Supporting Information for:

Structure-Function Relationship within Cu-peptoid Electrocatalysts for Water Oxidation

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Supporting Figures:

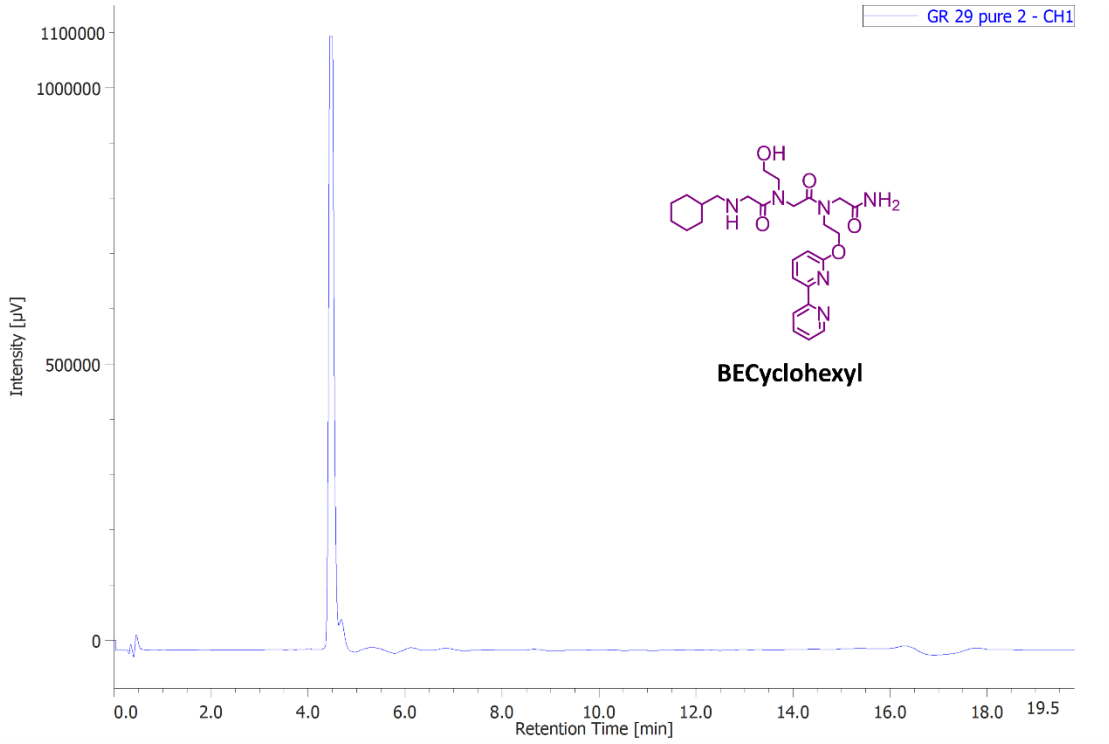


Figure S1. Analytical HPLC of preparative peptoid **BECyclohexyl**.

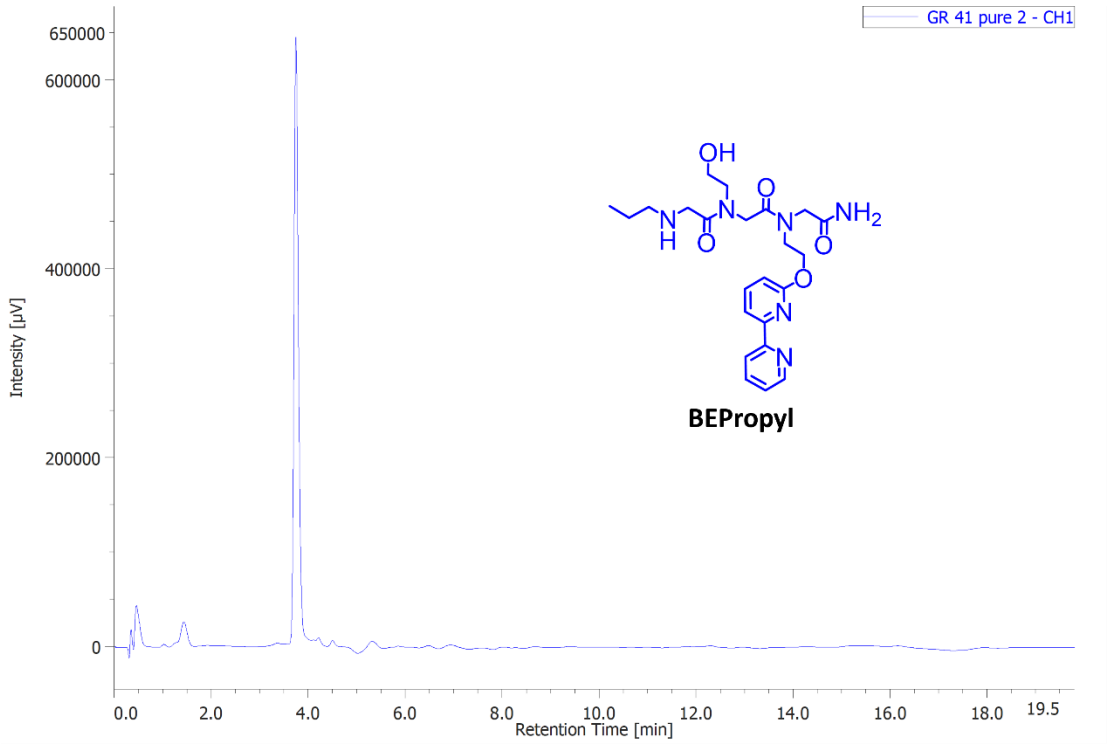


Figure S2. Analytical HPLC of preparative peptoid **BEPropyl**.

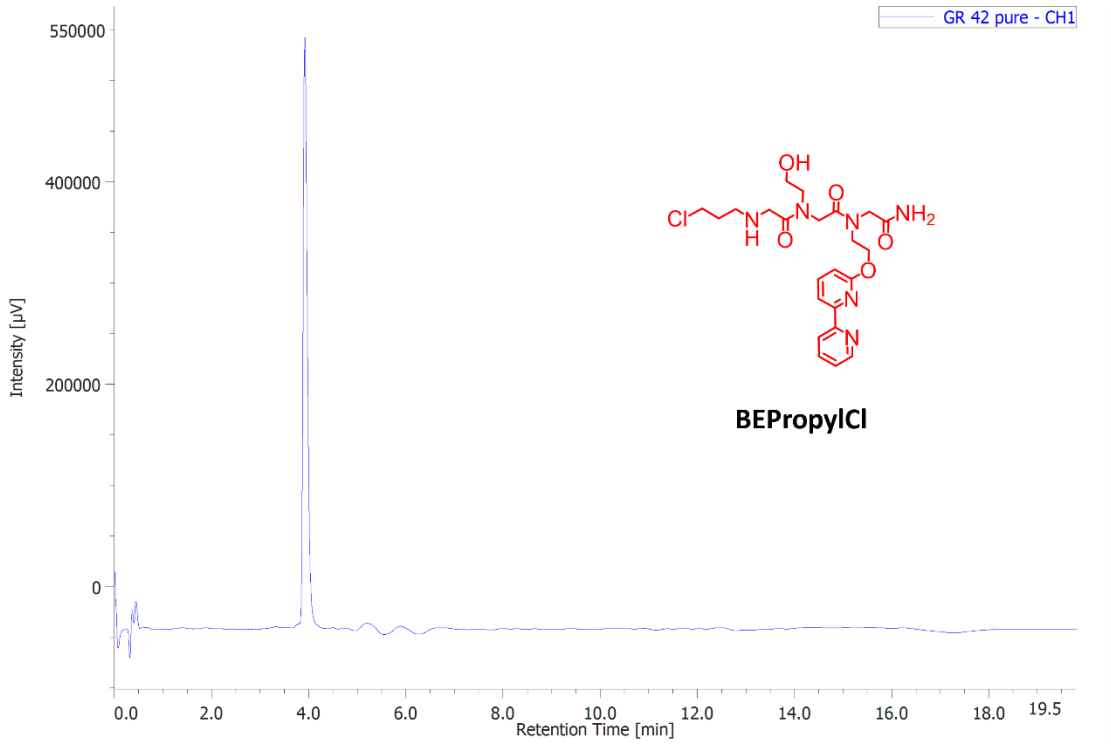


Figure S3. Analytical HPLC of preparative peptoid **BEPropylCl**.

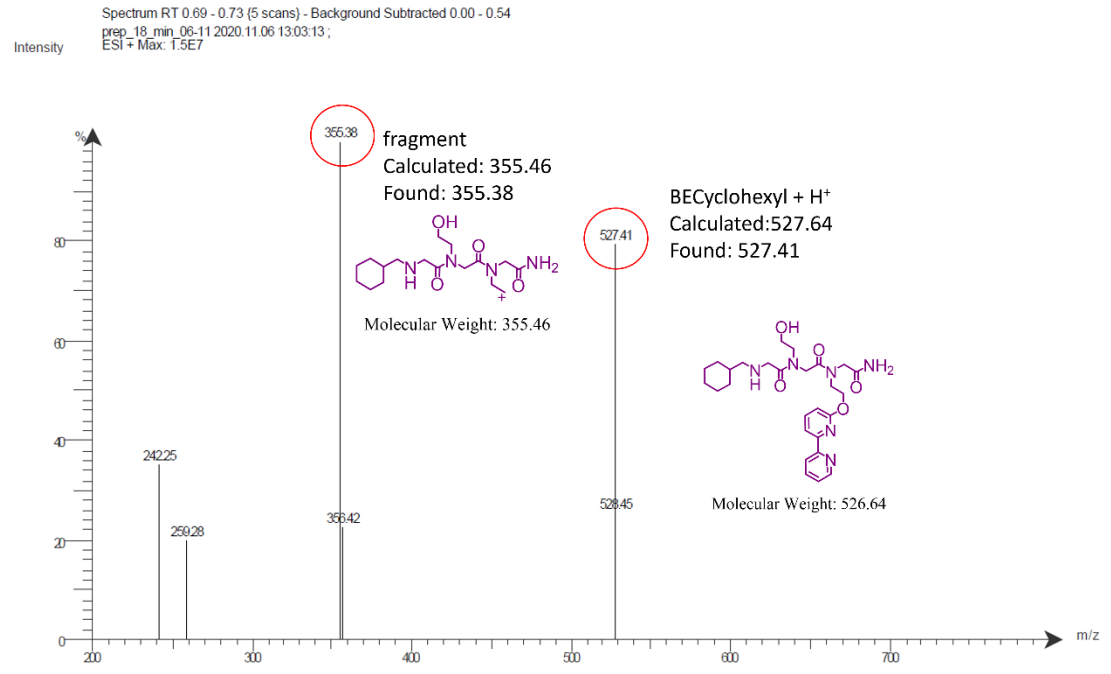


Figure S4. ESI-MS of preparative peptoid **BECyclohexyl**.

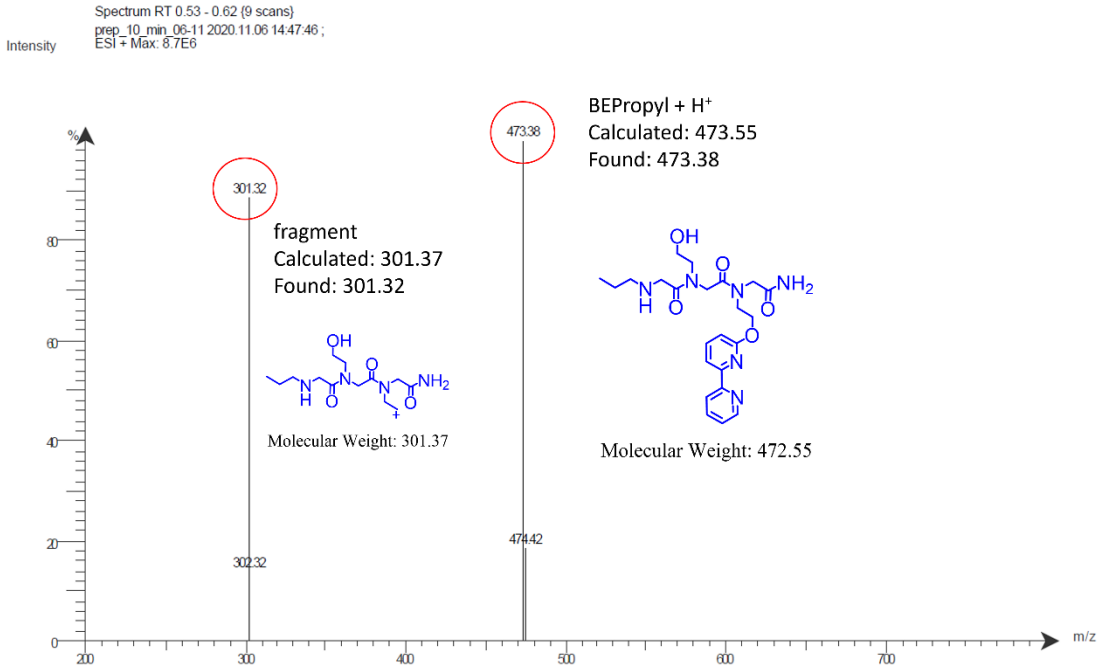


Figure S5. ESI-MS of preparative peptoid **BEPropyl**.

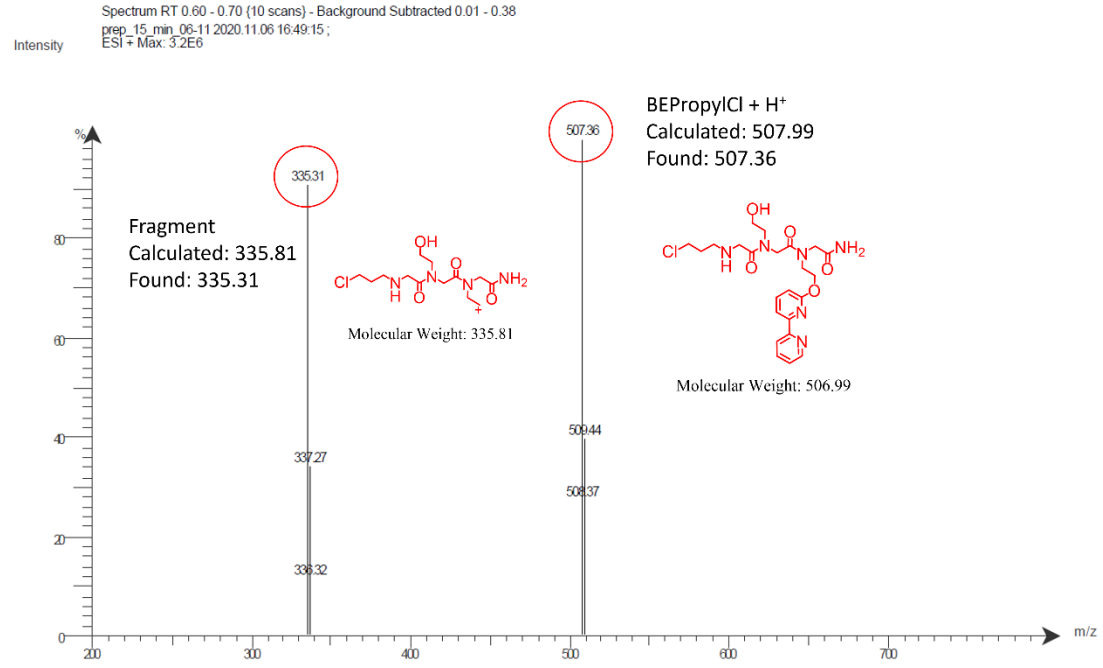


Figure S6. ESI-MS of preparative peptoid **BEPropylCl**.

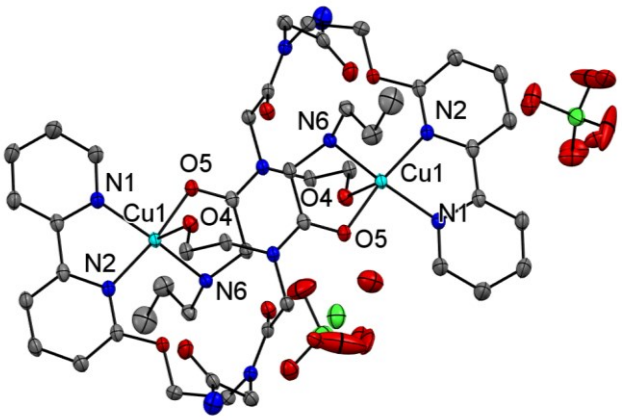


Figure S7. Crystal structure of complex Cu_2(**BEPropyl**)$_2$, hydrogen atoms are omitted for clarity.

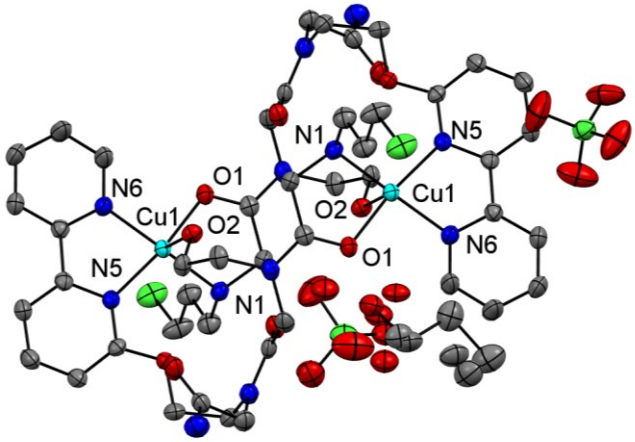


Figure S8. Crystal structure of complex Cu_2(**BEPropylCl**)$_2$, hydrogen atoms are omitted for clarity.

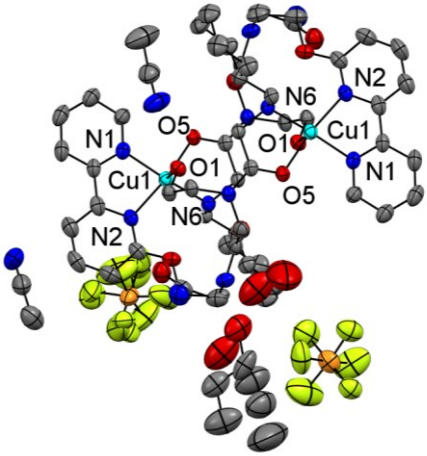


Figure S9. Crystal structure of complex Cu_2(**BECyclohexyl**)$_2$, hydrogen atoms are omitted for clarity.

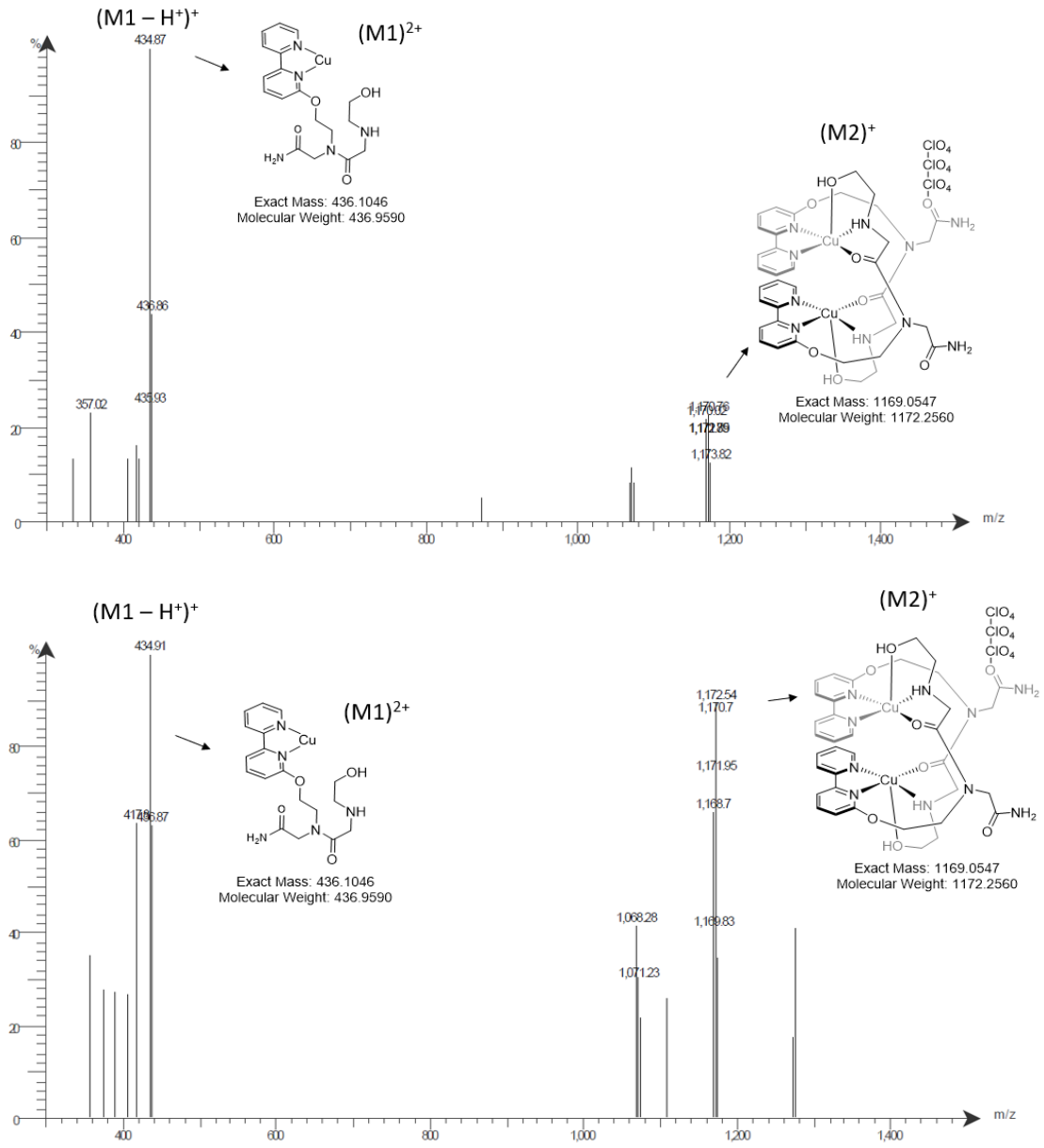


Figure S10. ESI-MS of isolated crystal re-dissolved in water, $\{[Cu_2(\mathbf{BE})_2](ClO_4)_3\}^+$. Top: ESI voltage = 3500 V; down: ESI voltage = 1500 V. **In ESI-MS, we observed the mass of both monomer (M1) and dimer (M2). However, in further study of this work, we understand that the self-assembled di-nuclear structure is possible to dissociate in specific conditions, but not in pure water which is the condition of this measurement. Since the flow of the ESI-MS instrument contains ACN with 0.1% formic acid, as well as high capillary temperature 250 ºC and high ESI voltage 3500 V, the dimer structure is very likely to be decomposed under such extreme conditions. To simply prove it, we decrease the ESI voltage from 3500 V (Top) to 1500 V (down) for another measurement. The ratio of the intensity between dimer and monomer increased from ~0.25 (~25% vs. 100%) to 0.9 (~90% vs. 100%). Therefore, the monomer signal seems inevitable, but it is mostly generated by the process of the ESI-MS measurement.*

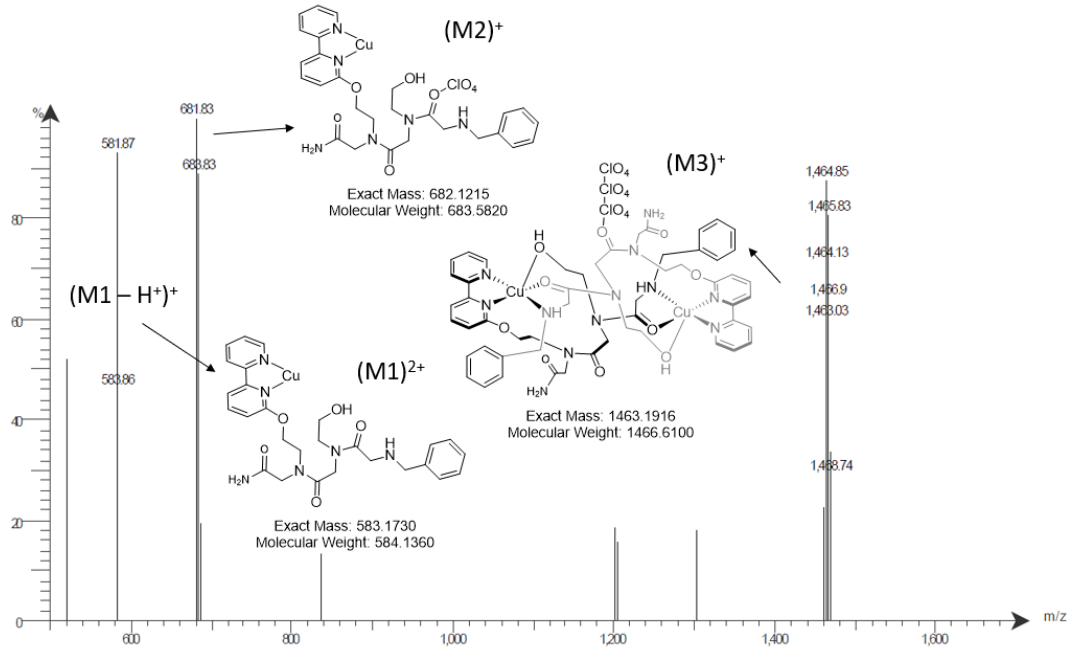


Figure S11. ESI-MS of isolated crystal re-dissolved in water, $\{[Cu_2(\mathbf{BEBenzyl})_2](ClO_4)_3\}^+$.

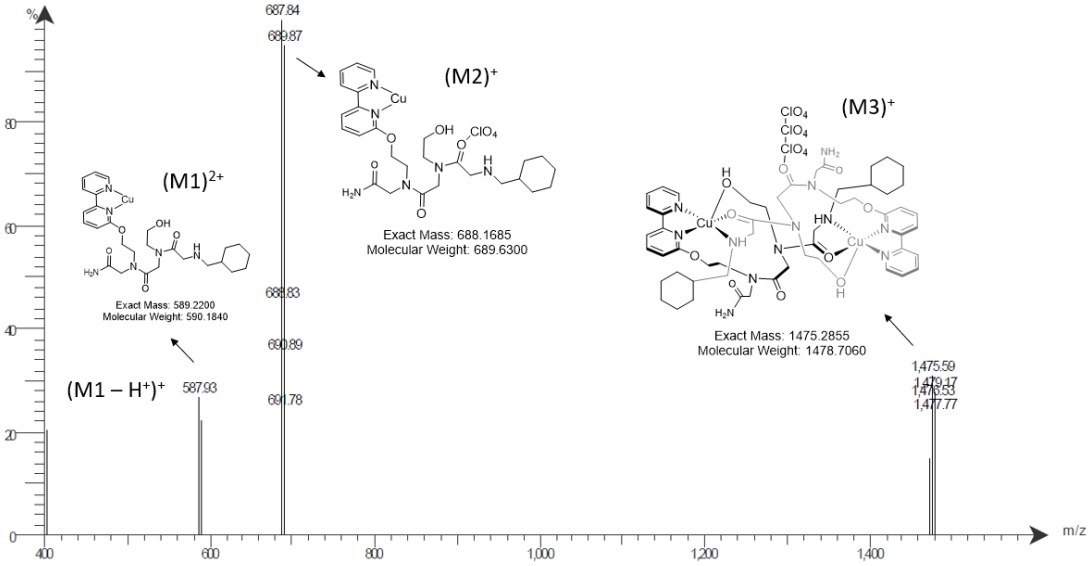


Figure S12. ESI-MS of isolated crystal re-dissolved in water, $\{[Cu_2(\mathbf{BECyclohexyl})_2](ClO_4)_3\}^+$.

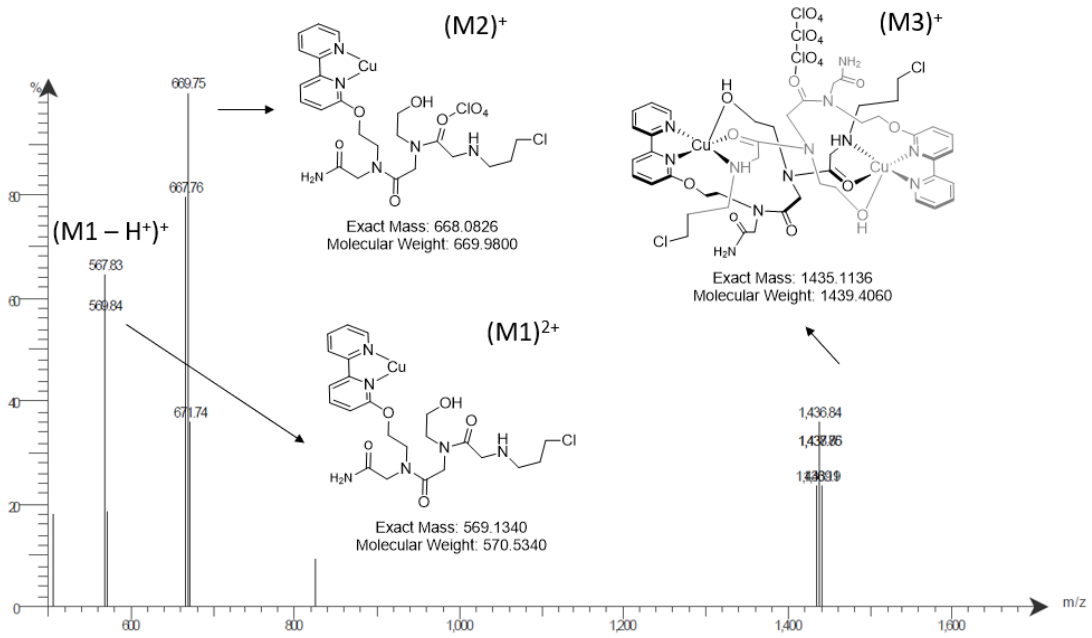


Figure S13. ESI-MS of isolated crystal re-dissolved in water, $\{[Cu_2(\mathbf{BEPropylCl})_2](ClO_4)_3\}^+$.

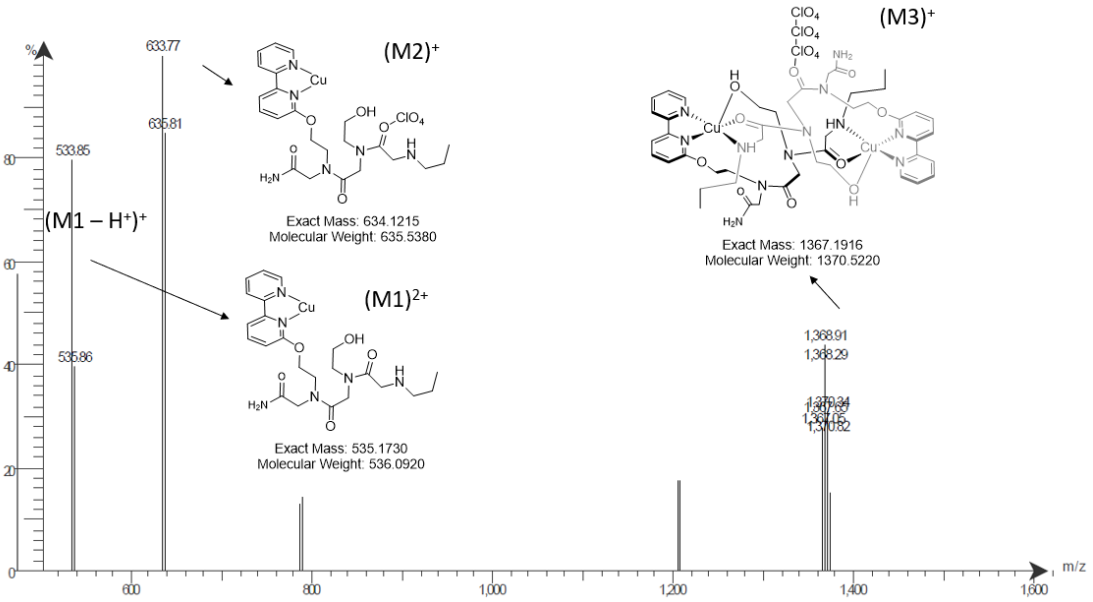


Figure S14. ESI-MS of isolated crystal re-dissolved in water, $\{[Cu_2(\mathbf{BEPropyl})_2](ClO_4)_3\}^+$.

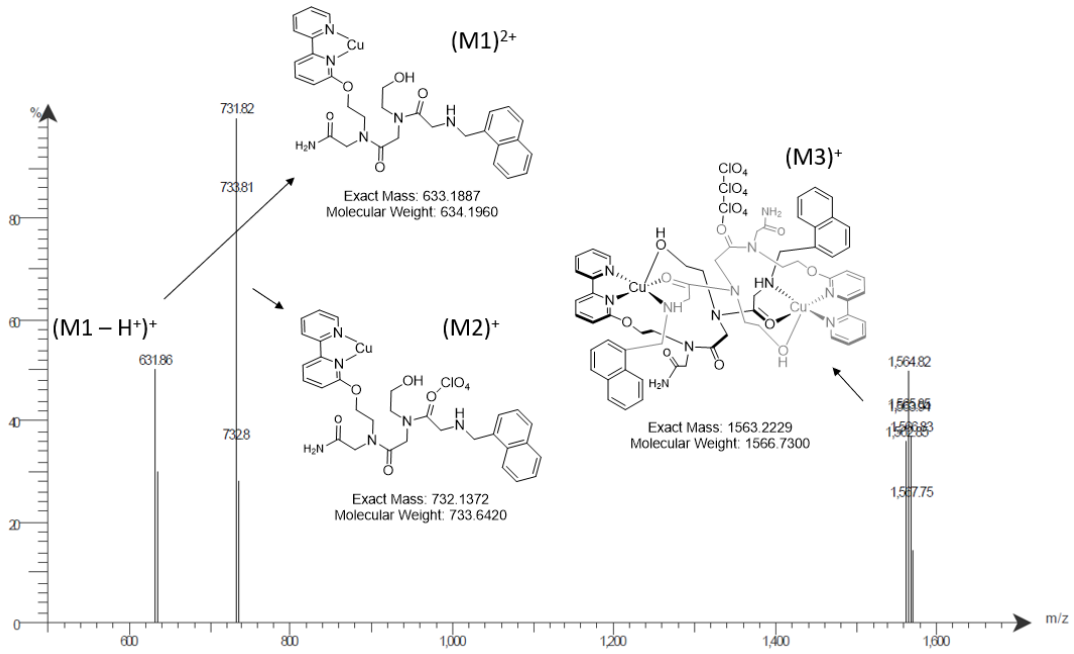


Figure S15. ESI-MS of isolated crystal re-dissolved in water, $\{[Cu_2(\mathbf{BENapthyl})_2](ClO_4)_3\}^+$.

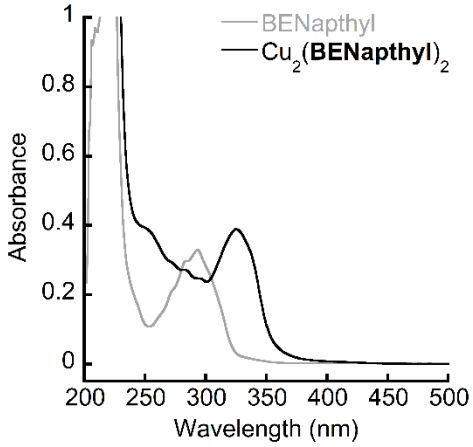


Figure S16. UV-Vis of 20 µM BENapthyl and 20 µM complex Cu_2(**BENapthyl**)$_2$ in water.

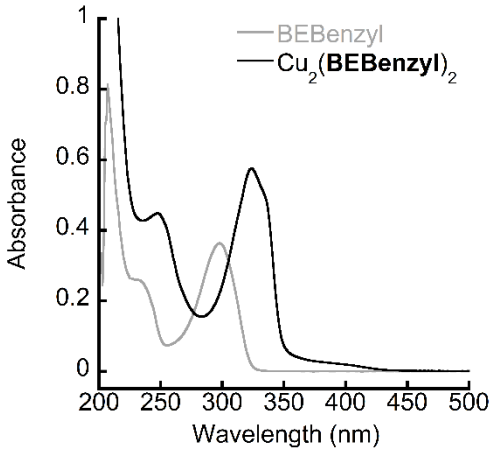


Figure S17. UV-Vis of 20 µM BEBenzyl and 20 µM complex Cu_2(**BEBenzyl**)$_2$ in water.

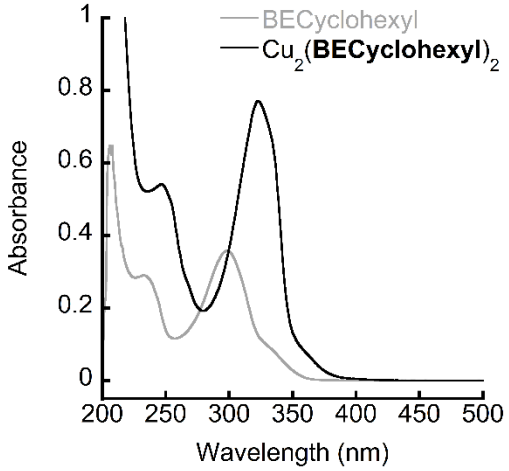


Figure S18. UV-Vis of 20 µM BECyclohexyl and 20 µM complex Cu_2(**BECyclohexyl**)$_2$ in water.

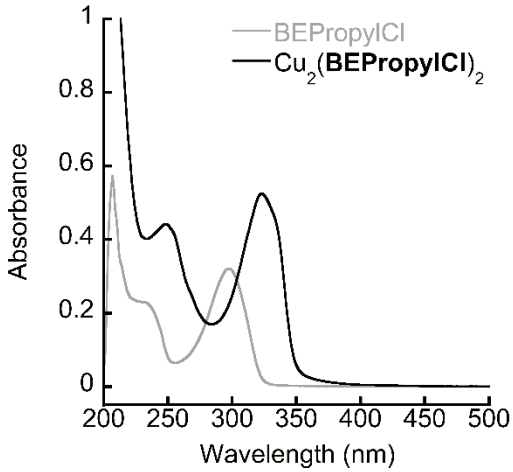


Figure S19. UV-Vis of 20 µM BEPropylCl and 20 µM complex Cu_2(**BEPropylCl**)$_2$ in water.

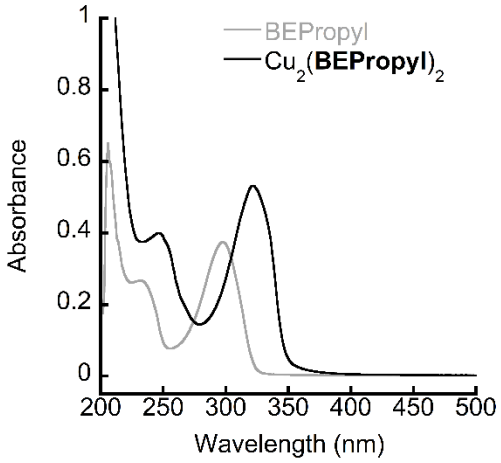


Figure S20. UV-Vis of 20 µM BEPropyl and 20 µM complex Cu_2(**BEPropyl**)$_2$ in water.

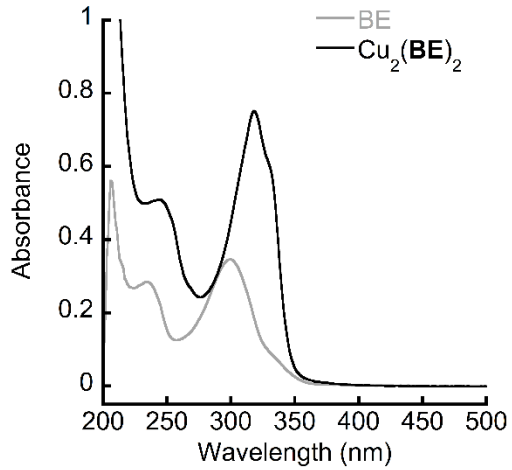


Figure S21. UV-Vis of 20 µM BE and 20 µM complex Cu_2(**BE**)$_2$ in water.

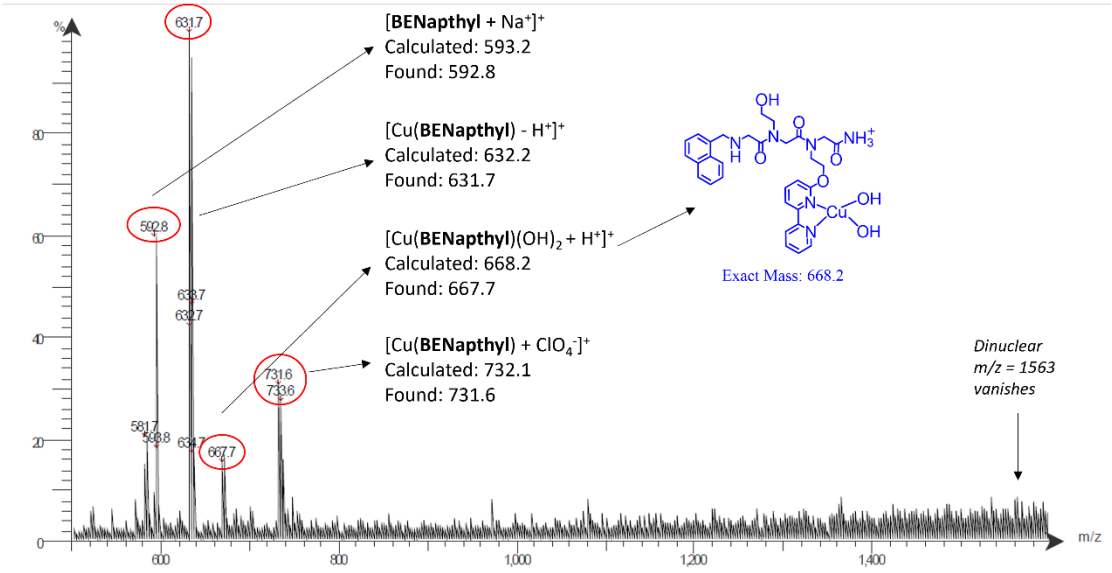


Figure S22. ESI-MS of Cu**BENapthyl** in 0.1 M PBS at pH 11.

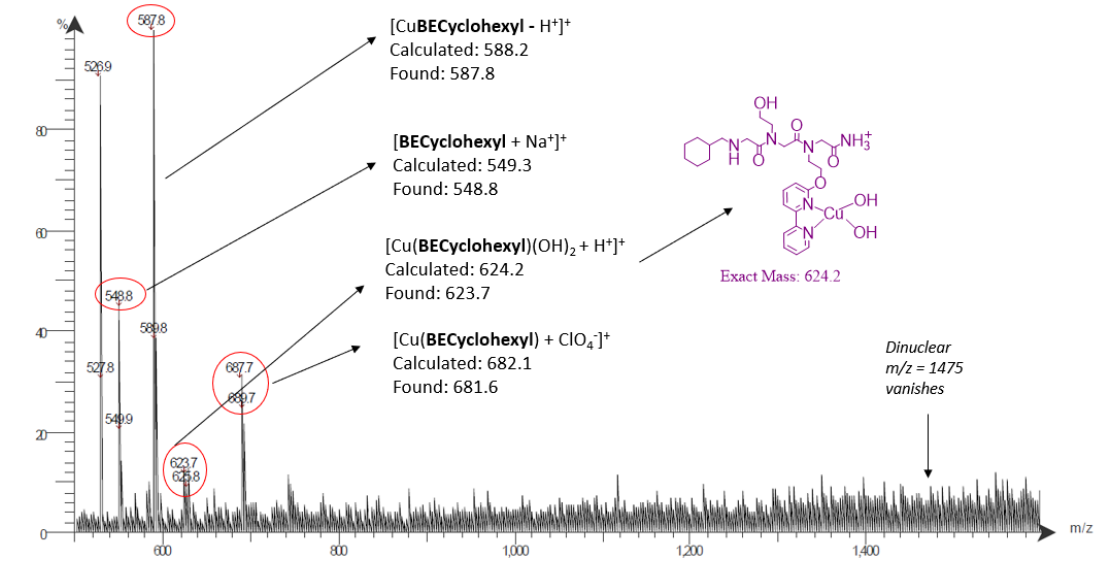


Figure S23. ESI-MS of Cu**BECyclohexyl** in 0.1 M PBS at pH 11.

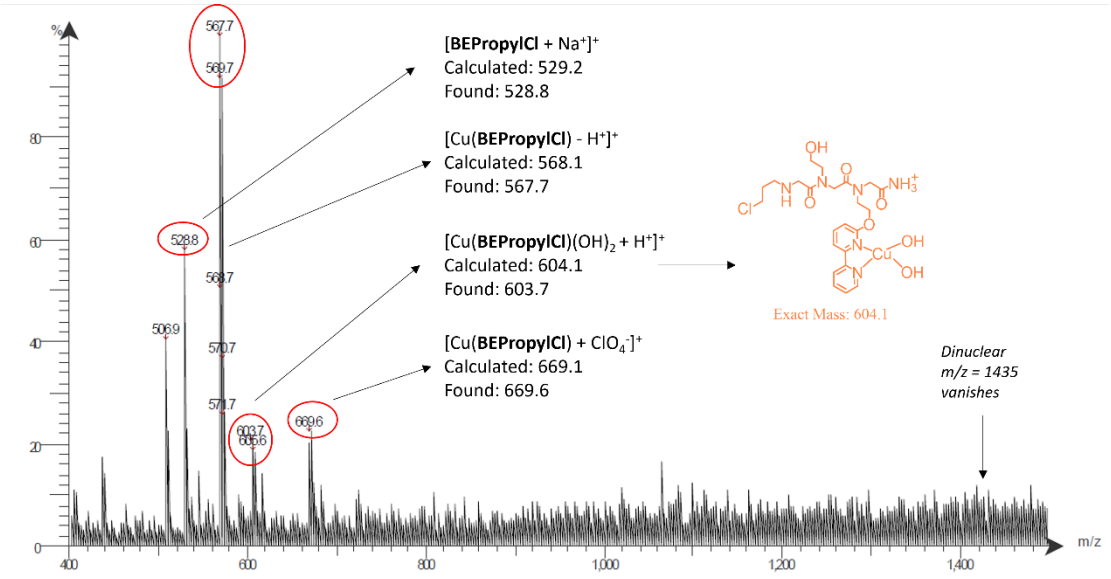


Figure S24. ESI-MS of Cu**BEPropylCl** in 0.1 M PBS at pH 11.

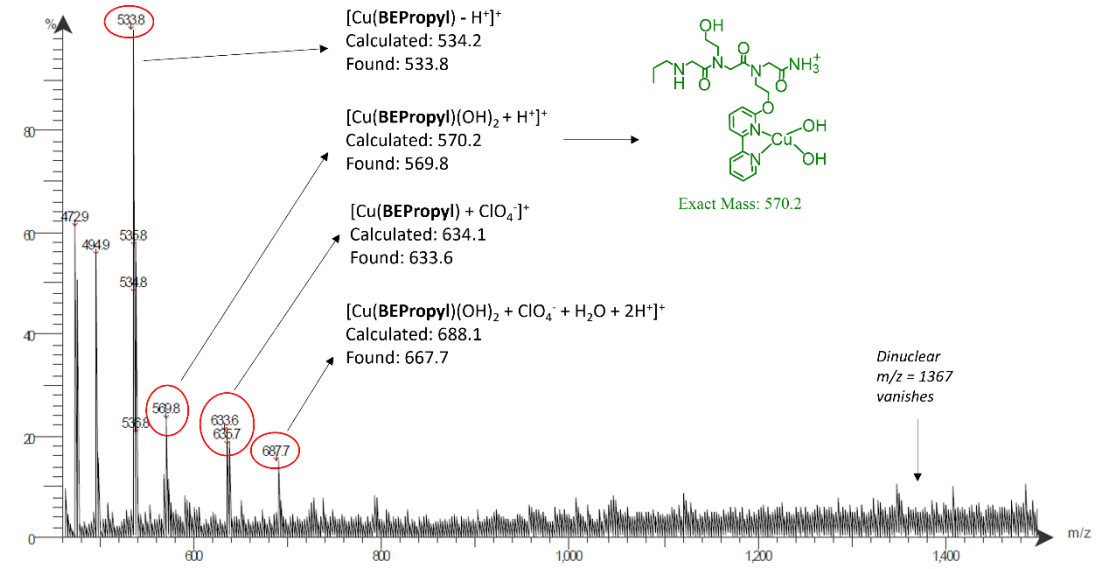


Figure S25. ESI-MS of Cu**BEPropyl** in 0.1 M PBS at pH 11.

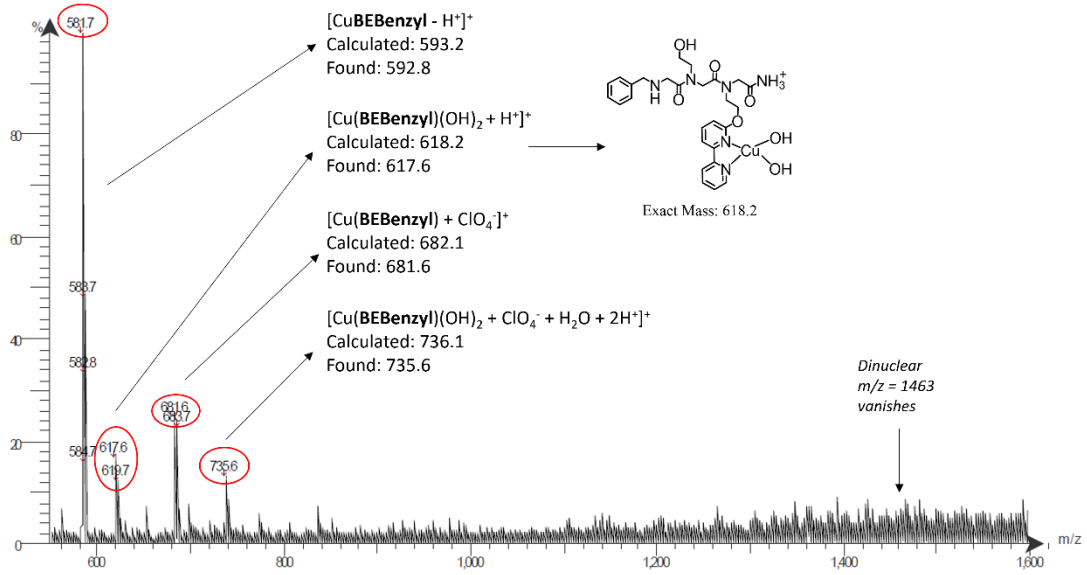


Figure S26. ESI-MS of Cu**BEBenzyl** in 0.1 M PBS at pH 11.

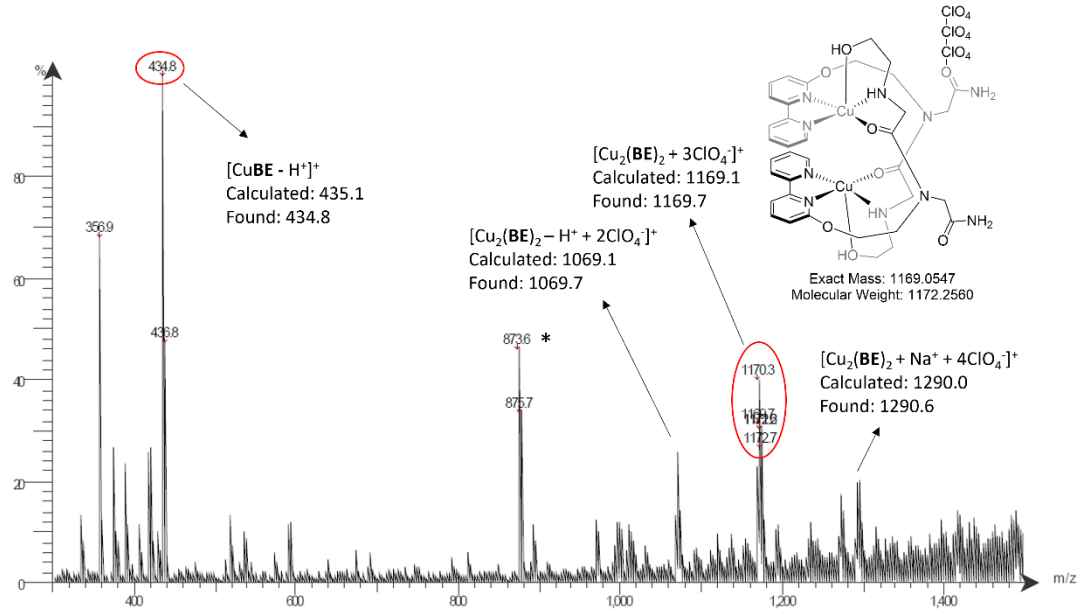


Figure S27. ESI-MS of Cu_2(**BE**)$_2$ in 0.1 M PBS at pH 11. *The mass signal marked with "*" is an unknown species. We suspected that it could be* $[Cu_2(\mathbf{BE})_2]^{4+}$ *whose calculated m/z is 872.2, but since ESI-MS present +1 signal, this hypothesis should be eliminated.*

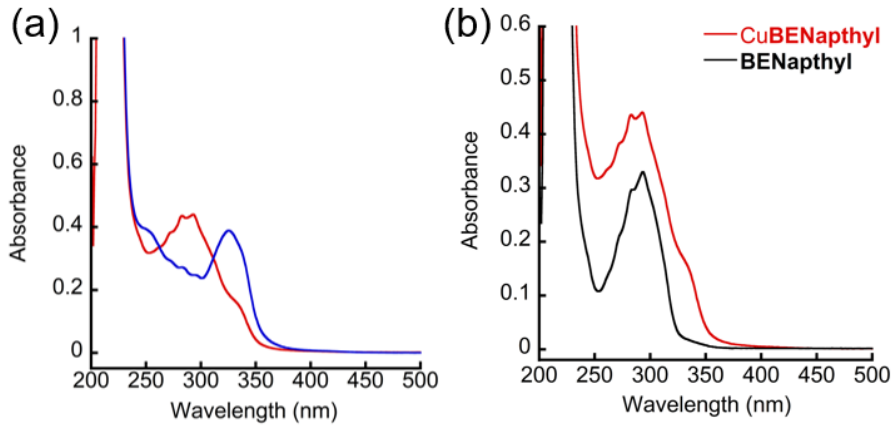


Figure S28. (a). UV-Vis of solid Cu_2(**BENapthyl**)$_2$ dissolved in water (blue line) and 0.1 M PBS at pH 11 (red line); (b) UV-Vis of comparison between ligand and complex in 0.1 M PBS at pH 11. All the concentrations are consistent with 20 μM.

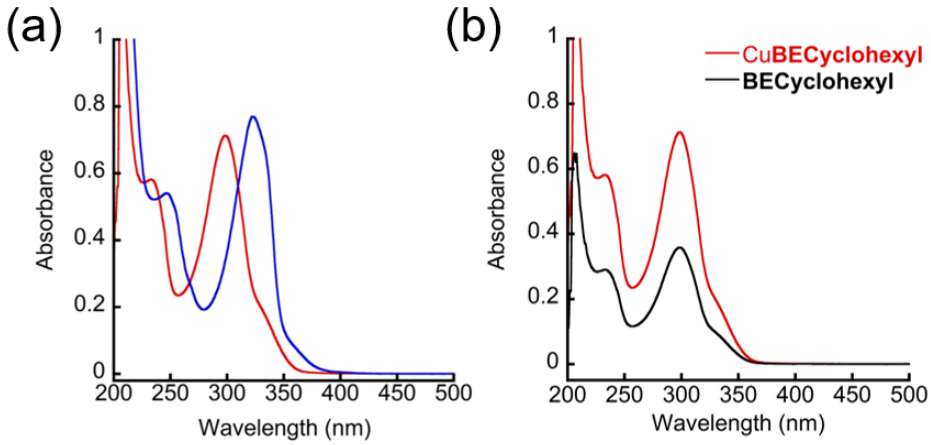


Figure S29. (a)UV-Vis of solid Cu_2(**BECyclohexyl**)$_2$ dissolved in water (blue line) and 0.1 M PBS at pH 11 (red line); (b) UV-Vis of comparison between ligand and complex in 0.1 M PBS at pH 11. All the concentrations are consistent with 20 μM.

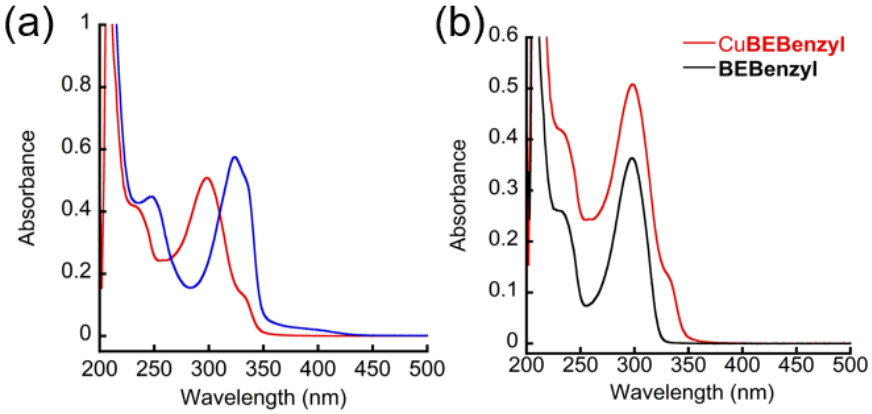


Figure S30. (a) UV-Vis of solid Cu_2(**BEBenzyl**)$_2$ dissolved in water (blue line) and 0.1 M PBS at pH 11 (red line). (b) UV-Vis of comparison between ligand and complex in 0.1 M PBS at pH 11. All the concentrations are consistent with 20 μM.

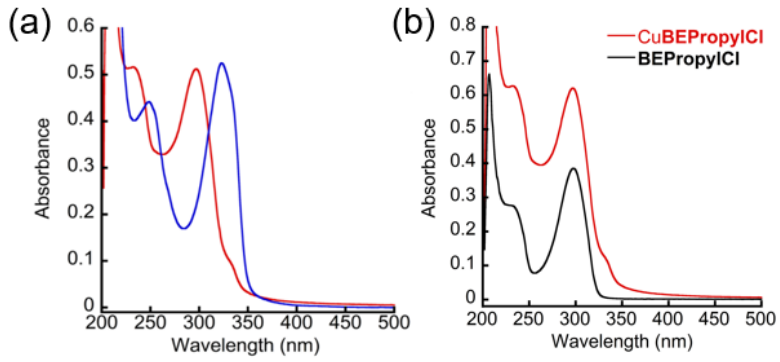


Figure S31. (a) UV-Vis of solid Cu_2(**BEPropylCl**)$_2$ dissolved in water (blue line) and 0.1 M PBS at pH 11 (red line). (b) UV-Vis of comparison between ligand and complex in 0.1 M PBS at pH 11. All the concentrations are consistent with ~ 20 μM.

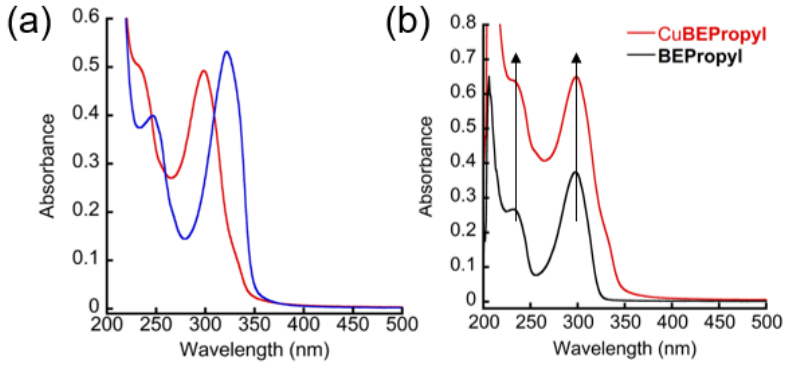


Figure S32. (a) UV-Vis of solid Cu_2(**BEPropyl**)$_2$ dissolved in water (blue line) and 0.1 M PBS at pH 11 (red line). (b) UV-Vis of comparison between ligand and complex in 0.1 M PBS at pH 11. All the concentrations are consistent with ~ 20 μM.

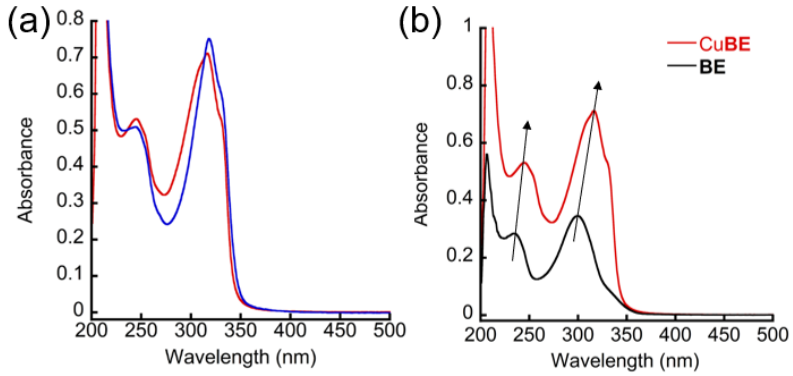


Figure S33. (a) UV-Vis of solid Cu_2(**BE**)$_2$ dissolved in water (blue line) and 0.1 M PBS at pH 11 (red line). (b) UV-Vis of comparison between ligand and complex in 0.1 M PBS at pH 11. All the concentrations are consistent with ~ 20 μM.

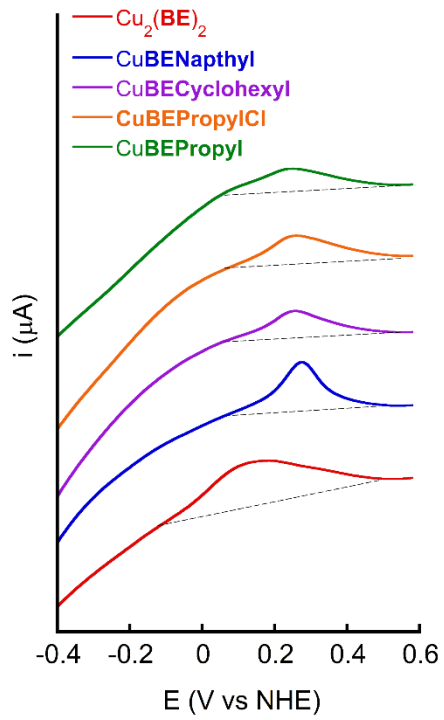


Figure S34. CV scans of 0.5 mM different catalysts under the same conditions that in 0.1 M PBS at pH 11 using glassy carbon as working electrode at scan rate 100 mV/s.

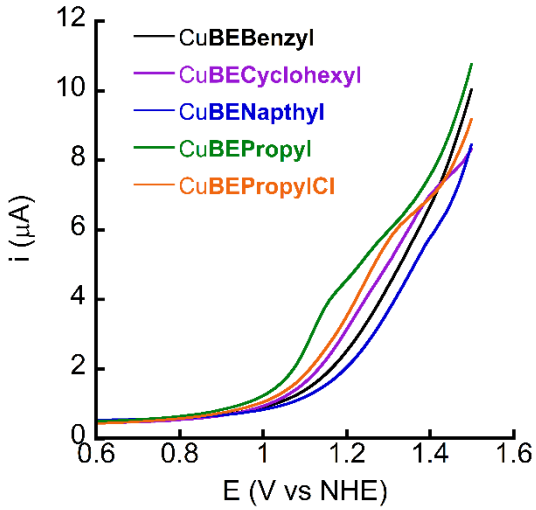


Figure S35. DPVs of 0.1 M phosphate buffer solution at pH 11 in the presence of 0.5 mM Cu**BENapthyl**, Cu**BECyclohexyl**, Cu**BEBenzyl**, Cu**BEPropylCl**, and Cu**BEPropyl**.

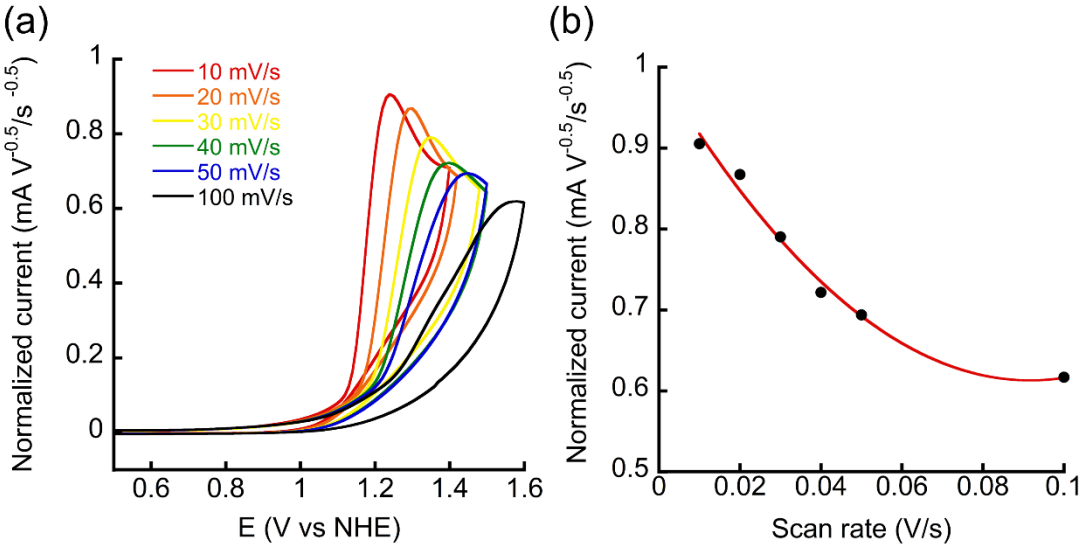


Figure S36. (a) Normalized CVs from the CVs of 0.5 mM Cu_2(**BE**)$_2$ at different scan rates in 0.1 M PBS at pH 11.0. (b) The normalized current of the catalytic peak versus corresponding scan rates. The normalized current is reverse dependent on the scan rate, indicating a catalytic behavior happens.

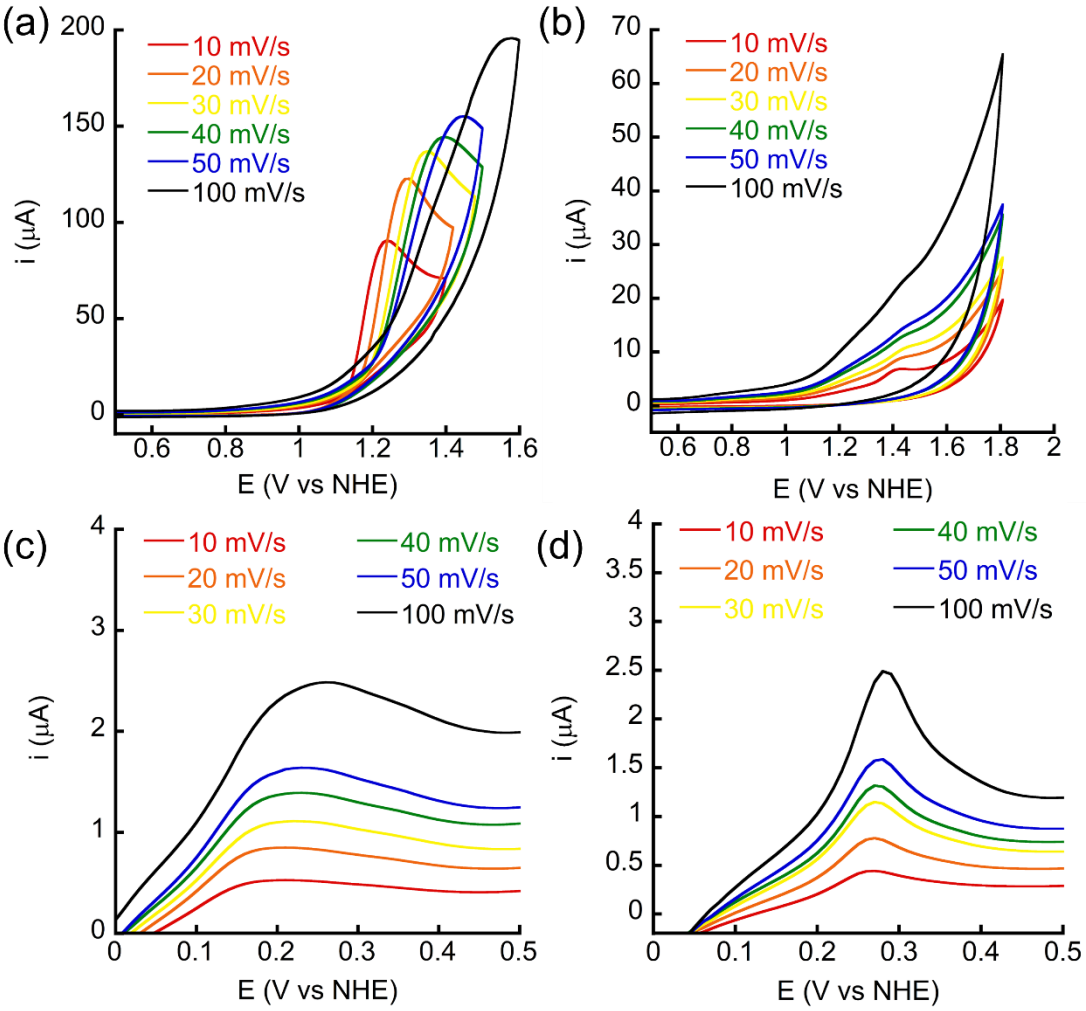


Figure S37. CVs of (a & c) 0.5 mM Cu_2(**BE**)$_2$ or (c & d) 0.5 mM Cu**BENapthyl** in 0.1 M PBS at pH 11 at various scan rates.

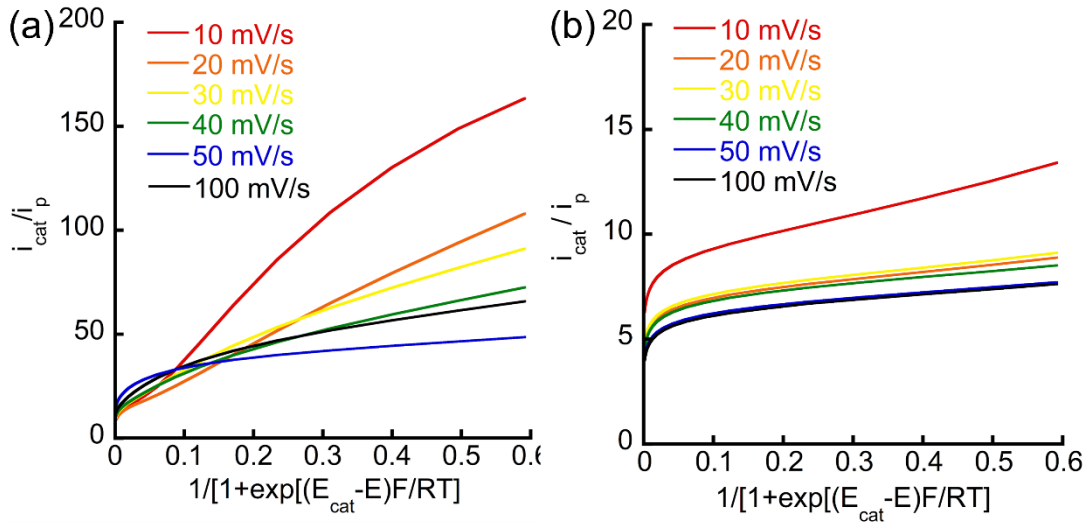


Figure S38. The experimental data of CVs of (a) 0.5 mM Cu_2(**BE**)$_2$ or (b) 0.5 mM Cu**BENapthyl** in 0.1 M PBS at pH 11 used for FOWA at various scan rates. The data are extracted for Figure 3b.

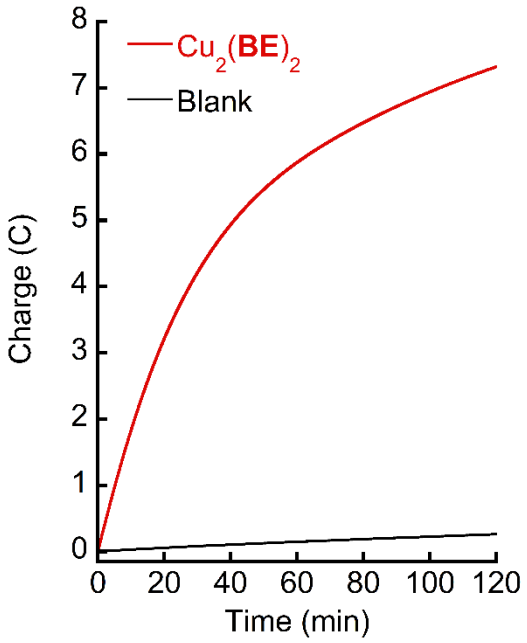


Figure S39. Accumulated charge of the CPE experiments using 0.5 mM Cu_2(**BE**)$_2$ or without any catalyst as blank in 0.1 M PBS at pH 11 using ITO as working electrode at applied potential +1.25 V vs NHE.

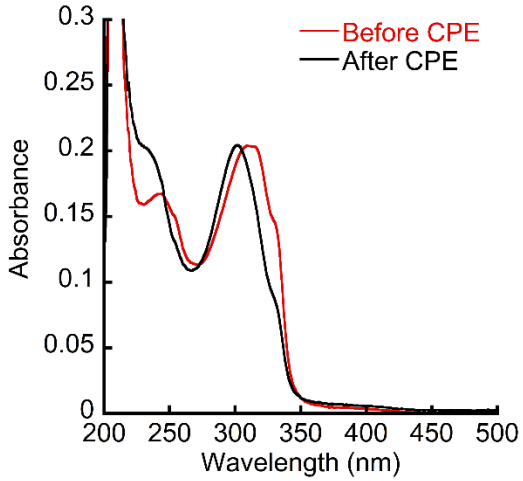


Figure S40. UV-Vis of 0.5 mM Cu_2(**BE**)$_2$ in 0.1 M PBS at pH 11 before and after the CPE experiment using ITO as working electrode at applied potential +1.25 V vs NHE.

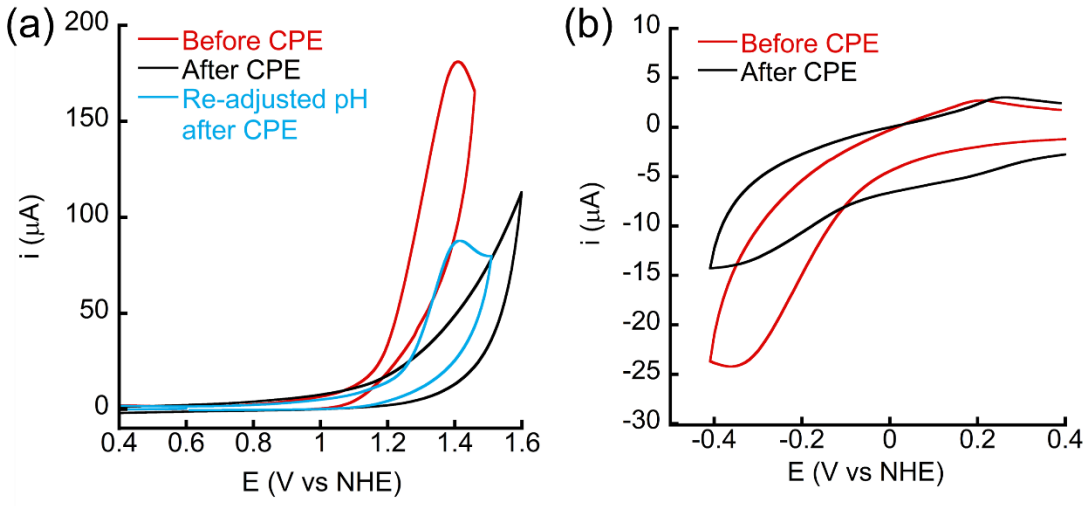


Figure S41. CVs of 0.5 mM Cu_2(**BE**)$_2$ in 0.1 M PBS at pH 11 before and after the CPE experiment using ITO as working electrode at applied potential +1.25 V vs NHE.

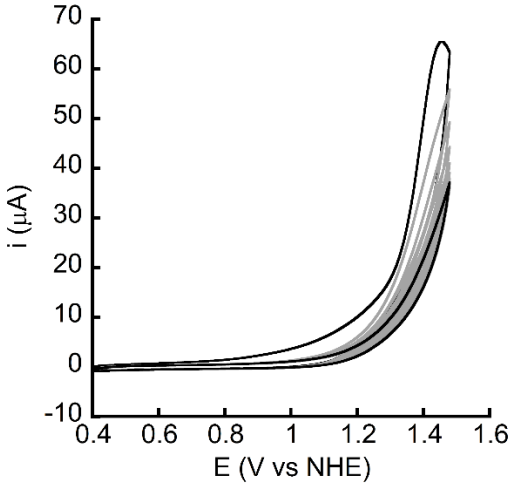


Figure S42. Ten continuous CV scans of a solution of 0.25 mM Cu_2(**BE**)$_2$ in 0.1 M PBS at pH 11 using glassy carbon as working electrode at scan rate 100 mV/s.

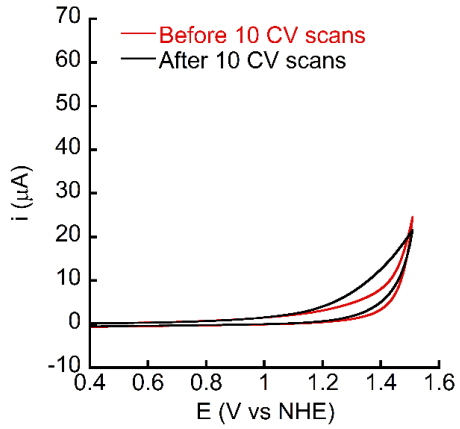


Figure S43. CVs of glassy carbon electrode in fresh 0.1 M PBS at pH 11 without catalyst before and after the ten continuous CV scans of a solution of 0.25 mM Cu_2(**BE**)$_2$ in Figure S42.

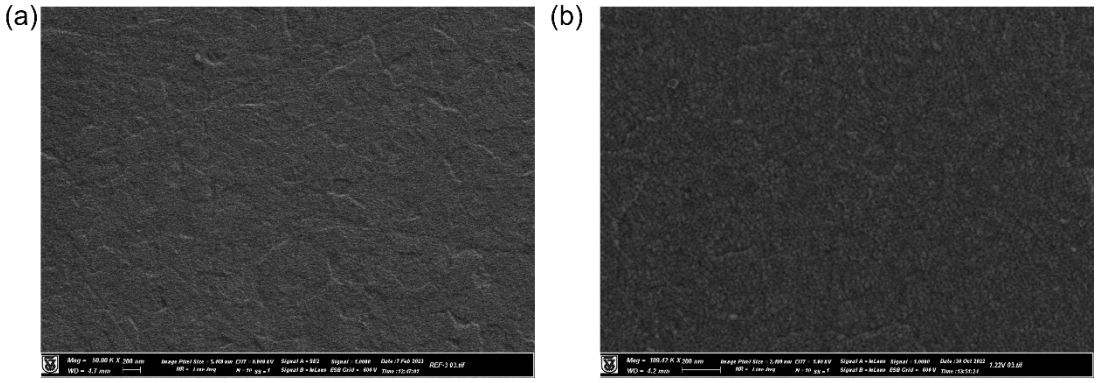


Figure S44. HR-SEM images of (a) the fresh ITO electrode and (b) the after 2-hour CPE experiment at +1.25 V applied potential in 0.1 M PBS at pH 11 containing 0.5 mM Cu_2(**BE**)$_2$.

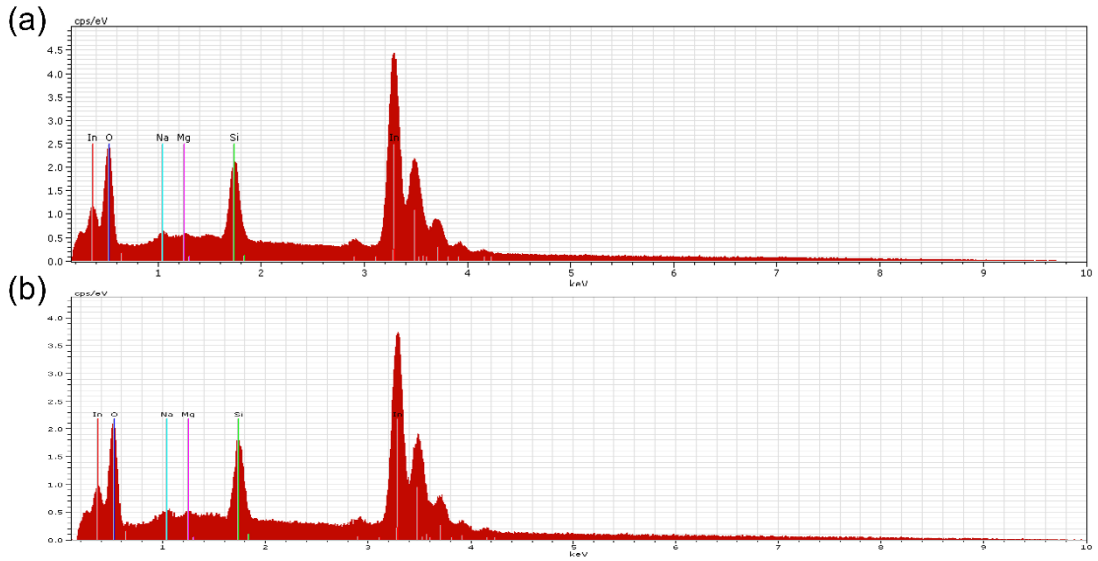


Figure S45. Energy-dispersive X-ray spectroscopy (EDX) analysis of the ITO electrode (a) before and (b) after electrolysis; no Cu element was detected at ~8 keV (Kα) and ~9 keV (Kβ). For confirmation of sample composition, an acceleration voltage of 10 kV (from 1kV) was used. This higher acceleration voltage was needed for sufficient X-ray emission from the specimens.

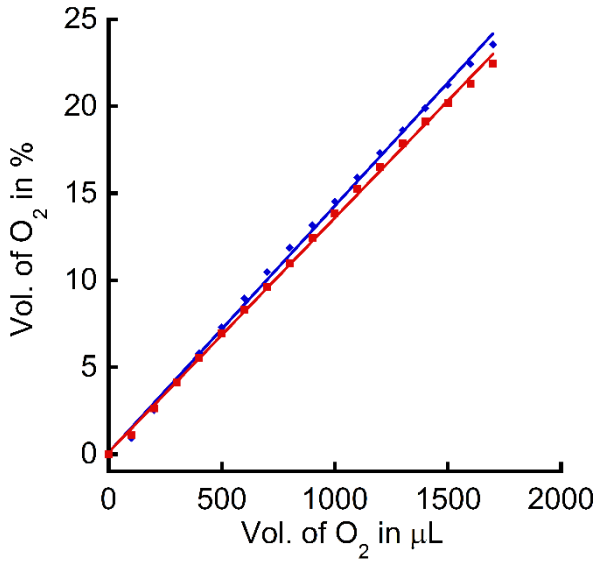


Figure S46. Calibration curve for the measure of evolved O_2 in µL from %. [Red line = experiment 1 and blue line = experiment 2 and then take the average].

Supporting Tables:

Table S1: Crystal data of complexes Cu_2(**BECyclohexyl**)$_2$, Cu_2(**BEPropylCl**)$_2$, Cu_2(**BEPropyl**)$_2$.

Complex	Cu_2(**BECyclohexyl**)$_2$	Cu_2(**BEPropylCl**)$_2$	Cu_2(**BEPropyl**)$_2$
Formula	$C_{68}H_{102}Cu_2F_{24}N_{16}O_{14}P_4$	$C_{52}H_{78}Cl_6Cu_2N_{12}O_{28}$	$C_{46}H_{64}Cl_4Cu_2N_{12}O_{26}$
Formula weight	2074.61	1659.04	1469.97
T (K)	100.15	100.15	100.15
Crystal color	blue	blue	blue
Crystal system	triclinic	triclinic	triclinic
Space group	P-1	P-1	P-1
a (Å)	13.4061(2)	11.5444(5)	11.1225(3)
b (Å)	13.5461(3)	12.1635(6)	12.4153(3)
c (Å)	13.6972(3)	13.7985(7)	13.9658(3)
α (°)	113.6275(19)	102.470(4)	103.308(2)
β (°)	101.1796(16)	111.799(5)	110.276(2)
γ (°)	95.4695(16)	100.241(4)	101.505(2)
V (Å^3)	2193.82(8)	1683.98(15)	1676.06(8)
Z	1	1	1
Crystal dimensions (mm)	0.36 × 0.33 × 0.24	0.24 × 0.18 × 0.15	0.21 × 0.18 × 0.15
D_c (g cm^{-3})	1.570	1.636	1.456
F (000)	1068.0	858.0	758.0
λ (Kα) (Å)	(Cu) 1.54184	(Mo) 0.71073	(Mo) 0.71073
θ Range (°)	6.85 to 161.444	4.522 to 59.662	5.27 to 60.14
Absorption correction	multi-scan	multi-scan	multi-scan
R factor (%)	8.40	8.54	4.00
wR_2 index (reflections)	0.2433	0.0936	0.1070
Goodness-of-fit	1.020	1.036	1.026

Cu_2(**BECyclohexyl**)$_2$:

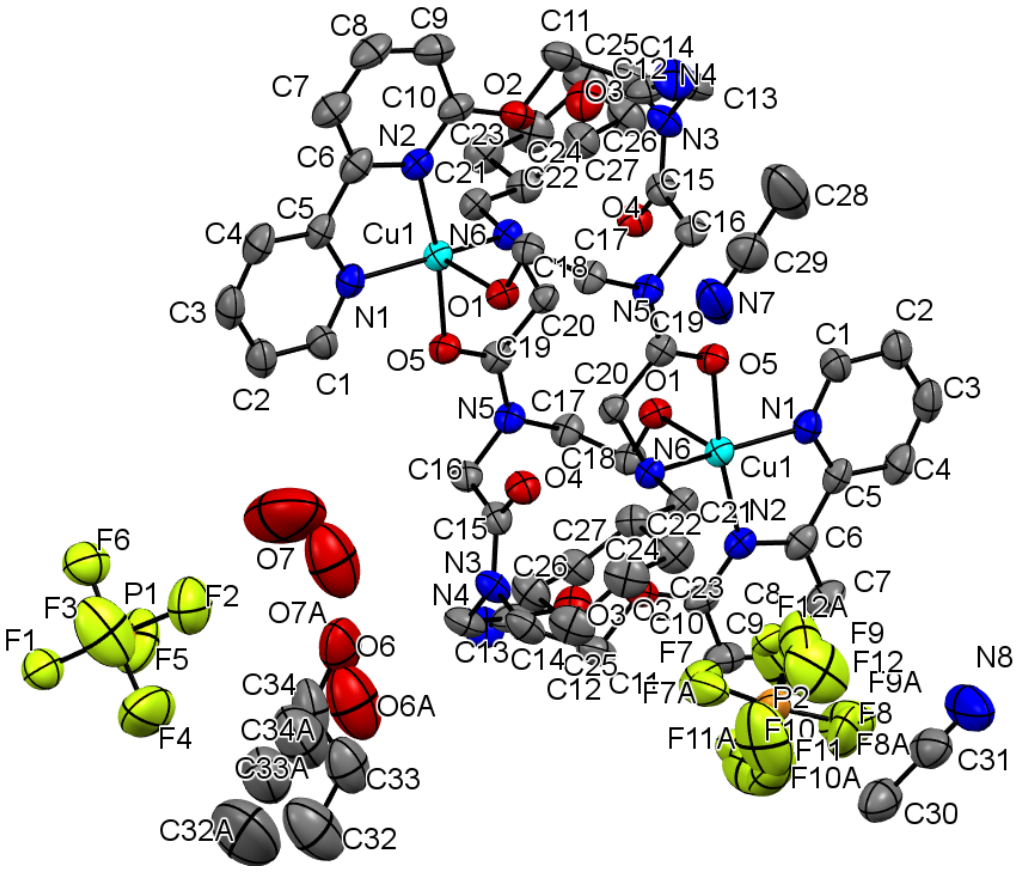


Table S2. Bond Lengths for Cu_2(**BECyclohexyl**)$_2$.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cu1	O1	2.249(2)	C17	C18	1.514(5)
Cu1	O5[1]	1.986(2)	C19	C20	1.497(5)
Cu1	N1	1.981(3)	C21	C22	1.537(5)
Cu1	N2	2.053(3)	C22	C23	1.534(5)
Cu1	N6[1]	2.002(3)	C22	C27	1.522(6)
O1	C18	1.428(4)	C23	C24	1.537(6)
O2	C10	1.356(5)	C24	C25	1.529(8)
O2	C11	1.448(5)	C25	C26	1.503(7)
O3	C14	1.239(6)	C26	C27	1.536(5)
O4	C15	1.223(4)	P1	F1	1.556(4)
O5	Cu1[1]	1.986(2)	P1	F2	1.649(5)
O5	C19	1.256(4)	P1	F3	1.503(5)
N1	C1	1.332(5)	P1	F4	1.602(6)
N1	C5	1.334(5)	P1	F5	1.567(5)
N2	C6	1.365(5)	P1	F6	1.559(4)
N2	C10	1.336(5)	P2	F7	1.491(9)
N3	C12	1.468(5)	P2	F7A	1.545(10)
N3	C13	1.451(5)	P2	F8	1.551(9)
N3	C15	1.349(5)	P2	F8A	1.546(11)
N4	C14	1.315(6)	P2	F9	1.648(9)
N5	C16	1.467(5)	P2	F9A	1.601(13)
N5	C17	1.478(4)	P2	F10	1.456(10)
N5	C19	1.334(4)	P2	F10A	1.490(11)
N6	Cu1[1]	2.002(3)	P2	F11	1.460(10)
N6	C20	1.474(4)	P2	F11A	1.568(10)
N6	C21	1.496(4)	P2	F12	1.479(9)
C1	C2	1.397(6)	P2	F12A	1.497(8)
C2	C3	1.387(7)	O6	C34	1.457(17)
C3	C4	1.368(7)	C32	C33	1.459(19)
C4	C5	1.410(5)	C33	C34	1.35(2)
C5	C6	1.476(6)	O6A	C34A	1.69(5)
C6	C7	1.367(6)	C32A	C33A	1.35(6)
C7	C8	1.379(8)	C33A	C34A	1.00(5)
C8	C9	1.378(7)	N7	C29	1.158(8)

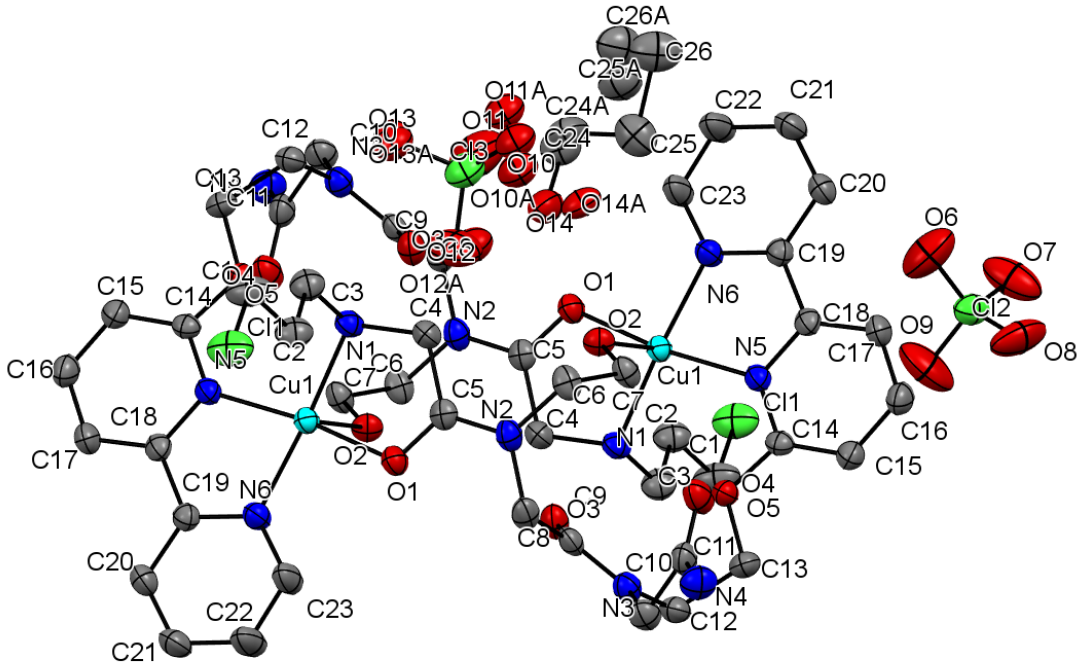
C9	C10	1.407(5)	C28	C29	1.425(10)
C11	C12	1.520(7)	N8	C31	1.114(9)
C13	C14	1.509(7)	C30	C31	1.437(9)
C15	C16	1.533(5)			

Table S3. Bond Angles for Cu_2(**BECyclohexyl**)$_2$.

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
O5[1]	Cu1	O1	87.25(10)	N6	C21	C22	115.7(3)
O5[1]	Cu1	N2	171.74(12)	C23	C22	C21	109.1(3)
O5[1]	Cu1	N6[1]	82.41(11)	C27	C22	C21	111.6(3)
N1	Cu1	O1	95.13(11)	C27	C22	C23	111.6(3)
N1	Cu1	O5[1]	89.86(12)	C22	C23	C24	111.0(4)
N1	Cu1	N2	81.92(13)	C25	C24	C23	111.1(4)
N1	Cu1	N6[1]	160.48(13)	C26	C25	C24	109.9(4)
N2	Cu1	O1	94.21(10)	C25	C26	C27	111.9(4)
N6[1]	Cu1	O1	102.33(11)	C22	C27	C26	112.1(3)
N6[1]	Cu1	N2	105.16(12)	F1	P1	F2	178.1(3)
C18	O1	Cu1	121.0(2)	F1	P1	F4	90.4(3)
C10	O2	C11	116.7(3)	F1	P1	F5	93.6(2)
C19	O5	Cu1[1]	114.1(2)	F1	P1	F6	92.2(2)
C1	N1	Cu1	124.7(3)	F3	P1	F1	95.3(3)
C1	N1	C5	120.2(3)	F3	P1	F2	84.3(3)
C5	N1	Cu1	115.1(3)	F3	P1	F4	92.6(5)
C6	N2	Cu1	111.6(3)	F3	P1	F5	170.7(3)
C10	N2	Cu1	128.2(2)	F3	P1	F6	92.7(3)
C10	N2	C6	120.2(3)	F4	P1	F2	87.8(3)
C13	N3	C12	118.6(3)	F5	P1	F2	86.8(3)
C15	N3	C12	118.9(3)	F5	P1	F4	84.8(4)
C15	N3	C13	122.2(3)	F6	P1	F2	89.7(2)
C16	N5	C17	117.0(3)	F6	P1	F4	173.9(4)
C19	N5	C16	119.8(3)	F6	P1	F5	89.5(3)
C19	N5	C17	123.2(3)	F7	P2	F8	165.3(11)
C20	N6	Cu1[1]	107.0(2)	F7	P2	F9	92.5(7)
C20	N6	C21	112.7(3)	F7A	P2	F8A	161.0(13)
C21	N6	Cu1[1]	111.2(2)	F7A	P2	F9A	92.9(14)
N1	C1	C2	122.4(4)	F7A	P2	F11A	92.6(10)

C3	C2	C1	117.7(4)	F8	P2	F9	88.5(9)
C4	C3	C2	119.9(4)	F8A	P2	F9A	73.7(16)
C3	C4	C5	119.4(4)	F8A	P2	F11A	100.2(13)
N1	C5	C4	120.4(4)	F10	P2	F7	91.4(9)
N1	C5	C6	115.8(3)	F10	P2	F8	103.3(11)
C4	C5	C6	123.8(4)	F10	P2	F9	81.7(9)
N2	C6	C5	115.5(3)	F10	P2	F11	90.8(9)
N2	C6	C7	121.5(4)	F10	P2	F12	168.3(9)
C7	C6	C5	122.9(4)	F10A	P2	F7A	87.8(8)
C6	C7	C8	118.6(4)	F10A	P2	F8A	79.1(10)
C9	C8	C7	120.8(4)	F10A	P2	F9A	90.5(11)
C8	C9	C10	118.3(4)	F10A	P2	F11A	86.7(9)
O2	C10	C9	125.3(4)	F10A	P2	F12A	176.4(7)
N2	C10	O2	114.0(3)	F11	P2	F7	94.3(9)
N2	C10	C9	120.6(4)	F11	P2	F8	86.7(10)
O2	C11	C12	108.0(3)	F11	P2	F9	170.0(10)
N3	C12	C11	113.4(4)	F11	P2	F12	100.9(9)
N3	C13	C14	111.6(4)	F11A	P2	F9A	173.7(12)
O3	C14	N4	123.5(5)	F12	P2	F7	88.9(9)
O3	C14	C13	119.7(4)	F12	P2	F8	76.5(12)
N4	C14	C13	116.8(4)	F12	P2	F9	86.5(8)
O4	C15	N3	123.1(4)	F12A	P2	F7A	88.8(7)
O4	C15	C16	118.1(3)	F12A	P2	F8A	104.0(10)
N3	C15	C16	118.8(3)	F12A	P2	F9A	88.6(8)
N5	C16	C15	111.3(3)	F12A	P2	F11A	94.5(5)
N5	C17	C18	113.4(3)	C34	C33	C32	112.1(15)
O1	C18	C17	112.0(3)	C33	C34	O6	113.7(10)
O5	C19	N5	120.9(3)	C34A	C33A	C32A	149(6)
O5	C19	C20	117.9(3)	C33A	C34A	O6A	139(6)
N5	C19	C20	121.2(3)	N7	C29	C28	175.3(9)
N6	C20	C19	109.3(3)	N8	C31	C30	178.8(8)

Cu_2(**BEPropylCl**)$_2$:


C26A
C26
C25A
O11A
C24A
C22
C21
C12
O13
O11
C10
C24
C25
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Cl3
O10
C23
C20
C13
N3
C11
O10A
O14A
O14
C9
O6
O7
C19
C15
C14
O4
O5
C3
O12A
O1
N6
Cl2
C4
N2
O2
C18
O9
C16
N5
C1
N1
C6
C5
Cu1
C7
Cu1
N5
C17
O8
C18
C6
C7
C2
Cl1
C14
C16
C17
O2
N2
C4
N1
C1
C15
C19
N6
O1
C3
O4
C9
O3
O5
C20
C8
C11
C10
C13
C22
C23
N3
N4
C12
C21

Table S4. Bond Lengths for Cu_2(**BEPropylCl**)$_2$.

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
Cu1	O1	1.960(4)	C6	C7	1.518(8)
Cu1	O2[1]	2.227(4)	C8	C9	1.515(9)
Cu1	N1	1.998(5)	C10	C11	1.537(9)
Cu1	N5[1]	2.032(5)	C12	C13	1.502(9)
Cu1	N6[1]	1.965(5)	C14	C15	1.381(8)
Cl1	C1	1.778(7)	C15	C16	1.373(9)
O1	C5	1.254(7)	C16	C17	1.384(9)
O2	Cu1[1]	2.227(4)	C17	C18	1.379(8)
O2	C7	1.423(7)	C18	C19	1.470(8)
O3	C9	1.237(8)	C19	C20	1.383(8)
O4	C11	1.223(8)	C20	C21	1.373(10)
O5	C13	1.451(7)	C21	C22	1.383(10)
O5	C14	1.343(7)	C22	C23	1.355(10)
N1	C3	1.469(8)	Cl2	O6	1.411(7)
N1	C4	1.467(8)	Cl2	O7	1.402(7)
N2	C5	1.330(8)	Cl2	O8	1.407(6)
N2	C6	1.470(8)	Cl2	O9	1.419(6)
N2	C8	1.465(8)	Cl3	O10	1.412(7)
N3	C9	1.339(8)	Cl3	O10A	1.493(16)
N3	C10	1.438(8)	Cl3	O11	1.411(8)
N3	C12	1.465(9)	Cl3	O11A	1.460(16)
N4	C11	1.336(9)	Cl3	O12	1.443(8)
N5	Cu1[1]	2.032(5)	Cl3	O12A	1.399(16)
N5	C14	1.349(8)	Cl3	O13	1.453(8)
N5	C18	1.362(7)	Cl3	O13A	1.458(17)
N6	Cu1[1]	1.965(5)	O14	C24	1.42(3)
N6	C19	1.344(8)	O14A	C24A	1.41(4)
N6	C23	1.355(8)	C24	C25	1.51(4)
C1	C2	1.505(10)	C24A	C25A	1.57(3)
C2	C3	1.506(10)	C25	C26	1.58(3)
C4	C5	1.501(8)	C25A	C26A	1.45(4)

Table S5 Bond Angles for Cu_2(**BEPropylCl**)$_2$.

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
O1	Cu1	O2[1]	87.50(17)	O4	C11	C10	121.7(6)
O1	Cu1	N1	83.60(19)	N4	C11	C10	114.3(6)
O1	Cu1	N5[1]	172.10(18)	N3	C12	C13	112.1(5)
O1	Cu1	N6[1]	90.47(19)	O5	C13	C12	107.4(5)
N1	Cu1	O2[1]	95.73(19)	O5	C14	N5	113.0(5)
N1	Cu1	N5[1]	102.9(2)	O5	C14	C15	124.3(5)
N5[1]	Cu1	O2[1]	96.26(18)	N5	C14	C15	122.6(5)
N6[1]	Cu1	O2[1]	104.5(2)	C16	C15	C14	118.9(6)
N6[1]	Cu1	N1	158.7(2)	C15	C16	C17	119.5(6)
N6[1]	Cu1	N5[1]	81.9(2)	C18	C17	C16	119.2(6)
C5	O1	Cu1	115.1(4)	N5	C18	C17	121.7(6)
C7	O2	Cu1[1]	123.1(4)	N5	C18	C19	115.2(5)
C14	O5	C13	116.4(4)	C17	C18	C19	123.1(5)
C3	N1	Cu1	114.6(4)	N6	C19	C18	115.1(5)
C4	N1	Cu1	109.1(4)	N6	C19	C20	121.4(6)
C4	N1	C3	112.9(5)	C20	C19	C18	123.5(5)
C5	N2	C6	123.2(5)	C21	C20	C19	119.3(6)
C5	N2	C8	119.6(5)	C20	C21	C22	118.7(6)
C8	N2	C6	117.2(5)	C23	C22	C21	120.2(7)
C9	N3	C10	123.3(6)	N6	C23	C22	121.3(6)
C9	N3	C12	119.6(5)	O6	Cl2	O9	111.2(6)
C10	N3	C12	117.1(5)	O7	Cl2	O6	108.1(5)
C14	N5	Cu1[1]	129.5(4)	O7	Cl2	O8	111.0(5)
C14	N5	C18	118.1(5)	O7	Cl2	O9	109.4(4)
C18	N5	Cu1[1]	112.4(4)	O8	Cl2	O6	107.7(4)
C19	N6	Cu1[1]	115.3(4)	O8	Cl2	O9	109.4(5)
C19	N6	C23	119.1(5)	O10	Cl3	O12	110.7(6)
C23	N6	Cu1[1]	125.5(4)	O10	Cl3	O13	107.7(14)
C2	C1	Cl1	111.0(5)	O11	Cl3	O10	117.4(6)
C1	C2	C3	110.6(6)	O11	Cl3	O12	111.1(6)
N1	C3	C2	112.0(6)	O11	Cl3	O13	105.2(10)
N1	C4	C5	111.0(5)	O11A	Cl3	O10A	92.1(14)
O1	C5	N2	121.3(6)	O12	Cl3	O13	103.6(13)
O1	C5	C4	118.3(5)	O12A	Cl3	O10A	94.5(17)

N2	C5	C4	120.4(5)	O12A	Cl3	O11A	125.9(15)
N2	C6	C7	114.0(5)	O12A	Cl3	O13A	118(4)
O2	C7	C6	113.2(5)	O13A	Cl3	O10A	111(4)
N2	C8	C9	110.7(5)	O13A	Cl3	O11A	109(4)
O3	C9	N3	122.2(6)	O14	C24	C25	108(3)
O3	C9	C8	118.6(6)	O14A	C24A	C25A	109(2)
N3	C9	C8	119.2(5)	C24	C25	C26	105.2(19)
N3	C10	C11	113.7(5)	C26A	C25A	C24A	111(2)
O4	C11	N4	124.0(6)				

Cu_2(**BEPropyl**)$_2$:

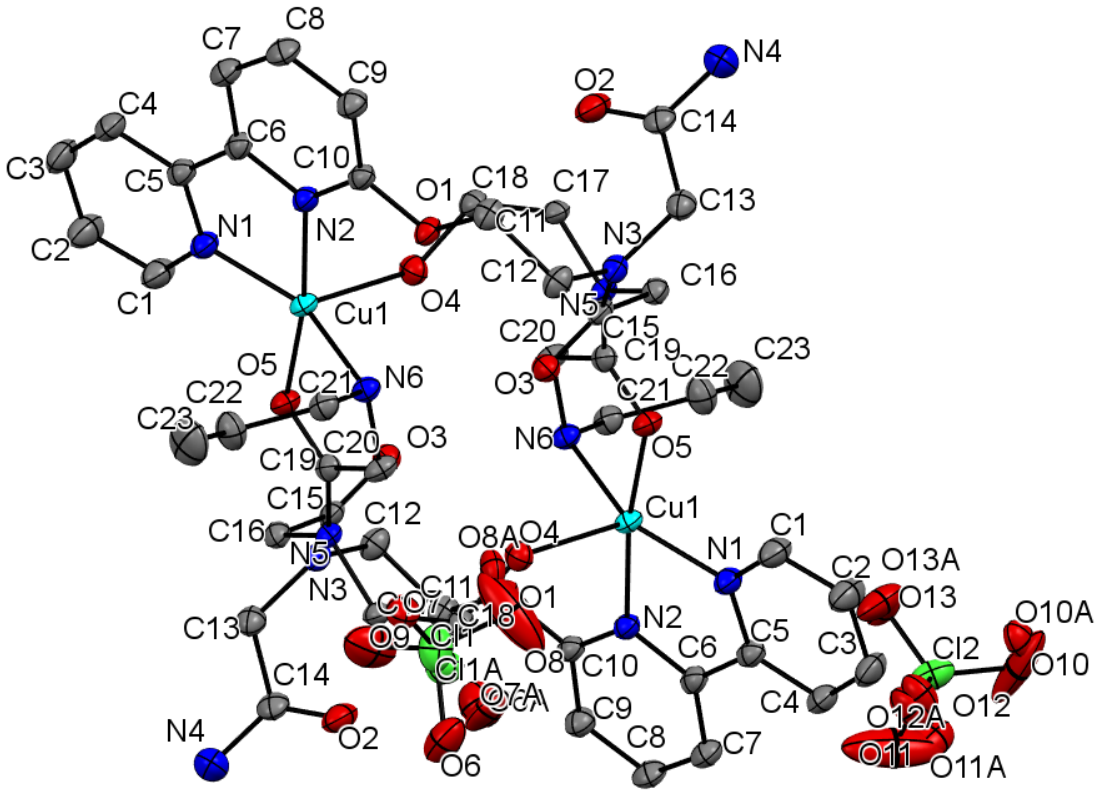

Table S6 Bond Lengths for Cu_2(**BEPropyl**)$_2$.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.385(3)	C19	N5	1.328(3)
C1	N1	1.342(3)	C19	O5	1.259(3)
C2	C3	1.390(4)	C20	N6	1.484(3)
C3	C4	1.383(4)	C21	C22	1.518(3)
C4	C5	1.381(3)	C21	N6	1.491(3)
C5	C6	1.480(3)	C22	C23	1.519(4)
C5	N1	1.351(3)	Cu1	N1[1]	1.9820(19)
C6	C7	1.379(3)	Cu1	N2[1]	2.0305(17)
C6	N2	1.365(3)	Cu1	N6	2.0008(18)
C7	C8	1.388(3)	Cu1	O4[1]	2.2256(15)
C8	C9	1.378(3)	Cu1	O5	1.9647(15)
C9	C10	1.398(3)	Cl2	O10	1.375(9)
C10	N2	1.340(3)	Cl2	O12	1.436(9)
C10	O1	1.345(3)	Cl2	O13	1.428(10)
C11	C12	1.516(3)	Cl2	O11	1.476(10)
C11	O1	1.447(3)	Cl2	O10A	1.482(6)
C12	N3	1.465(3)	Cl2	O11A	1.406(7)
C13	C14	1.532(3)	Cl2	O12A	1.426(12)
C13	N3	1.457(3)	Cl2	O13A	1.430(10)
C14	N4	1.337(3)	O7	Cl1	1.425(3)
C14	O2	1.219(3)	O7	Cl1A	2.067(7)
C15	C16	1.526(3)	O9	Cl1	1.429(2)
C15	N3	1.346(3)	O9	Cl1A	1.296(4)
C15	O3	1.231(3)	Cl1	O6	1.492(4)
C16	N5	1.463(3)	Cl1	O8	1.346(5)
C17	C18	1.523(3)	Cl1A	O6A	1.147(9)
C17	N5	1.477(3)	Cl1A	O7A	1.439(11)
C18	O4	1.432(3)	Cl1A	O8A	1.751(10)
C19	C20	1.508(3)			

Table S7. Bond Angles for Cu_2(**BEPropyl**)$_2$.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	C1	C2	121.9(2)	C1	N1	Cu1[1]	125.29(15)
C1	C2	C3	118.6(2)	C5	N1	Cu1[1]	115.04(15)
C4	C3	C2	119.4(2)	C6	N2	Cu1[1]	112.82(14)
C5	C4	C3	119.2(2)	C10	N2	C6	117.97(18)
C4	C5	C6	123.7(2)	C10	N2	Cu1[1]	129.21(14)
N1	C5	C4	121.3(2)	C13	N3	C12	117.02(18)
N1	C5	C6	114.93(19)	C15	N3	C12	119.40(18)
C7	C6	C5	122.7(2)	C15	N3	C13	123.45(18)
N2	C6	C5	115.08(18)	C16	N5	C17	117.31(17)
N2	C6	C7	122.2(2)	C19	N5	C16	119.69(17)
C6	C7	C8	119.0(2)	C19	N5	C17	122.95(18)
C9	C8	C7	119.7(2)	C20	N6	C21	112.59(16)
C8	C9	C10	118.3(2)	C20	N6	Cu1	109.54(13)
N2	C10	C9	122.85(19)	C21	N6	Cu1	113.30(13)
N2	C10	O1	113.68(17)	C10	O1	C11	117.24(16)
O1	C10	C9	123.5(2)	C18	O4	Cu1[1]	124.70(12)
O1	C11	C12	107.93(17)	C19	O5	Cu1	114.96(14)
N3	C12	C11	112.34(18)	O10	Cl2	O12	108.1(12)
N3	C13	C14	113.41(19)	O10	Cl2	O13	114.1(9)
N4	C14	C13	113.6(2)	O10	Cl2	O11	114.3(7)
O2	C14	C13	122.5(2)	O12	Cl2	O11	104.0(12)
O2	C14	N4	123.9(2)	O13	Cl2	O12	114.1(14)
N3	C15	C16	118.38(18)	O13	Cl2	O11	101.8(11)
O3	C15	C16	119.00(18)	O11A	Cl2	O10A	107.0(4)
O3	C15	N3	122.6(2)	O11A	Cl2	O12A	112.6(13)
N5	C16	C15	110.88(17)	O11A	Cl2	O13A	116.5(9)
N5	C17	C18	113.96(17)	O12A	Cl2	O10A	109.1(14)
O4	C18	C17	112.82(17)	O12A	Cl2	O13A	107.7(18)
N5	C19	C20	119.72(18)	O13A	Cl2	O10A	103.5(10)
O5	C19	C20	118.99(18)	O7	Cl1	O9	108.73(18)
O5	C19	N5	121.3(2)	O7	Cl1	O6	102.12(18)
N6	C20	C19	110.50(17)	O9	Cl1	O6	105.1(2)
N6	C21	C22	112.65(18)	O8	Cl1	O7	110.3(3)
C21	C22	C23	111.1(2)	O8	Cl1	O9	117.6(3)
N1[1]	Cu1	N2[1]	81.81(7)	O8	Cl1	O6	111.9(4)
N1[1]	Cu1	N6	157.36(8)	O9	Cl1A	O7	83.9(3)
N1[1]	Cu1	O4[1]	105.10(7)	O9	Cl1A	O7A	99.5(5)
N2[1]	Cu1	O4[1]	97.59(6)	O9	Cl1A	O8A	100.6(4)

N6	Cu1	N2[1]	101.88(7)	O6A	Cl1A	O7	88.0(6)
N6	Cu1	O4[1]	96.60(7)	O6A	Cl1A	O9	150.9(7)
O5	Cu1	N1[1]	90.60(7)	O6A	Cl1A	O7A	90.2(7)
O5	Cu1	N2[1]	171.91(7)	O6A	Cl1A	O8A	103.3(8)
O5	Cu1	N6	84.06(7)	O7A	Cl1A	O7	175.8(4)
O5	Cu1	O4[1]	87.08(6)	O7A	Cl1A	O8A	104.7(5)
C1	N1	C5	119.57(19)	O8A	Cl1A	O7	72.1(4)