Supporting Information

Enhancement of Anion Recognition Exhibited by a Zinc−Imidazole-Based Ion-Pair Receptor Composed of C-H Hydrogen- and Halogen-Bond Donor Groups.

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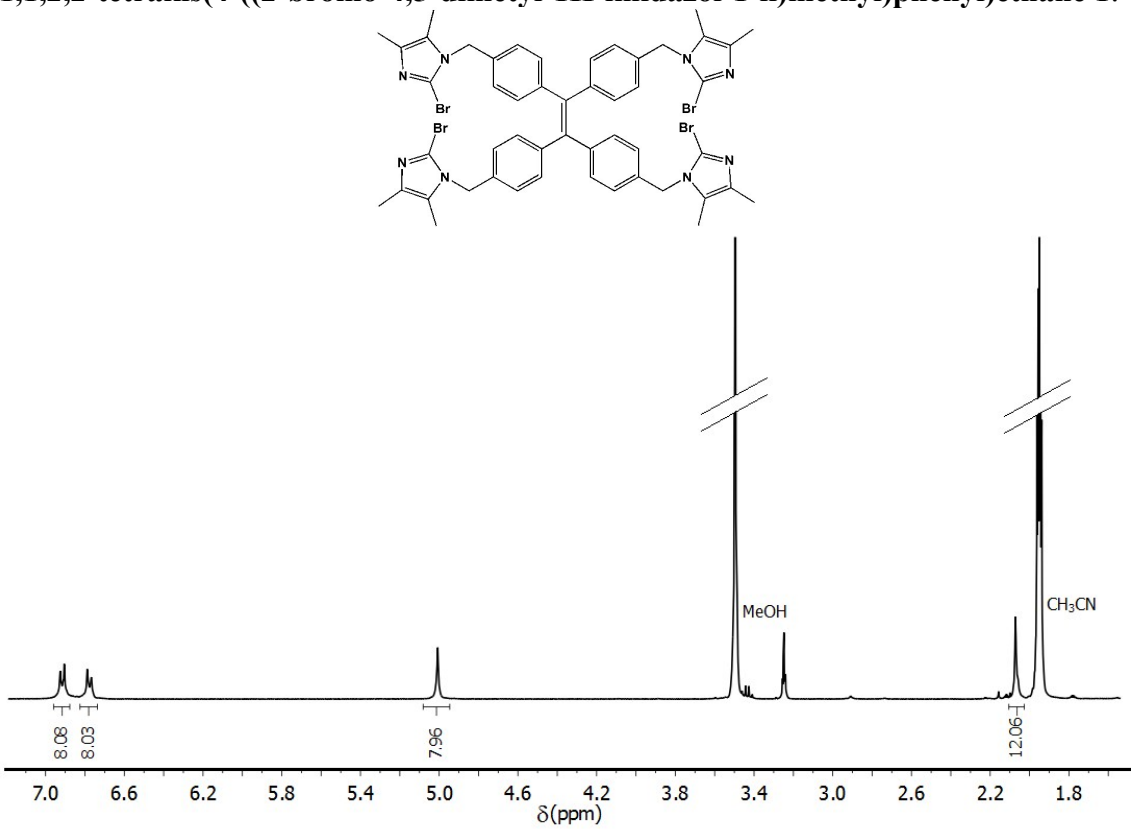


Figure S1. ^{1}H NMR spectra of 1,1,2,2-tetrakis(4-((2-bromo-4,5-dimetyl-1H-imidazol-1-il)methyl)phenyl)ethane **1**.

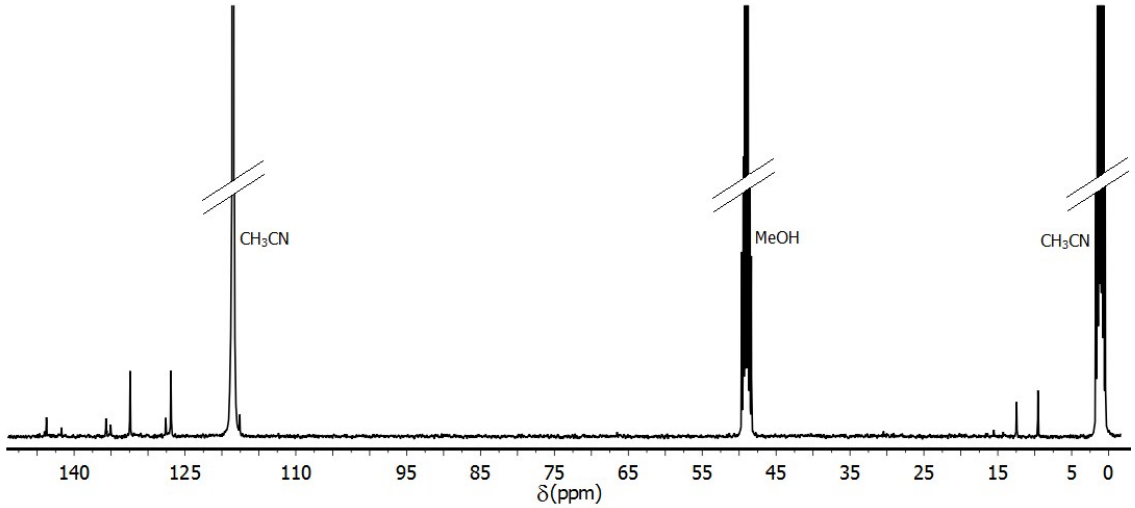


Figure S2. ^{13}C NMR spectra of 1,1,2,2-tetrakis(4-((2-bromo-4,5-dimetyl-1H-imidazol-1-il)methyl)phenyl)ethane **1**.

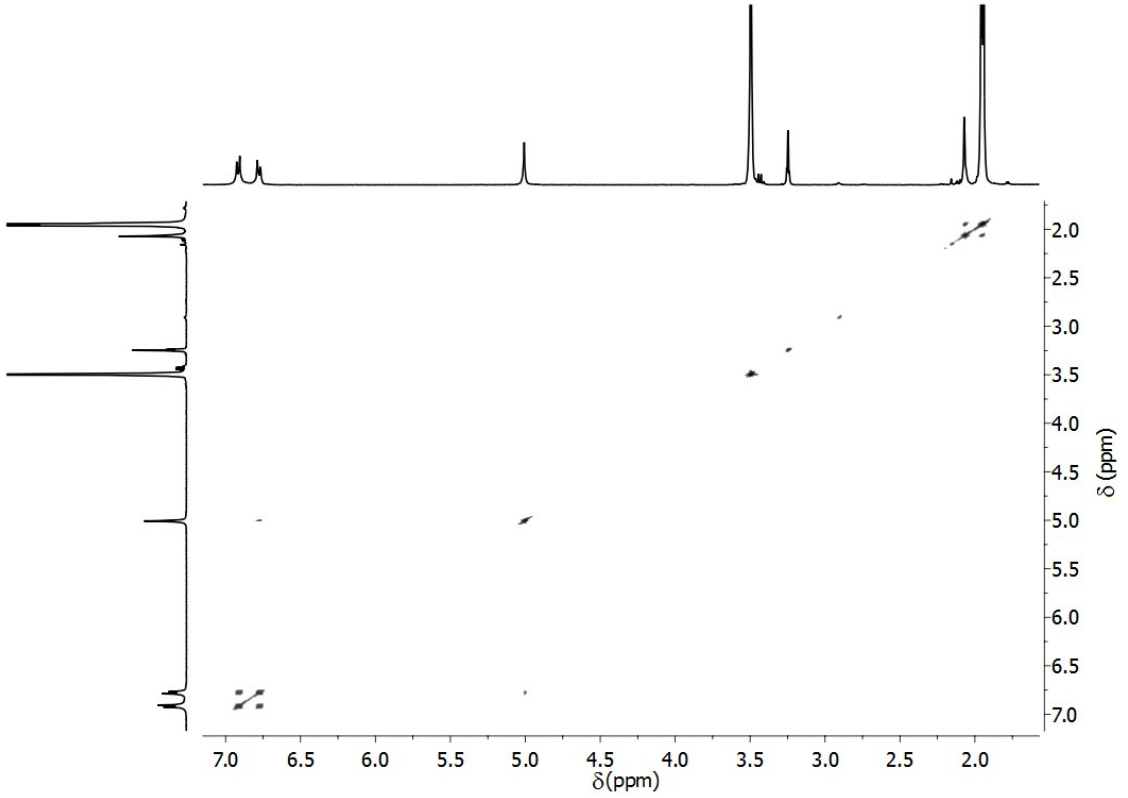


Figure S3. COSY NMR spectra of 1,1,2,2-tetrakis(4-((2-bromo-4,5-dimetyl-1H-imidazol-1-il)methyl)phenyl)ethane **1**.

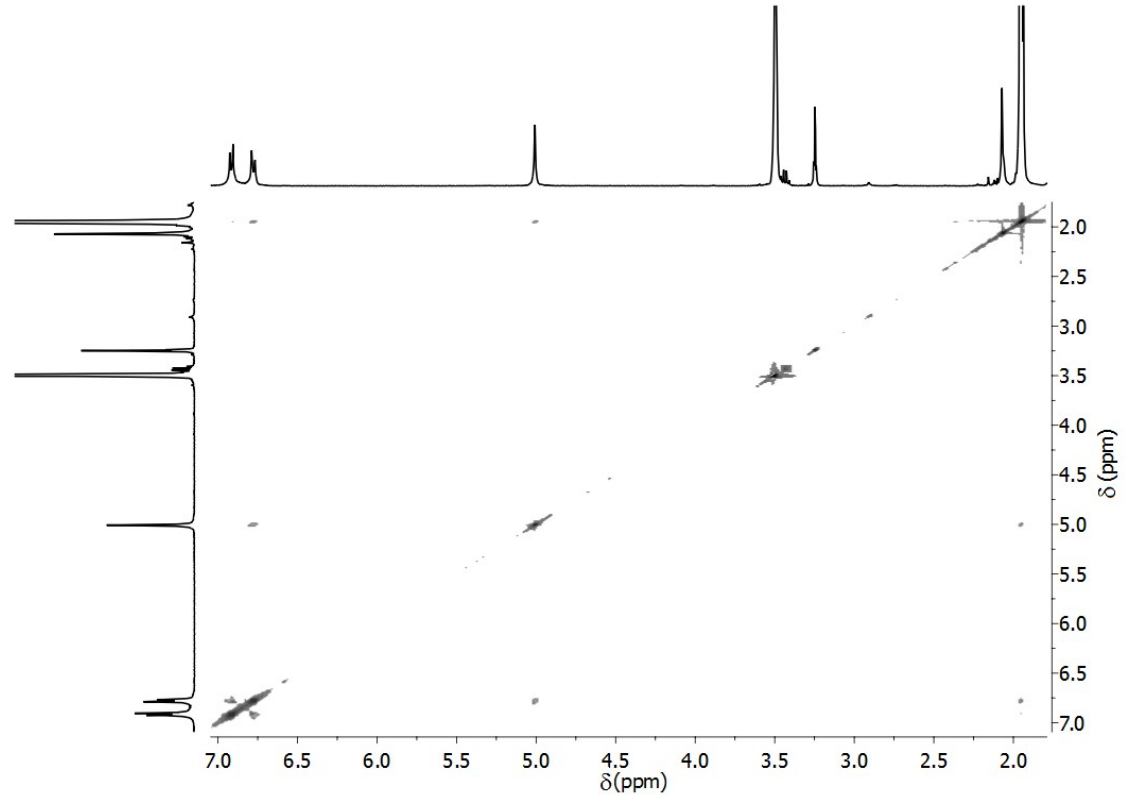


Figure S4. NOESY NMR spectra of 1,1,2,2-tetrakis(4-((2-bromo-4,5-dimetyl-1H-imidazol-1-il)methyl)phenyl)ethane **1**.

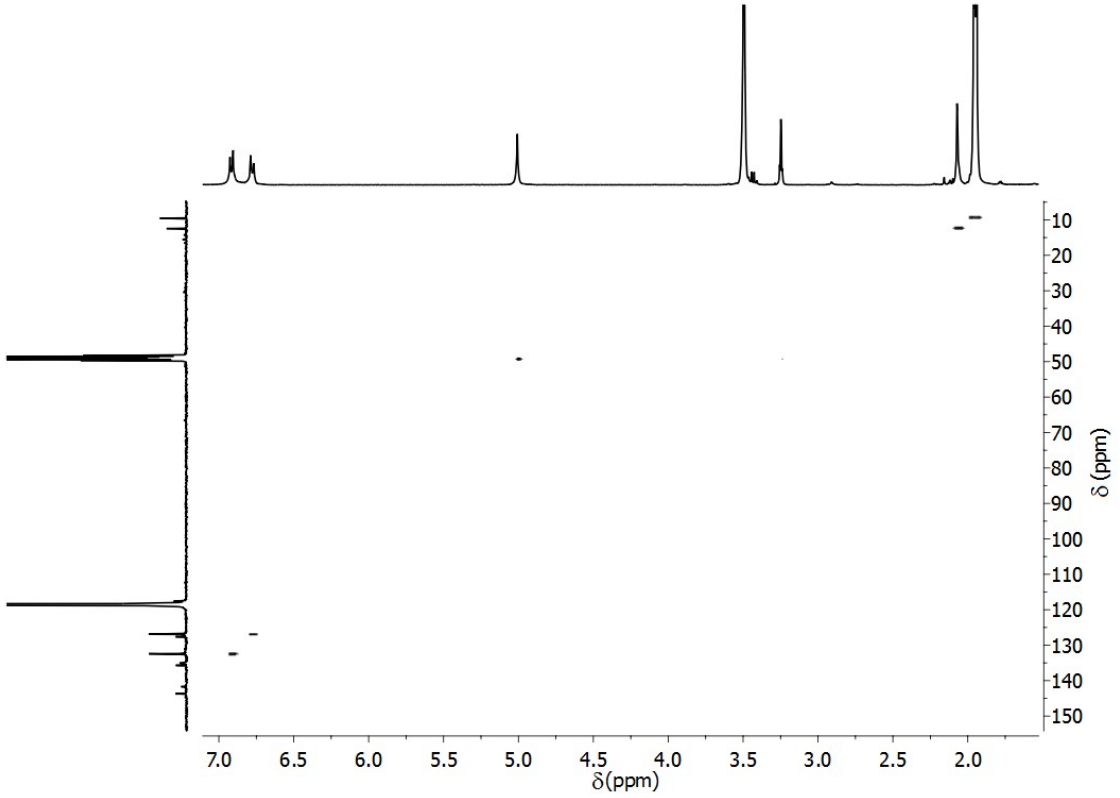


Figure S5. HSQC NMR spectra of 1,1,2,2-tetrakis(4-((2-bromo-4,5-dimetyl-1H-imidazol-1-il)methyl)phenyl)ethane **1**.

1,1,2,2-tetrakis(4-((4,5-dimetyl-1H-imidazol-1-il)methyl)phenyl)ethane 2:

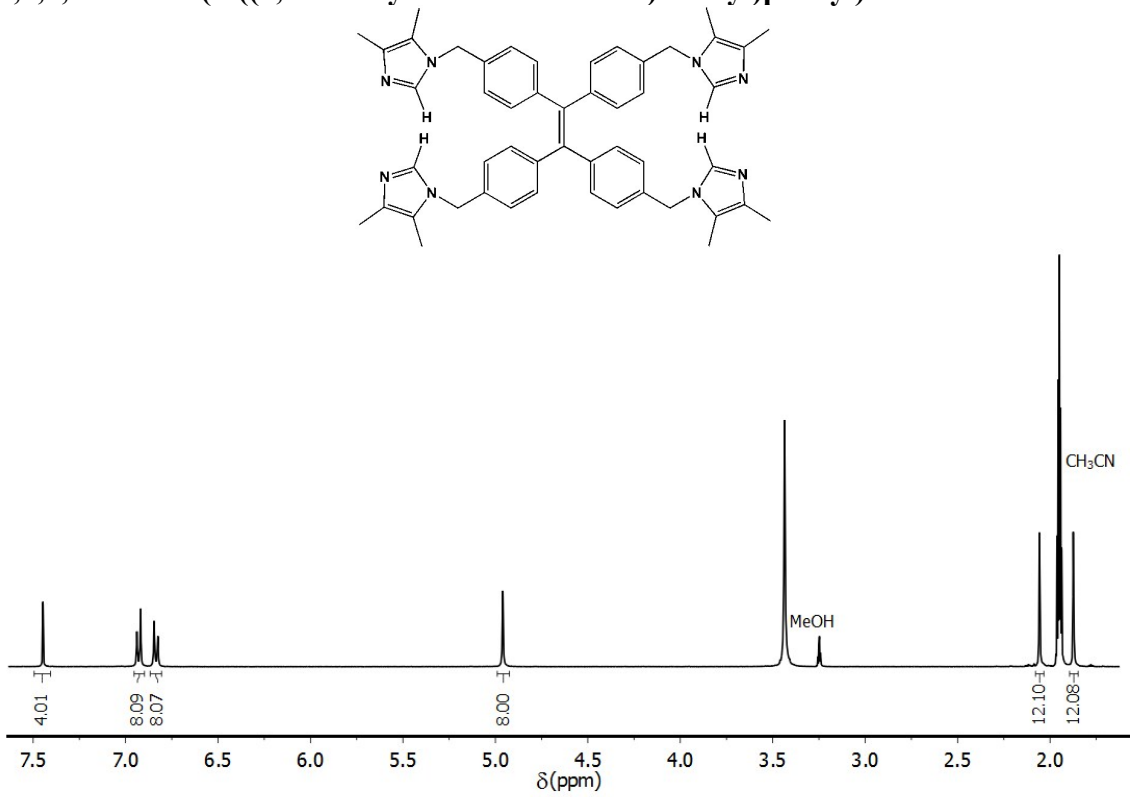


Figure S6. ^{1}H NMR spectra of 1,1,2,2-tetrakis(4-((4,5-dimetyl-1H-imidazol-1-il)methyl)phenyl)ethane **2**.

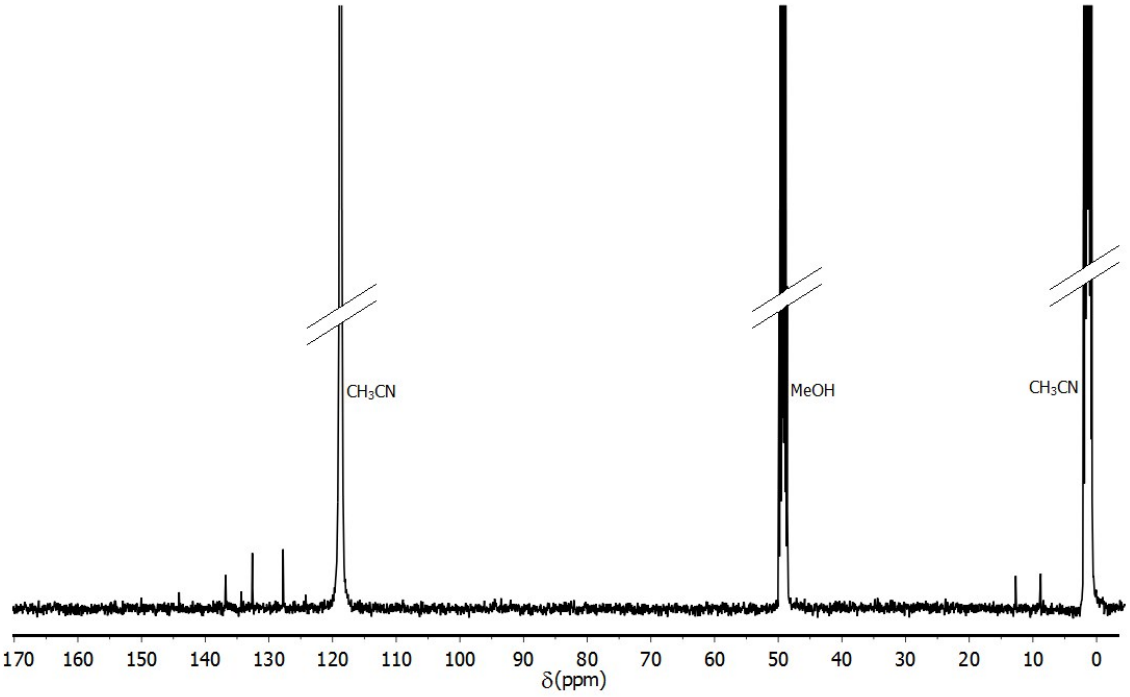


Figure S7. ^{13}C NMR spectra of 1,1,2,2-tetrakis(4-((4,5-dimetyl-1H-imidazol-1-il)methyl)phenyl)ethane **2**.

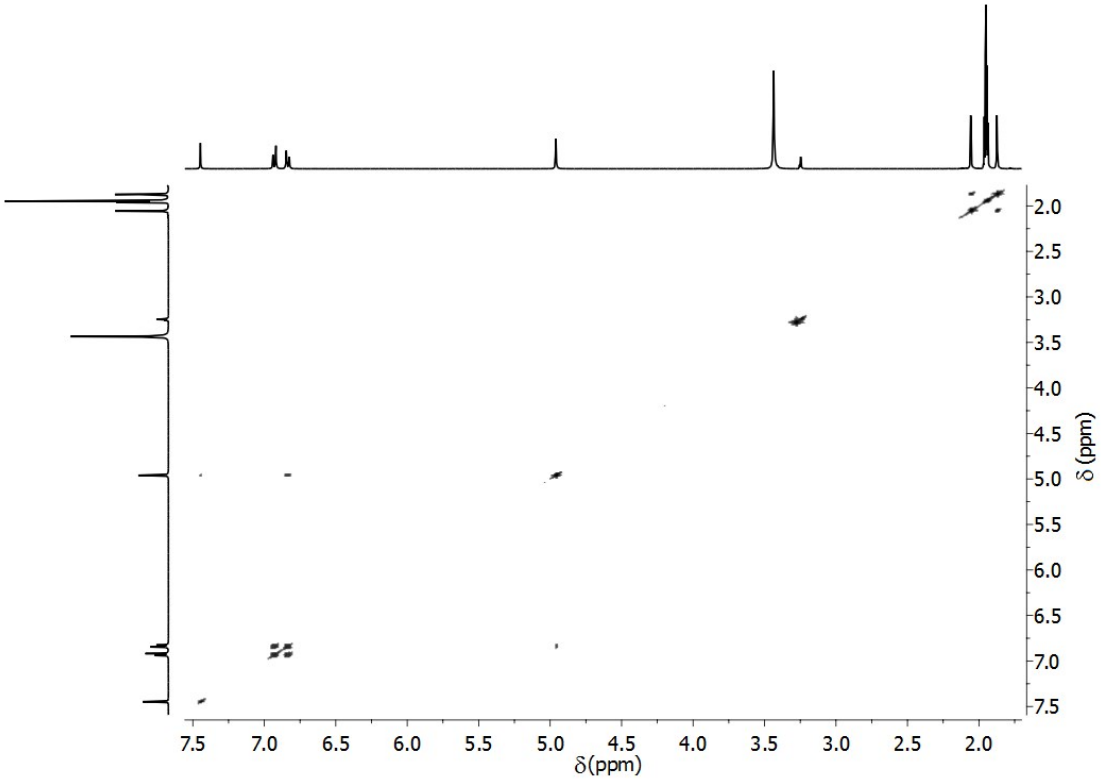


Figure S8. COSY NMR spectra of 1,1,2,2-tetrakis(4-((4,5-dimetyl-1H-imidazol-1-il)methyl)phenyl)ethane **2**.

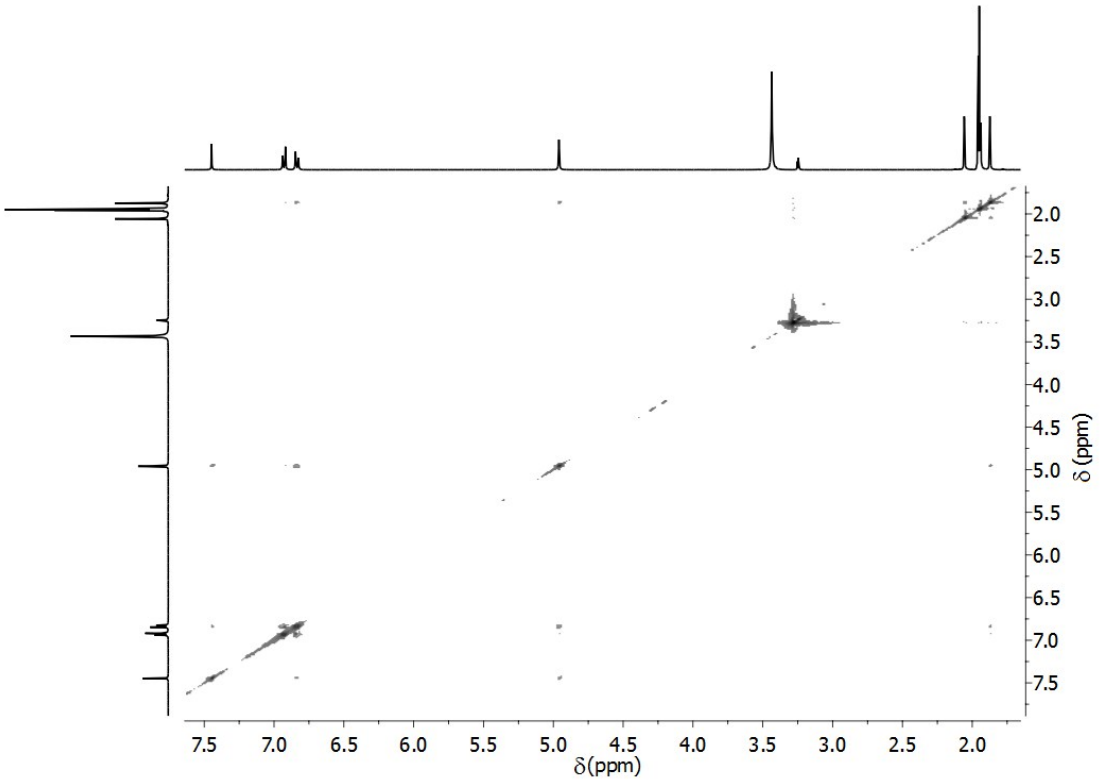
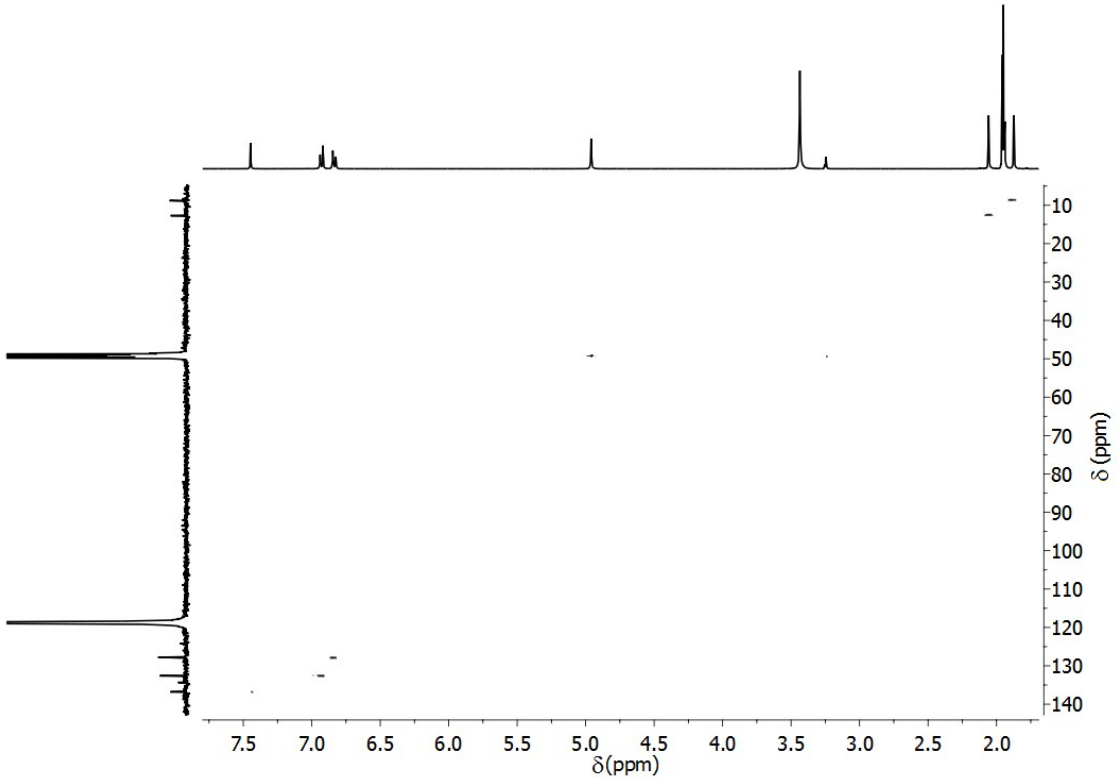


Figure S9. NOESY NMR spectra of 1,1,2,2-tetrakis(4-((4,5-dimetyl-1H-imidazol-1-il)methyl)phenyl)ethane **2**.



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PART II: Fluorescence Anion Binding Studies

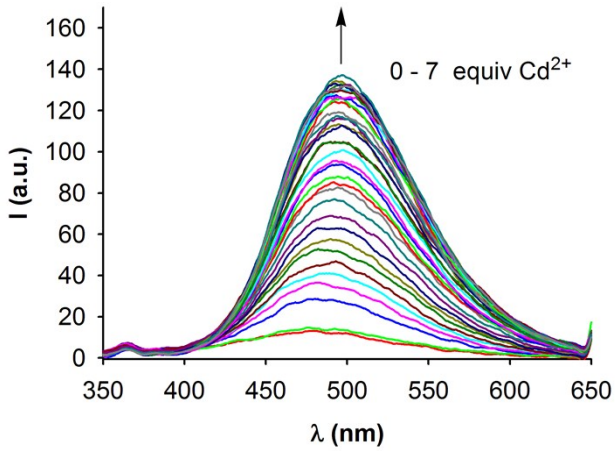


Figure S11. Changes in the fluorescence spectra of receptor **1** ($c = 1 \cdot 10^{-5}$ M in CH_3CN) upon addition of Cd^{2+} cations at 20 °C.

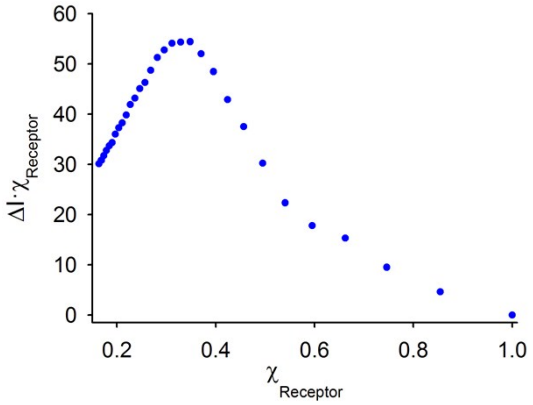


Figure S12. Job plot experiment, using the fluorescence titration data, with a maximum at 0.33 indicating 1:2 stoichiometry for receptor **1** and Zn^{2+} in CH_3CN.

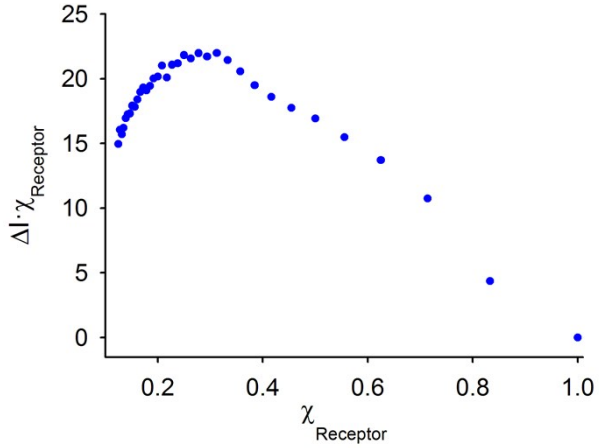


Figure S13. Job plot experiment, using the fluorescence titration data, with a maximum at 0.33 indicating 1:2 stoichiometry for receptor **1** and Cd^{2+} in CH_3CN.

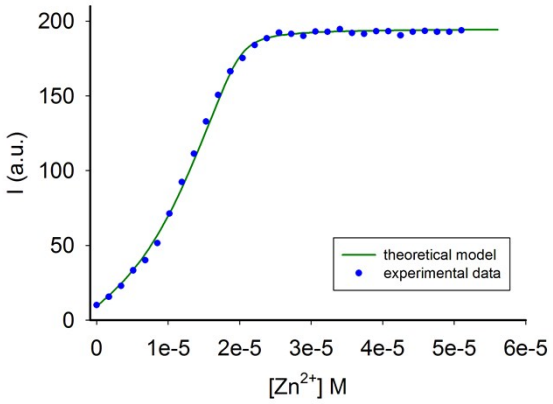


Figure S14. Changes in the emission intensity of the receptor **1** (c = $1 \cdot 10^{-5}$ M in CH_3CN) upon addition of increasing amounts of Zn^{2+}. Data points represent experimental data, continuous lines represent calculated curves.

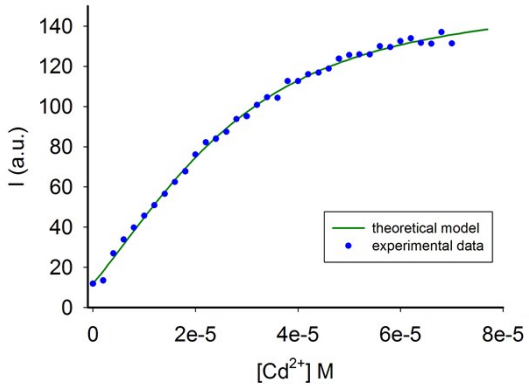
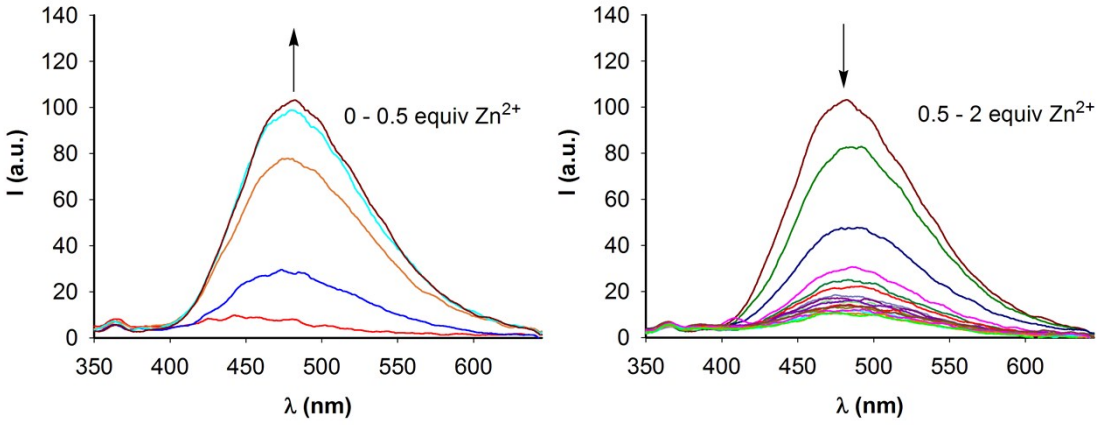


Figure S15. Changes in the emission intensity of the receptor **1** (c = $1 \cdot 10^{-5}$ M in CH_3CN) upon addition of increasing amounts of Cd^{2+}. Data points represent experimental data, continuous lines represent calculated curves.



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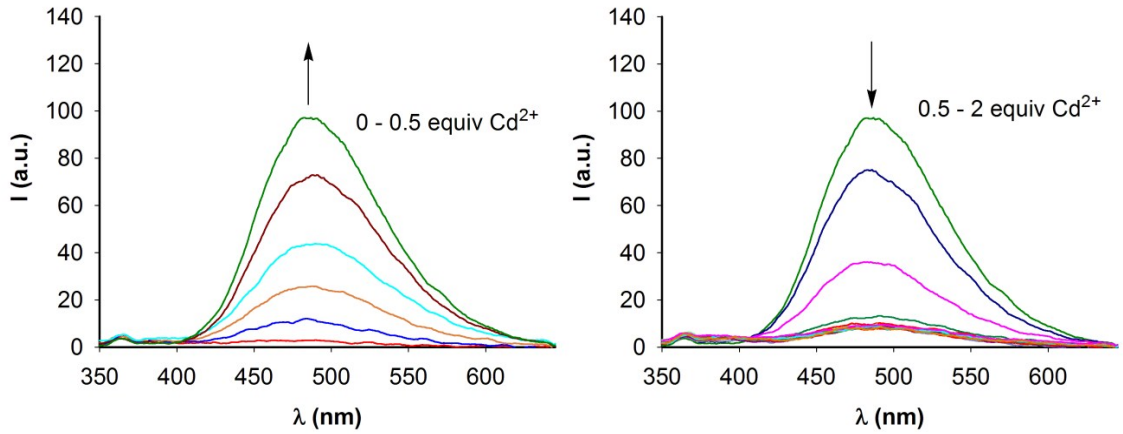

Figure S17. Changes in the fluorescence spectra of receptor **2** ($c = 1 \cdot 10^{-5}$ M in CH_3CN) upon addition of Cd^{2+} cations at 20 °C.

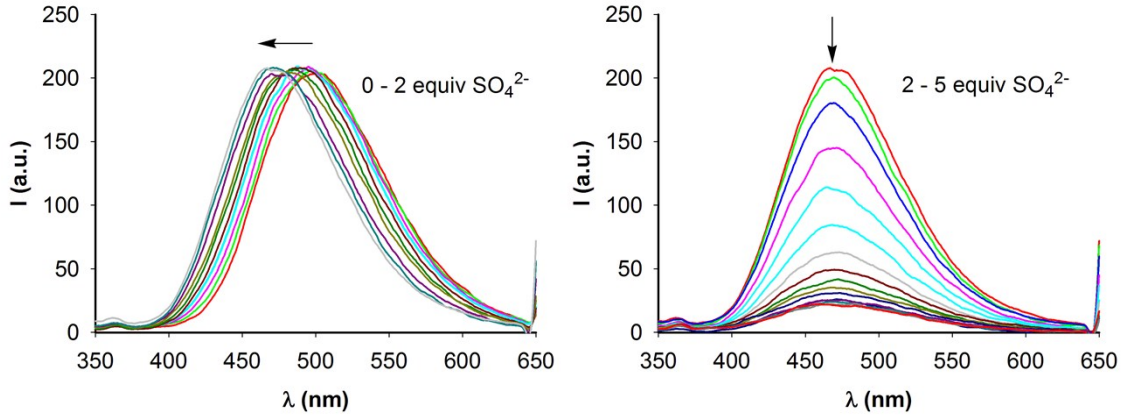

Figure S18. Changes in the fluorescence spectra of receptor $[\mathbf{1}\cdot 2Zn]^{4+}$ ($c = 1 \cdot 10^{-5}$ M in CH_3CN) upon addition of SO_4^{2-} anions at 20 °C.

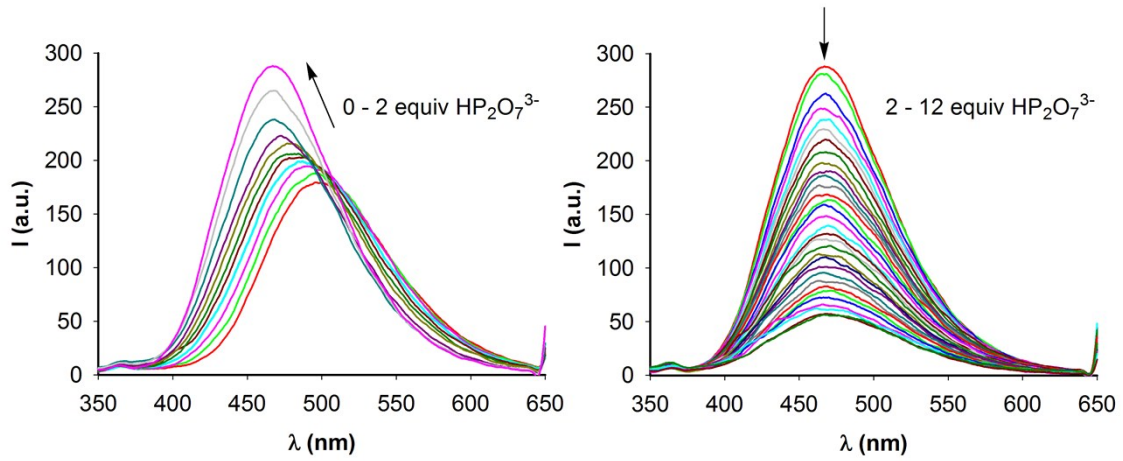

Figure S19. Changes in the fluorescence spectra of receptor $[\mathbf{1}\cdot 2Zn]^{4+}$ ($c = 1 \cdot 10^{-5}$ M in CH_3CN) upon addition of $HP_2O_7^{3-}$ anions at 20 °C.

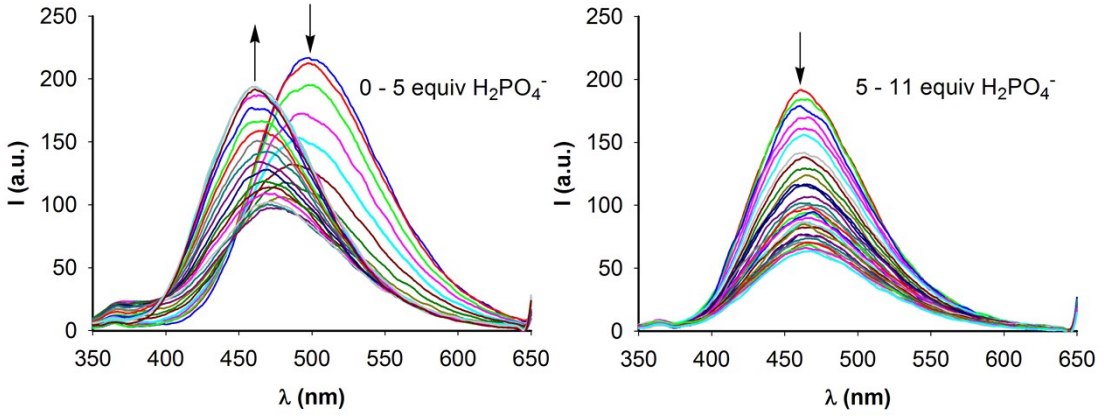

Figure S20. Changes in the fluorescence spectra of receptor $[\mathbf{1}\cdot 2Zn]^{4+}$ ($c = 1\cdot 10^{-5}$ M in CH_3CN) upon addition of $H_2PO_4^-$ anions at 20 °C.

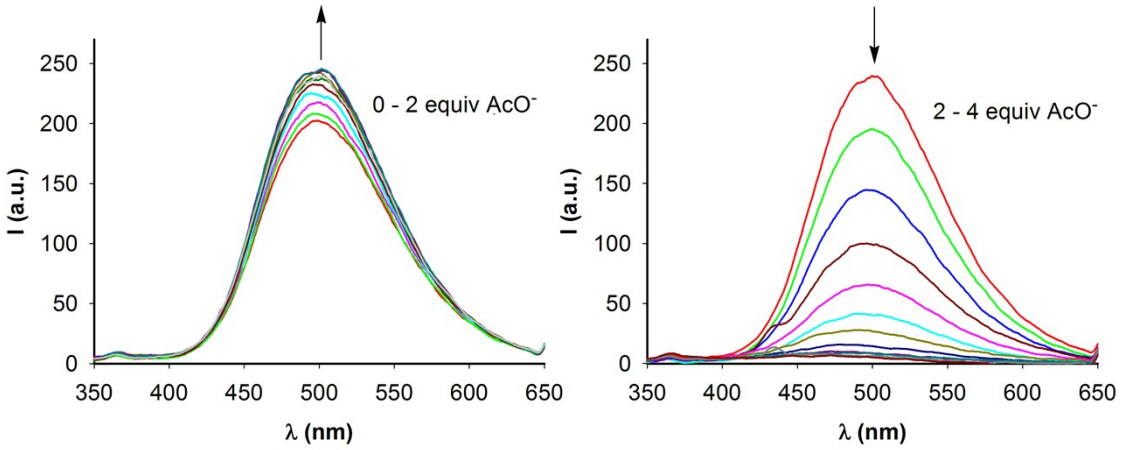

Figure S21. Changes in the fluorescence spectra of receptor $[\mathbf{1}\cdot 2Zn]^{4+}$ ($c = 1\cdot 10^{-5}$ M in CH_3CN) upon addition of AcO^- anions at 20 °C.

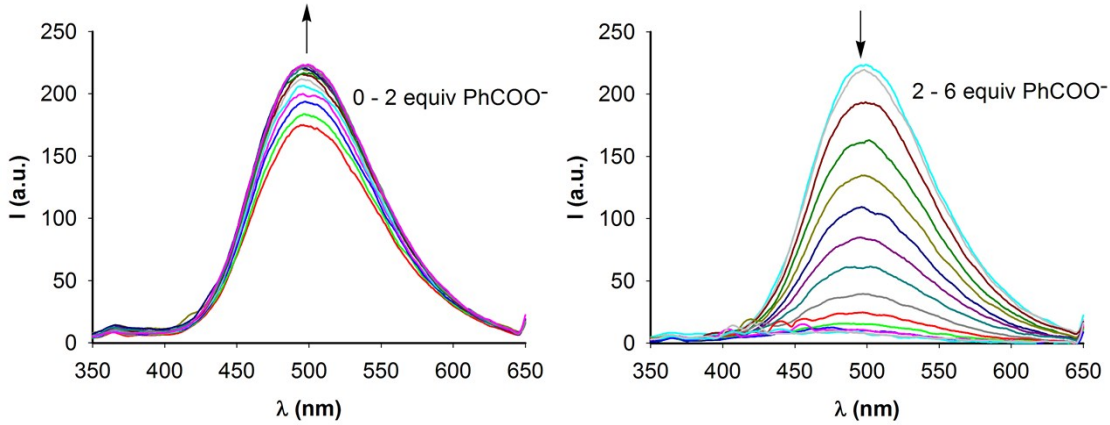

Figure S22. Changes in the fluorescence spectra of receptor $[\mathbf{1}\cdot 2Zn]^{4+}$ ($c = 1\cdot 10^{-5}$ M in CH_3CN) upon addition of $PhCOO^-$ anions at 20 °C.

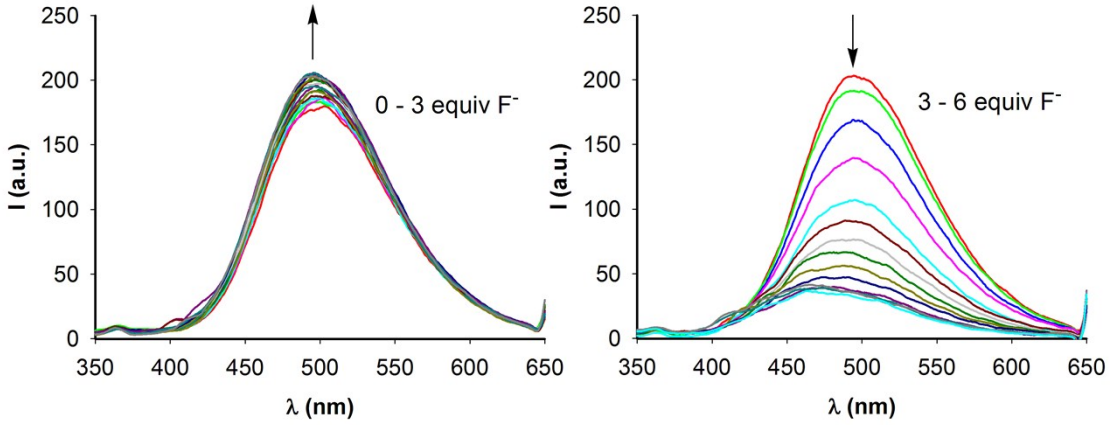

Figure S23. Changes in the fluorescence spectra of receptor $[\mathbf{1}\cdot 2Zn]^{4+}$ ($c = 1\cdot 10^{-5}$ M in CH_3CN) upon addition of F^- anions at 20 °C.

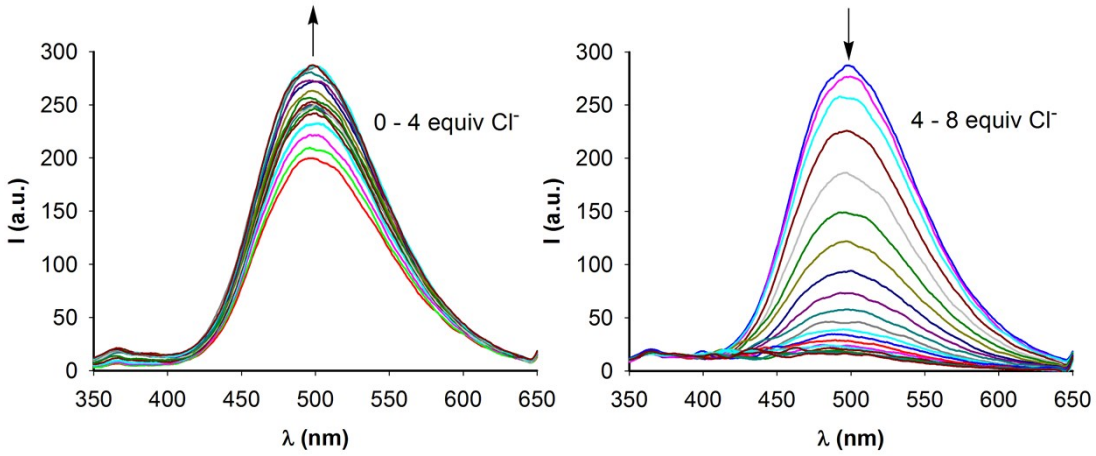

Figure S24. Changes in the fluorescence spectra of receptor $[\mathbf{1}\cdot 2Zn]^{4+}$ ($c = 1\cdot 10^{-5}$ M in CH_3CN) upon addition of Cl^- anions at 20 °C.

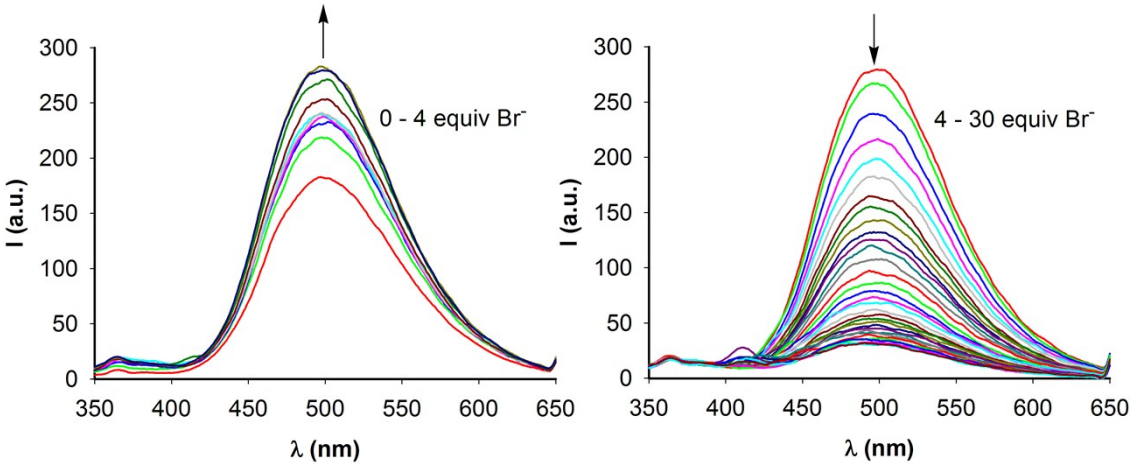

Figure S25. Changes in the fluorescence spectra of receptor $[\mathbf{1}\cdot 2Zn]^{4+}$ (c = $1\cdot 10^{-5}$ M in CH_3CN) upon addition of Br^- anions at 20 °C.

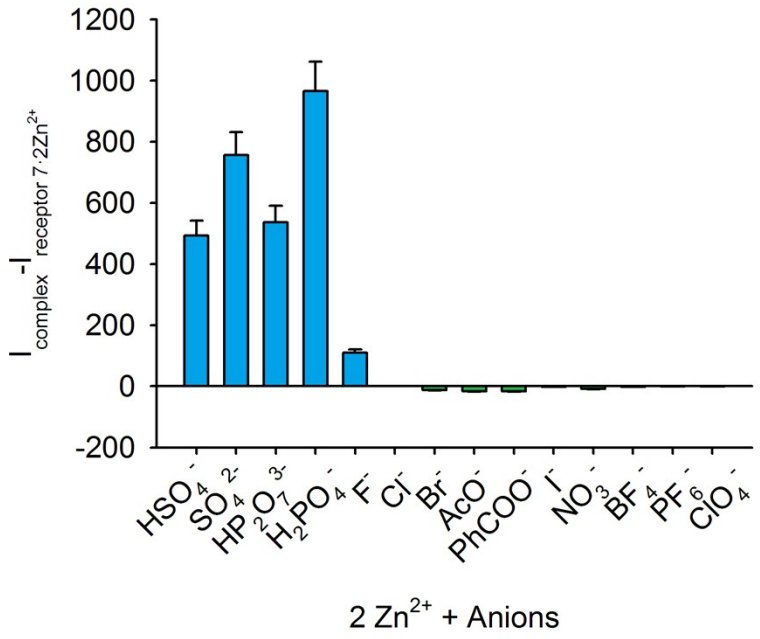

Figure S26. Increase or decrease of the intensity of the emission band of the complex $[2\cdot 2Zn]^{4+}$ at $\lambda = 480$ nm upon addition of several anions.

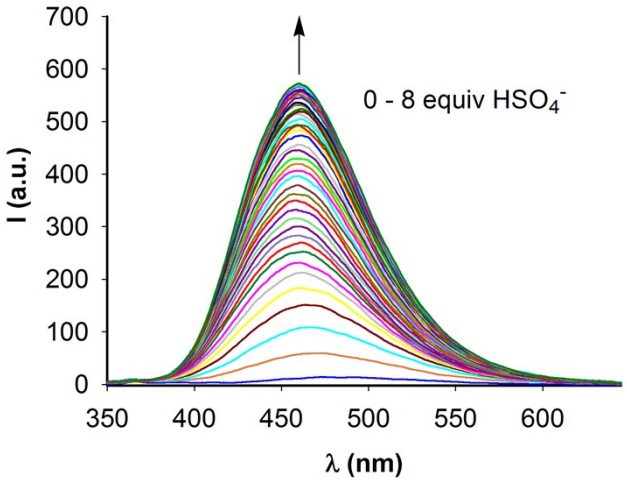

Figure S27. Changes in the fluorescence spectra of receptor $[\mathbf{2}\cdot 2Zn]^{4+}$ ($c = 1\cdot 10^{-5}$ M in CH_3CN) upon addition of HSO_4^- anions at 20 °C.

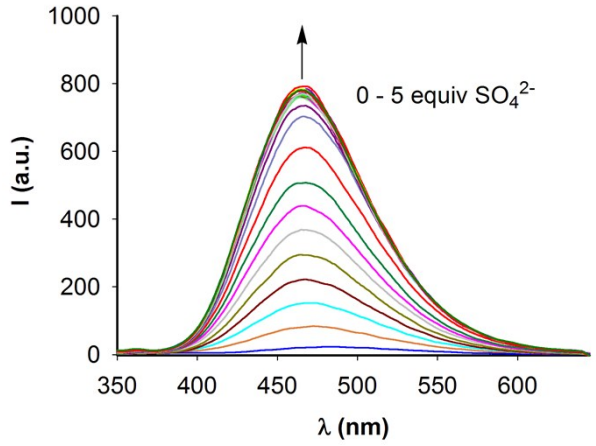

Figure S28. Changes in the fluorescence spectra of receptor $[\mathbf{2}\cdot 2Zn]^{4+}$ ($c = 1\cdot 10^{-5}$ M in CH_3CN) upon addition of SO_4^{2-} anions at 20 °C.

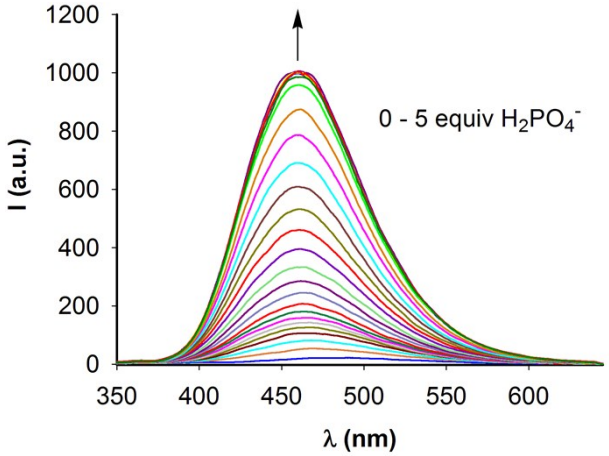

Figure S29. Changes in the fluorescence spectra of receptor $[\mathbf{2}\cdot 2Zn]^{4+}$ ($c = 1\cdot 10^{-5}$ M in CH_3CN) upon addition of $H_2PO_4^-$ anions at 20 °C.

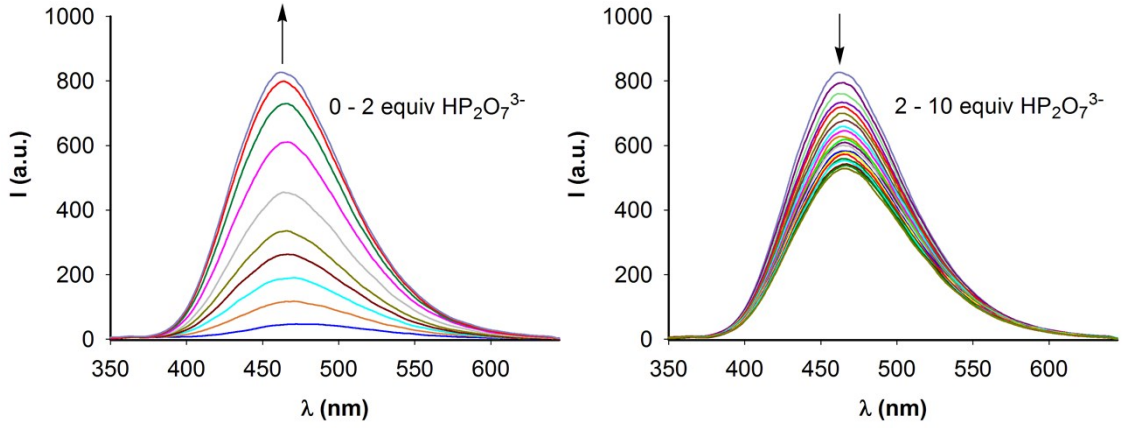

Figure S30. Changes in the fluorescence spectra of receptor $[\mathbf{2}\cdot 2Zn]^{4+}$ ($c = 1\cdot 10^{-5}$ M in CH_3CN) upon addition of $HP_2O_7^{3-}$ anions at 20 °C.

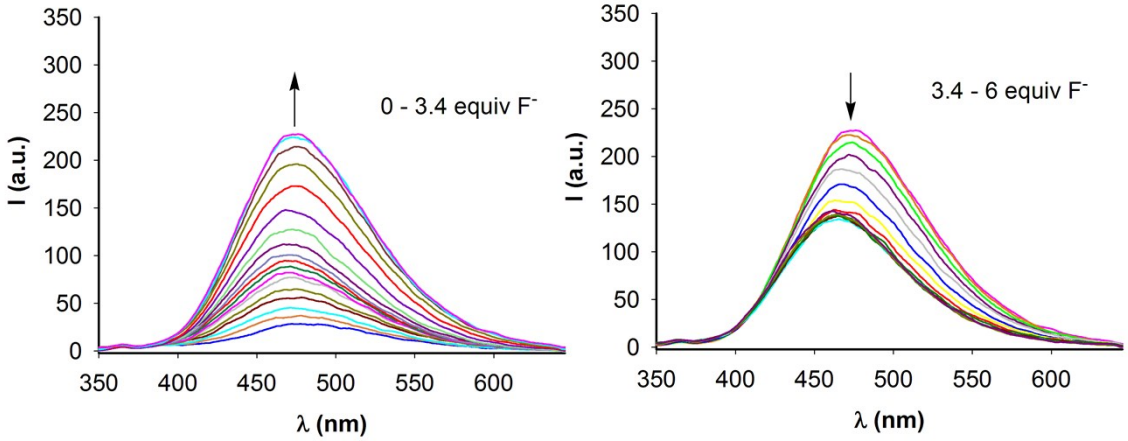

Figure S31. Changes in the fluorescence spectra of receptor $[\mathbf{2}\cdot 2Zn]^{4+}$ ($c = 1\cdot 10^{-5}$ M in CH_3CN) upon addition of F^- anions at 20 °C.

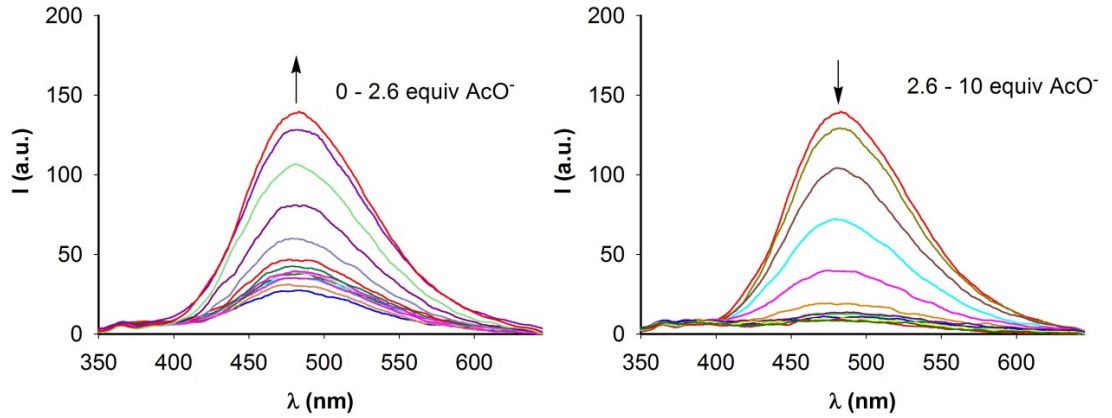

Figure S32. Changes in the fluorescence spectra of receptor $[\mathbf{2}\cdot 2Zn]^{4+}$ ($c = 1\cdot 10^{-5}$ M in CH_3CN) upon addition of AcO^- anions at 20 °C.

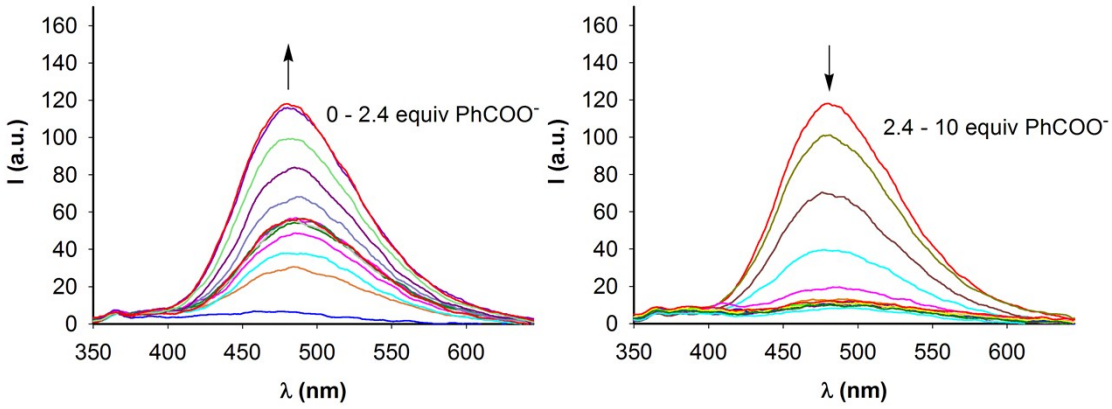

Figure S33. Changes in the fluorescence spectra of receptor $[\mathbf{2}\cdot 2Zn]^{4+}$ ($c = 1\cdot 10^{-5}$ M in CH_3CN) upon addition of $PhCOO^-$ anions at 20 °C.

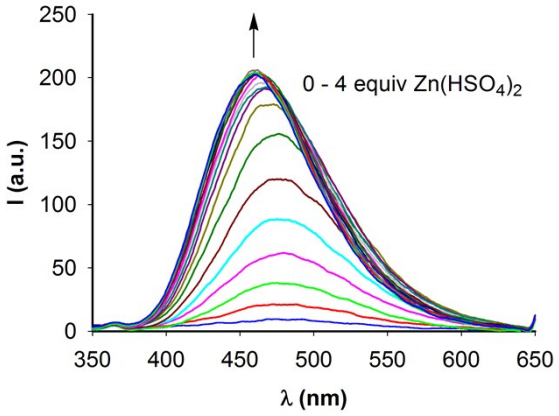

Figure S34. Changes in the fluorescence spectra of receptor **1** ($c = 1 \cdot 10^{-5}$ M in CH_3CN) upon addition of $Zn(HSO_4)_2$ at 20 °C.

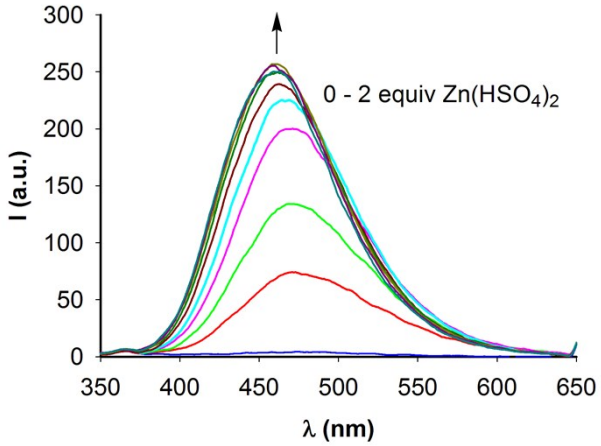

Figure S35. Changes in the fluorescence spectra of receptor **2** ($c = 1 \cdot 10^{-5}$ M in CH_3CN) upon addition of $Zn(HSO_4)_2$ anions at 20 °C.

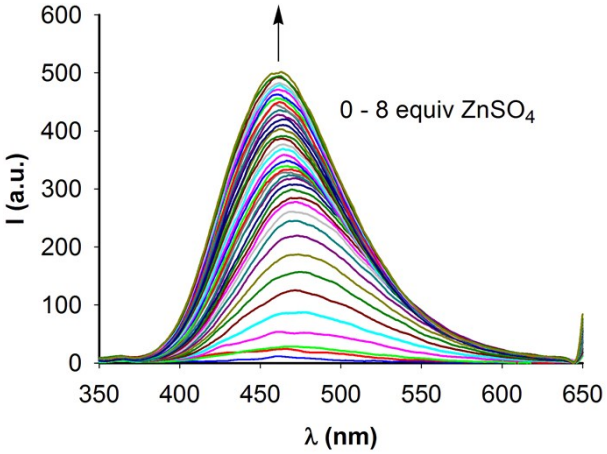

Figure S36. Changes in the fluorescence spectra of receptor **2** ($c = 1 \cdot 10^{-5}$ M in CH_3CN) upon addition of $ZnSO_4$ anions at 20 °C.

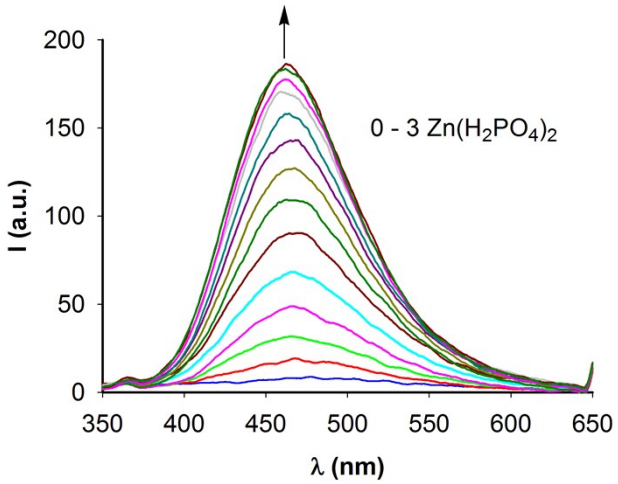

Figure S37. Changes in the fluorescence spectra of receptor **2** ($c = 1 \cdot 10^{-5}$ M in CH_3CN) upon addition of $Zn(H_2PO_4)_2$ anions at 20 °C.

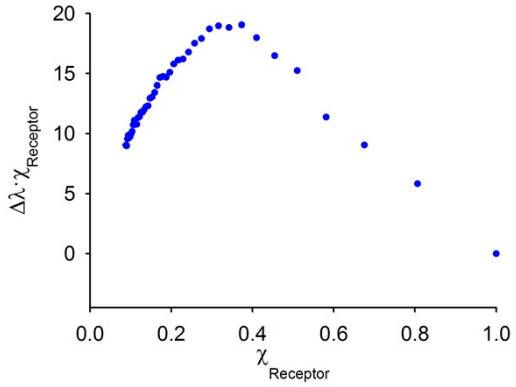

Figure S38. Job plot experiment, using the fluorescence titration data, with a maximum at 0.33 indicating 1:2 stoichiometry for receptor $[\mathbf{1}\cdot 2Zn]^{4+}$ and HSO_4^- in CH_3CN.

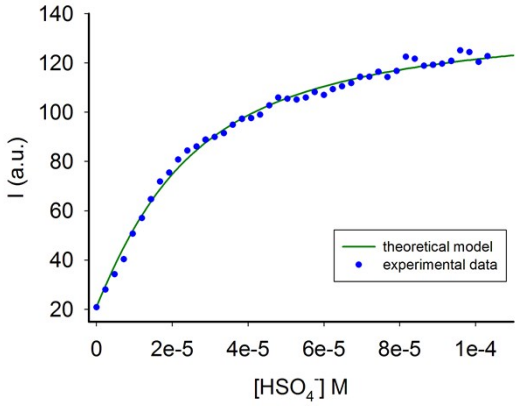

Figure S39. Changes in the emission intensity of the receptor $[\mathbf{1}\cdot 2Zn]^{4+}$ ($c = 1 \cdot 10^{-5}$ M in CH_3CN) upon addition of increasing amounts of HSO_4^-. Data points represent experimental data, continuous lines represent calculated curves.

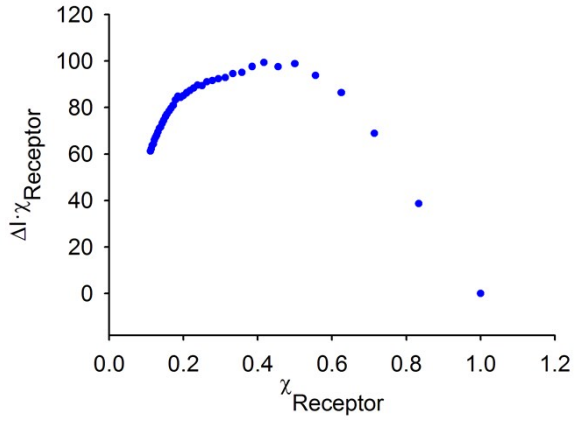

Figure S40. Job plot experiment, using the fluorescence titration data, with a maximum at 0.33 indicating 1:2 stoichiometry for receptor $[\mathbf{2}\cdot 2Zn]^{4+}$ and HSO_4^- in CH_3CN.

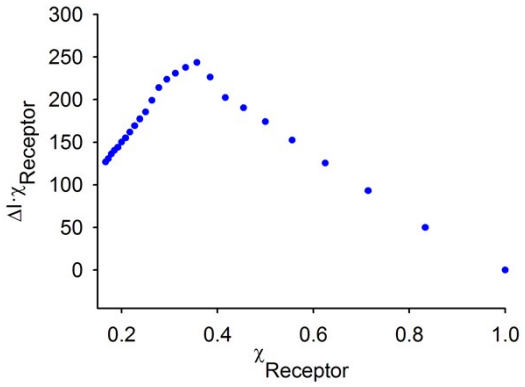

Figure S41. Job plot experiment, using the fluorescence titration data, with a maximum at 0.33 indicating 1:2 stoichiometry for receptor $[\mathbf{2}\cdot 2Zn]^{4+}$ and SO_4^{2-} in CH_3CN.

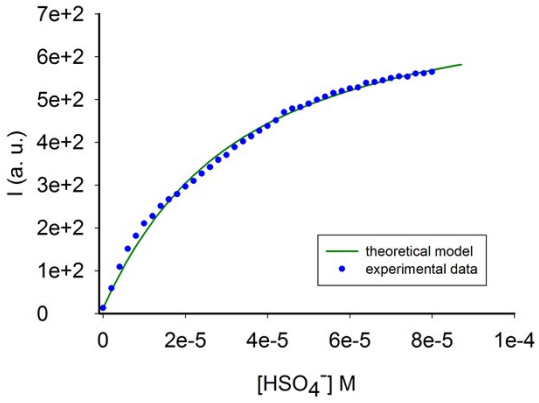

Figure S42. Changes in the emission intensity of the receptor $[\mathbf{2}\cdot 2Zn]^{4+}$ ($c = 1\cdot 10^{-5}$ M in CH_3CN) upon addition of increasing amounts of HSO_4^-. Data points represent experimental data, continuous lines represent calculated curves.

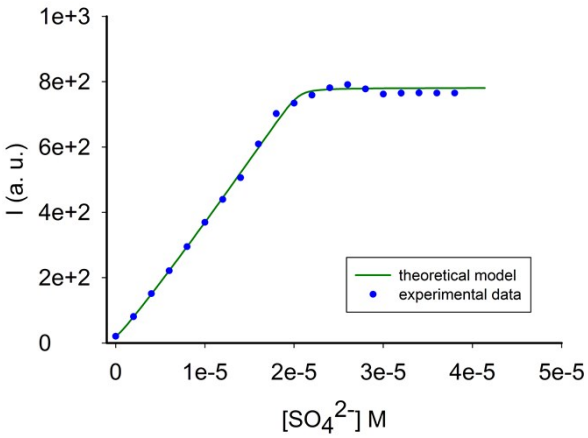

Figure S43. Changes in the emission intensity of the receptor $[\mathbf{2}\cdot 2Zn]^{4+}$ ($c = 1\cdot 10^{-5}$ M in CH_3CN) upon addition of increasing amounts of SO_4^{2-}. Data points represent experimental data, continuous lines represent calculated curves.

Table S1. Association constants (M^{-1}) of receptor **1** with Zn^{2+} and Cd^{2+} in CH_3CN obtained from the fluorescence titration data. The corresponding errors are in brackets.

Compound	Zn^{2+}	Cd^{2+}
1	$K_1 = 4.3x10^7$ (16%) $K_2 = 5.3x10^6$ (14%)	$K_1 = 8.2x10^4$ (7%) $K_2 = 6.5x10^4$ (4%)

Table S2. Association constants (M^{-1}) of the complex $[\mathbf{1}\cdot 2Zn]^{4+}$ and $[\mathbf{2}\cdot 2Zn]^{4+}$ with different anions in CH_3CN obtained from the fluorescence titration data. The corresponding errors are in brackets.

Compound	HSO_4^-	SO_4^{2-}	$H_2PO_4^-$
$[\mathbf{1}\cdot 2Zn]^{4+}$	$K_1 = 2.2x10^5$ (9%) $K_2 = 3.4x10^4$ (4%)	-	-
$[\mathbf{2}\cdot 2Zn]^{4+}$	$K_1 = 5.3x10^5$ (12%)[a] $K_2 = 2.3x10^4$ (2%)[a]	$K_1 = 1.5\cdot 10^6$ (25%) $K_2 = 4.4\cdot 10^7$(23%)	-

a Errors (in percent) are given in parenthesis

PART III: ^{1}H-NMR Anion Binding Studies.

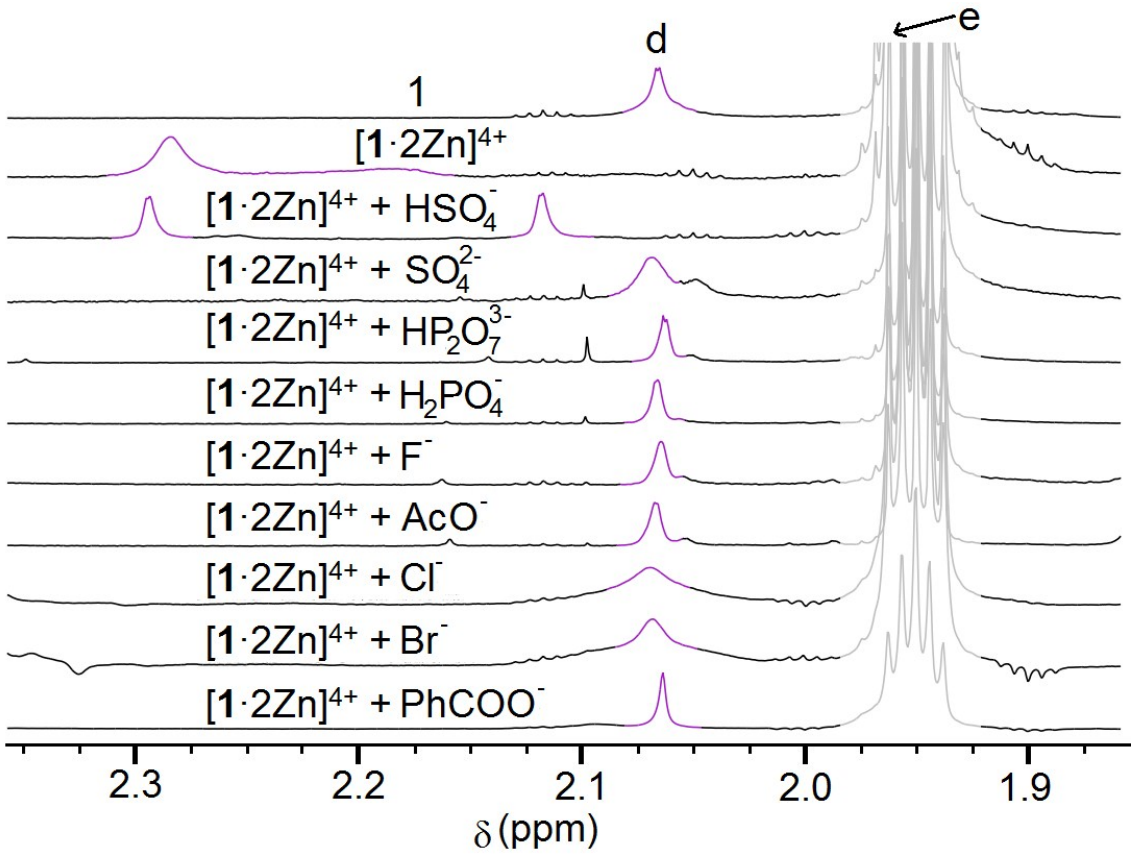

Figure S44. Changes in the ^{1}H NMR spectrum of **1** in CD_3CN/CD_3OD (9:1 v/v) in the presence of the indicated species.

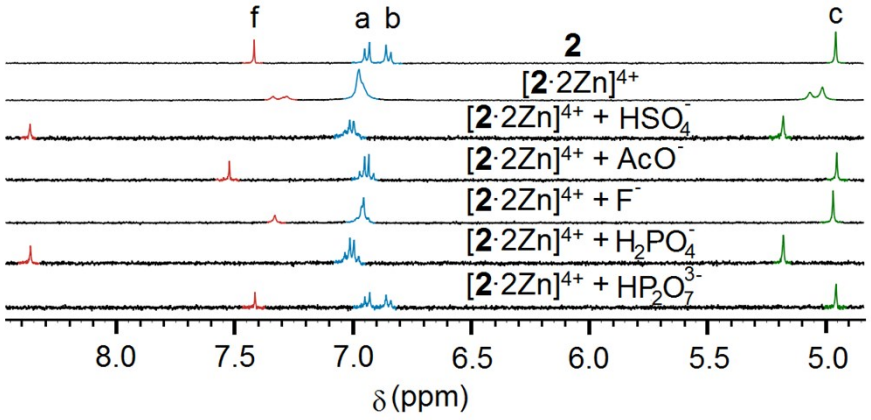

Figure S45. Changes in the ^{1}H NMR spectrum of **2** in CD_3CN/CD_3OD (9:1 v/v) in the presence of the indicated species.

PART IV: Computational Results.

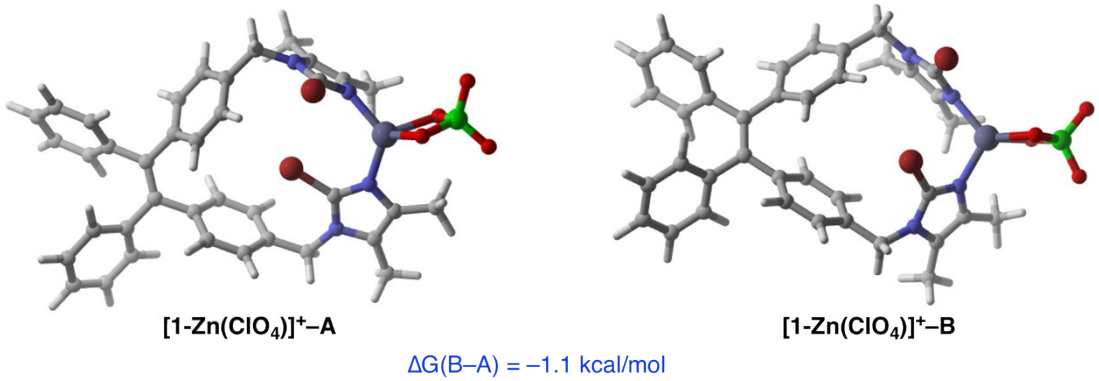

Figure S46. Computed most stable conformations for species **[1-Zn(ClO$_4$)]$^+$**. Relative free energies are given in kcal/mol. All data have been computed at the B3LYP-D3/def2-SVPP level.

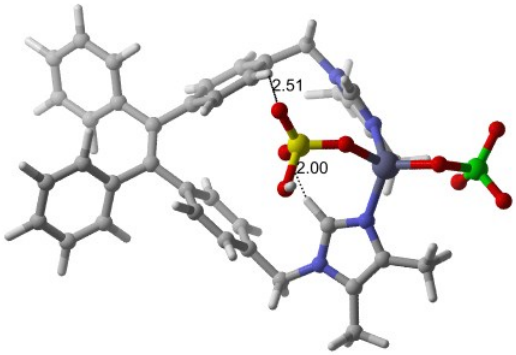

Figure S47. Optimized geometry for the **[2-Zn(ClO$_4$)](HSO$_4$)** complex. Bond lengths are given in angstroms. All data have been computed at the B3LYP-D3/def2-SVPP level.

Cartesian coordinates (in Å) and free energies (in a.u.) of all the stationary points discussed in the text. All calculations have been performed at the B3LYP-D3/def2-SVPP level.

[1-Zn(ClO$_4$)]$^+$: G= -9372.987824

C	-2.406666000	-1.266762000	-0.876083000
C	-3.383558000	-1.385466000	0.131823000
C	-3.187384000	-2.365163000	1.121499000
C	-2.037626000	-3.159018000	1.133520000
C	-1.056785000	-3.018337000	0.141842000
C	-1.269602000	-2.075166000	-0.877714000
H	-2.559777000	-0.547396000	-1.684228000
H	-3.951482000	-2.508804000	1.890201000
H	-1.915094000	-3.910271000	1.919946000
H	-0.548446000	-1.981780000	-1.695278000
C	-4.639240000	-0.580952000	0.081624000
C	-4.628153000	0.773740000	-0.102619000
C	-5.897200000	-1.370358000	0.220592000
C	-6.918611000	-0.952589000	1.094089000
C	-6.074053000	-2.569926000	-0.494421000
C	-8.088065000	-1.701529000	1.234131000
H	-6.790190000	-0.029398000	1.665048000
C	-7.249372000	-3.313615000	-0.363772000
H	-5.285347000	-2.915687000	-1.169451000
C	-8.261007000	-2.881308000	0.500856000
H	-8.869850000	-1.362671000	1.920613000
H	-7.376078000	-4.235543000	-0.939458000
C	-5.840330000	1.567645000	-0.449896000
C	-6.092645000	2.800673000	0.181858000
C	-6.736666000	1.127572000	-1.443136000
C	-7.223531000	3.553248000	-0.143982000
H	-5.400958000	3.166637000	0.946469000
C	-7.859057000	1.885816000	-1.778025000
H	-6.547215000	0.181001000	-1.955220000
C	-8.111365000	3.097995000	-1.124623000
H	-7.411408000	4.501421000	0.368965000
H	-8.541585000	1.528950000	-2.555222000
C	-3.381051000	1.581731000	0.057083000
C	-2.713130000	1.627699000	1.294097000
C	-2.902659000	2.389308000	-0.990276000
C	-1.589026000	2.434886000	1.470265000
H	-3.095107000	1.030364000	2.126303000
C	-1.756478000	3.165642000	-0.825956000
H	-3.436130000	2.398216000	-1.944893000
C	-1.078718000	3.186990000	0.402468000
H	-1.085982000	2.457677000	2.442825000
H	-1.380873000	3.759330000	-1.665778000
C	0.189634000	3.981556000	0.560074000
H	0.206614000	4.816335000	-0.157985000
H	0.242341000	4.416811000	1.571276000
C	0.219632000	-3.837626000	0.173744000
H	0.456793000	-4.254902000	-0.815992000
H	0.136927000	-4.679207000	0.876217000
N	1.473196000	3.246805000	0.368528000

C	1.747356000	1.948705000	0.100892000
C	2.700187000	3.913172000	0.496993000
C	3.683911000	2.973735000	0.301132000
N	1.379129000	-3.024325000	0.588628000
C	1.658154000	-2.631460000	1.902316000
C	2.246092000	-2.374704000	-0.219888000
C	2.700711000	-1.738333000	1.822468000
C	0.902242000	-3.140229000	3.083319000
H	-0.130962000	-2.751738000	3.102157000
H	0.851215000	-4.243530000	3.095947000
H	1.401377000	-2.822169000	4.011385000
C	3.415966000	-0.960320000	2.878890000
H	4.508820000	-1.089316000	2.786561000
H	3.199821000	0.121444000	2.782240000
H	3.111245000	-1.272298000	3.889300000
C	2.791365000	5.373910000	0.790783000
H	2.300897000	5.984788000	0.011393000
H	2.326203000	5.631932000	1.759592000
H	3.847089000	5.680525000	0.837867000
C	5.171743000	3.106345000	0.303297000
H	5.627722000	2.535287000	1.130258000
H	5.602343000	2.710681000	-0.632581000
H	5.478026000	4.158797000	0.399227000
N	3.048755000	-1.589454000	0.486210000
N	3.068190000	1.750590000	0.062890000
Br	2.334398000	-2.537983000	-2.077484000
Br	0.528806000	0.569692000	-0.247448000
Zn	4.059941000	0.026402000	-0.085659000
O	5.556408000	-0.062107000	-1.474879000
Cl	6.728056000	-0.137009000	-0.433997000
O	7.385555000	-1.429294000	-0.504811000
O	5.913817000	-0.008922000	0.892279000
O	7.614393000	1.005004000	-0.600105000
H	-9.180035000	-3.465350000	0.607627000
H	-8.994592000	3.689334000	-1.384250000

[1-Zn(ClO_4)](HSO_4): G= -10072.459548

C	-2.435245000	1.034261000	0.982551000
C	-3.386988000	1.563153000	0.092933000
C	-3.129921000	2.824951000	-0.478058000
C	-1.952791000	3.518528000	-0.186441000
C	-1.006557000	2.980066000	0.701196000
C	-1.270362000	1.733356000	1.284360000
H	-2.589316000	0.077564000	1.482944000
H	-3.869167000	3.272067000	-1.148953000
H	-1.785689000	4.503803000	-0.635388000
H	-0.589684000	1.283362000	2.005284000
C	-4.675838000	0.849135000	-0.145285000
C	-4.715613000	-0.491180000	-0.408480000
C	-5.904326000	1.689130000	-0.040202000
C	-6.913188000	1.622344000	-1.019145000
C	-6.067076000	2.594328000	1.025427000
C	-8.056107000	2.418837000	-0.926238000
H	-6.794179000	0.932499000	-1.858762000
C	-7.214824000	3.384686000	1.125156000
H	-5.285729000	2.667216000	1.787517000
C	-8.214834000	3.299683000	0.149771000
H	-8.827848000	2.352263000	-1.699712000
H	-7.328723000	4.071932000	1.969622000
C	-5.956838000	-1.312646000	-0.360537000

C	-6.204571000	-2.289294000	-1.344582000
C	-6.887016000	-1.174380000	0.688304000
C	-7.359916000	-3.073496000	-1.303550000
H	-5.482800000	-2.426918000	-2.154831000
C	-8.035489000	-1.965584000	0.736385000
H	-6.698610000	-0.439919000	1.474978000
C	-8.281919000	-2.914044000	-0.263464000
H	-7.538567000	-3.817650000	-2.086380000
H	-8.741609000	-1.844022000	1.563912000
C	-3.478325000	-1.236034000	-0.794376000
C	-2.850257000	-0.957444000	-2.017476000
C	-2.939154000	-2.243590000	0.022121000
C	-1.700956000	-1.651194000	-2.401719000
H	-3.268905000	-0.184783000	-2.668791000
C	-1.773797000	-2.909942000	-0.346308000
H	-3.406596000	-2.469638000	0.984110000
C	-1.136446000	-2.617090000	-1.560024000
H	-1.230580000	-1.422520000	-3.362511000
H	-1.339248000	-3.631005000	0.346741000
H	-9.184045000	-3.532829000	-0.226103000
C	0.162169000	-3.303131000	-1.933624000
H	0.095383000	-4.387758000	-1.770783000
H	0.395260000	-3.141815000	-2.998318000
C	0.270747000	3.721058000	1.044911000
H	0.482038000	3.655579000	2.123087000
H	0.197399000	4.787013000	0.784873000
N	1.324979000	-2.841660000	-1.152422000
C	1.918912000	-1.638714000	-1.253157000
C	1.948448000	-3.521837000	-0.104588000
C	2.918813000	-2.678286000	0.384855000
N	1.458749000	3.186598000	0.351609000
C	1.893107000	3.543852000	-0.930428000
C	2.249496000	2.179332000	0.777802000
C	2.953018000	2.718318000	-1.226290000
C	1.243869000	4.625915000	-1.726515000
H	0.192687000	4.380076000	-1.959165000
H	1.254221000	5.596048000	-1.196245000
H	1.778514000	4.761857000	-2.679279000
C	3.838006000	2.646127000	-2.428176000
H	4.899339000	2.659631000	-2.126088000
H	3.679197000	1.705468000	-2.986419000
H	3.653711000	3.488737000	-3.112889000
C	1.550679000	-4.888028000	0.338303000
H	0.541264000	-4.883152000	0.779787000
H	1.589722000	-5.622998000	-0.486889000
H	2.241765000	-5.228698000	1.124470000
C	3.793513000	-2.803402000	1.587779000
H	4.744768000	-2.260781000	1.443707000
H	3.257918000	-2.372665000	2.455759000
H	4.029616000	-3.856666000	1.809637000
N	3.145377000	1.861016000	-0.151069000
N	2.896904000	-1.511760000	-0.365273000
Br	2.170920000	1.309066000	2.419400000
Br	1.486307000	-0.339006000	-2.522870000
Zn	4.030210000	0.079353000	-0.147468000
O	5.818454000	0.032658000	0.893424000
Cl	6.728635000	0.161190000	-0.368709000
O	7.399630000	1.456709000	-0.375329000
O	5.667631000	0.104592000	-1.496559000
O	7.634453000	-0.975302000	-0.450376000
O	0.318172000	-1.175996000	1.053554000

S	0.098007000	-1.548732000	2.465981000
O	-0.168557000	-3.222289000	2.360850000
H	-0.346164000	-3.519946000	3.272433000
O	1.294381000	-1.441967000	3.339194000
O	-1.140909000	-1.014956000	3.068052000
H	-9.112157000	3.922009000	0.224934000

[2-Zn(ClO$_4$)](HSO$_4$): G= -4925.941120

C	2.371200000	-1.543588000	0.906647000
C	3.302321000	-1.585953000	-0.143037000
C	3.158305000	-2.582385000	-1.125719000
C	2.069411000	-3.456451000	-1.098262000
C	1.123901000	-3.384533000	-0.063002000
C	1.311725000	-2.445260000	0.956852000
H	2.465342000	-0.790201000	1.691559000
H	3.898087000	-2.655911000	-1.928425000
H	1.956881000	-4.203172000	-1.891436000
H	0.610984000	-2.374261000	1.790617000
C	4.450357000	-0.634384000	-0.149108000
C	4.248997000	0.716390000	-0.108004000
C	5.800789000	-1.264748000	-0.158406000
C	6.825055000	-0.783801000	-0.996568000
C	6.069220000	-2.389864000	0.644521000
C	8.081164000	-1.392111000	-1.013894000
H	6.627507000	0.077824000	-1.639348000
C	7.329758000	-2.991990000	0.636629000
H	5.279866000	-2.786950000	1.289201000
C	8.341717000	-2.494959000	-0.192025000
H	8.862117000	-1.003736000	-1.675272000
H	7.521742000	-3.856966000	1.279413000
C	5.335364000	1.689375000	0.206536000
C	5.496526000	2.860094000	-0.558763000
C	6.200078000	1.481673000	1.297871000
C	6.509874000	3.775473000	-0.264265000
H	4.822348000	3.045878000	-1.399918000
C	7.206198000	2.400989000	1.599651000
H	6.075832000	0.586432000	1.912326000
C	7.370259000	3.548993000	0.815793000
H	6.626617000	4.672960000	-0.880081000
H	7.864969000	2.221420000	2.455102000
C	2.928850000	1.343403000	-0.425535000
C	2.313894000	1.112212000	-1.668524000
C	2.339443000	2.283565000	0.438413000
C	1.186333000	1.839052000	-2.057365000
H	2.752773000	0.379073000	-2.350542000
C	1.195814000	2.986265000	0.063014000
H	2.792935000	2.470685000	1.415626000
C	0.625480000	2.800810000	-1.205512000
H	0.745202000	1.664486000	-3.044765000
H	0.741845000	3.691432000	0.765738000
H	8.160655000	4.268604000	1.051130000
C	-0.593005000	3.593845000	-1.625238000
H	-0.558791000	4.606226000	-1.190683000
H	-0.624391000	3.707566000	-2.723170000
C	-0.146013000	-4.213404000	-0.072781000
H	-0.354347000	-4.630464000	0.925391000
H	-0.078997000	-5.054136000	-0.779443000
N	-1.848534000	2.969511000	-1.185947000
C	-1.964800000	1.722962000	-0.699829000
C	-3.113596000	3.560419000	-1.165830000

C	-3.966730000	2.610950000	-0.640180000
N	-1.309907000	-3.394961000	-0.444929000
C	-1.705031000	-3.054239000	-1.738498000
C	-2.020572000	-2.636277000	0.412278000
C	-2.678380000	-2.087456000	-1.595932000
C	-1.118504000	-3.689443000	-2.955180000
H	-0.040949000	-3.466398000	-3.054004000
H	-1.235130000	-4.789368000	-2.944236000
H	-1.624765000	-3.313613000	-3.857686000
C	-3.483400000	-1.372934000	-2.631912000
H	-4.549997000	-1.642849000	-2.555701000
H	-3.428961000	-0.281162000	-2.477822000
H	-3.123646000	-1.603737000	-3.647337000
C	-3.350962000	4.954534000	-1.643100000
H	-2.789748000	5.698438000	-1.046022000
H	-3.052524000	5.086514000	-2.700195000
H	-4.420374000	5.204510000	-1.564795000
C	-5.436339000	2.664627000	-0.379901000
H	-5.984114000	1.990801000	-1.059402000
H	-5.665267000	2.316437000	0.641355000
H	-5.828906000	3.687109000	-0.498378000
N	-2.853335000	-1.841197000	-0.241697000
N	-3.222246000	1.474462000	-0.357272000
H	-1.892101000	-2.652361000	1.492568000
H	-1.129262000	1.047486000	-0.532651000
Zn	-3.646679000	-0.211047000	0.664004000
O	-5.461992000	-0.261154000	1.450048000
Cl	-6.591357000	-0.614703000	0.411587000
O	-7.036463000	-1.983588000	0.682050000
O	-5.939822000	-0.503287000	-0.930751000
O	-7.658430000	0.377837000	0.581408000
O	-0.349138000	-0.041402000	0.947055000
S	-0.943667000	0.065786000	2.285535000
O	-0.842198000	1.685913000	2.601546000
H	-1.173270000	1.835835000	3.508382000
O	-2.443342000	-0.201825000	2.282071000
O	-0.278104000	-0.642707000	3.378867000
H	9.327831000	-2.969755000	-0.203202000