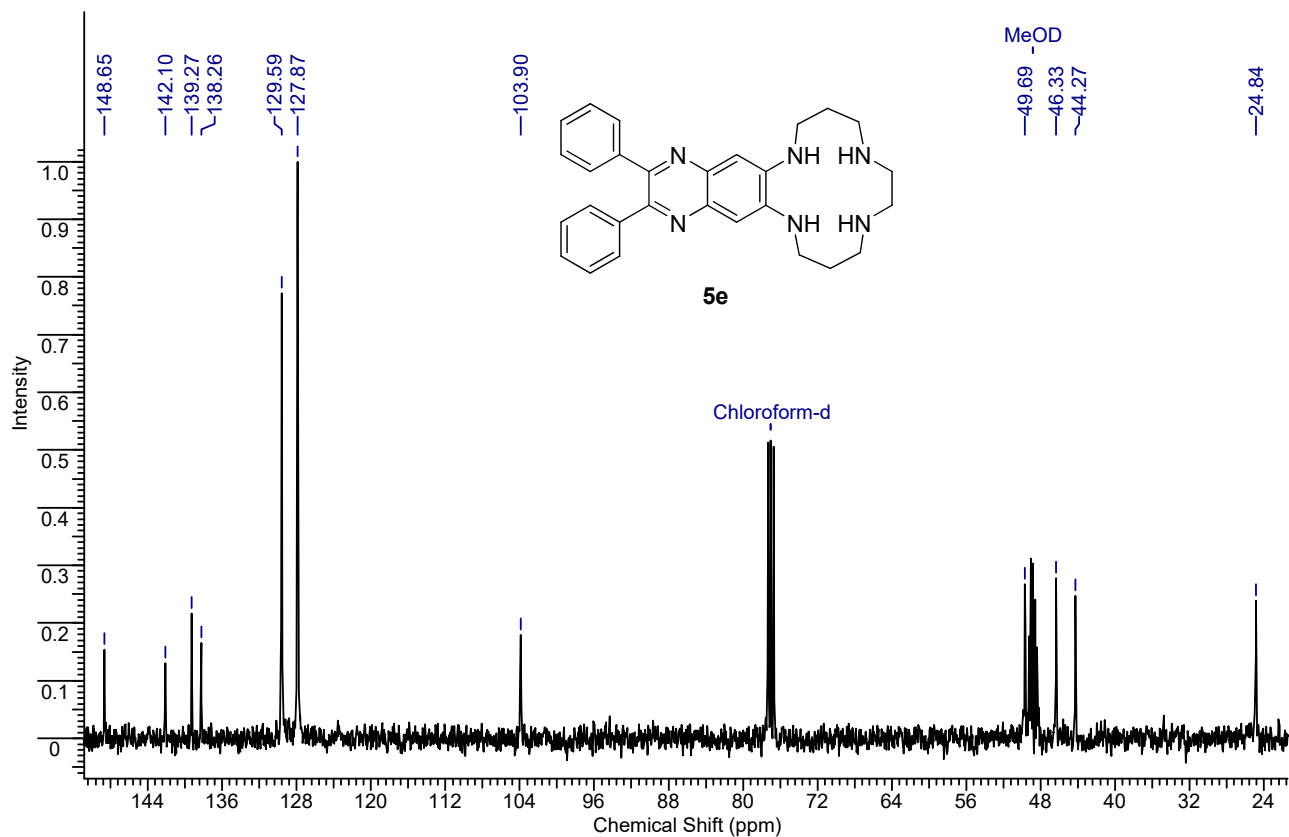


Figure S58. ^{13}C NMR spectrum of the compound **5e** ($\text{CDCl}_3/\text{CD}_3\text{OD}$, 5:1 v/v, 100.6 MHz, 300 K).

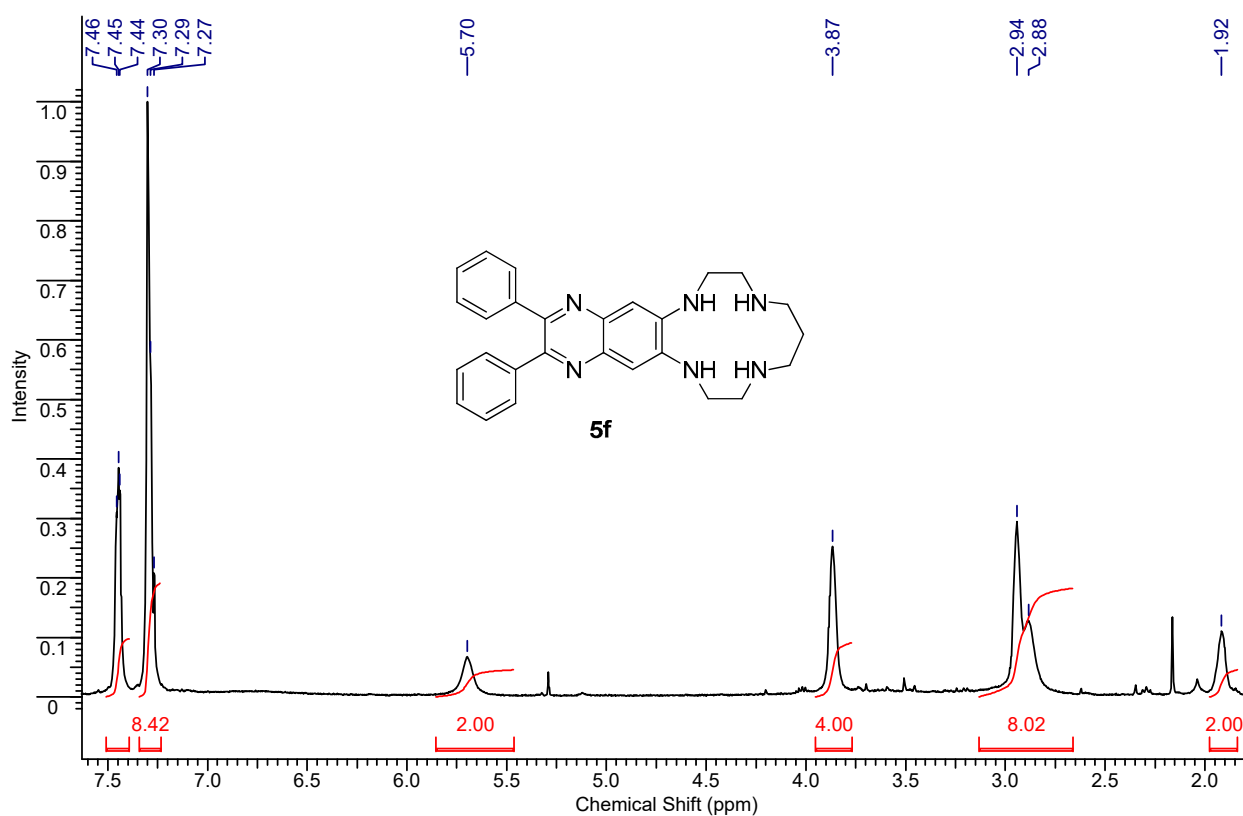


Figure S59. ¹H NMR spectrum of the compound **5f** (CDCl₃/CD₃OD, 5:1 v/v, 400 MHz, 300 K).

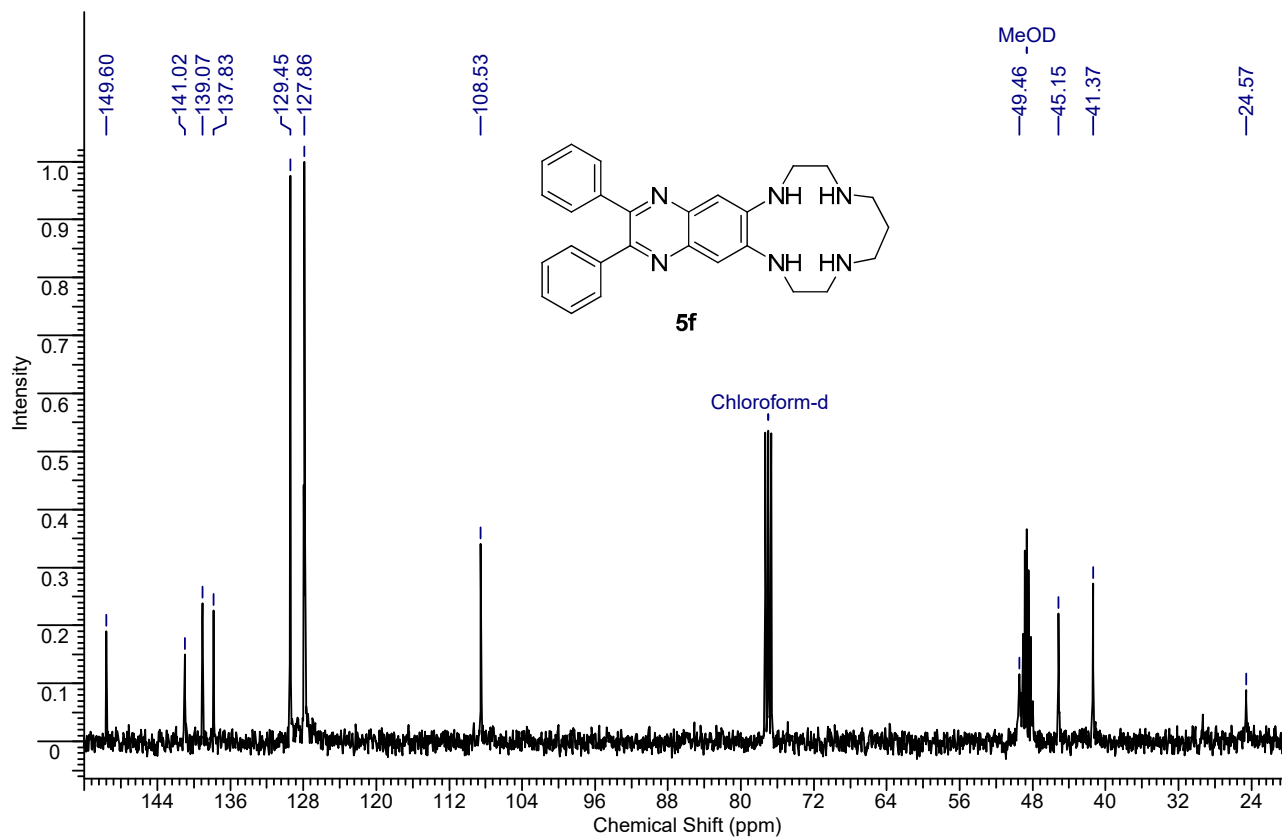


Figure S60. ¹³C NMR spectrum of the compound **5f** (CDCl₃/CD₃OD, 5:1 v/v, 100.6 MHz, 300 K).

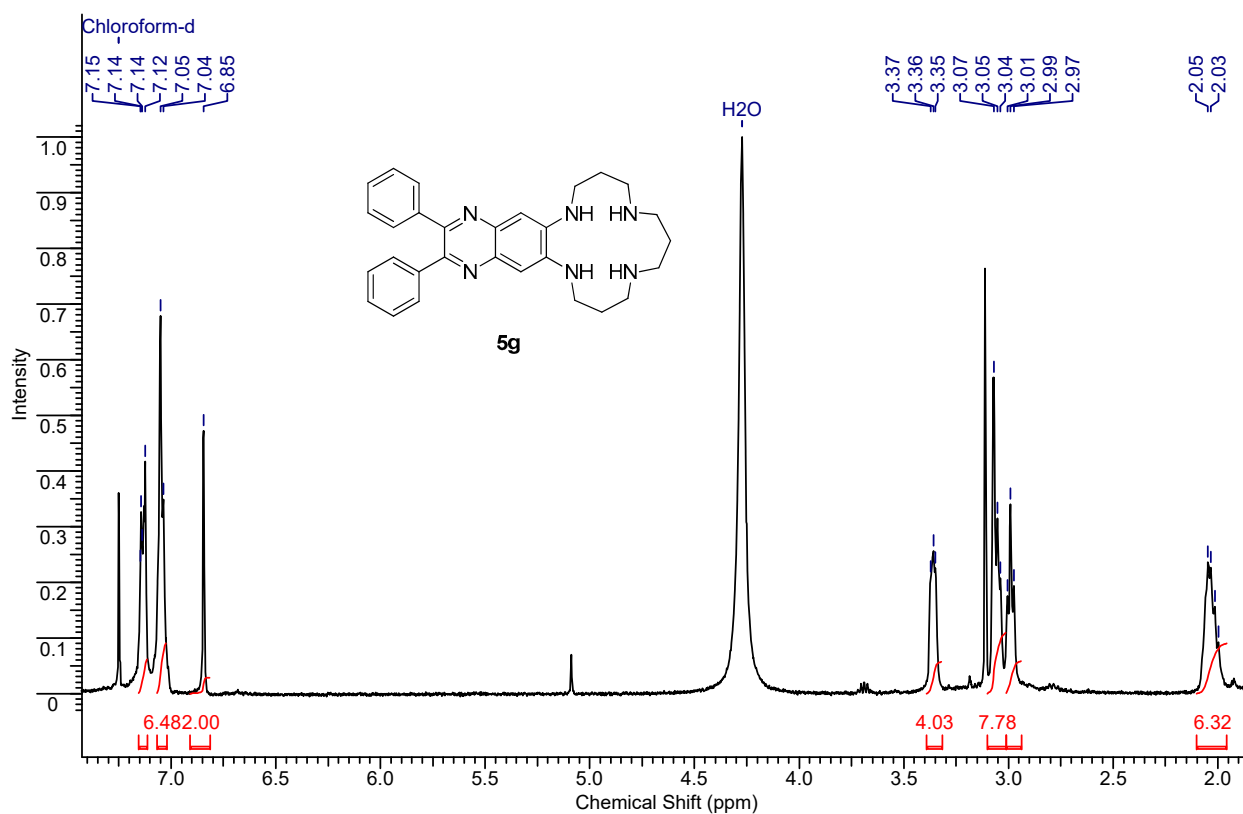


Figure S61. ¹H NMR spectrum of the compound **5g** (CDCl₃/CD₃OD, 5:1 v/v, 400 MHz, 300 K).

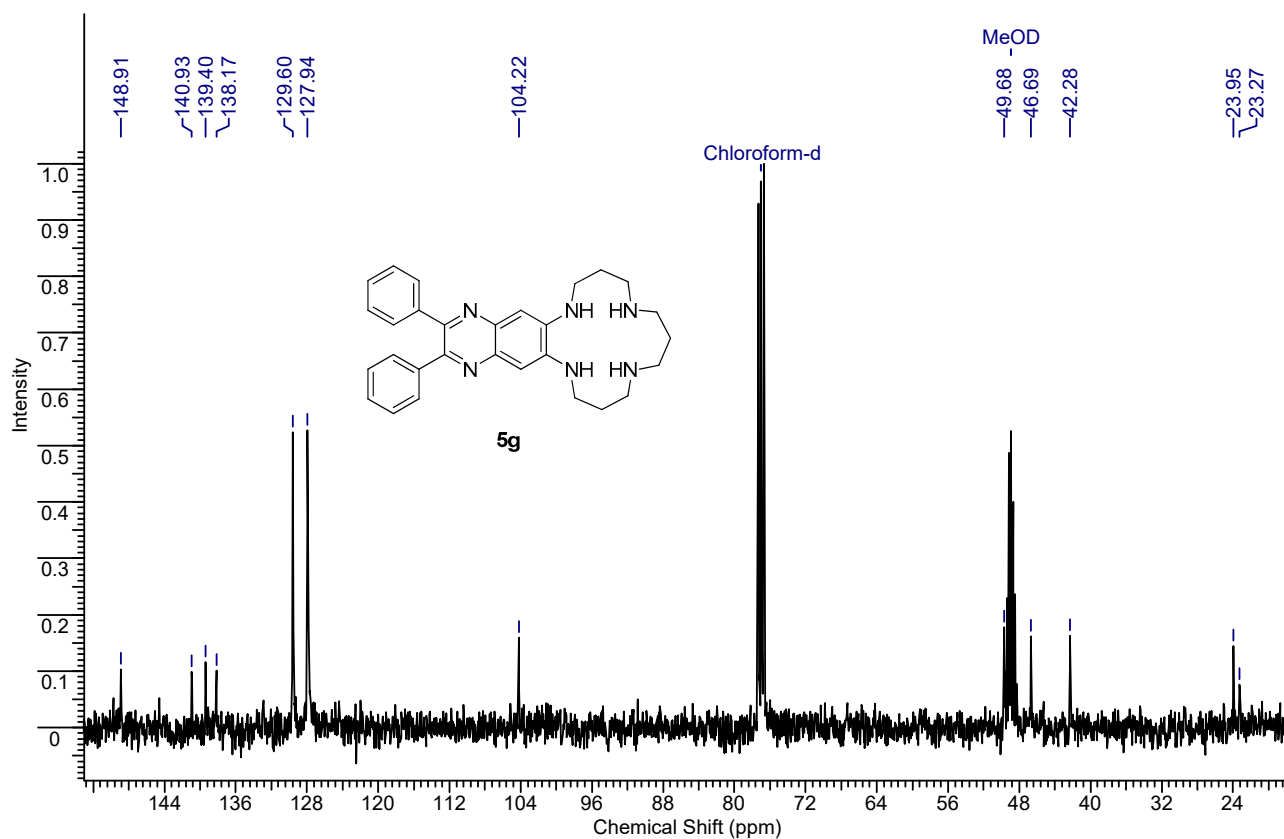


Figure S62. ¹³C NMR spectrum of the compound **5g** (CDCl₃/CD₃OD, 5:1 v/v, 100.6 MHz, 300 K).

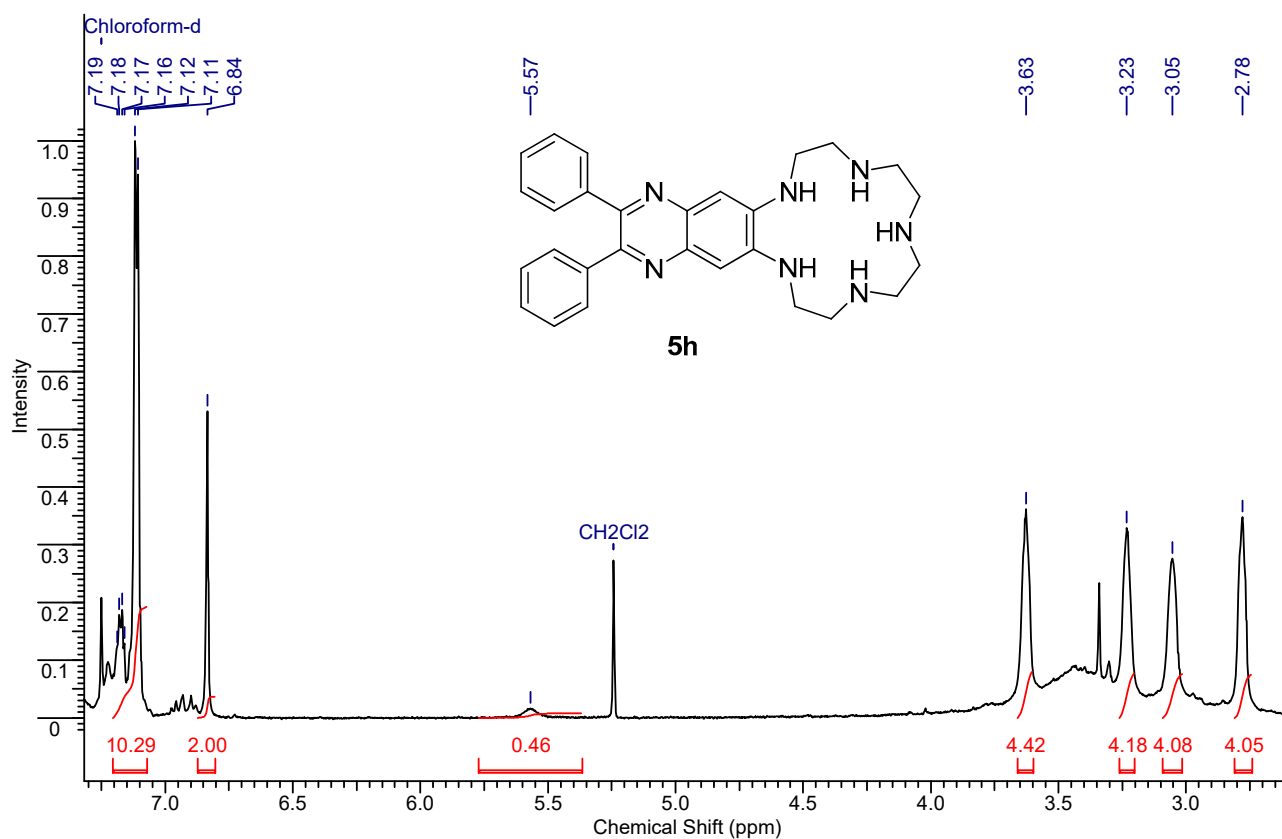


Figure S63. ¹H NMR spectrum of the compound **5h** (CDCl₃/CD₃OD, 10:1 v/v, 400 MHz, 300 K).

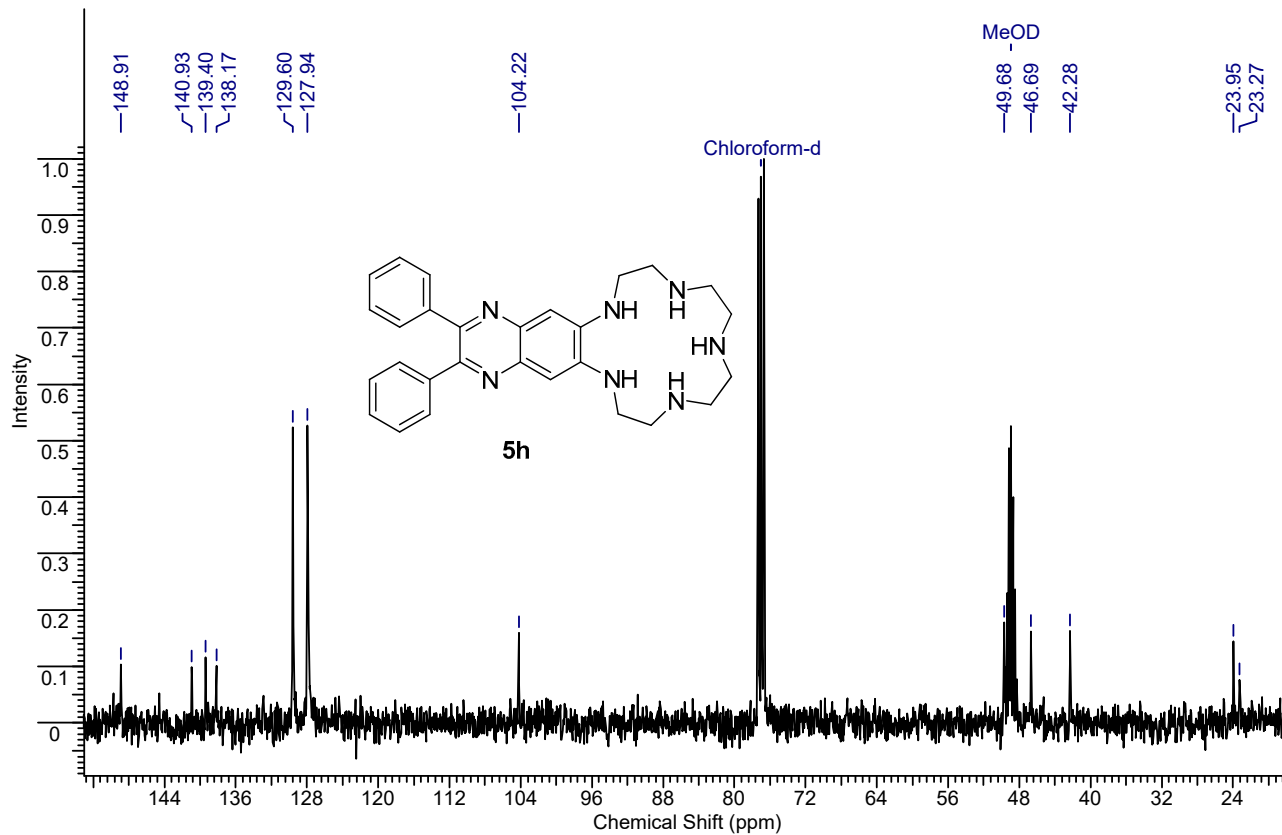


Figure S64. ¹³C NMR of the compound **5h** (CDCl₃/CD₃OD, 10:1 v/v, 100.6 MHz, 300 K).

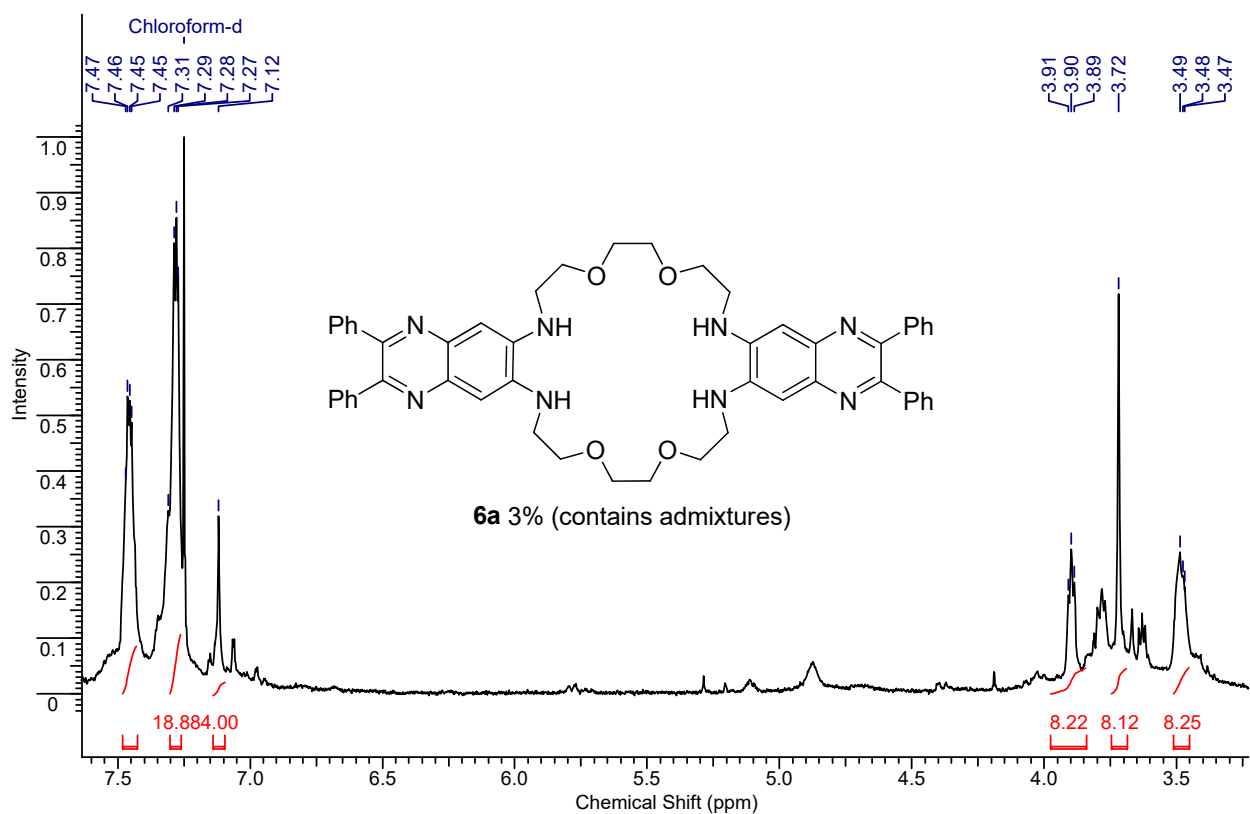


Figure S65. ¹H NMR spectrum of the compound **6a** (contains admixtures **5a**), (CDCl₃, 400 MHz, 300 K).

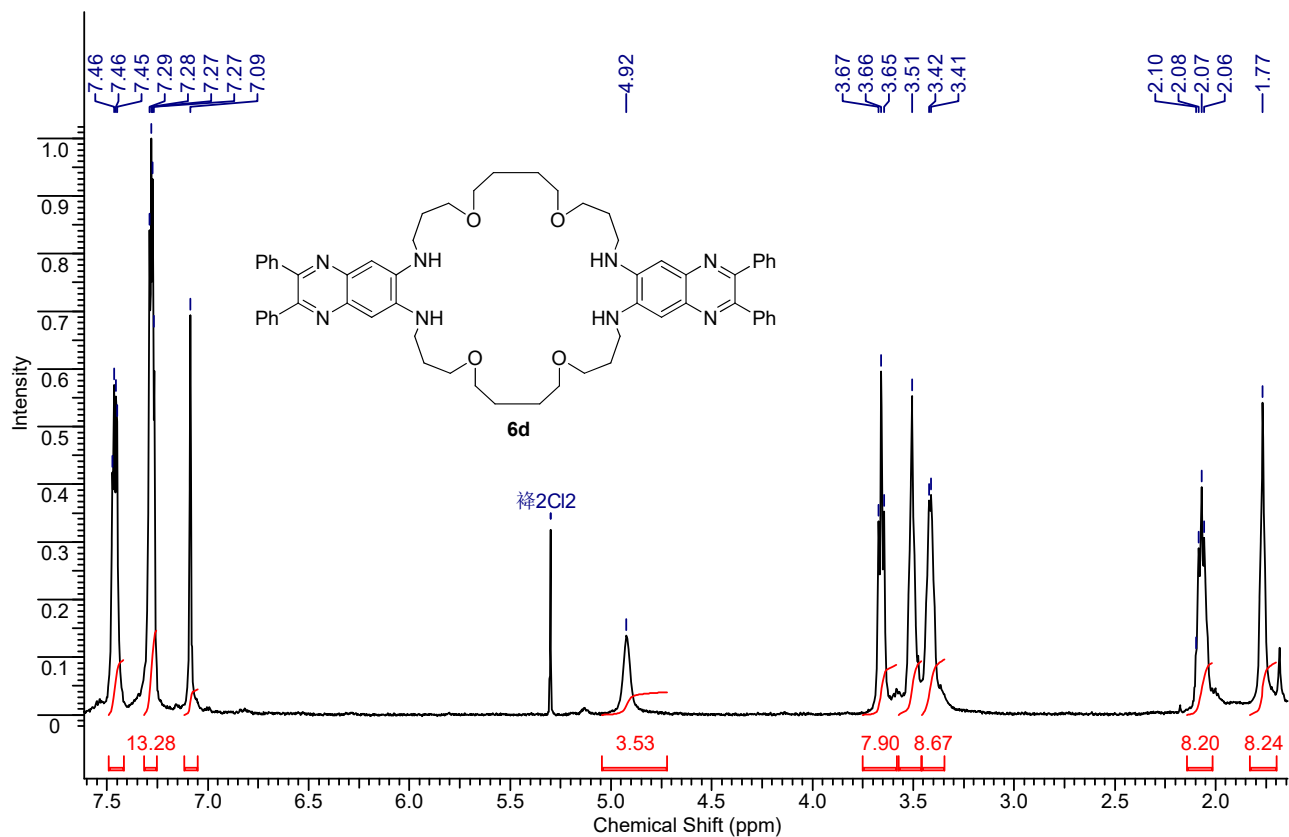


Figure S66. ¹H NMR spectrum of the compound **6d** (CDCl₃, 400 MHz, 300 K).

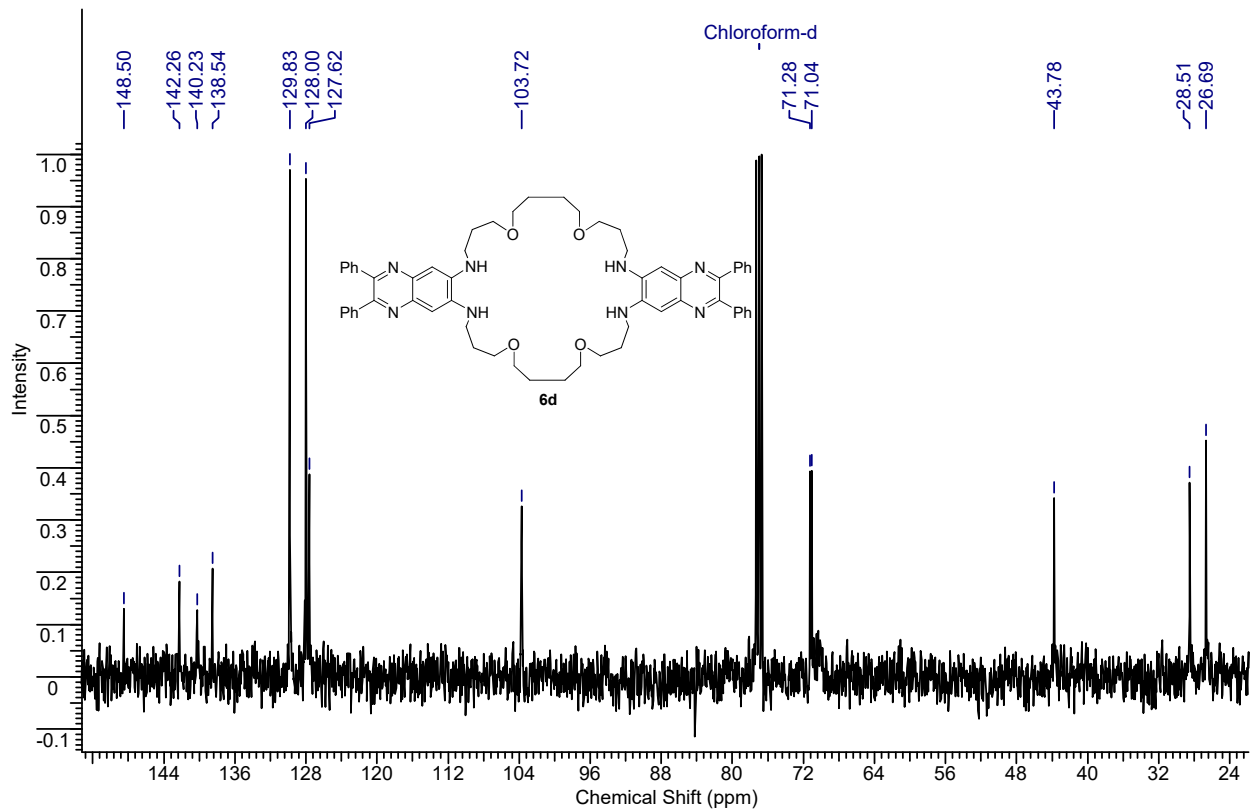


Figure S67. ¹³C NMR spectrum of the compound **6d** (CDCl₃, 100.6 MHz, 300 K).

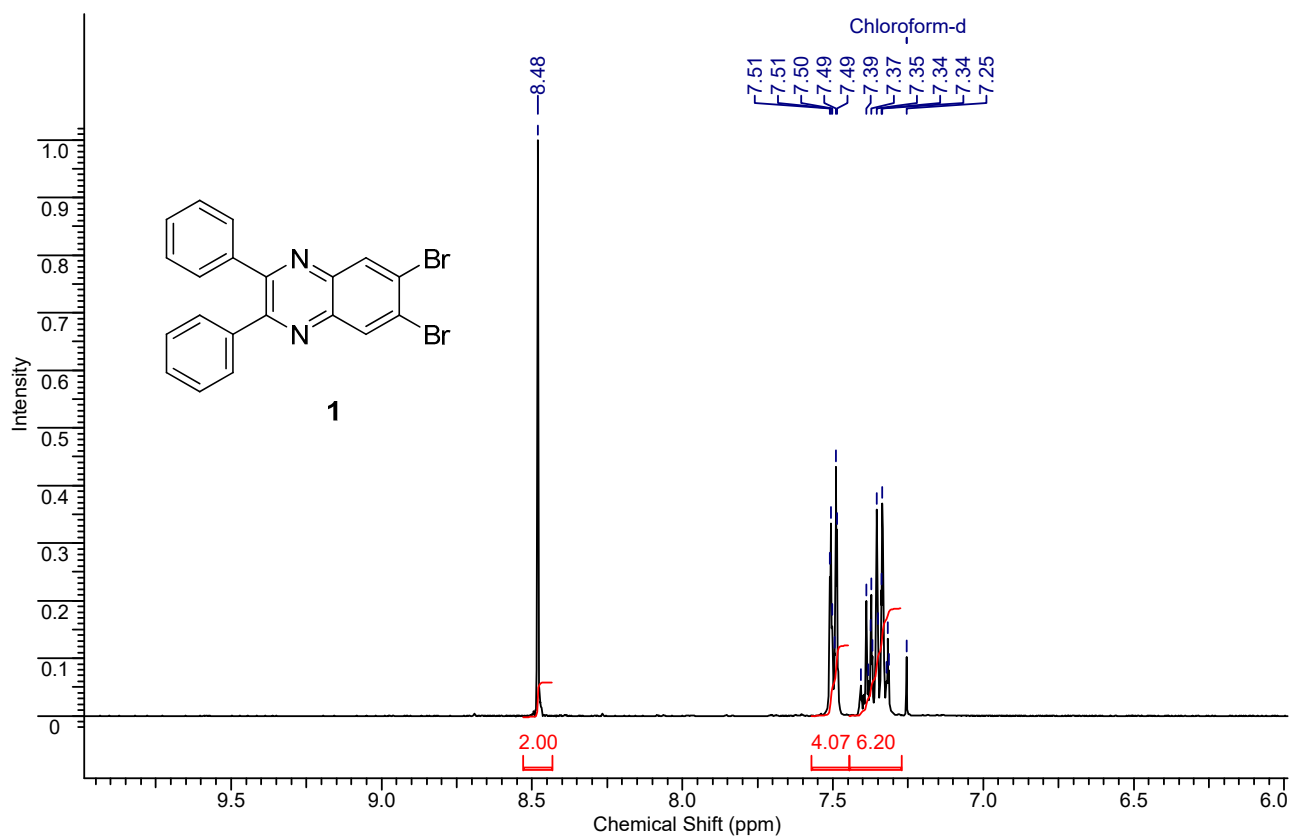


Figure S68. ¹H NMR spectrum of the compound **1** (CDCl₃, 400 MHz, 300 K).

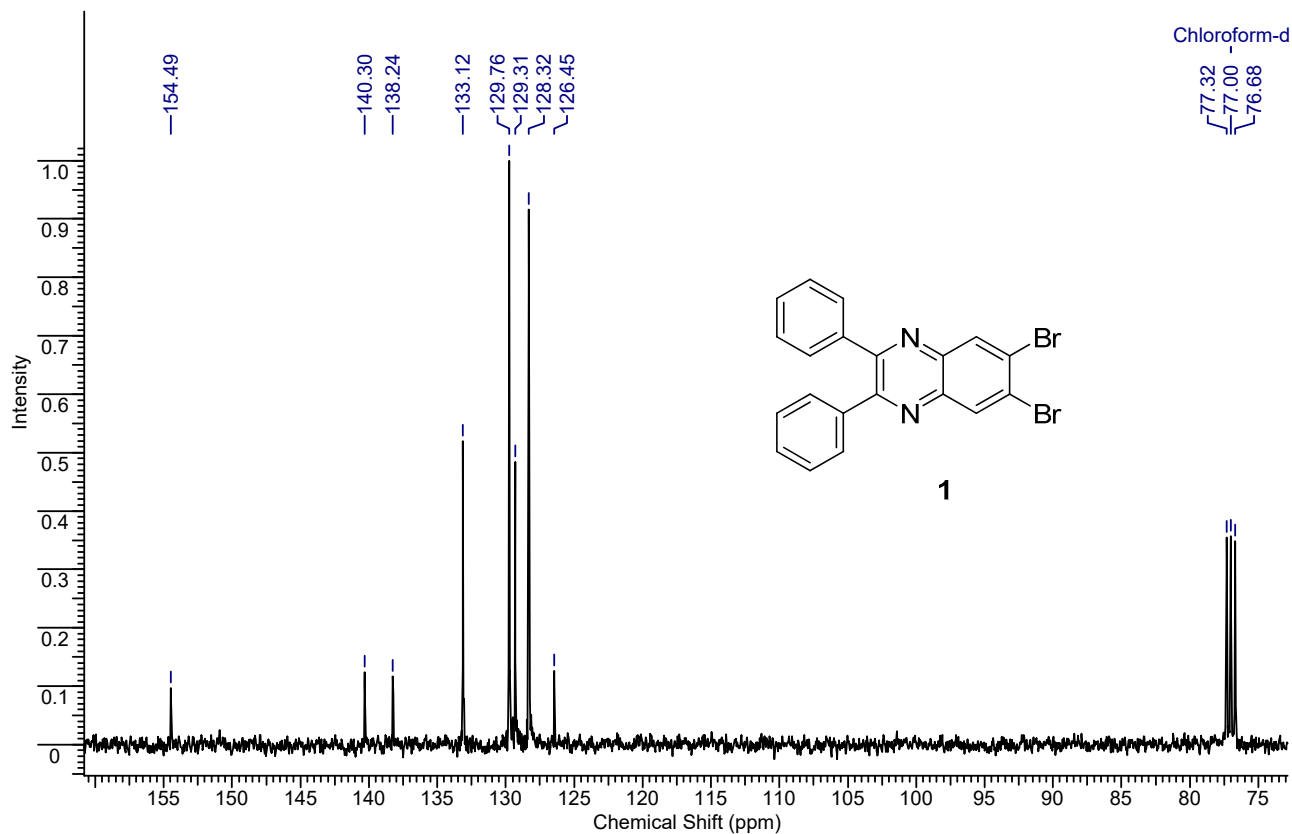


Figure S69. ^{13}C NMR spectrum of the compound **1** (CDCl_3 , 100.6 MHz, 300 K).

6. References

1. Wong, K.-L.; Bünzli, J.-C.G.; Tanner, P.A. Quantum yield and brightness. *J. Lumin.* **2020**, *224*, 117256, doi:10.1016/j.jlumin.2020.117256.
2. Gans, P.; Sabatini, A.; Vacca, A. Investigation of equilibria in solution. Determination of equilibrium constants with the HYPERQUAD suite of programs. *Talanta* **1996**, *43*, 1739–1753, doi:10.1016/0039-9140(96)01958-3.