Supporting materials

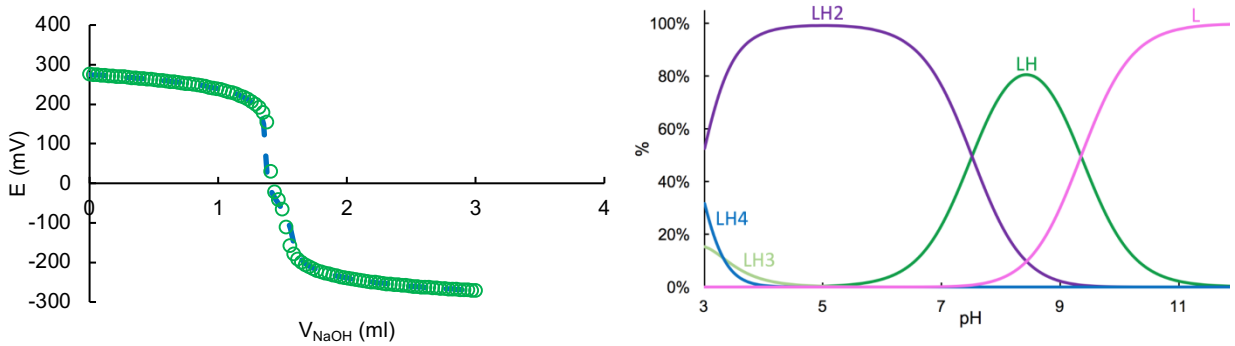

Fig. S1. L2 titration curve (left) and its protonated forms at various pH values (right).

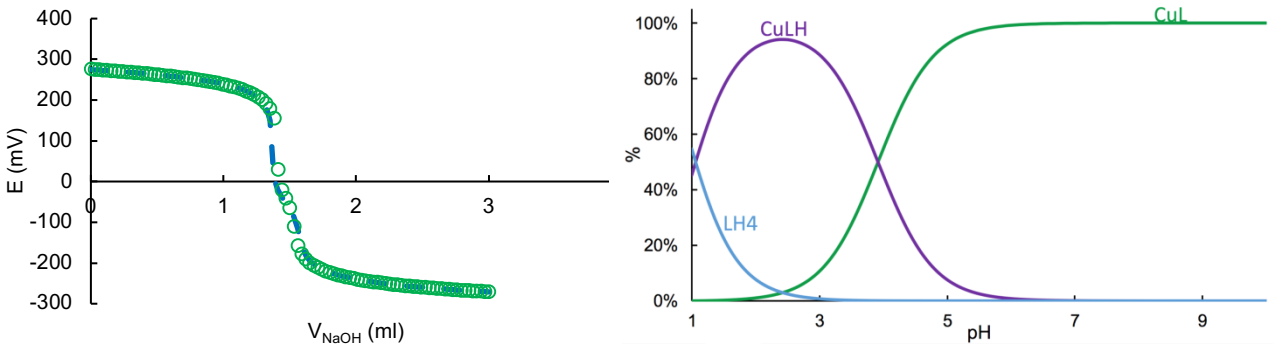

Fig. S2. CuL2 titration curve (left) and the complex forms at various pH values (right)

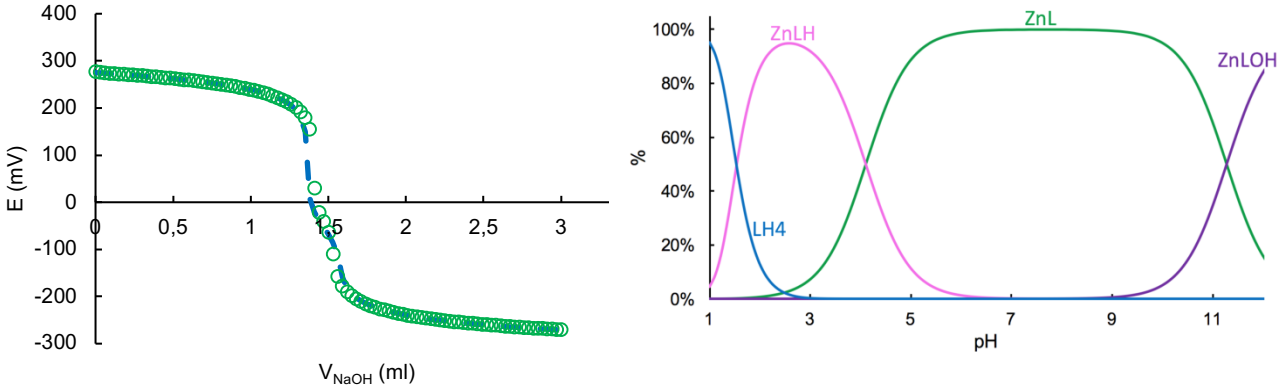

Fig. S3. ZnL2 titration curve (left) and the complex forms at various pH values (right)

Table S1. *In vivo* biodistribution of [^{65}Zn]Zn blank, [^{65}Zn]ZnL1, and [^{65}Zn]ZnL2

	Zn blank		ZnL1		ZnL2	
	1 h	6 h	1 h	6 h	1 h	6 h
Liver	7.45±1.31	11.12±0.8	3.22±0.16	3.31±1.01	2.72±0.32	0.98±0.38
Kidneys	3.54±0.56	8.1±0.91	6.01±1.13	2.58±1.4	3.76±0.64	1.14±0.56
Pancreas	11.71±1.24	13.56±3.54	4.32±0.98	3.04±1.9	1.06±0.71	0.57±0.29
Spleen	7.66±1.59	5.35±0.5	2.32±0.19	1.69±0.94	0.41±0.16	0.36±0.11
Lungs	0.68±0.17	3.75±2.11	1.42±0.02	0.97±0.65	0.46±0.05	0.18±0.06
Heart	0.38±0.08	2.7±1.03	0.78±0.04	0.38±0.33	0.26±0.04	0.12±0.06
Brain	0.13±0.03	0.62±0.24	0.22±0.02	0.07±0.13	0.09±0.03	0.04±0.03
Femur	1.26±0.88	5.59±0.52	1.18±0.36	1.2±1.04	0.7±0.02	0.47±0.4
Blood	0.28±0.02	0.33	0.54±0.09	0.05±0.09	0.42±0.27	0.03±0.01
Urea	27.96	20.13	439±339	71	286±153	152±23
Rest of body	1.78±0.22	2.47±1.1	1.09±0.09	1±0.13	0.94±0.13	0.4±0.17

Table S2. ^{1}H NMR (400 MHz, 298 K) chemical shifts (ppm) of **L1** recorded in D_2O solution at different pD values in the absence and presence of Zn^{2+} (1.5 equiv.). See Figure 2 for proton labeling and pD values.

	L1^{3-}	**H**$^{+}$	**Zn**$^{2+}$
H_1	8.13	8.08 ($\Delta\delta$ = –0.05)	8.01 ($\Delta\delta$ = –0.12)
H_2	8.15	8.08 ($\Delta\delta$ = –0.07)	8.04 ($\Delta\delta$ = –0.11); 8.07 ($\Delta\delta$ = –0.08)
H_{5a}	3.46	3.84 ($\Delta\delta$ = 0.38)	3.70 ($\Delta\delta$ = 0.24)
H_{5e}			3.35 ($\Delta\delta$ = –0.11)
H_{6a}	2.75	2.98 ($\Delta\delta$ = 0.23)	2.90 ($\Delta\delta$ = 0.15)
H_{6e}			2.67 ($\Delta\delta$ = –0.08)
H_{7a}	2.66	3.28 ($\Delta\delta$ = 0.62)	2.87 ($\Delta\delta$ = 0.21)
H_{7e}			2.74 ($\Delta\delta$ = 0.08)
H_{8a}	2.66	3.50 ($\Delta\delta$ = 0.84)	3.07 ($\Delta\delta$ = 0.41)
H_{8e}			2.97 ($\Delta\delta$ = 0.31)
H_{9x}	3.12	3.84 ($\Delta\delta$ = 0.72)	3.57 ($\Delta\delta$ = 0.45)
H_{9y}			3.10 ($\Delta\delta$ = –0.02)
H_{11x}	2.99	3.27 ($\Delta\delta$ = 0.28)	3.42 ($\Delta\delta$ = 0.43)
H_{11y}			3.18 ($\Delta\delta$ = 0.19)

Table S3. ^{1}H NMR (400 MHz, 298 K) chemical shifts (δ, ppm) of **L2** recorded in D_2O solution at different pD values in the absence and presence of Zn^{2+} (1.5 equiv.). See Figure 3 for proton labeling and pD values.

	L2^{3-}	**H**$^{+}$	**Zn**$^{2+}$
H_1	6.94	7.00 (Δδ = 0.06)	6.97 (Δδ = 0.03)
H_2	6.94	7.00 (Δδ = 0.06)	6.97 (Δδ = 0.03)
H_{4a}	4.02	4.36 (Δδ = 0.34)	4.23 (Δδ = 0.21)
H_{4e}			3.96 (Δδ = –0.06)
H_{5a}	3.02	3.79 (Δδ = 0.77)	3.41 (Δδ = 0.39)
H_{5e}			3.22 (Δδ = 0.20)
H_{6a}	2.69	3.51 (Δδ = 0.82)	2.90 (Δδ = 0.21)
H_{6e}			2.63 (Δδ = –0.06)
H_{7a}	2.61	3.17 (Δδ = 0.56)	3.22 (Δδ = 0.61)
H_{7e}			2.90 (Δδ = 0.29)
H_{8x}	3.15	3.85 (Δδ = 0.70)	3.35 (Δδ = 0.20)
H_{8y}			3.16 (Δδ = 0.01)
H_{10x}	3.04	3.15 (Δδ = 0.11)	3.34 (Δδ = 0.30)
H_{10y}			3.17 (Δδ = 0.13)