

# Supramolecular Detection of a Nerve Agent Simulant by Fluorescent Zn–Salen Oligomer Receptors

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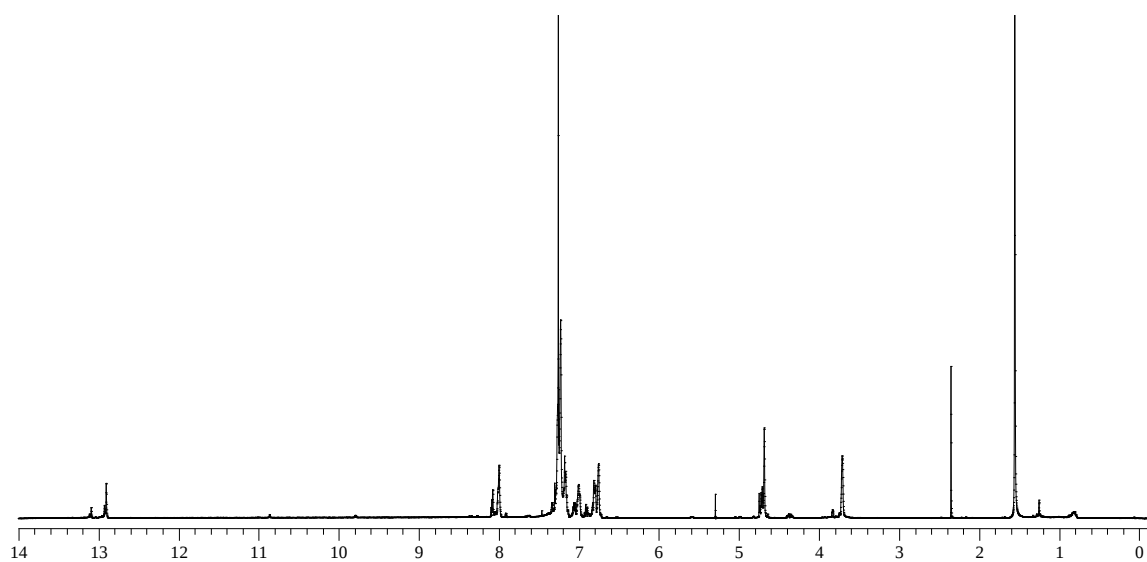


Figure S1.  $^1\text{H}$  NMR spectrum of Oligo-Salen-A in  $\text{CDCl}_3$

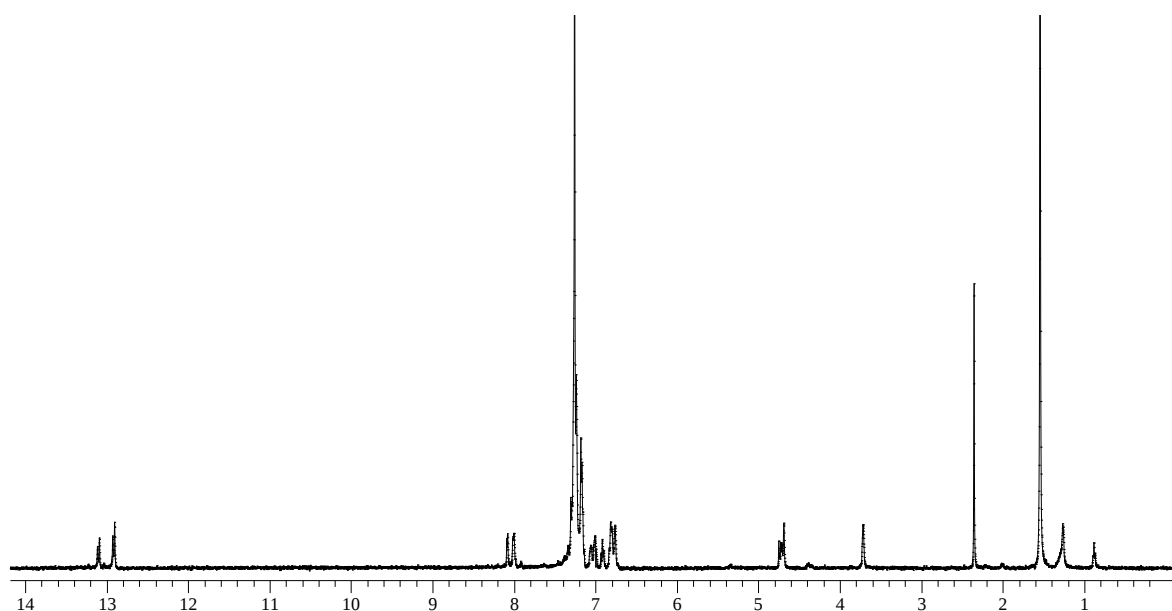


Figure S2.  $^1\text{H}$  NMR spectrum of Oligo-Salen-B in  $\text{CDCl}_3$

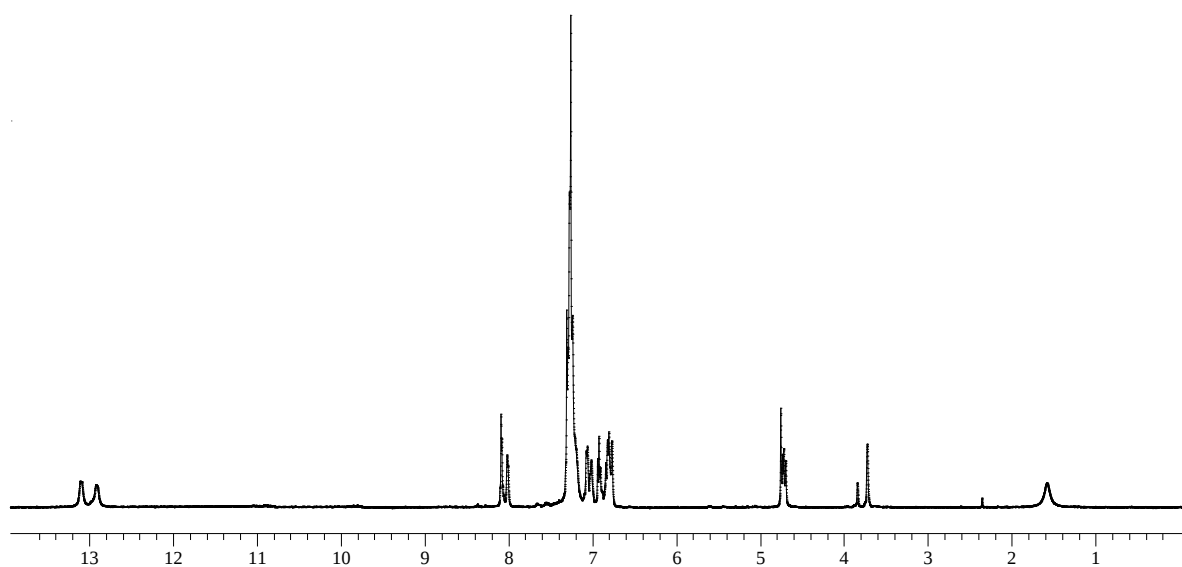


Figure S3.  $^1\text{H}$  NMR spectrum of Oligo-Salen-C in  $\text{CDCl}_3$

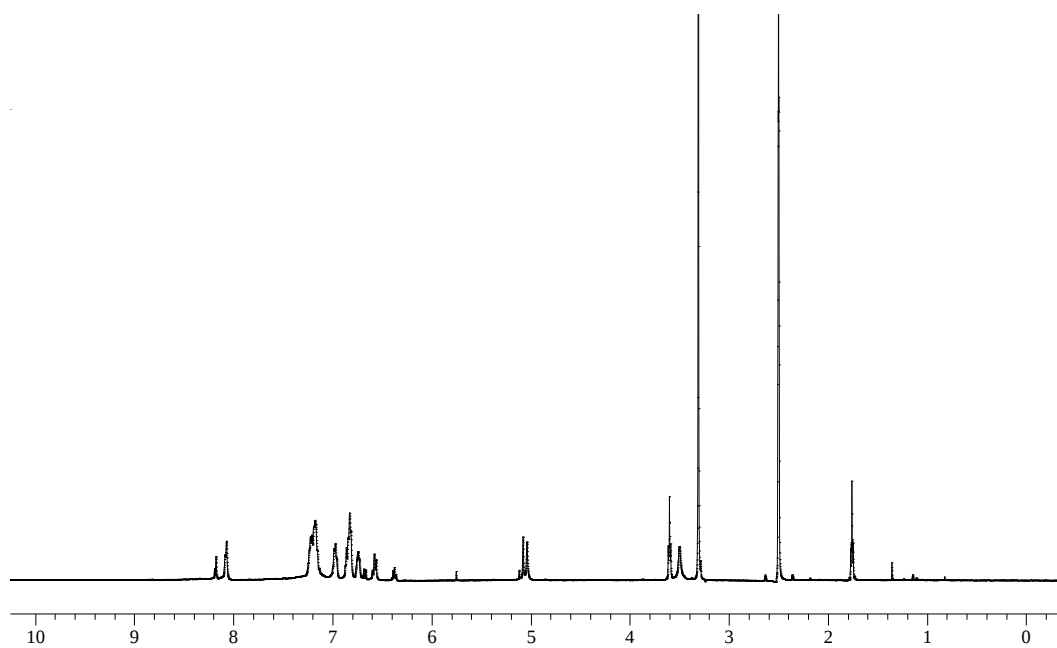


Figure S4.  $^1\text{H}$  NMR spectrum of Zn-Oligo-A in  $\text{DMSO}-d_6$

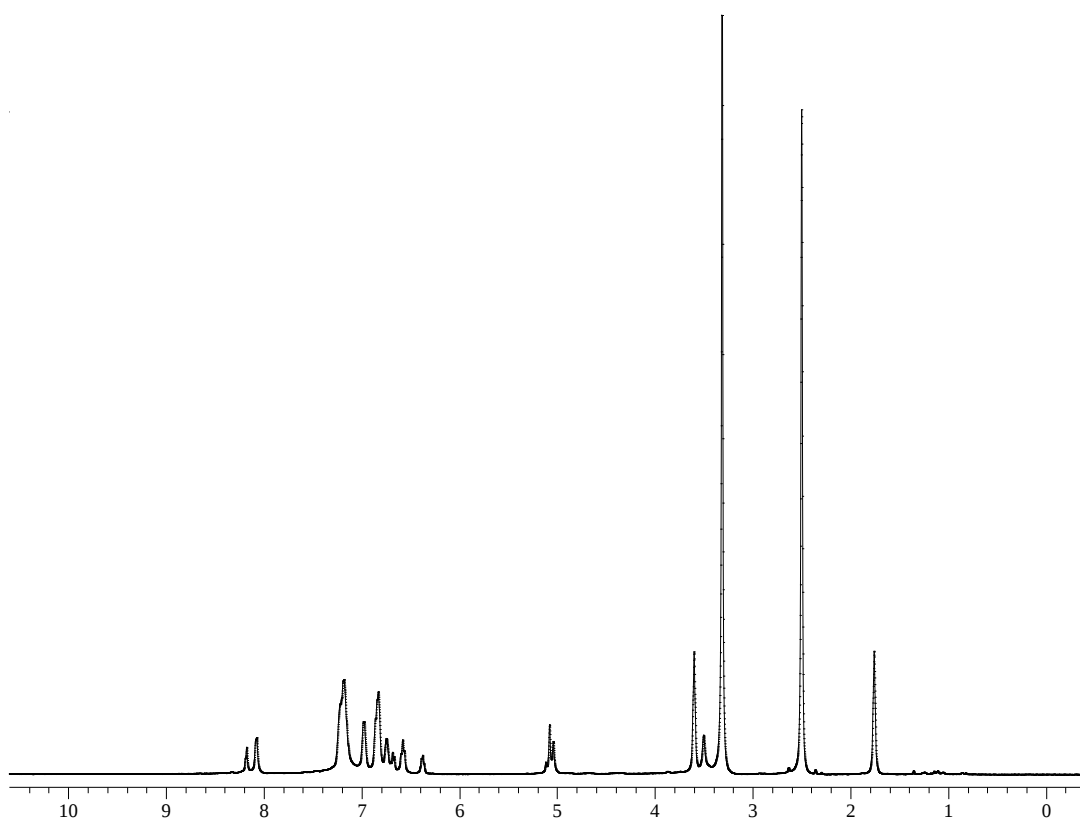


Figure S5.  $^1\text{H}$  NMR spectrum of Zn-Oligo-B in  $\text{DMSO-}d_6$

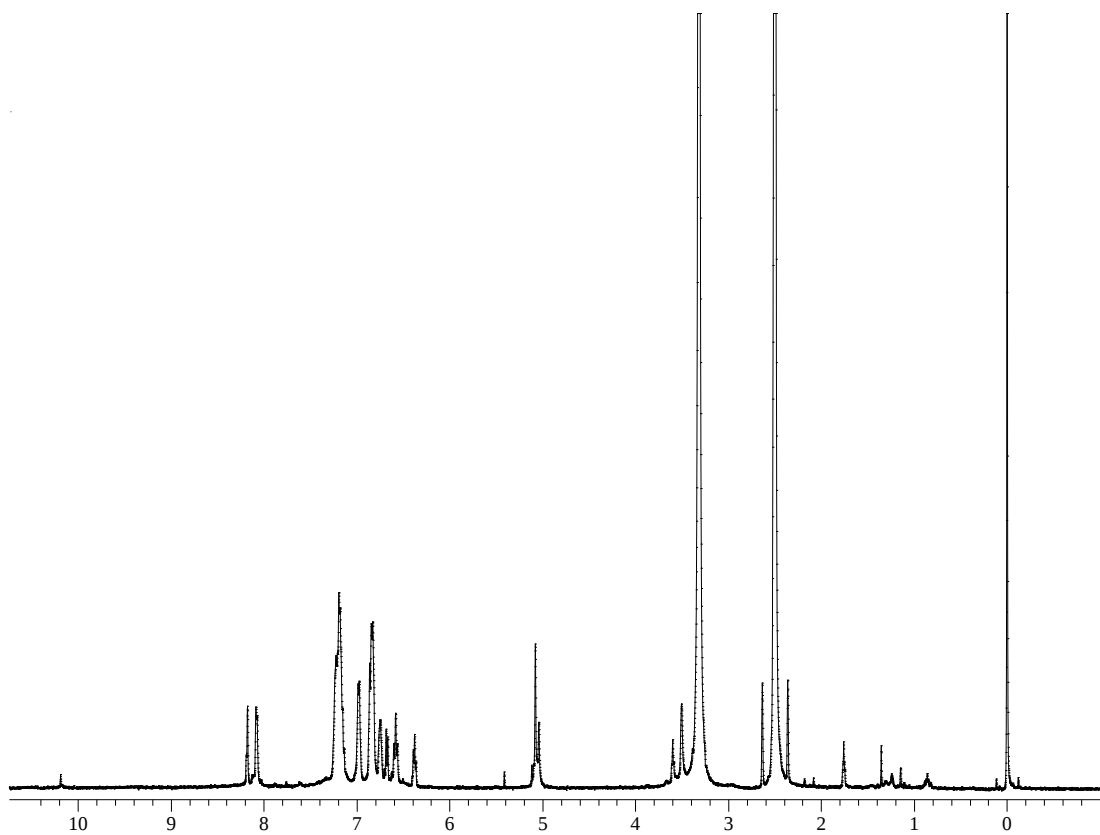


Figure S6.  $^1\text{H}$  NMR spectrum of Zn-Oligo-C in  $\text{DMSO-}d_6$

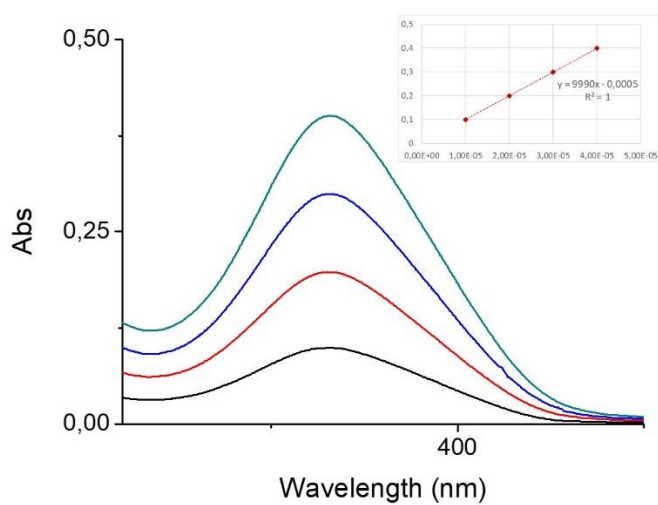


Figure S7. UV-Vis spectra of Zn-Oligo-A in DMSO ( $1 \times 10^{-5}$  M –  $4 \times 10^{-5}$  M). Inset shows  $\epsilon$  calculation.

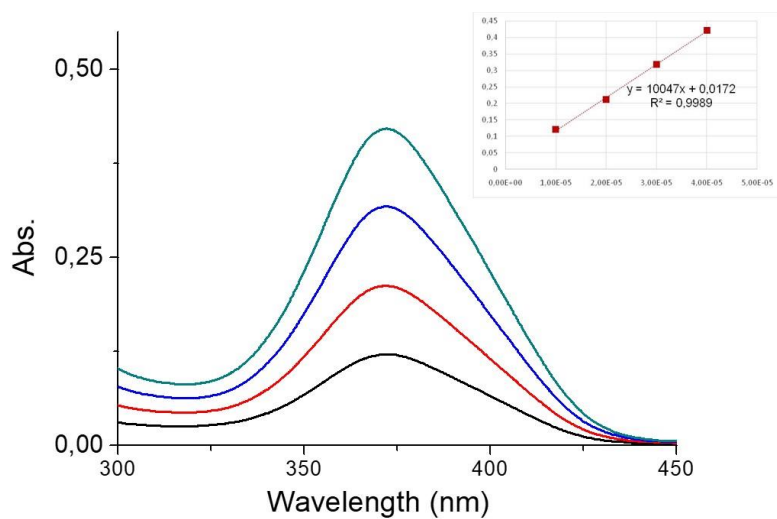


Figure S8. UV-Vis spectra of Zn-Oligo-B in DMSO ( $1 \times 10^{-5}$  M –  $4 \times 10^{-5}$  M). Inset shows  $\epsilon$  calculation.

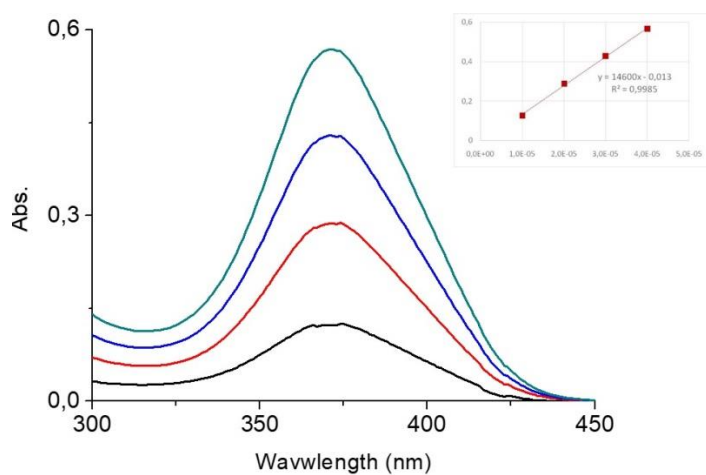


Figure S9. UV-Vis spectra of Zn-Oligo-C in DMSO ( $1 \times 10^{-5}$  M –  $4 \times 10^{-5}$  M). Inset shows  $\epsilon$  calculation.

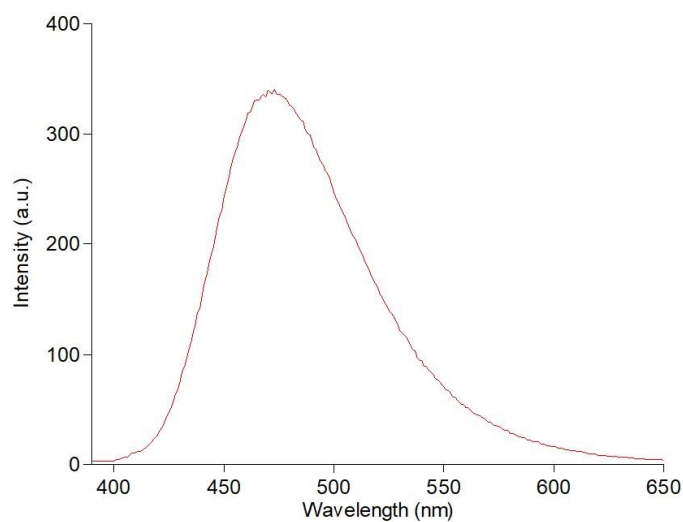


Figure S10. Fluorescence spectra of Zn-Oligo-A in DMSO ( $1 \times 10^{-5}$  M)

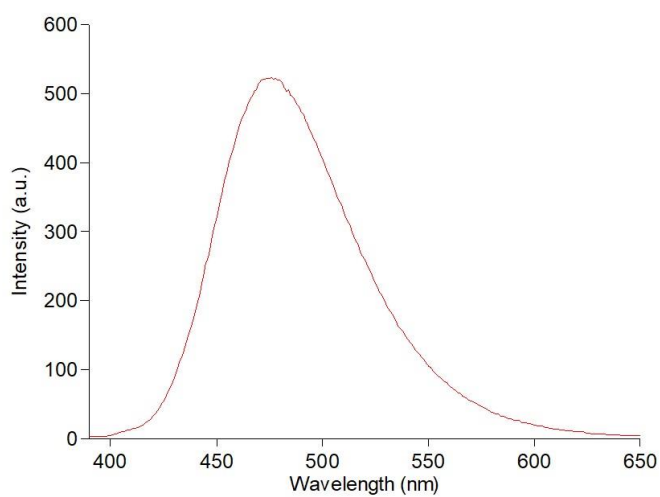


Figure S11. Fluorescence spectra of Zn-Oligo-B in DMSO ( $1 \times 10^{-5}$  M)

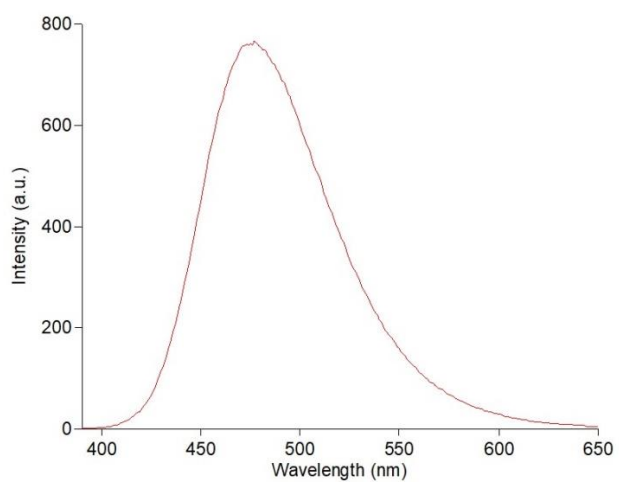


Figure S12. Fluorescence spectra of Zn-Oligo-C in DMSO ( $1 \times 10^{-5}$  M)

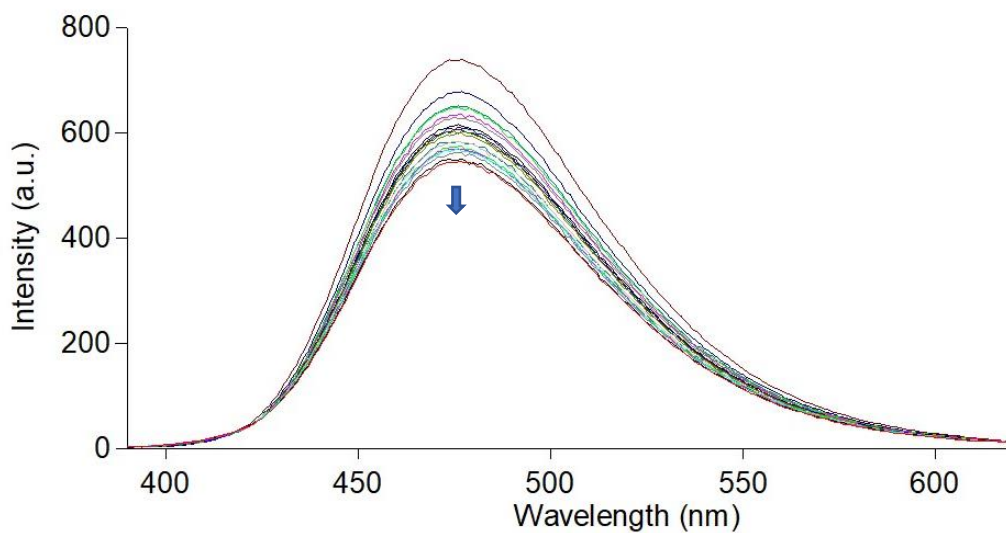


Figure S13. Representative fluorescence titration of Zn–Oligo–C vs DMMP in DMSO ( [Host] =  $1 \times 10^{-5}$  M, [Guest] = from 1 to 6 eq.)

#### BINDING CONSTANT CALCULATION

Host: Zn–Oligo–A; Guest DMMP

HypSpec output file:

Converged in 1 iterations with sigma = 0,030713

| Log beta | value  | standard deviation |
|----------|--------|--------------------|
| AB       | 4.8567 | 0.0698             |

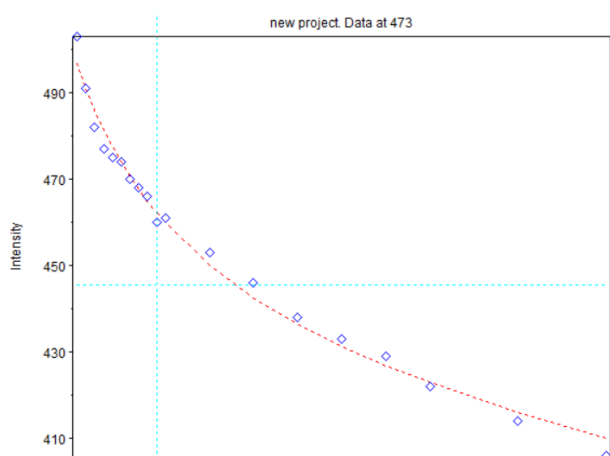


Figure S14.

Host: Zn–Oligo–B; Guest: DMMP

HypSpec output file:

Converged in 1 iterations with sigma = 0,030713

| Log beta | value  | standard deviation |
|----------|--------|--------------------|
| AB       | 4.9756 | 0.098              |

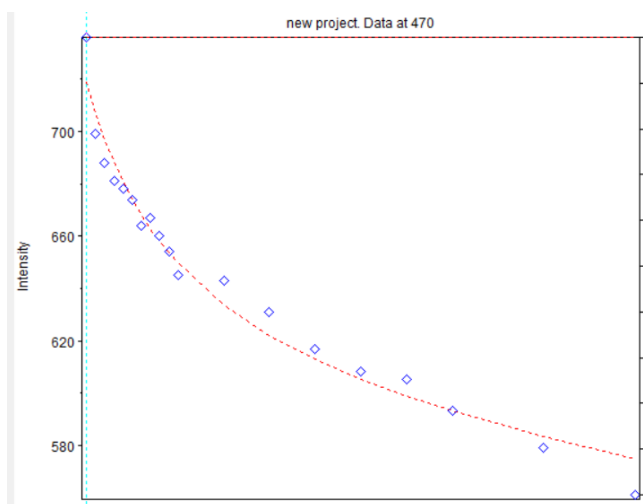


Figure S15.

Host: Zn–Oligo–C; Guest: DMMP

HypSpec output file:

Converged in 1 iterations with sigma = 0,030713

| Log beta | value  | standard deviation |
|----------|--------|--------------------|
| AB       | 5.6891 | 0.0409             |

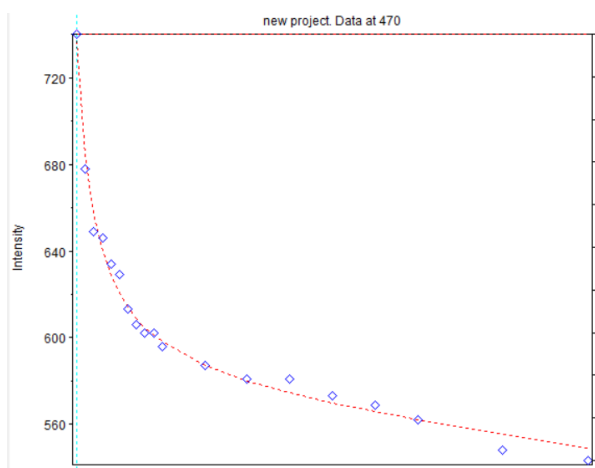


Figure S16.

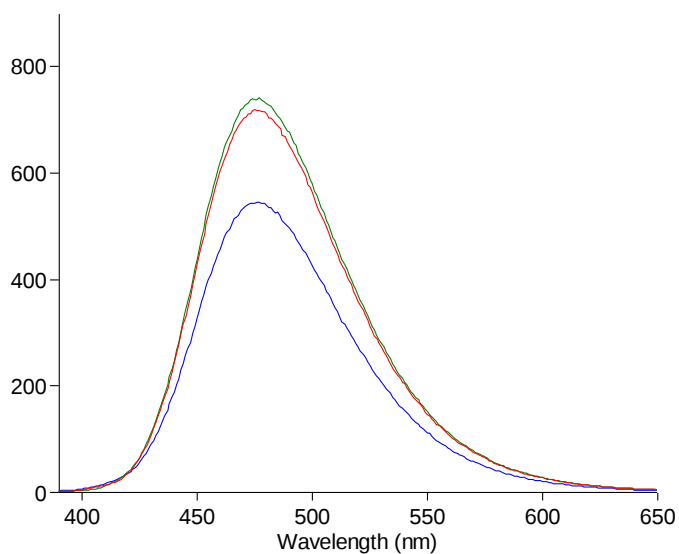


Figure S17. Selectivity tests. Emission spectra of: *i*) Zn–Oligo–C (red line,  $1 \times 10^{-5}$  M in DMSO), *ii*) Zn–Oligo–C after 10 minutes of air bubbling (green line), *iii*) Zn–Oligo–C after 10 minutes of air bubbling and 6 eq. of DMMP (blue line).

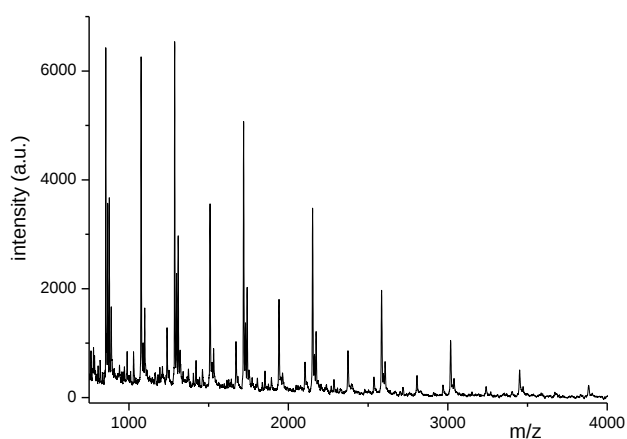


Figure S18: MALDI-TOF spectrum of Oligo–Salen–C.