Electronic Supplementary Material (ESI) for

Effect of the type of N-substituent in the benzo-18-azacrown-6 compound on copper (II) chelation: complexation, radiolabeling, stability in vitro and biodistribution in vivo

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Content:

Table S1 ^{1}H NMR chemical shifts (δ, ppm) of **H_4BATPic** recorded in D_2O solution at different pH values.

proton	pH							
	9,8	**8,3**	**7,3**	**6,0**	**4,6**	**3,5**	**3,0**	**2,1**
H_1	6,88	6,86	6,83	6,83	6,80	6,80	6,81	6,81
H_2	6,88	6,86	6,77	6,75	6,69	6,67	6,66	6,66
H_4	4,06	4,13	4,13	4,14	4,13	4,13	4,13	4,15
H_5	2,95	3,19	3,34	3,41	3,50	3,56	3,56	3,63
H_6	2,66	3,19	3,34	3,41	3,50	3,52	3,56	3,55
H_7	2,61	3,10	3,21	3,30	3,47	3,52	3,56	3,63
H_8	2,56	3,19	3,34	3,41	3,47	3,49	3,49	3,46
H_9	3,71	3,99	4,09	4,18	4,32	4,40	4,45	4,51
H_{10}	3,55	3,96	4,09	4,14	4,21	4,26	4,29	4,29
H_{12}	7,30	7,34	7,31	7,32	7,43	7,52	7,59	7,63
H_{13}	7,66	7,64	7,64	7,68	7,75	7,86	7,94	7,97
H_{14}	7,66	7,64	7,64	7,65	7,66	7,76	7,86	7,91
H_{18}	7,11	7,19	7,23	7,26	7,36	7,48	7,57	7,59
H_{19}	7,57	7,64	7,59	7,65	7,73	7,84	7,86	7,91
H_{20}	7,64	7,64	7,59	7,62	7,66	7,70	7,74	7,80

MS data

BATPic·Cu^{2+}: MS (ESI): m/z $[M - 2H + 2Cu]^{2+}$ calcd for $C_{44}H_{48}N_8O_{10}$ - $2H^+$ + $2Cu^{2+}$: 486.0964; found: 486.0950; $[M - 3H + 2Cu]^+$ calcd for $C_{44}H_{48}N_8O_{10}$ - $3H^+$ + $2Cu^{2+}$: 971.1851; found: 971.1824.

BATPy·Cu^{2+}: MS (ESI): m/z m/z $[M + Cu]^{2+}$ calcd for $C_{40}H_{48}N_8O_2$ + Cu^{2+}: 367.6598; found: 367.6581; $[M + Cu + ClO_4]^+$ calcd for $C_{40}H_{48}N_8O_2$ + Cu^{2+} + ClO_4^-: 834.2681; found: 834.2616; $[M + 2Cu + 2ClO_4]^{2+}$ calcd for $C_{40}H_{48}N_8O_2$ + $2Cu^{2+}$ + $2ClO_4^-$: 498.0731; found: 498.0716.

BATA·Cu^{2+}: MS (ESI): m/z $[M - 3H + Cu]^-$ calcd for $C_{24}H_{36}N_4O_{10}$ - $3H^+$ + Cu^{2+}: 600.1493; found: 600.1478, m/z $[M - 2H + Cu + ClO_4]^-$ calcd for $C_{24}H_{36}N_4O_{10}$ - $2H^+$ + Cu^{2+} + ClO_4^-: 700.1056; found: 699.0356.

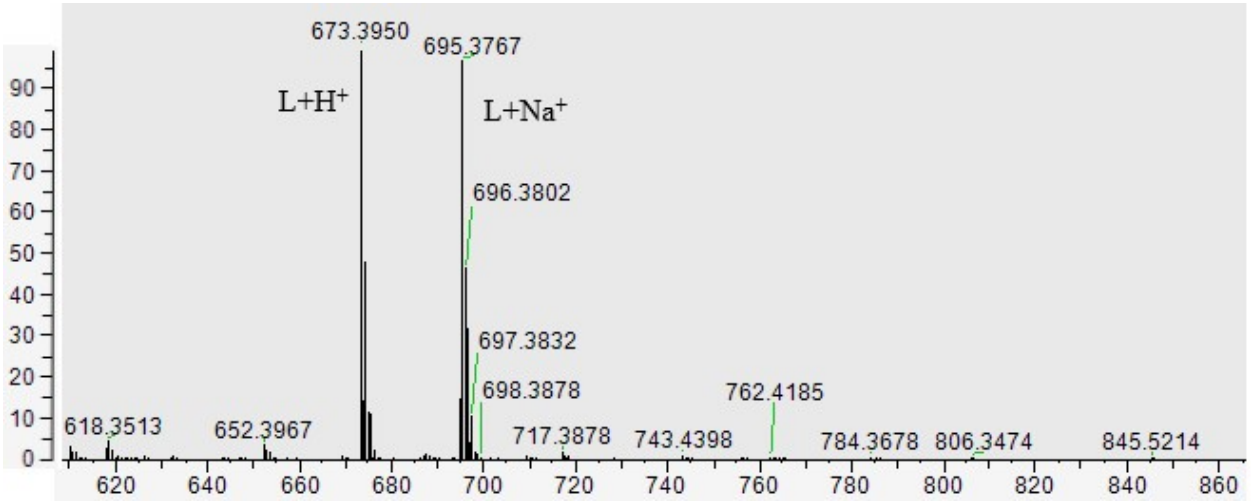


Fig. S1 ESI-MS spectra of **BATPy**.

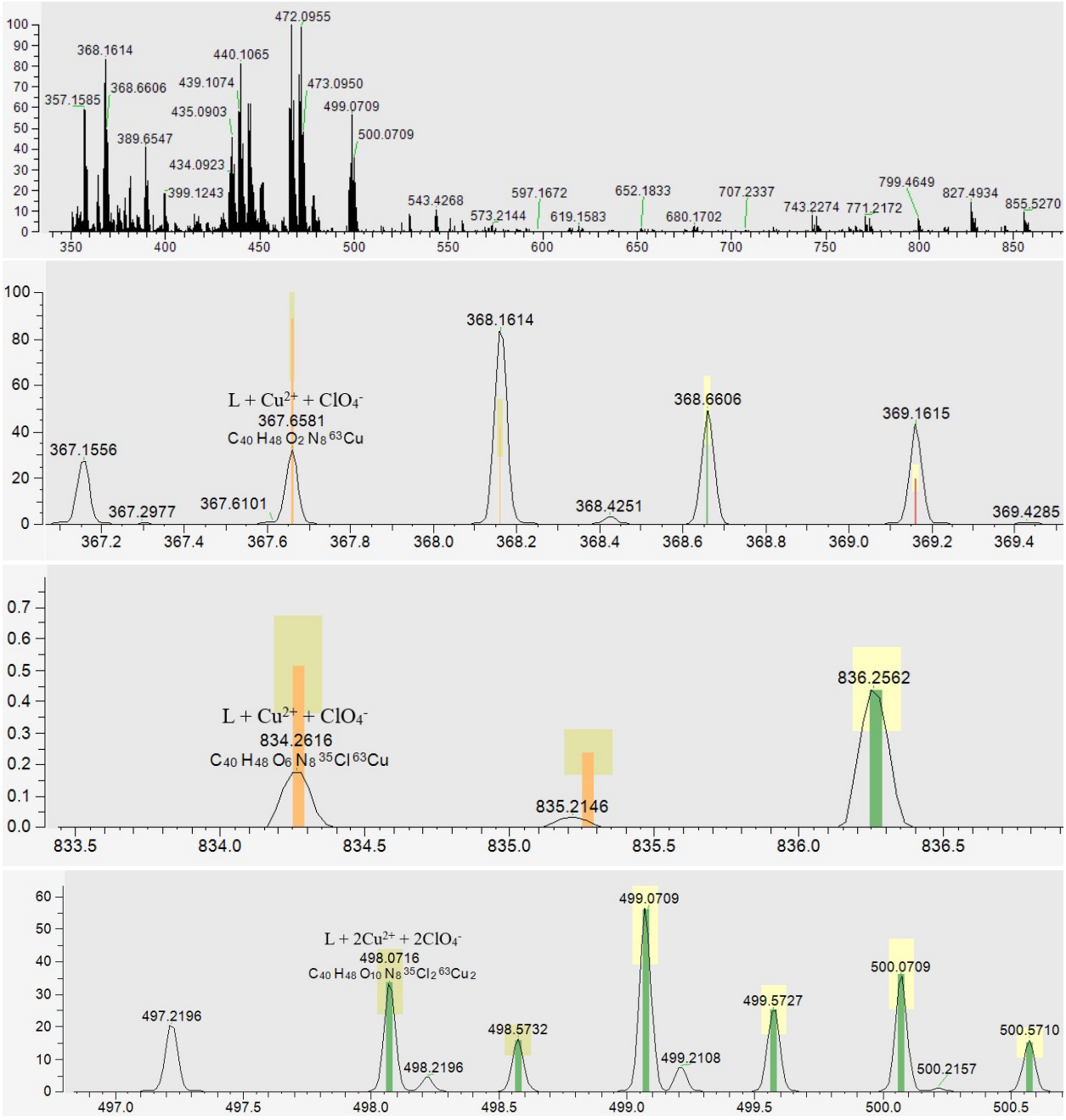


Fig. S2. ESI-MS spectra of **BATPy**·Cu.

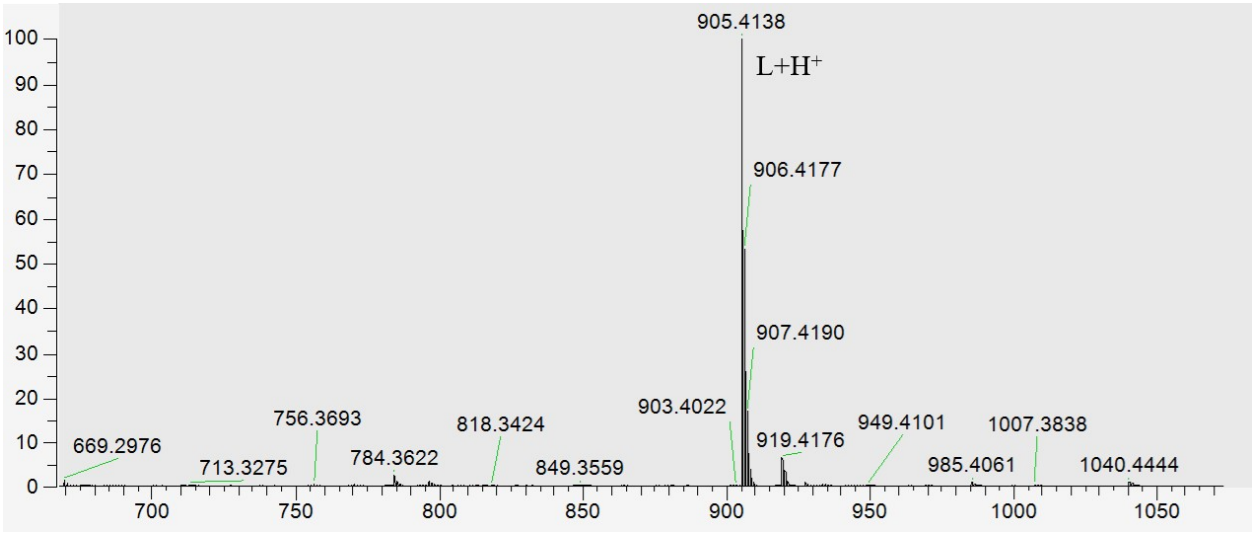


Fig. S3 ESI-MS spectra of compound **Me_4BATPic**.

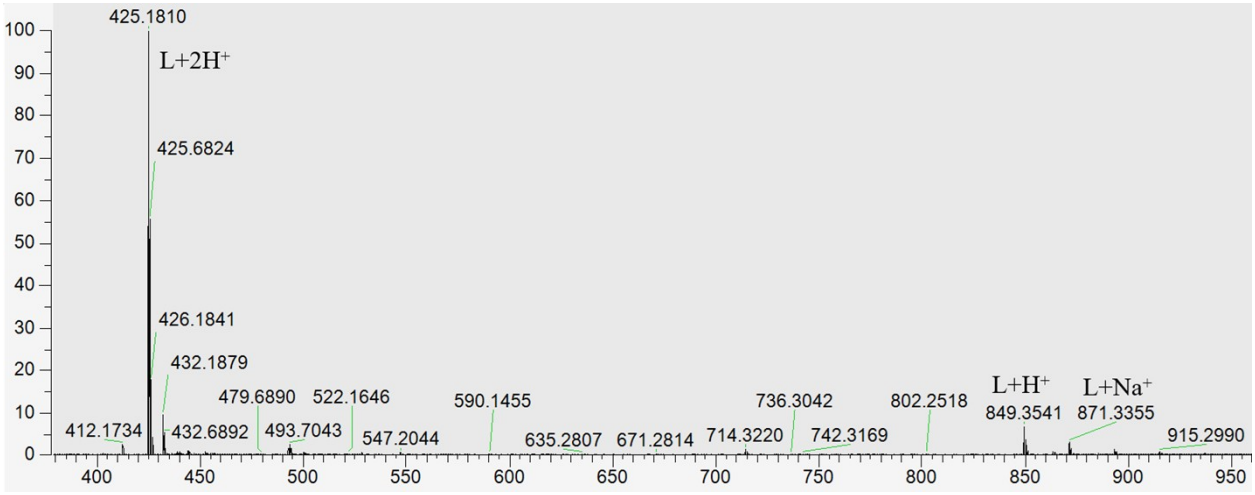


Fig. S4 ESI-MS spectra of **H_4BATPic**.

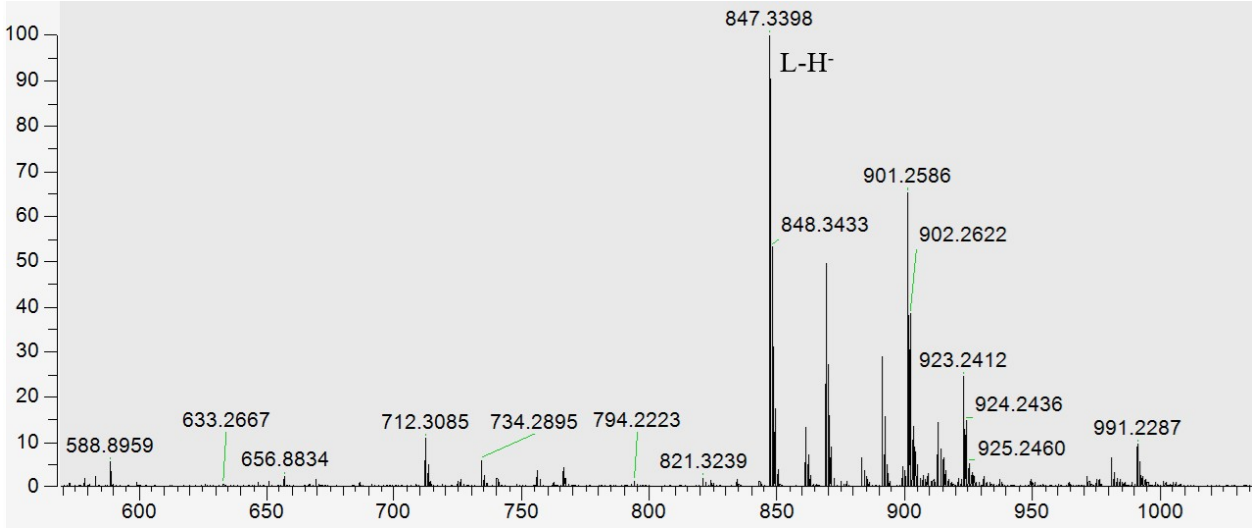


Fig. S5 ESI-MS spectra of **H_4BATPic.**

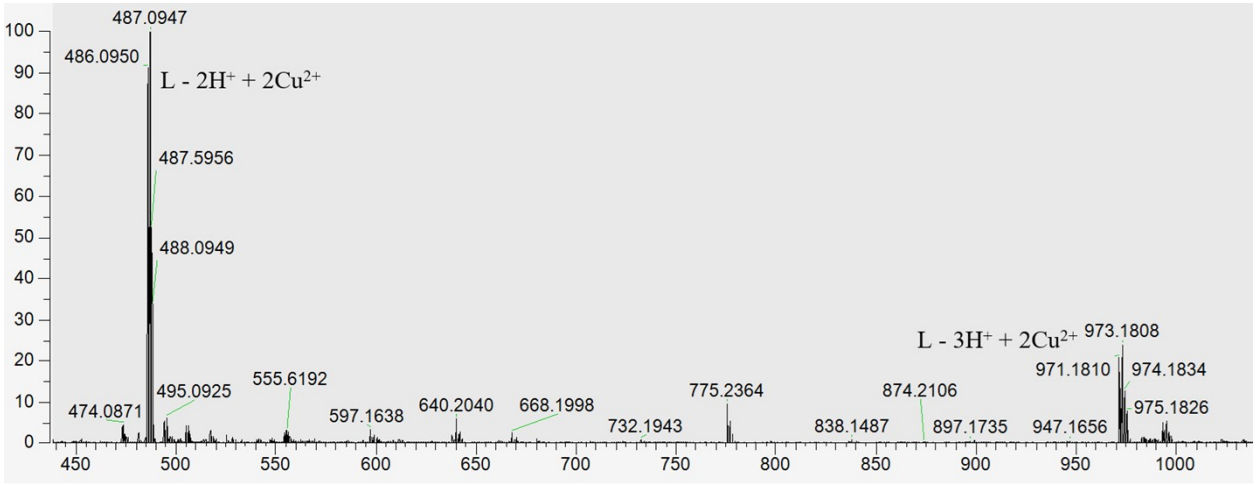


Fig. S6 ESI-MS spectra of **H_4BATPic**·Cu.

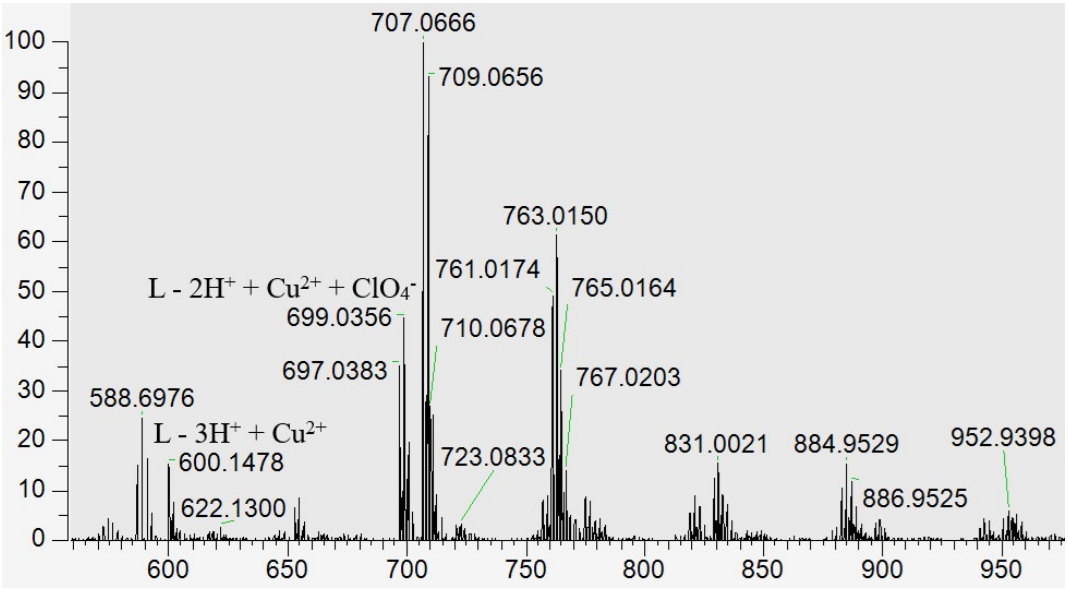


Fig. S7 ESI-MS spectra of **H_4BATA**·Cu.

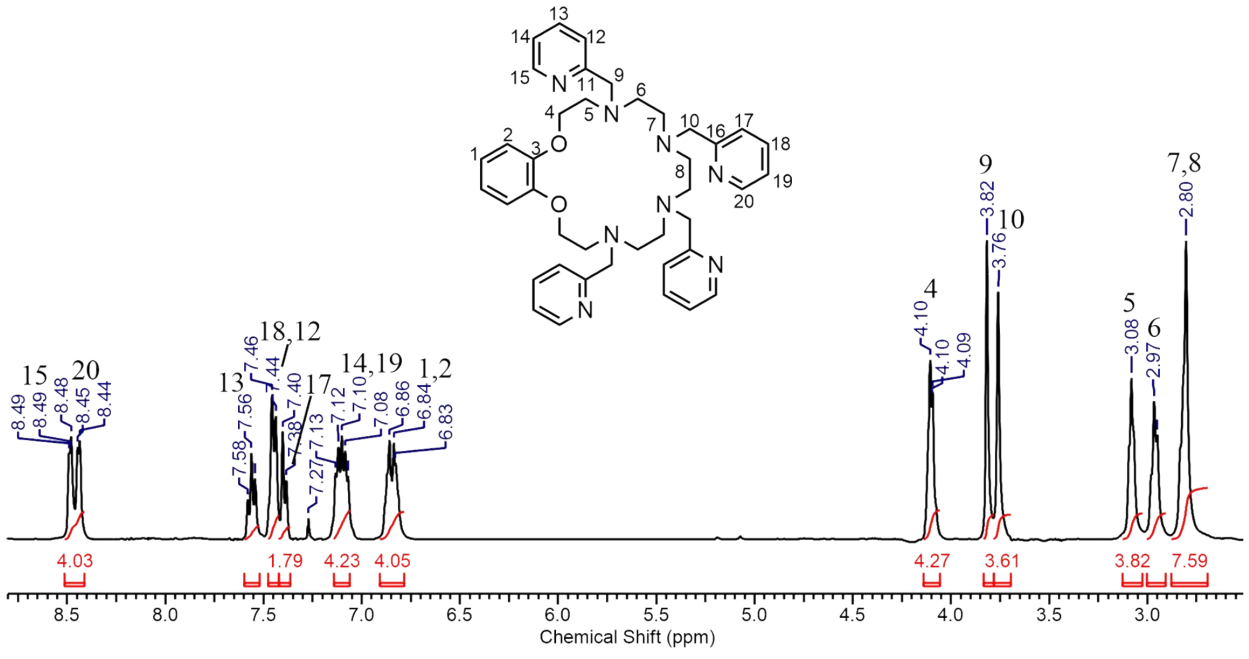


Fig. S8 ^{1}H NMR spectra of **BATPy.**

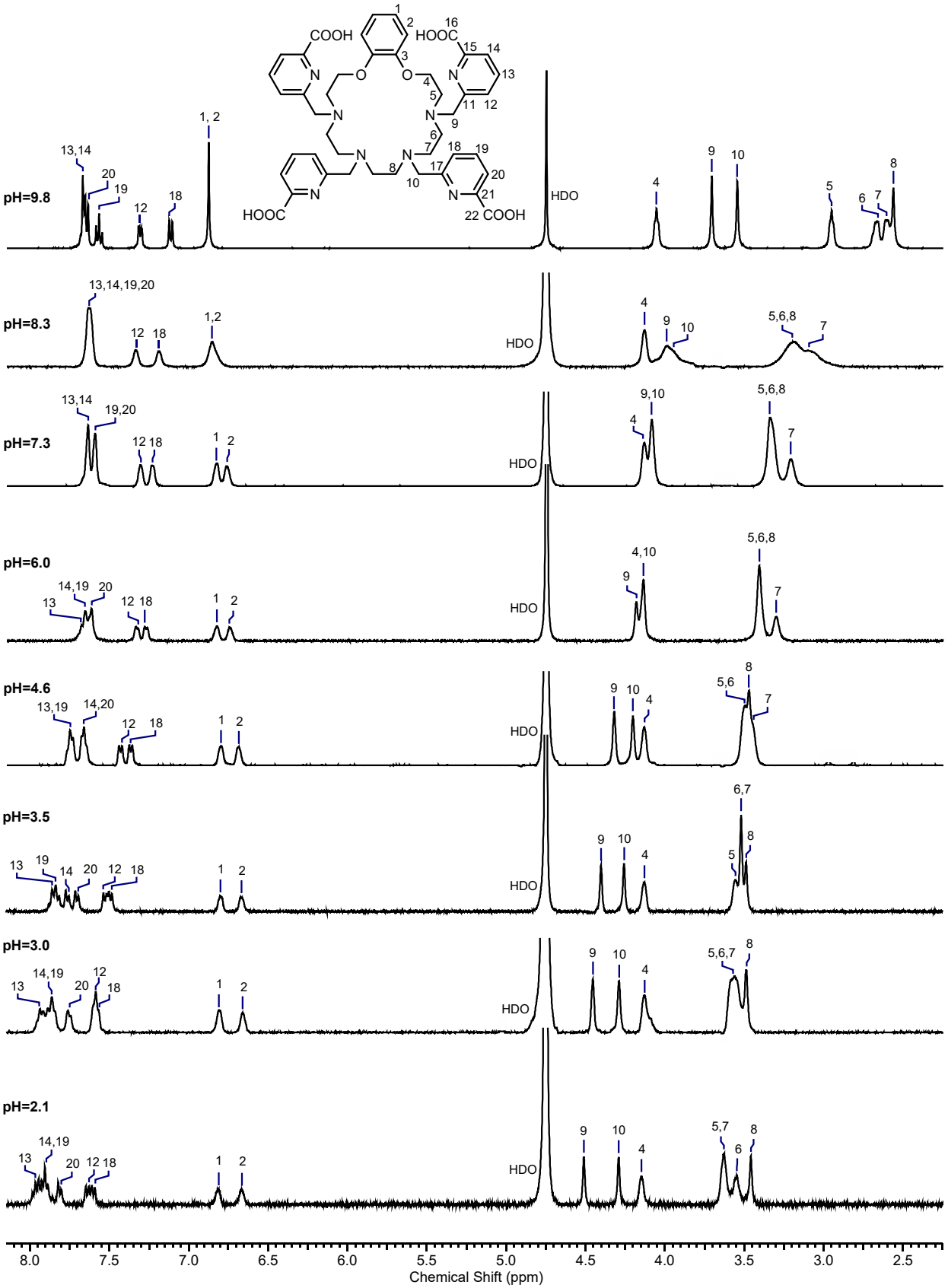


Fig. S9 ^{1}H NMR spectra of **H_4BATPic** recorded in D_2O solution at different pH values.

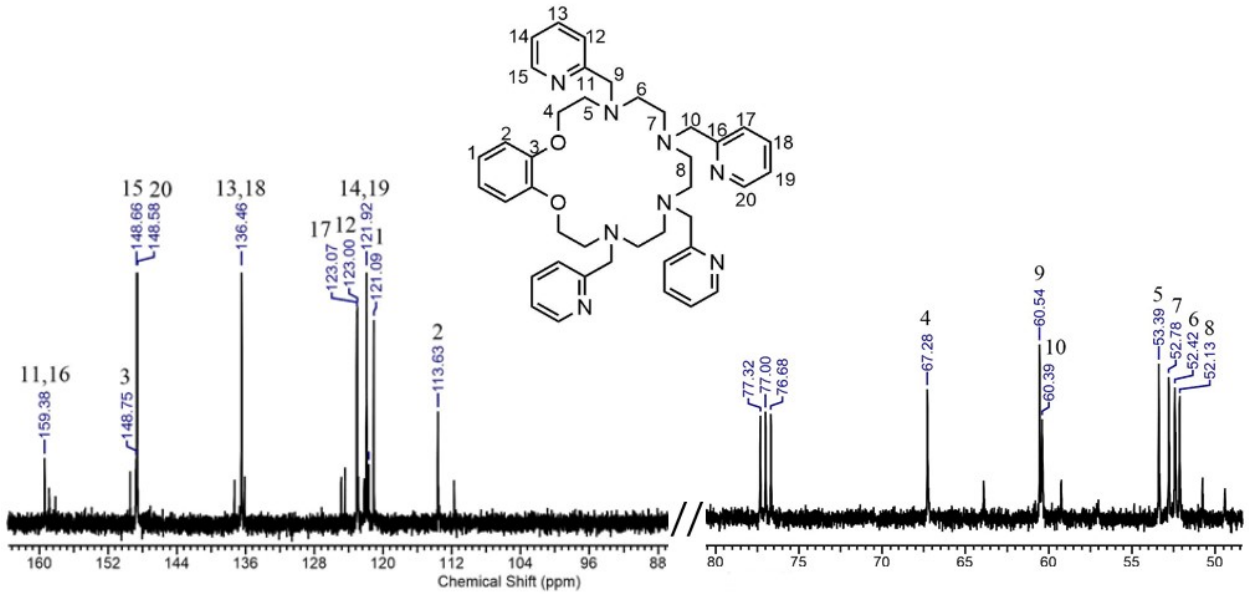


Fig. S10 ^{13}C NMR spectra of **BATPy**.

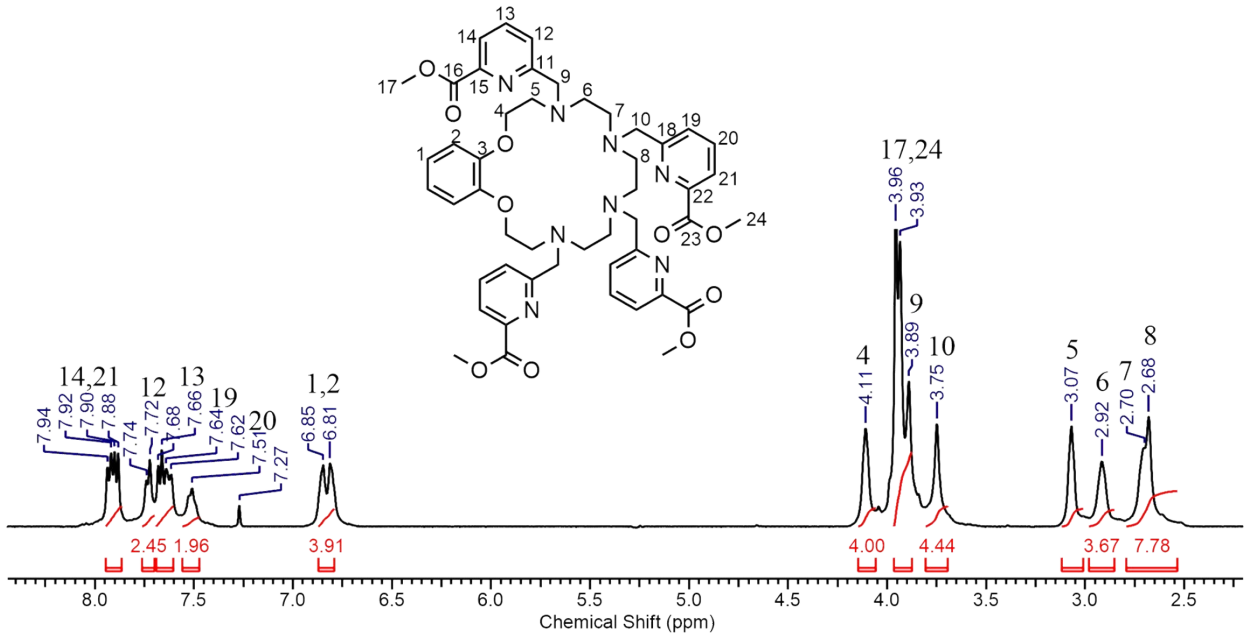


Fig. S11 ^{1}H NMR spectra of compound **Me_4BATPic**.

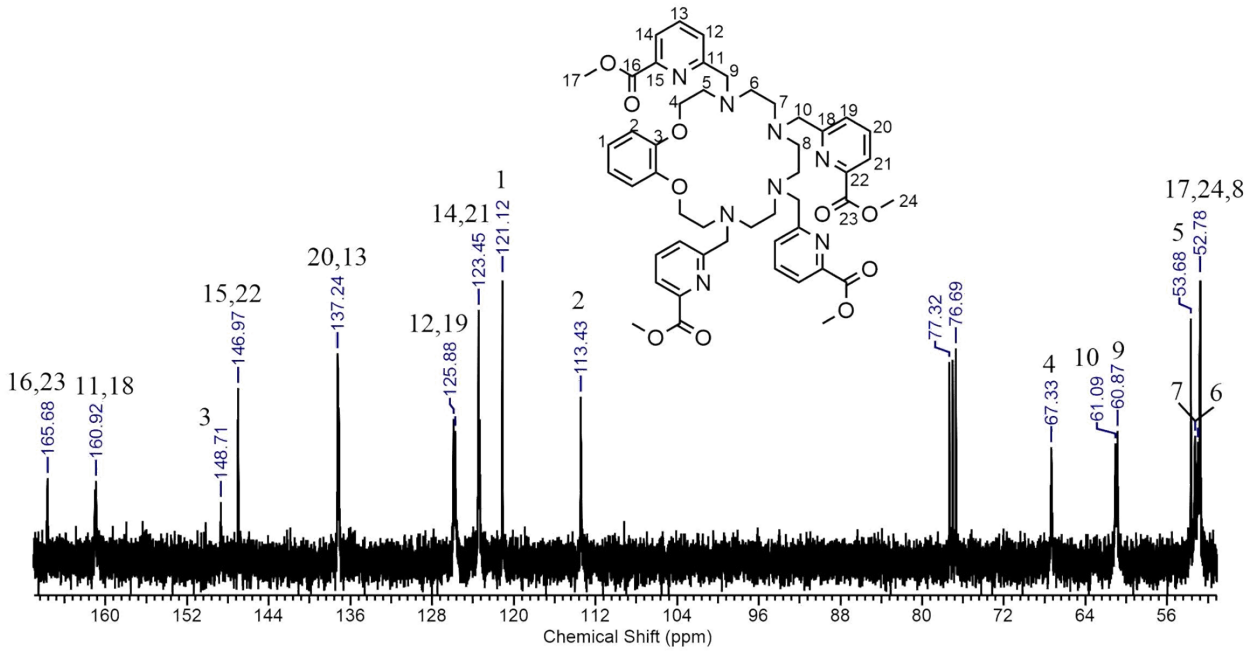


Fig. S12 ^{13}C NMR spectra of compound **Me_4BATPic**.

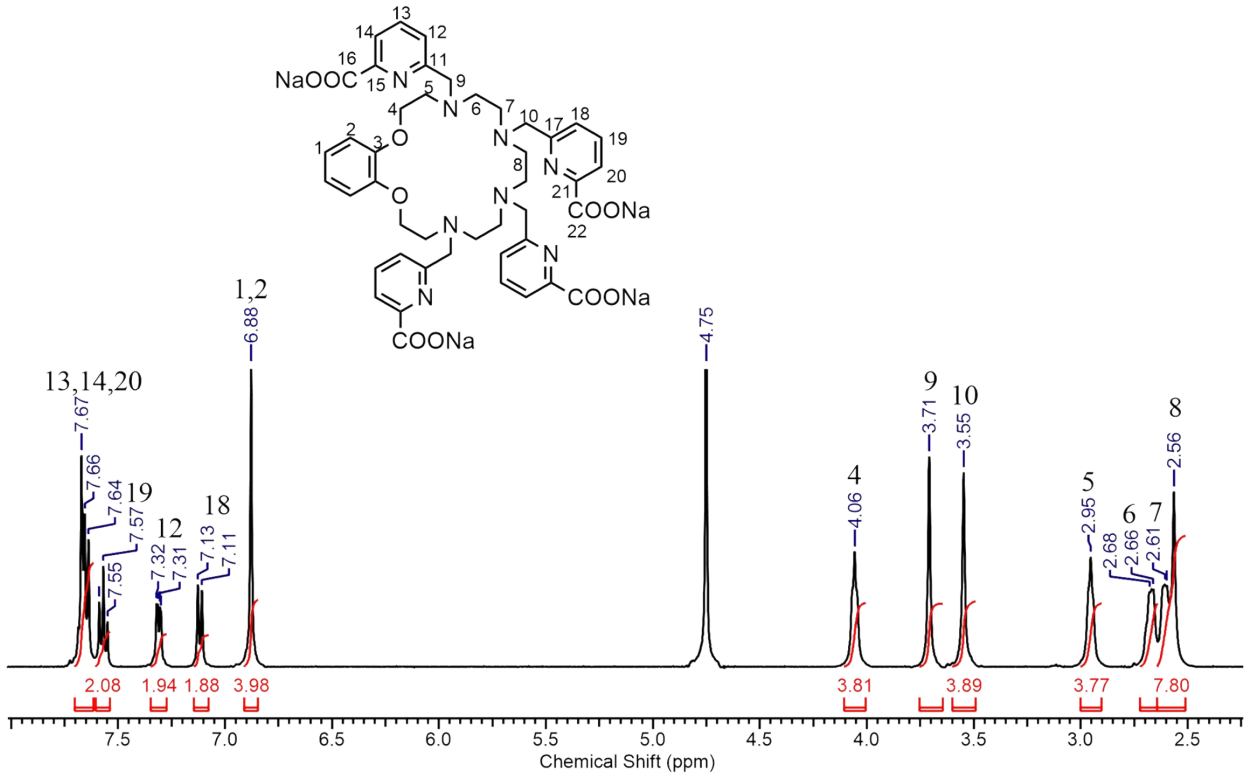


Fig. S13 ^{1}H NMR spectra of **H_4BATPic**.

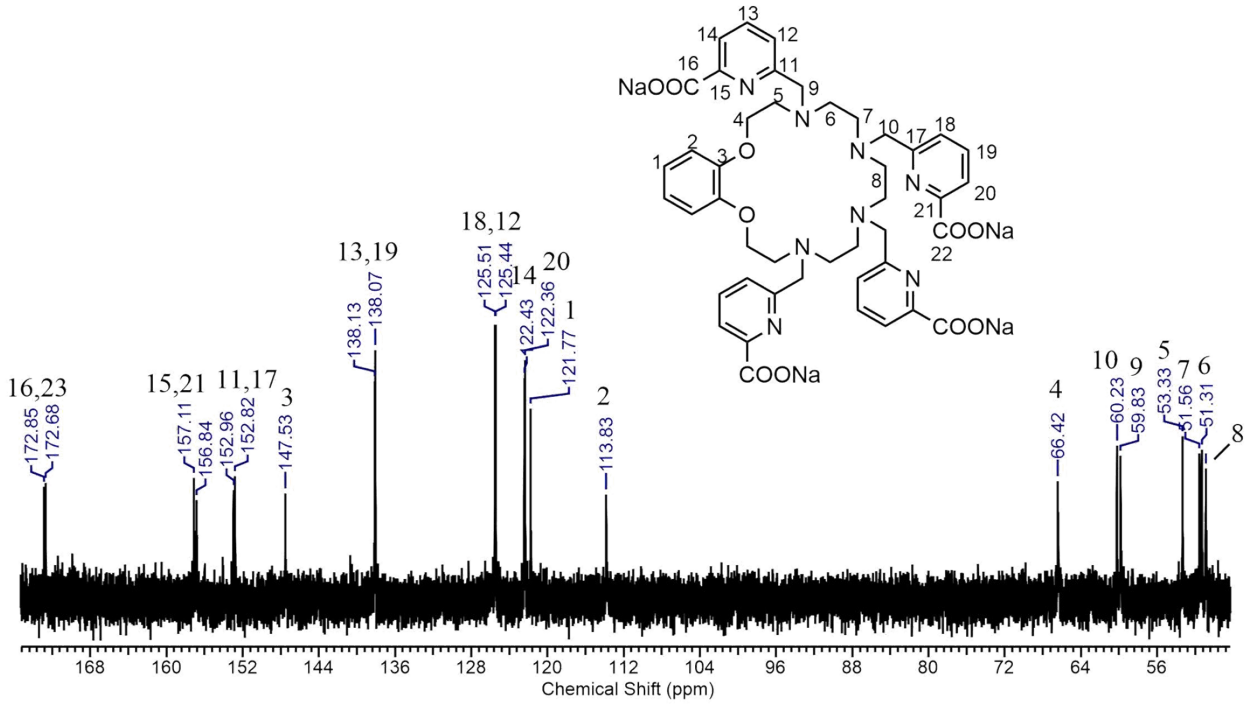


Fig. S14 ^{13}C NMR spectra of **H_4BATPic**.

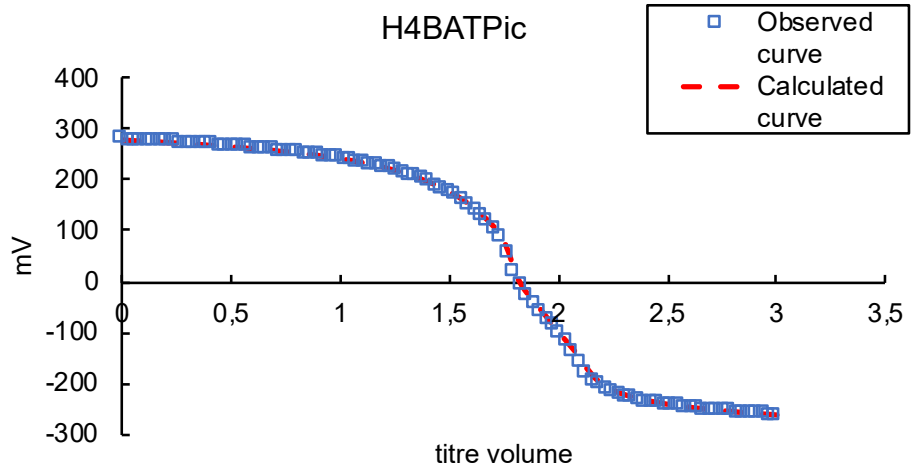


Fig. S15 Potentiometric titration of **H_4BATPic**: observed data and calculated fitting in HYPERQUAD.

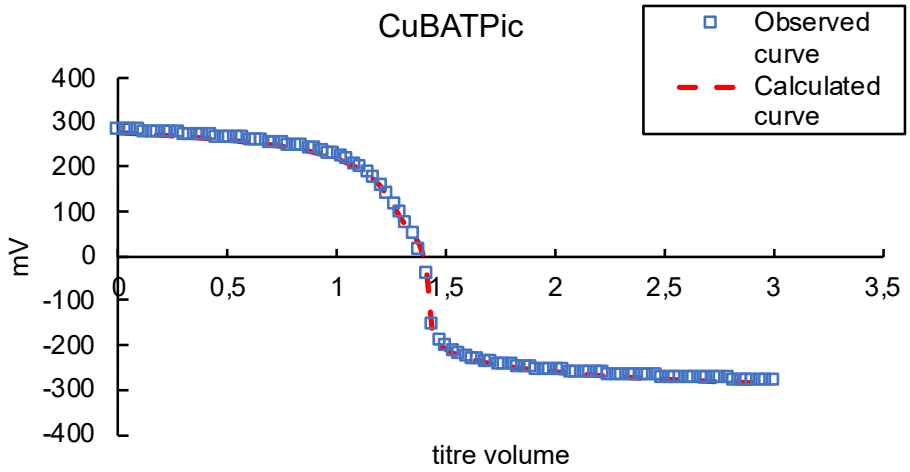


Fig. S16 Potentiometric titration of Cu^{2+} with **H_4BATPic** (equimolar): observed data and calculated fitting in HYPERQUAD.

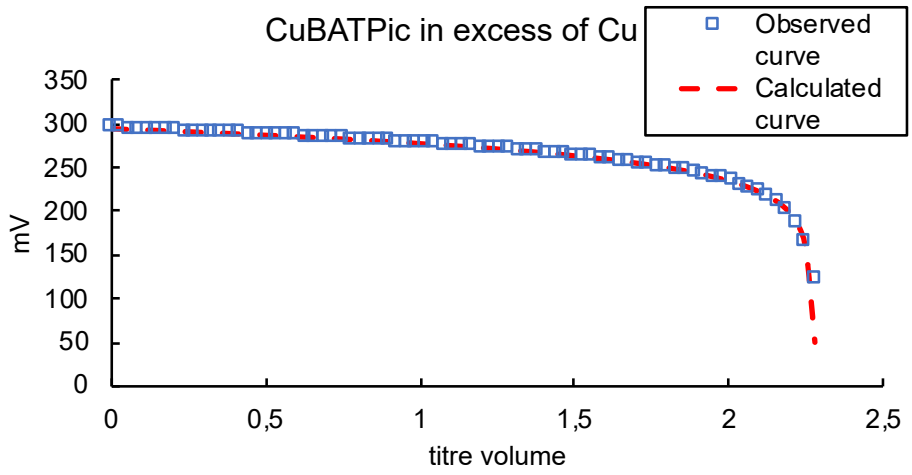


Fig. S17 Potentiometric titration of Cu^{2+} (3-fold excess of Cu^{2+}) with **H_4BATPic**: observed data and calculated fitting in HYPERQUAD.

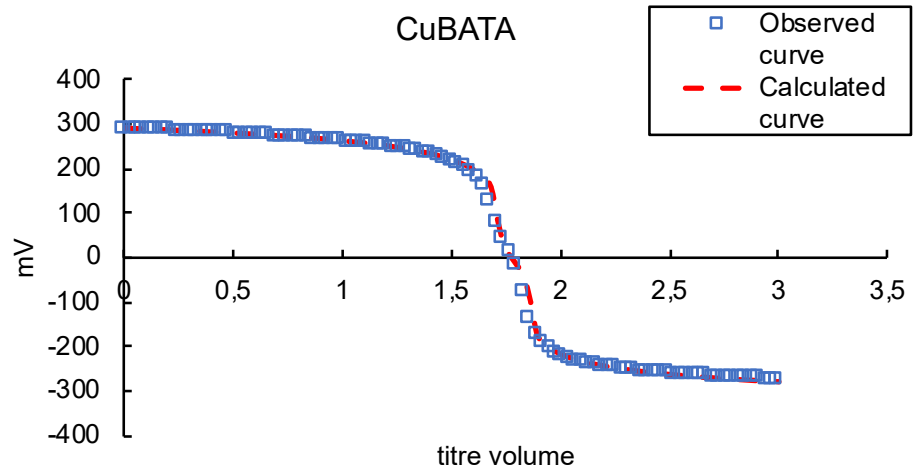


Fig. S18 Potentiometric titration of Cu^{2+} with **H_4BATA** (equimolar): observed data and calculated fitting in HYPERQUAD.

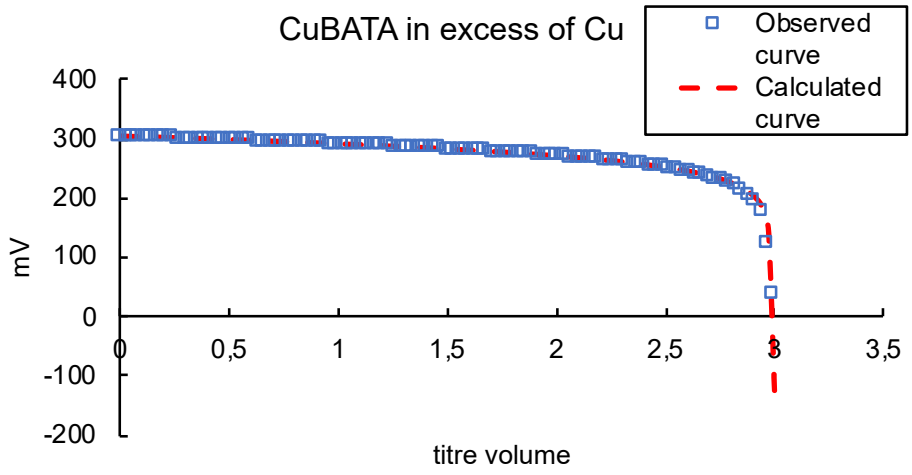


Fig. S19 Potentiometric titration of Cu^{2+} (2-fold excess of Cu^{2+}) with **H_4BATA**: observed data and calculated fitting in HYPERQUAD.

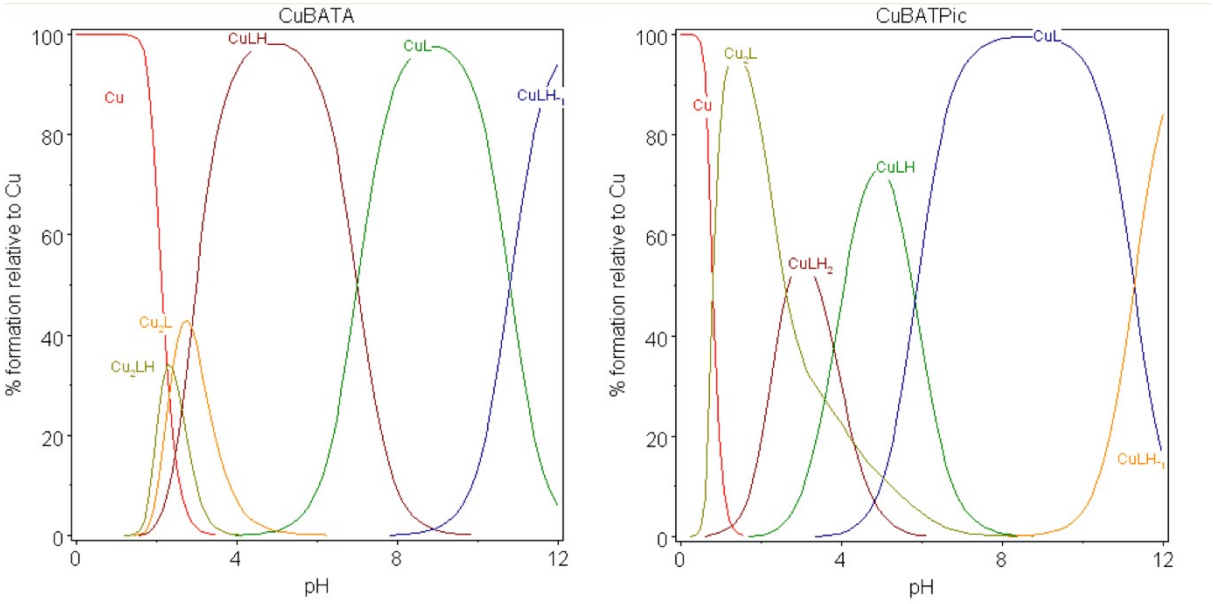


Fig. S20. pH distribution diagrams for copper species in the presence of equimolar content of ligand c(L)=c(Cu2+)=1 mM: simulated at pH from 0 to 12 with Hyss.

Table. Potentiometric titration parameters.

Titration curve	Slope factor	Standard potential, mV	c(NaOH), M
H_4BATPic	1.0046	411.3	0.0926
CuBATPic	1.0057	410.3	0.107
CuBATPic in excess of Cu^{2+}	1.0055	409.3	0.087
CuBATA	1.0122	412.6	0.1025
CuBATA in excess of Cu^{2+}	1.0078	411.87	0.103

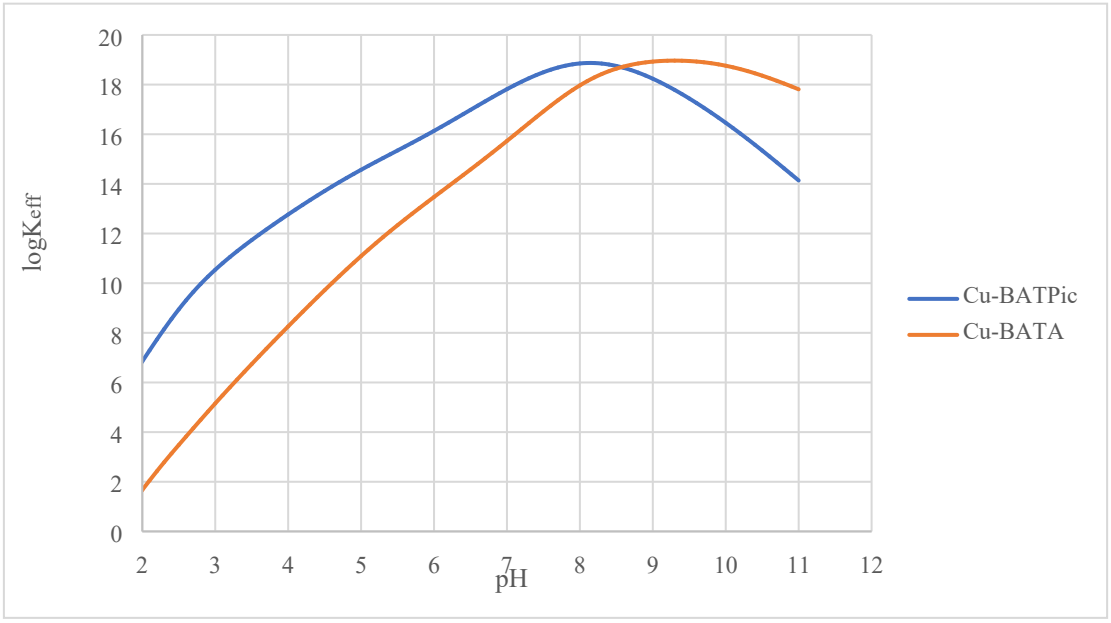


Fig. S21. The dependence of logKeff from pH for Cu-BATA and Cu-BATPic complexes

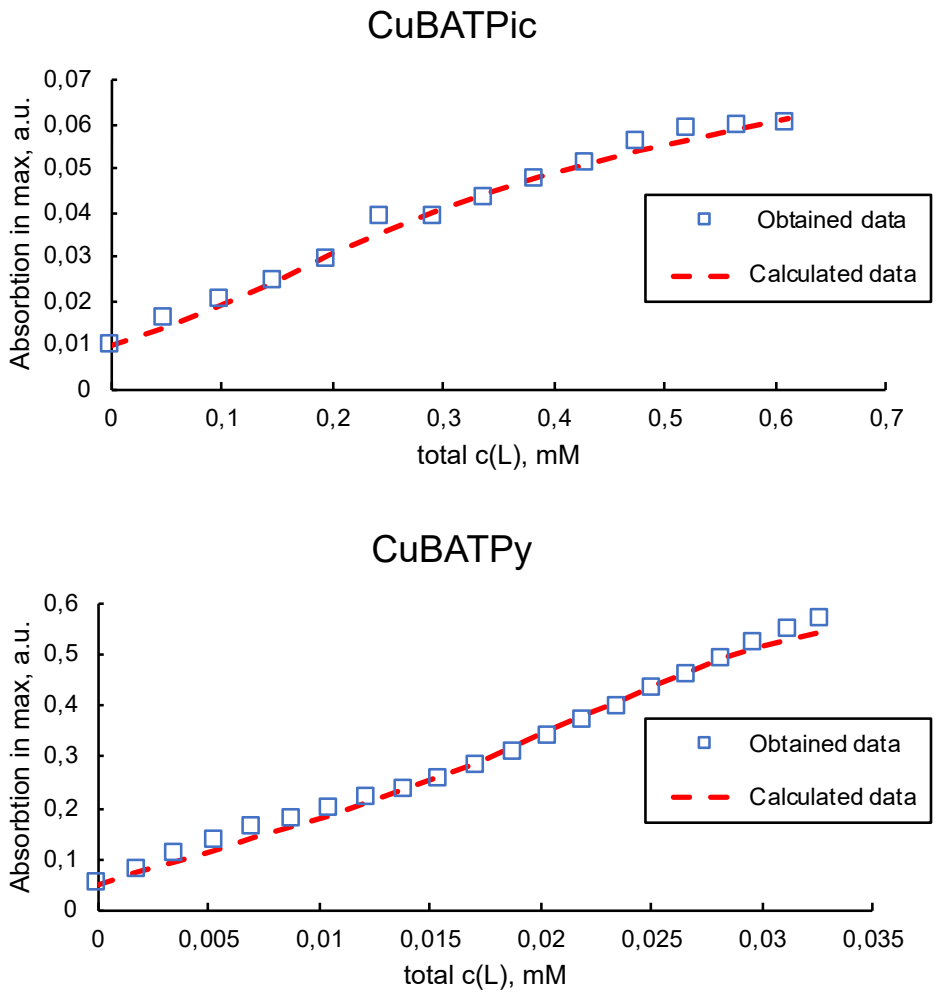


Fig. S22. Spectrophotometric titration of Cu^{2+} with **H_4BATPic** ($c(Cu^{2+})$=0.5 mM, c(L)=0÷0.6 mM) and **H_4BATPy** ($c(Cu^{2+})$=0.03 mM, c(L)=0÷0.033 mM): observed data and calculated fitting in HYPSPEC.

Table. Spectrophotometric details for Fig S22

CuBATPic				**CuBATPy**			
Point	c(Cu), mM	c(L), mM	C(Cu)/C(L)	Point	c(L), mM	c(Cu), mM	c(Cu)/C(L)
1	0,50	0,00		1	0,000	0,030	
2	0,50	0,05	10,00	2	0,002	0,030	16,67
3	0,50	0,10	5,00	3	0,004	0,030	8,33
4	0,49	0,15	3,33	4	0,005	0,030	5,56
5	0,49	0,20	2,50	5	0,007	0,029	4,17
6	0,49	0,24	2,00	6	0,009	0,029	3,33
7	0,49	0,29	1,67	7	0,010	0,029	2,78
8	0,48	0,34	1,43	8	0,012	0,029	2,38
9	0,48	0,38	1,25	9	0,014	0,029	2,08
10	0,48	0,43	1,11	10	0,016	0,029	1,85
11	0,48	0,48	1,00	11	0,017	0,029	1,67
12	0,47	0,52	0,91	12	0,019	0,028	1,52
13	0,47	0,57	0,83	13	0,020	0,028	1,39
14	0,47	0,61	0,77	14	0,022	0,028	1,28
				15	0,024	0,028	1,19
				16	0,025	0,028	1,11
				17	0,027	0,028	1,04
				18	0,028	0,028	0,98
				19	0,030	0,028	0,93
				20	0,031	0,027	0,88
				21	0,033	0,027	0,83

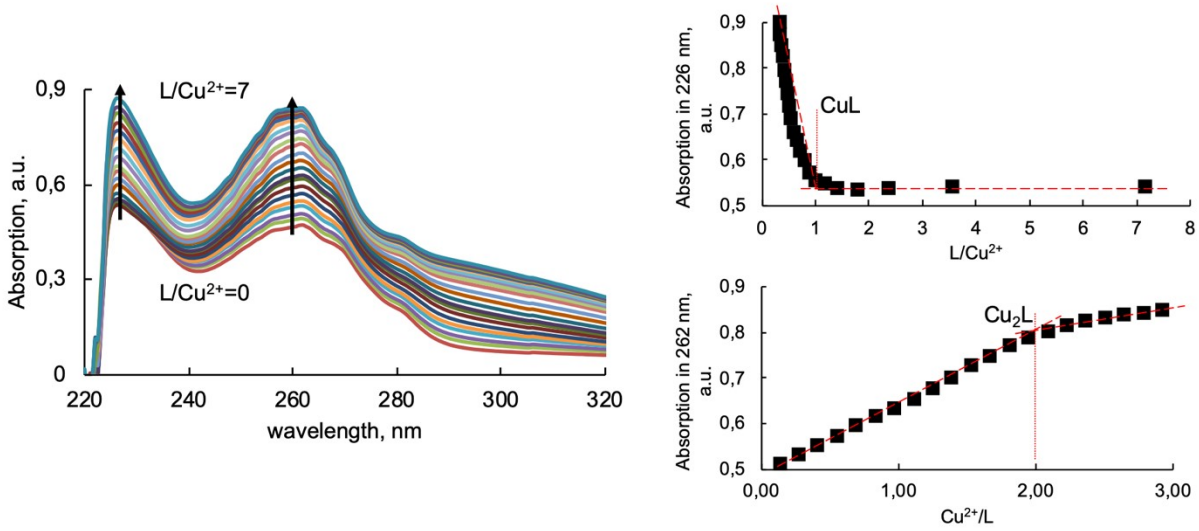


Fig. S23 Spectrophotometric titration of Cu^{2+} with **BATPy**: spectra and functions of absorption at 226 from L/Cu^{2+} ratio and 262 nm from Cu^{2+}/L ratio ($c(L)_0=4\times10^{-5}$ M $V_0=1.78$ mL, Cu^{2+} addition by 10 µL, $c(Cu^{2+})=0.001$ M).

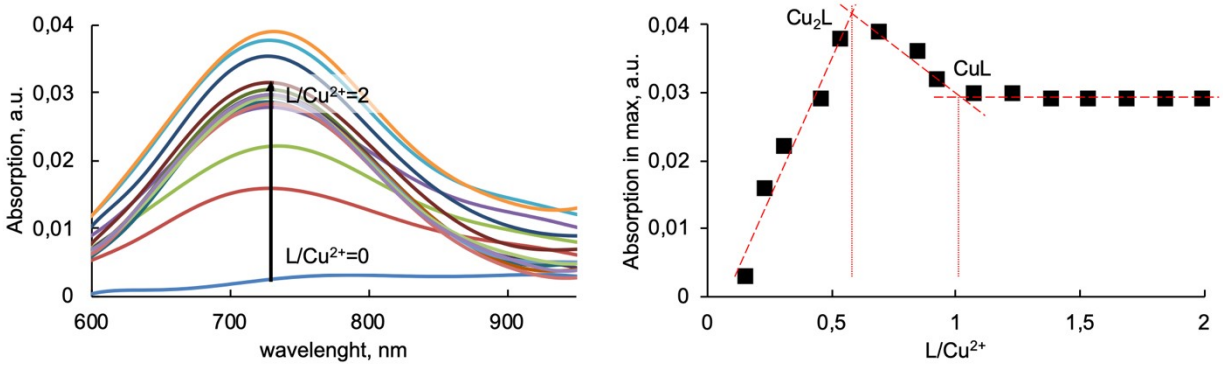


Fig. S24. Spectrophotometric titration of Cu^{2+} with **H_4BATPic**: spectra and functions of absorption at 730 from L/Cu^{2+} ratio ($c(Cu^{2+})_0=0.001$ M $V_0=1.5$ mL, L addition by 10 µL, $c(L)=0.011$ M)

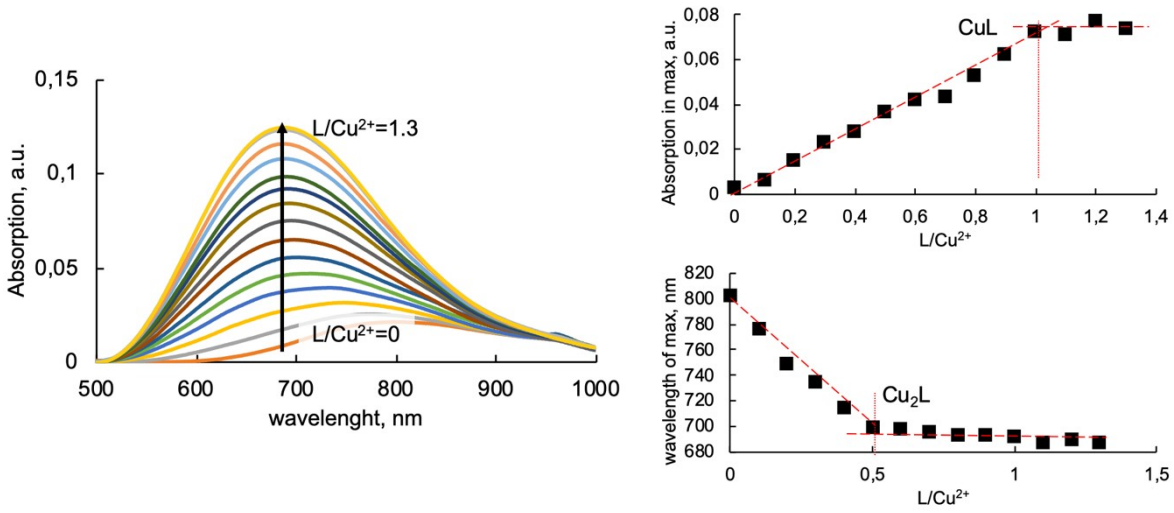
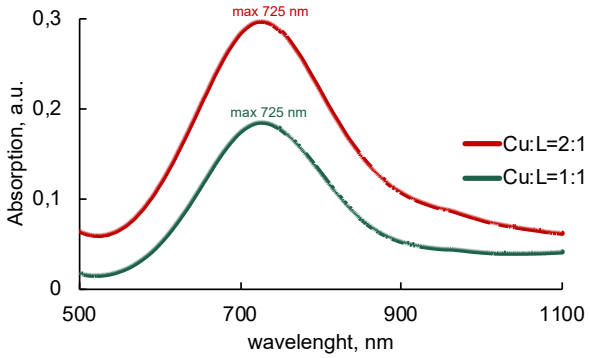
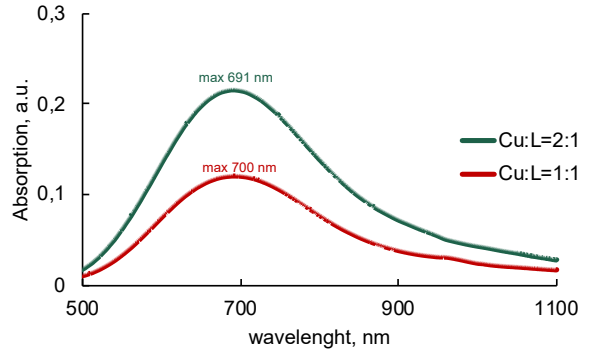


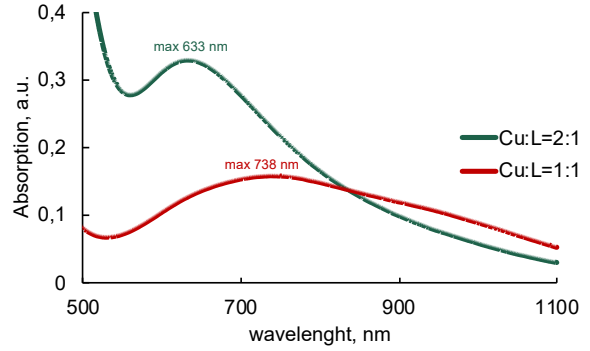
Fig. S25. Spectrophotometric titration of Cu^{2+} with **H_4BATA**: spectra and functions of maximum absorption and wavelength of maximum absorption from L/Cu^{2+} ratio ($c(Cu^{2+})_0=0.001$ M $V_0=1.5$ mL, L addition by 10 µL, $c(L)=0.03$ M).



(a)



(b)

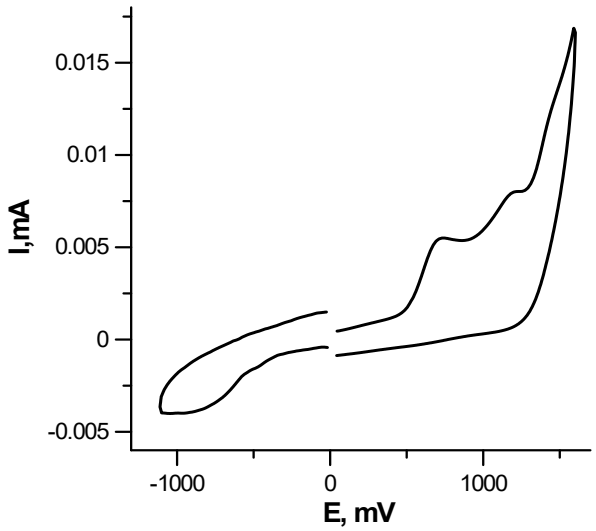


(c)

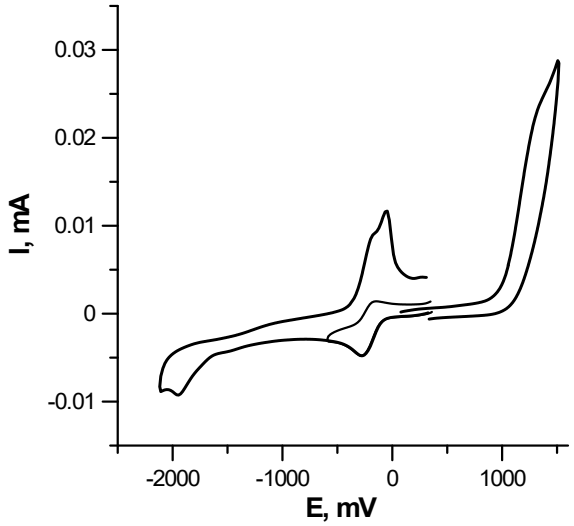
Fig. S26. Spectrophotometric data for Cu:L 1:1 and 2:1 forms: (a) Cu**BATPic**, (b) Cu**BATA,** (c) Cu**BATPy.**

Table S2. UV_Vis absorption wavelengths and molar absorptivities for Cu^{2+} complexes with H_4**BATPic** and H_4**BATA**

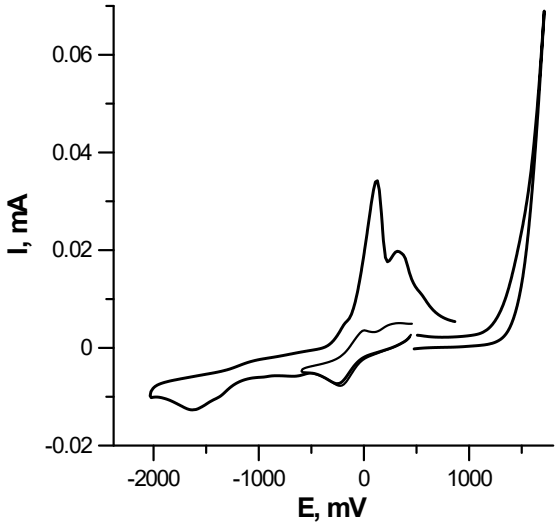
	Cu**BATPic**	Cu_2**BATPic**	Cu**BATA**	Cu_2**BATA**	Cu**BATPy**	Cu_2**BATPy**
Wl, nm	725	725	692	690	738	633
ε, $mM^{-1}\cdot cm^{-1}$	0.186	0.3101	0.115	0.208	0.1511	0.326
$\varepsilon(M_2L)/\ \varepsilon(ML)$		1.7		1.8		2.2



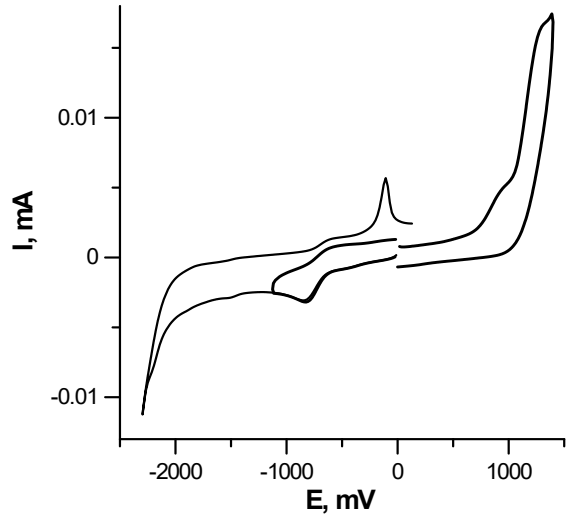
(a) Cu**BATA**$^{2-}$



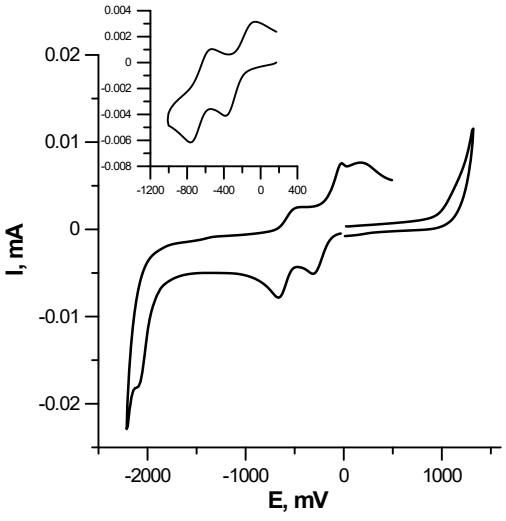
(b) Cu**BATPy**$^{2+}$



(c) Cu_2**BATPy**$^{4+}$



(d) Cu**BATPic**$^{2-}$



(e) Cu_2**BATPic**

Fig. S27. Cyclic voltammograms: copper complexes of (a) **H_4BATA**, (b, c) **BATPy**, (d, e) **H_4BATPic**, GC electrode, 0.1 M Bu_4NClO_4.

Table S3. Electrochemical potentials of ligands and complexes 1a–c, 2a–c, and 3a–c in DMSO in the presence of 0.1 M Bu_4NClO_4 on GC electrodes relative to Ag/AgCl/KCl (sat.). The potential scan rate was 100 mV s^{-1}

	compound	E_{pc}, V	E_{pa}, V
1a	**H_4BATA**	–2.16	0.95; 1.21
1b	Cu**BATA**$^{2-}$	–0.77	0.70; 1.19; 1.43
1c	Cu_2**BATA**	insoluble	–
2a	**Na_4BATPic**	–	0.77; 1.32
2b	Cu**BATPic**$^{2-}$	–0.83; –2.21/0.11 desorption peak	0.94; 1.28
2c	Cu_2**BATPic**	–0.37/–0.08; –0.76/–0.56; –2.13/–0.03 desorption peak	1.09
3a	**BATPy**	–	1.56
3b	Cu**BATPy**$^{2+}$	–0.27/–0.16; –1.95/0.06 desorption peak	1.36
3c	Cu_2**BATPy**$^{4+}$	–0.23/0; 0.27 –1.36; –1.63/0.12 desorption peak	–

Table S4. Biodistribution (% ID/g) of the Cu^{2+} complexes with **H_4BATPic** in mice at 1 and 6 hours after injection

Tissue	CuBATPic 1hour, % ID/g	Cu blank 1hour, % ID/g	CuBATPic 6 hours, % ID/g	Cu blank 6 hours, % ID/g
blood	1.8±0.5	1.4±0.2	0.7±0.06	1.6±0.6
heart	2.6±0.3	2.2±0.2	2±0.3	3.1±1.2
lungs	6.6±2.9	5±2	2.8±0.3	6.2±1.2
pancreas	1.9±0.8	1.8±0.7	0.8±0.4	3.2±0.9
spleen	2.0±1.6	1.75±0.01	0.8±0.7	1.8±1.4
liver	11.4±1.3	16.6±4.3	6.9±1.6	13.1±0.9
kidneys	4.9±1.7	4.5±0.7	3.0±0.3	5.6±0.5
femur	1.3±0.9	1.3±0.1	0.5±0.2	0.8±0.5
brain	0.3±0.2	0.2±0.1	0.11±0.07	0.3±0.2
bladder	27.2±1.6	4.4±0.3	5.7±4.5	1.2±1.3
rest of the body	2.2±0.2	1.5±0.8	1.3±0.4	1.8±0.2

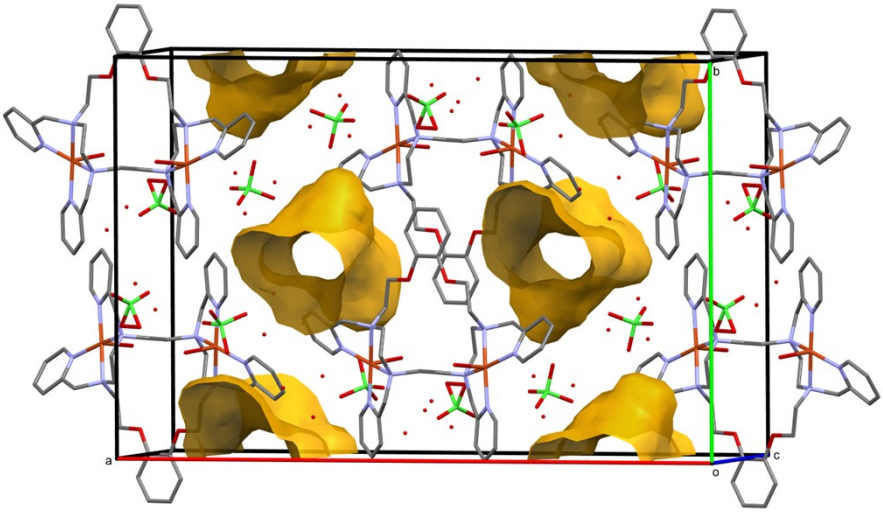


Fig. S28. The representation of the squeezed void in the form of infinite channels in the crystal structure Cu_2**BATPy**$^{4+}$**.**

Table S5. Selected interatomic distances in calculated geometries of Copper complexes

	CuBATA	Cu_2BATA	CuBATPic	Cu_2BATPic
N1	Cu1-3.96	Cu1-2.05	Cu1-2.15	Cu1-2.11
N2	Cu1-3.01	Cu1-2.03	Cu1-2.02	Cu1-2.04
N3			Cu1-1.91	Cu1-1.89
N4			Cu1-2.19ax	Cu1-2.22ax
N7	Cu1-2.27ax	Cu2-2.03		Cu2-3.09
N8	Cu1-2.18	Cu2-2.05		Cu2-2.43ax
N9				Cu2-1.96
N10				Cu2-1.95
O5	Cu1-1.95	Cu1-1.93	Cu1-2.00	Cu1-1.96
O6	Cu1-1.97	Cu1-1.93		
O11		Cu2-1.93		Cu2-2.02
O12	Cu1-2.00	Cu2-1.93		Cu2-1.99
Ow		Cu1-2.42ax		
Ow		Cu2-2.42ax		
Cu-Cu		7.05		8.40

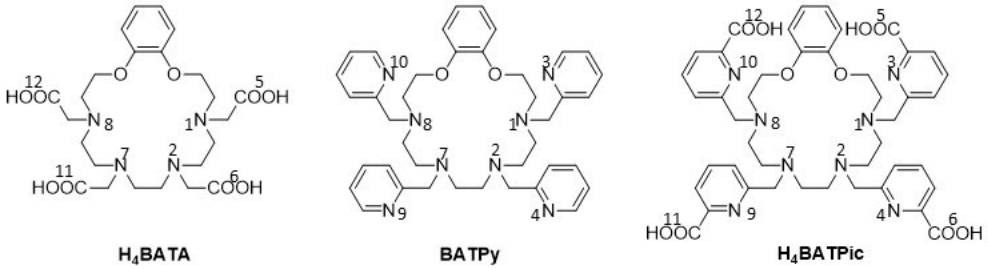


Fig. S29. Numbers of atoms used for the Table S5

Table S6 Coordinates in Angstroem of optimized geometries of complexes

Cu_2BATA

Cu	12.0620530000	4.8318510000	0.5478240000
Cu	18.6328880000	4.7627090000	3.0966260000
O	14.3255890000	9.1024810000	1.1596020000
O	13.0906900000	4.7196460000	-1.6419270000
H	12.8575700000	3.7828380000	-1.4970420000
H	12.3163570000	5.0769660000	-2.1013310000
N	12.3288730000	6.7608000000	1.2035910000
N	13.4301480000	4.3088000000	1.9587790000
C	14.7937780000	12.7414950000	1.6081330000
H	14.3460370000	13.6821330000	1.3133160000
C	14.2220480000	11.5439650000	1.1708480000
H	13.3420620000	11.5672670000	0.5417120000
C	14.7861410000	10.3321340000	1.5398480000
C	13.1363150000	9.0392270000	0.3777100000
H	13.2808940000	9.5659590000	-0.5721670000
H	12.3059460000	9.5154460000	0.9096010000
C	12.8692580000	7.5734040000	0.0857060000
H	12.1457830000	7.4970510000	-0.7264610000
H	13.7951030000	7.1071580000	-0.2557680000
C	13.2004540000	6.7101760000	2.4066470000
H	12.8961690000	7.4552150000	3.1463000000
H	14.2103170000	6.9757310000	2.1010290000
C	13.1649910000	5.3129920000	3.0140010000
H	13.8690020000	5.2400580000	3.8499050000
H	12.1696480000	5.0921770000	3.4056460000
C	14.7633990000	4.4068640000	1.3226480000
H	14.7932900000	5.3287740000	0.7404740000
H	14.8279780000	3.5830310000	0.6107440000
C	10.9115450000	7.1001740000	1.4752590000
H	10.7678660000	8.1701170000	1.6419670000
H	10.5998240000	6.5678040000	2.3777080000
C	13.0885790000	2.9095900000	2.3031650000
H	12.2766480000	2.9253210000	3.0330710000
H	13.9316350000	2.3707860000	2.7393010000
O	16.3867540000	9.0650880000	2.6850180000
N	18.3681730000	6.7201690000	2.5303510000
N	17.2563710000	4.3047560000	1.6712070000
C	15.9225880000	12.7219910000	2.4087560000
H	16.3713430000	13.6472450000	2.7474190000
C	16.4929930000	11.5045270000	2.7891680000
H	17.3727620000	11.4970470000	3.4189320000
C	15.9277340000	10.3120000000	2.3634040000
C	17.5754170000	8.9627050000	3.4636170000
H	17.4314410000	9.4440210000	4.4374490000
H	18.4068080000	9.4623570000	2.9553600000
C	17.8399440000	7.4842580000	3.6875960000
H	18.5693470000	7.3704360000	4.4900770000
H	16.9153350000	7.0056120000	4.0147890000
C	17.4833530000	6.7241790000	1.3362420000
H	17.7759370000	7.5050330000	0.6296500000
H	16.4765380000	6.9703100000	1.6672440000
C	17.5154170000	5.3576760000	0.6630950000
H	16.8062980000	5.3245310000	-0.1709220000
H	18.5082360000	5.1561830000	0.2548990000
C	15.9244230000	4.3678370000	2.3158220000
H	15.9009190000	5.2450270000	2.9642370000
H	15.8546990000	3.4951470000	2.9661270000
C	19.7829310000	7.0700350000	2.2591460000
H	19.9267150000	8.1468530000	2.1458250000

H	20.0830730000	6.5846370000	1.3268320000
C	17.5969100000	2.9235910000	1.2594200000
H	18.4065070000	2.9730680000	0.5283670000
H	16.7514080000	2.4071540000	0.8010640000
O	17.6226090000	4.5567200000	5.2849680000
H	17.8517520000	3.6269500000	5.0945820000
H	18.3985790000	4.8889450000	5.7600050000
C	10.0346120000	6.6163560000	0.2934760000
O	9.0303660000	7.2379090000	0.0034640000
O	10.4798740000	5.5428240000	-0.2921870000
C	12.5839780000	2.1682620000	1.0424590000
O	12.7212210000	0.9656360000	0.9604670000
O	12.0117470000	2.9392910000	0.1582500000
C	18.1045450000	2.1241700000	2.4831160000
O	17.9679300000	0.9189250000	2.5093370000
O	18.6782350000	2.8535140000	3.4011980000
C	20.6737280000	6.5253750000	3.4034330000
O	21.6856170000	7.1275550000	3.7077420000
O	20.2319970000	5.4266400000	3.9428110000

Cu_2BATPy^{4+}

Cu	12.0266800000	4.8094810000	0.5748570000
Cu	18.7397020000	4.7597590000	3.3900270000
O	14.2461580000	9.1121390000	1.3986950000
O	13.2291440000	5.0705240000	-1.4276060000
H	13.4557970000	4.2829010000	-1.9419670000
H	13.0024090000	5.7412900000	-2.0879160000
N	12.2827360000	6.7298890000	1.3464270000
N	13.4422160000	4.2309080000	2.0244000000
N	10.1987980000	5.5243040000	0.1099940000
N	11.9865200000	2.8220510000	0.2395290000
C	14.7995660000	12.7574230000	1.7225910000
H	14.3163020000	13.6949760000	1.4810540000
C	14.1727330000	11.5578520000	1.3931860000
H	13.2098870000	11.5864990000	0.9015150000
C	14.7826360000	10.3483710000	1.6966360000
C	13.0192120000	9.1038330000	0.6795750000
H	13.1093570000	9.6987260000	-0.2356020000
H	12.2162710000	9.5399350000	1.2840460000
C	12.7255930000	7.6686630000	0.2707660000
H	11.9333630000	7.6763370000	-0.4802320000
H	13.6246580000	7.2445950000	-0.1777470000
C	13.2541760000	6.6370280000	2.4739040000
H	13.0461350000	7.3947140000	3.2325970000
H	14.2415720000	6.8634990000	2.0770160000
C	13.1945520000	5.2492930000	3.0801310000
H	13.8933980000	5.1589710000	3.9165280000
H	12.1985610000	5.0480720000	3.4791390000
C	14.8178050000	4.2594040000	1.4523370000
H	14.8957030000	5.1569100000	0.8396680000
H	14.8905160000	3.4054740000	0.7765610000
C	10.9145400000	7.0602780000	1.8286280000
H	10.8257530000	8.1240260000	2.0612690000
H	10.7446450000	6.5138940000	2.7608510000
C	9.8908790000	6.6373550000	0.8123010000
C	8.6891190000	7.3033250000	0.6372910000
H	8.4741950000	8.1951850000	1.2130770000
C	7.7654650000	6.8061210000	-0.2776990000
H	6.8176980000	7.3086260000	-0.4281560000
C	8.0807600000	5.6577510000	-0.9947580000

H	7.3926220000	5.2359080000	-1.7155810000
C	9.3052660000	5.0494340000	-0.7744530000
H	9.5813250000	4.1548700000	-1.3136020000
C	13.0213280000	2.8659890000	2.4297110000
H	12.2095050000	2.9702430000	3.1543230000
H	13.8283380000	2.3253840000	2.9320590000
C	12.5213140000	2.0886400000	1.2373950000
C	12.5503000000	0.7031200000	1.1874310000
H	12.9744980000	0.1399760000	2.0099280000
C	12.0114140000	0.0504180000	0.0831490000
H	12.0099330000	-1.0315680000	0.0307900000
C	11.4820100000	0.8097340000	-0.9549170000
H	11.0647750000	0.3450030000	-1.8388310000
C	11.4932170000	2.1894190000	-0.8398480000
H	11.1046050000	2.8159720000	-1.6319200000
O	16.5558480000	9.0933320000	2.6307820000
N	18.4982850000	6.6937840000	2.6478620000
N	17.3229530000	4.2141640000	1.9285520000
N	20.5716620000	5.4558010000	3.8687440000
N	18.7691570000	2.7657080000	3.6885570000
C	16.0359020000	12.7475970000	2.3549910000
H	16.5277040000	13.6774200000	2.6088670000
C	16.6517190000	11.5381020000	2.6685920000
H	17.6147560000	11.5514920000	3.1605370000
C	16.0308130000	10.3383450000	2.3493020000
C	17.7829390000	9.0639720000	3.3490790000
H	17.6987040000	9.6467910000	4.2725500000
H	18.5894950000	9.5012190000	2.7502580000
C	18.0641520000	7.6205880000	3.7373730000
H	18.8569600000	7.6108050000	4.4876960000
H	17.1616060000	7.1977980000	4.1801270000
C	17.5255090000	6.6264980000	1.5197930000
H	17.7381760000	7.3956350000	0.7740400000
H	16.5400560000	6.8528290000	1.9216860000
C	17.5759720000	5.2489280000	0.8902600000
H	16.8761070000	5.1768630000	0.0529880000
H	18.5703410000	5.0484790000	0.4869050000
C	15.9473090000	4.2399320000	2.5013100000
H	15.8778420000	5.1211030000	3.1384950000
H	15.8661460000	3.3684830000	3.1532620000
C	19.8689650000	7.0197340000	2.1698970000
H	19.9662960000	8.0858500000	1.9518480000
H	20.0346790000	6.4849250000	1.2302520000
C	20.8889040000	6.5750650000	3.1805960000
C	22.0957830000	7.2292320000	3.3644480000
H	22.3182000000	8.1265340000	2.8000400000
C	23.0148420000	6.7135270000	4.2737640000
H	23.9664920000	7.2065470000	4.4309290000
C	22.6898560000	5.5590770000	4.9766140000
H	23.3740050000	5.1230410000	5.6927650000
C	21.4606820000	4.9632060000	4.7480530000
H	21.1768190000	4.0643910000	5.2759650000
C	17.7358830000	2.8544800000	1.4986250000
H	18.5476510000	2.9668250000	0.7751240000
H	16.9252310000	2.3276430000	0.9874440000
C	18.2326980000	2.0533340000	2.6763410000
C	18.1996180000	0.6672020000	2.6992490000
H	17.7742780000	0.1214590000	1.8656740000
C	18.7358910000	-0.0085050000	3.7908310000
H	18.7343060000	-1.0913100000	3.8219340000
C	19.2667370000	0.7288630000	4.8438800000

H	19.6820230000	0.2457510000	5.7188040000
C	19.2597000000	2.1105490000	4.7557240000
H	19.6496150000	2.7201960000	5.5602310000
O	17.5367620000	4.9961320000	5.3938860000
H	17.3048160000	4.2021980000	5.8960620000
H	17.7679250000	5.6551770000	6.0643790000

Cu_2BATPic

Cu	1.5428750000	26.1698940000	20.7727280000
Cu	0.8688760000	21.4989080000	13.8243230000
C	-1.0834030000	24.3747620000	11.4800010000
H	-0.8499250000	25.3326360000	11.0316840000
C	-2.3477320000	23.8026710000	11.3372320000
C	-2.6484270000	22.6097390000	11.9851870000
O	-2.9216990000	20.2407010000	13.6826750000
N	-0.4234950000	22.5293120000	12.7853710000
H	3.4731880000	23.0243050000	13.4353600000
H	3.6019620000	25.4479430000	12.8391330000
H	4.9036790000	24.8852190000	13.9039090000
C	4.5578770000	27.7964360000	13.5113310000
H	5.0884330000	27.0726730000	12.9070550000
C	4.7457140000	29.1607570000	13.2805900000
H	5.4154630000	29.4790550000	12.4915260000
C	1.2617860000	24.2004800000	12.5456650000
H	1.9732010000	23.7090790000	11.8743370000
H	1.3163140000	25.2845950000	12.3795070000
C	-0.1256370000	23.7047040000	12.2289350000
C	-1.6480040000	22.0010760000	12.7288190000
C	-1.8400420000	20.8039550000	13.6455010000
O	2.2504580000	27.8022650000	16.3089520000
O	3.4463800000	26.0580660000	14.8108090000
O	-1.4466980000	25.0891660000	23.1305570000
O	0.2625180000	24.9824940000	21.6685360000
O	2.6117990000	28.1807680000	23.6968960000
O	4.2438650000	28.7395200000	22.2182100000
O	2.3446960000	21.1594140000	12.4936920000
O	4.2242040000	19.9266910000	12.3142010000
O	-0.7944660000	20.5442150000	14.3691270000
N	2.0420560000	27.7781080000	19.4988050000
N	2.5134640000	24.9520330000	19.4488610000
N	1.1753400000	22.7070400000	16.6549380000
N	1.6201910000	23.8040180000	13.9155150000
N	0.4955060000	27.5366860000	21.5619570000
N	3.4790410000	25.8378690000	21.7986540000
N	2.0917080000	20.5696510000	15.0395290000
C	4.0800520000	30.0937190000	14.0561120000
H	4.2148080000	31.1533890000	13.8791340000
C	3.2273250000	29.6724470000	15.0788220000
H	2.7042950000	30.4084860000	15.6745800000
C	3.0444400000	28.3185610000	15.3223740000
C	1.5841880000	28.7038650000	17.1925800000
H	2.2719470000	29.4855670000	17.5323480000
H	0.7494300000	29.1801540000	16.6672510000
C	1.0903600000	27.8716020000	18.3698350000
H	0.8559340000	26.8750030000	17.9951930000
H	0.1677050000	28.2911100000	18.7725970000
C	3.4046670000	27.3343590000	19.1417180000
H	3.8514050000	27.9543010000	18.3555390000
H	4.0086290000	27.4380720000	20.0416220000
C	3.3635280000	25.8860140000	18.6279540000

H	4.3856760000	25.5038980000	18.5749180000
H	2.9657560000	25.8935870000	17.6146490000
C	1.5191660000	24.2164120000	18.6233460000
H	0.9013210000	23.6320780000	19.3068740000
H	0.8687460000	24.9589060000	18.1610870000
C	2.1408650000	23.3453030000	17.5256320000
H	2.7576180000	22.5580850000	17.9646340000
H	2.8161480000	23.9735490000	16.9352110000
C	0.1997320000	23.5379790000	15.9764290000
H	-0.4813440000	22.8655870000	15.4517410000
H	-0.4208360000	24.1374220000	16.6639600000
C	0.8375070000	24.4994620000	14.9665390000
H	0.0269870000	25.0562640000	14.4883770000
H	1.4631600000	25.2372760000	15.4711970000
C	3.0746780000	23.7800430000	14.1164480000
H	3.2651780000	23.4354920000	15.1312240000
C	3.8253870000	25.0734310000	13.8430180000
C	3.7060880000	27.3668480000	14.5199510000
C	1.9440020000	28.9928850000	20.3575430000
H	2.8700840000	29.0902460000	20.9454470000
H	1.8199330000	29.8973570000	19.7528830000
C	0.7918610000	28.8122420000	21.3214030000
C	0.0816610000	29.7979550000	21.9936610000
H	0.3026630000	30.8450400000	21.8308250000
C	-0.8975130000	29.4044540000	22.9045070000
H	-1.4475390000	30.1614530000	23.4509640000
C	-1.1764580000	28.0561550000	23.1224700000
H	-1.9338300000	27.7228410000	23.8190540000
C	-0.4426120000	27.1231060000	22.4096880000
C	-0.5842110000	25.6063230000	22.4415480000
C	3.2915870000	23.9920610000	20.2654610000
H	2.5714420000	23.2724510000	20.6661880000
H	4.0140430000	23.4452990000	19.6491410000
C	4.0013280000	24.6692950000	21.4069590000
C	5.1040900000	24.1006700000	22.0209480000
H	5.5055300000	23.1574580000	21.6699230000
C	5.6723570000	24.7734800000	23.1027530000
H	6.5231670000	24.3476110000	23.6224330000
C	5.1620010000	26.0021880000	23.4815100000
H	5.6062720000	26.5744910000	24.2854120000
C	4.0724860000	26.5329650000	22.7860400000
C	3.5818670000	27.9594070000	22.9611650000
C	0.8496190000	21.3204320000	16.9627480000
H	0.7637670000	21.1331720000	18.0401200000
H	-0.1058150000	21.0666560000	16.4993800000
C	1.9209320000	20.4354540000	16.3641130000
C	2.7632690000	19.6046510000	17.0880360000
H	2.6142210000	19.4890170000	18.1548670000
C	3.7980010000	18.9388210000	16.4294230000
H	4.4613610000	18.2856200000	16.9844780000
C	3.9878540000	19.1420230000	15.0704970000
H	4.7950850000	18.6887530000	14.5109130000
C	3.1030890000	19.9765190000	14.3979170000
C	3.2559440000	20.3544700000	12.9281920000
H	-3.1049290000	24.3108880000	10.7517870000
H	-3.6298890000	22.1552730000	11.9571080000

CuBATA^{2-}

Cu	0.7923600000	-1.1558740000	-1.4701180000
C	-1.5896650000	3.1067180000	0.4152740000

C	-1.1482360000	4.1795340000	-0.3466860000
C	0.1147030000	4.1324990000	-0.9193390000
C	0.9082330000	3.0092710000	-0.7173210000
C	0.4797400000	1.9285140000	0.0515900000
C	-0.8124700000	1.9652180000	0.6344290000
O	-1.4380200000	1.0274350000	1.3844860000
O	1.2498030000	0.8221410000	0.2449240000
C	-0.7978020000	-0.1470090000	1.9371500000
C	-1.8507900000	-1.2301690000	2.1515800000
C	2.6631000000	0.8728030000	0.0465770000
C	3.1197080000	0.4756270000	-1.3555970000
N	-2.2349090000	-1.9375310000	0.9583870000
N	2.9542180000	-0.9615950000	-1.6575850000
N	-0.6943380000	-3.7291830000	-0.9873470000
N	1.0759690000	-2.5505460000	-3.2397470000
C	-2.2851090000	-3.3730090000	0.9511440000
C	-2.0091120000	-3.9996910000	-0.4235410000
C	3.2222110000	-1.2059650000	-3.0969170000
C	2.4968950000	-2.4510240000	-3.6294140000
C	-0.6263790000	-4.2156050000	-2.3573870000
C	0.6925890000	-3.9605130000	-3.0810320000
C	-3.0017450000	-1.2654910000	-0.0620210000
C	-2.1502990000	-1.1311610000	-1.3442890000
C	0.3718670000	-4.1607800000	-0.0945200000
C	0.8033470000	-3.0462790000	0.8600060000
C	0.2092620000	-1.8312970000	-4.1841350000
C	0.4717490000	-0.3214010000	-4.1487600000
C	3.8413270000	-1.7636020000	-0.7573800000
C	4.2586610000	-3.1454300000	-1.3183570000
O	-1.0288400000	-0.5853390000	-1.0927450000
O	-2.5835970000	-1.5478760000	-2.4291080000
O	1.1049640000	-1.9259420000	0.3123730000
O	0.4118110000	0.3339120000	-5.1925800000
O	0.7422060000	0.1519760000	-2.9839570000
O	3.4937010000	-4.1163850000	-1.0920170000
H	-2.5745880000	3.1126030000	0.8688490000
H	-1.7958000000	5.0371800000	-0.4965250000
H	0.4768240000	4.9403830000	-1.5452930000
H	1.8700000000	2.9467970000	-1.2081450000
H	-0.3745190000	0.1438460000	2.9085630000
H	-0.0182030000	-0.5238150000	1.2885280000
H	-1.3868310000	-1.9554480000	2.8250840000
H	-2.7209440000	-0.7869910000	2.6792240000
H	3.0288340000	1.8814200000	0.2696460000
H	3.0617930000	0.1806270000	0.7885970000
H	4.1856080000	0.7517260000	-1.4400470000
H	2.5460420000	1.0247860000	-2.1023740000
H	-3.2849080000	-3.7669200000	1.2520320000
H	-1.5602560000	-3.7461570000	1.6783360000
H	-2.7551390000	-3.6525990000	-1.1426160000
H	-2.1603790000	-5.0953090000	-0.2973790000
H	2.9016750000	-0.3203270000	-3.6396130000
H	4.2962800000	-1.3564600000	-3.2544060000
H	2.5893130000	-2.4423930000	-4.7264780000
H	3.0046910000	-3.3410890000	-3.2680880000
H	-0.7901240000	-5.3143370000	-2.4115450000
H	-1.4537880000	-3.7412680000	-2.8928520000
H	1.5109310000	-4.4472320000	-2.5491860000
H	0.6158050000	-4.4495230000	-4.0690820000
H	-3.9336540000	-1.8075560000	-0.2871240000
H	-3.2577090000	-0.2607320000	0.2834890000

H	1.2747350000	-4.4047640000	-0.6568180000
H	0.0803700000	-5.0461570000	0.4922290000
H	-0.8335140000	-1.9641750000	-3.8789270000
H	0.3506740000	-2.1991330000	-5.2114460000
H	3.3152560000	-1.8954860000	0.1853410000
H	4.7669920000	-1.1915660000	-0.6069400000
O	0.8899400000	-3.2679280000	2.0757040000
O	5.3461820000	-3.1604270000	-1.9594720000
O	5.0932610000	-5.8287320000	-2.7304230000
H	5.4656880000	-4.9220080000	-2.6426930000
H	4.3384970000	-5.6874720000	-2.1276680000

CuBATPy^{2+}

Cu	12.3342840000	4.8236830000	0.9959710000
O	14.2109550000	9.3021200000	0.8809320000
O	12.8430440000	4.9621450000	-1.3270590000
H	13.4600220000	4.3578120000	-1.7599080000
H	12.4687550000	5.5060970000	-2.0323600000
N	12.5270960000	6.8520170000	1.5257650000
N	14.0536810000	4.5616110000	2.1053210000
N	10.3603480000	5.3333420000	0.9038180000
N	12.5130990000	2.8168010000	0.7685450000
C	14.6650420000	12.9763840000	0.8929800000
H	14.1468060000	13.8811900000	0.6031140000
C	14.0534780000	11.7376350000	0.6880140000
H	13.0688420000	11.6960550000	0.2400990000
C	14.7125360000	10.5758400000	1.0547270000
C	12.8732500000	9.1634220000	0.4524760000
H	12.7196550000	9.6381380000	-0.5243840000
H	12.1853130000	9.6373180000	1.1642260000
C	12.6223620000	7.6728250000	0.2850250000
H	11.6858470000	7.5263700000	-0.2574990000
H	13.4331080000	7.2565030000	-0.3129280000
C	13.7199560000	6.9584690000	2.4183390000
H	13.5975660000	7.7679870000	3.1414480000
H	14.5773530000	7.2288370000	1.8077580000
C	13.9429480000	5.6348560000	3.1232430000
H	14.8346370000	5.6855380000	3.7548750000
H	13.0959820000	5.3800540000	3.7652880000
C	15.2662110000	4.6783400000	1.2546790000
H	15.1477980000	5.5416620000	0.5988770000
H	15.2860210000	3.7857140000	0.6266670000
C	11.2699670000	7.1189880000	2.2562590000
H	11.1086180000	8.1914160000	2.3976160000
H	11.3585990000	6.6747760000	3.2519540000
C	10.1000710000	6.4898180000	1.5455020000
C	8.8240070000	7.0319200000	1.5845050000
H	8.6497360000	7.9669710000	2.1022660000
C	7.7827290000	6.3572440000	0.9574140000
H	6.7781540000	6.7612850000	0.9765170000
C	8.0521440000	5.1596800000	0.3050640000
H	7.2715390000	4.6011850000	-0.1940980000
C	9.3531110000	4.6846580000	0.3003300000
H	9.6058340000	3.7562890000	-0.1934810000
C	13.9531610000	3.1949280000	2.6702330000
H	13.2698690000	3.2268190000	3.5234740000
H	14.9257040000	2.8294550000	3.0109320000
C	13.4050340000	2.2703280000	1.6189450000
C	13.7841870000	0.9393730000	1.5226910000
H	14.5412740000	0.5519450000	2.1907840000

C	13.2057220000	0.1426490000	0.5425280000
H	13.4841640000	-0.8997460000	0.4491980000
C	12.2802830000	0.7073380000	-0.3293100000
H	11.8145370000	0.1245290000	-1.1129380000
C	11.9712410000	2.0498670000	-0.1903670000
H	11.2888630000	2.5423620000	-0.8706210000
O	16.5314470000	9.4299340000	1.9919590000
N	18.6059210000	7.1177990000	2.1783400000
N	17.7482460000	4.5513780000	1.2547290000
N	18.7592790000	5.2897800000	4.2523660000
N	17.1282030000	1.7085140000	2.5931640000
C	15.9262930000	13.0389400000	1.4599450000
H	16.4078610000	13.9955140000	1.6172460000
C	16.5903210000	11.8698490000	1.8355950000
H	17.5749780000	11.9331380000	2.2784620000
C	15.9876250000	10.6340100000	1.6428270000
C	17.7715680000	9.4431930000	2.7084110000
H	17.6709350000	10.0903270000	3.5861990000
H	18.5732380000	9.8300680000	2.0707100000
C	18.0496930000	8.0160250000	3.1639000000
H	18.7522990000	8.0582300000	3.9970030000
H	17.1117310000	7.6187200000	3.5807220000
C	18.0044070000	6.9965320000	0.8729980000
H	18.4598800000	7.6640100000	0.1234000000
H	16.9673320000	7.3262740000	0.9649120000
C	18.0574250000	5.5768380000	0.2795820000
H	17.3834800000	5.5770560000	-0.5967710000
H	19.0543360000	5.3609820000	-0.1136790000
C	16.5783440000	4.7757710000	2.0630210000
H	16.6795390000	5.7494010000	2.5390280000
H	16.5730300000	4.0334140000	2.8596910000
C	19.8874720000	6.5277390000	2.4511480000
H	20.6671470000	7.2958260000	2.5769900000
H	20.1905020000	5.9372880000	1.5843470000
C	19.9179690000	5.6247280000	3.6787070000
C	21.1499380000	5.1851390000	4.1663160000
H	22.0695190000	5.4962560000	3.6828350000
C	21.1801180000	4.3609730000	5.2814340000
H	22.1242520000	4.0111930000	5.6819700000
C	19.9763970000	4.0058870000	5.8812970000
H	19.9485550000	3.3737090000	6.7597810000
C	18.8023230000	4.4976690000	5.3296810000
H	17.8430480000	4.2497950000	5.7752890000
C	17.9682270000	3.1715410000	0.8372930000
H	18.8488690000	3.1647830000	0.1926310000
H	17.1310480000	2.7571240000	0.2515240000
C	18.2063920000	2.2800380000	2.0321220000
C	19.4922730000	2.0995990000	2.5351350000
H	20.3329830000	2.5877190000	2.0582150000
C	19.6781980000	1.2902420000	3.6462640000
H	20.6699950000	1.1290870000	4.0498790000
C	18.5676540000	0.6910210000	4.2284840000
H	18.6623750000	0.0467510000	5.0932190000
C	17.3212530000	0.9358580000	3.6700910000
H	16.4319310000	0.4877360000	4.1047890000

CuBATPic^{2-}

Cu	1.5212760000	26.1690650000	20.7374420000
C	-1.2767180000	23.7550670000	12.3435780000
H	-1.1820730000	24.8333950000	12.2654600000

C	-2.5024520000	23.1177020000	12.1595350000
C	-2.5584260000	21.7390960000	12.2619150000
O	-2.5042190000	18.9888570000	12.1974050000
N	-0.2245690000	21.6442880000	12.7725670000
H	3.5355160000	22.9798170000	13.9739940000
H	3.3298360000	25.2816110000	12.9001140000
H	4.7144170000	25.0575780000	14.0035720000
C	4.1940520000	27.8159290000	13.2824710000
H	4.5949450000	27.0508950000	12.6315860000
C	4.4382970000	29.1644650000	13.0097000000
H	5.0244860000	29.4308370000	12.1376430000
C	1.1898840000	23.6047360000	12.8680400000
H	1.9313920000	23.0105700000	12.3256920000
H	1.1744830000	24.6217350000	12.4266860000
C	-0.1656000000	22.9749970000	12.6466670000
C	-1.3936600000	21.0246690000	12.5772660000
C	-1.4632700000	19.4838040000	12.6970370000
O	2.2473800000	27.9981350000	16.3249320000
O	3.1471310000	26.1853280000	14.7568820000
O	-1.5532130000	26.3069470000	23.2879350000
O	-0.1323700000	25.5815990000	21.6929490000
O	2.8805230000	27.2780240000	23.8807240000
O	4.5072960000	28.3575330000	22.7222050000
O	4.8277000000	22.8465270000	17.9553990000
O	6.4501850000	21.6056630000	16.9849280000
O	-0.5763810000	18.9462120000	13.3925640000
N	2.4441390000	27.5994430000	19.4281070000
N	1.9448080000	24.8004300000	19.3201200000
N	0.1896660000	22.5151500000	16.8727650000
N	1.5896660000	23.6200260000	14.2642550000
N	1.1369970000	27.8125260000	21.6413270000
N	3.3728200000	25.4254250000	21.6233510000
N	2.9352380000	21.3772290000	16.6564020000
C	3.9413740000	30.1487580000	13.8455520000
H	4.1279460000	31.1959550000	13.6379590000
C	3.1946120000	29.7921580000	14.9732280000
H	2.8038180000	30.5617850000	15.6265960000
C	2.9494640000	28.4565020000	15.2514430000
C	1.8739070000	28.9177650000	17.3411080000
H	2.7298330000	29.5460470000	17.6168640000
H	1.0711620000	29.5715680000	16.9772050000
C	1.3873090000	28.0916630000	18.5245660000
H	0.8216470000	27.2427130000	18.1381610000
H	0.7049170000	28.6885220000	19.1327780000
C	3.4736520000	26.7430750000	18.8020040000
H	3.9757140000	27.2374100000	17.9635730000
H	4.2191360000	26.5411720000	19.5686440000
C	2.8396780000	25.4511020000	18.2941280000
H	3.6213600000	24.7457160000	17.9888750000
H	2.2352130000	25.6741360000	17.4167910000
C	0.7251700000	24.2196330000	18.6742510000
H	0.0274930000	23.9427100000	19.4665110000
H	0.2654180000	25.0167020000	18.0841160000
C	1.1589630000	23.0360800000	17.8155650000
H	1.4301490000	22.2092340000	18.4713070000
H	2.1066880000	23.3091870000	17.3385020000
C	-0.3210750000	23.4584260000	15.8898660000
H	-0.9077830000	22.8927830000	15.1666630000
H	-1.0213020000	24.1419380000	16.3952460000
C	0.7001850000	24.3452160000	15.1588660000
H	0.1457720000	25.1319650000	14.6208130000

H	1.3112370000	24.8660490000	15.8961390000
C	3.0127530000	23.8049570000	14.4679040000
H	3.2369750000	23.7158280000	15.5328440000
C	3.6205820000	25.0998090000	13.9407150000
C	3.4463340000	27.4473380000	14.3951530000
C	2.9295640000	28.6642820000	20.3293770000
H	3.8587530000	28.3433390000	20.8114970000
H	3.1345600000	29.5995900000	19.7936990000
C	1.8981920000	28.8799920000	21.4179530000
C	1.7098090000	30.0159820000	22.1900400000
H	2.3391630000	30.8855070000	22.0493720000
C	0.7206070000	29.9911850000	23.1705070000
H	0.5732050000	30.8631130000	23.7981500000
C	-0.0726050000	28.8628890000	23.3551730000
H	-0.8546170000	28.8119850000	24.1007740000
C	0.1705690000	27.7621360000	22.5517090000
C	-0.5867550000	26.4414370000	22.5448260000
C	2.7101700000	23.7335880000	20.0311570000
H	1.9937640000	23.1898250000	20.6545100000
H	3.1817790000	23.0582910000	19.3082760000
C	3.7636900000	24.3582110000	20.8977190000
C	5.0588410000	23.8697160000	20.9100220000
H	5.3260250000	23.0662390000	20.2316330000
C	5.9845020000	24.5135390000	21.7306540000
H	7.0148230000	24.1737690000	21.7553550000
C	5.5899540000	25.6190580000	22.4646340000
H	6.2892340000	26.1875030000	23.0645980000
C	4.2658380000	26.0637280000	22.3914130000
C	3.8427230000	27.3523260000	23.0968520000
C	0.5399470000	21.1663110000	16.3838970000
H	0.4020130000	20.4827660000	17.2327460000
H	-0.1772180000	20.8826020000	15.6132340000
C	1.9524990000	20.9507110000	15.8586800000
C	2.2017040000	20.3256250000	14.6360250000
H	1.3773230000	20.0049400000	14.0049550000
C	3.5339710000	20.1388930000	14.2770840000
H	3.7709300000	19.6357390000	13.3433820000
C	4.5548400000	20.6150910000	15.0967550000
H	5.6037840000	20.5111330000	14.8467890000
C	4.2108450000	21.2700750000	16.2790640000
C	5.2674500000	21.9669690000	17.1534410000
H	-3.3938660000	23.6968210000	11.9337320000
H	-3.4641660000	21.1691080000	12.0990900000