Supporting Information for

Synthesis and structural characterization of copper-cuprizone complexes

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Table S1. Assignment of ions as well as the product ions and neutral losses generated by collision-induced dissociation of [$Cu^{III}(CPZmh_2)_{-4H}$]. Colours correspond to the fragmentation pathway colour scheme in Figure S2.

annotation	Assignment	neutral losses	Th. *m/z*	Obs *m/z*
	Positive Ion Mode MS/MS			
[($^{63}Cu^{III}$)M+2Na]$^+$	**$^{63}Cu^{III}C_{16}H_{24}N_8O_4Na_2$**	**–**	**501.1**	**501.1**
	$^{63}Cu^{III}C_{12}H_{13}N_7O_4Na_2$	*501* – $C_4H_{11}N$	428.0	428.0
	$^{63}Cu^{III}C_{10}H_{12}N_8O_4Na_2$	*501* – C_6H_{12}	417.0	417.3
	385 m/z + H_2O capture	–	–	403.3
	$^{63}Cu^{III}C_9H_6N_7O_4Na_2$	*428* – C_3H_7	385.0	385.1
	$^{63}Cu^{III}C_9H_{13}N_5O_3Na_2$	*501* – $C_7H_{11}N_3O$	348.0	347.9
	305 m/z + H_2O capture	–	–	323.2
	$^{63}Cu^{III}C_4N_6O_4Na_2$	*417* – $C_6H_{12}N_2$	304.9	305.1
	$^{63}Cu^{III}C_6H_6N_5O_3Na_2$	*348* – C_3H_7	305.0	305.1
	$^{63}Cu^{III}C_6H_5N_4O_3Na_2$	*385* – $C_3HN_3O_2$	290.0	289.6
	247 m/z + H_2O capture	–	–	265.0
	$^{63}Cu^{III}C_4N_3O_3Na_2$	*290* – C_2H_5N	246.9	246.9
	$^{63}Cu^{III}C_3H_3N_5O_3Na$	*348* – $C_6H_{10}Na$	243.0	243.2
	$^{63}Cu^{III}C_2N_2O_2Na_2$	*385* – $C_7H_6N_5O_2$	192.9	193.1
	$^{63}Cu^{III}C_2N_2O_2Na_2$	*305* – $C_2N_4O_2$	192.9	193.1
	$^{63}Cu^{III}C_2N_3Ona$	*247* – C_2O_2Na	167.9	168.0
	$^{63}Cu^{III}C_2N_3Ona$	*305* – $C_4H_6N_2O_2Na$	167.9	168.0
	$^{63}Cu^{III}C_2N_3Ona$	*243* – $CH_3N_2O_2$	167.9	168.0

Table S2. EXAFS multiple scattering parameters of the best-fit models representing the blue and green products arising from the reaction of Cu(II) with cuprizone.[a]

path [b]	*N*	*R*	σ^2	ΔE_0	*F*
Blue Product; *$Cu^{III}N_4$ environment, 12 variables used for EXAFS curve fitting*					
Cu – N	4	1.908(2)	0.0028	+3.4(2)	**0.3300**
Cu · C	2	2.71(6)	0.0040		
Cu · C	2	2.73	0.0040		
Cu · C · N	4	2.93(3)	0.0041		
Cu · C · N	4	2.94	0.0041		
Cu · N	2	2.925(7)	0.0035		
Cu · N	2	2.9774	0.0035		
Cu · N · N	4	3.04(4)	0.0037		
Cu · N · N	4	3.08	0.0037		
Cu · C	2	3.19(2)	0.0034		
Cu · O	2	3.86(5)	0.0031		
Cu · N · N	4	3.87	0.0055		
Cu · N · Cu · N	4	3.89	0.0055		
Cu · O · C	4	3.92	0.0031		
Cu · O	2	3.94	0.0031		
Cu · C · O · C	2	3.95	0.0035		
Cu · O · C	4	3.97	0.0031		
Cu · C · O · C	2	3.99	0.0033		
Cu · C	1	4.02	0.0034		
Cu · O · N	4	4.14(4)	0.0034		
Cu · O · N	4	4.16	0.0034		
Cu · C · O · N	4	4.18	0.0035		
Cu · C · N	4	4.18	0.0037		
Cu · C · O · N	4	4.18	0.0033		
Cu · N · C · N	4	4.5(1)	0.0042		
Cu · C · O · C · N	4	4.5(2)	0.0042		
Green Product; *$Cu^{II}N_2O_2$ environment, 11 variables used for EXAFS curve fitting*					
Cu – N	1	1.945(8)	0.0035	+1.3(4)	**0.3384**
Cu – N	1	1.963	0.0035		
Cu – O	1	1.977	0.0038		
Cu – O	1	1.980	0.0038		
Cu · C	1	2.70(1)	0.0036		
Cu · C	1	2.73	0.0036		
Cu · C	1	2.87	0.0034		
Cu · C	1	2.87	0.0034		
Cu · C · O	2	2.93(2)	0.0034		
Cu · C · O	2	2.95	0.0034		
Cu · C · N	2	3.01	0.0034		
Cu · C · N	2	3.02	0.0034		

Cu · N	1	3.03(1)	0.0035
Cu · N	1	3.09	0.0035
Cu · N · N	2	3.11	0.0033
Cu · N · N	2	3.17	0.0033
Cu · C	1	3.28(2)	0.0035
Cu · C	1	3.44	0.0043
Cu · C	1	3.47	0.0043
Cu · C	1	3.68	0.0043
Cu · N · N	2	3.81(1)	0.0044
Cu · N	1	3.85	0.0034
Cu · N · Cu · N	2	3.85	0.0045
Cu · O	1	3.87	0.0034
Cu · O	1	3.88	0.0034
Cu · O · O	2	3.93	0.0043
Cu · O · Cu · O	2	3.95	0.0044
Cu · C · N	2	3.97	0.0035
Cu · O · C	2	4.00	0.0035
Cu · C · N · C	1	4.00	0.0033
Cu · N	1	4.00	0.0033
Cu · O · C	2	4.01	0.0034
Cu · C · N	2	4.02	0.0036
Cu · C · O · C	1	4.05(1)	0.0033
Cu · C · N · C	1	4.06(1)	0.0032
Cu · C · O · C	1	4.07	0.0030
Cu · N · O	2	4.13	0.0033
Cu · O · N	2	4.15	0.0030
Cu · C · N · O	2	4.16	0.0033
Cu · O · N	2	4.17	0.0030
Cu · N · O	2	4.17	0.0033
Cu · C · O · N	2	4.17	0.0030
Cu · C · N · O	2	4.19	0.0032
Cu · C · O · N	2	4.20	0.0030
Cu · N	1	4.52(4)	0.0031
Cu · N · O	2	4.56	0.0032
Cu · N · O	2	4.62	0.0031
Cu · Cu	1	4.80	0.0035
Cu · Cu	1	4.80	0.0035
Cu · Cu · N	2	4.80	0.0038
Cu · Cu · N	2	4.80	0.0038
Cu · C · C	2	4.87(3)	0.0036
Cu · C · C	2	4.90	0.0036
Cu · C · C	2	4.98	0.0036

a. Coordination numbers N, interatomic distances R (Å), Debye-Waller factors (the mean-square deviations in interatomic distance) σ^2 (Å^2), and threshold energy shifts ΔE_0 (eV). The values in parentheses are the estimated standard deviations in the last digit obtained from the diagonal elements of the covariance matrix. The fit-error function F is defined by $F = \sqrt{\sum k^6 \left(\chi(k)_{calcd} - \chi(k)_{\mathrm{expt}}\right)^2 / \sum \chi(k)^2_{\mathrm{expt}}}$ where $\chi(k)$ are the EXAFS oscillations and k is the photo-electron wave number given by $k = \sqrt{\frac{2m_e}{\hbar^2}\left(E - E_0\right)}$. Values in parentheses are the estimated standard deviations obtained from the diagonal elements of the covariance matrix; these are precisions and are distinct from the accuracies which are expected to be larger (*ca* ±0.02 Å for R, and ±20% for N and σ^2), although relative accuracies (e.g. comparing two different Cu—O/N scattering interactions) will be more similar to the precisions. Parameters without standard deviation values specified in parentheses are linked as variables to a preceding value in the fit, which will have a value defined if it was permitted to vary during the curve fitting procedure. The k-range of the data fitted was from 1.0 to 15.75 Å^{-1}.

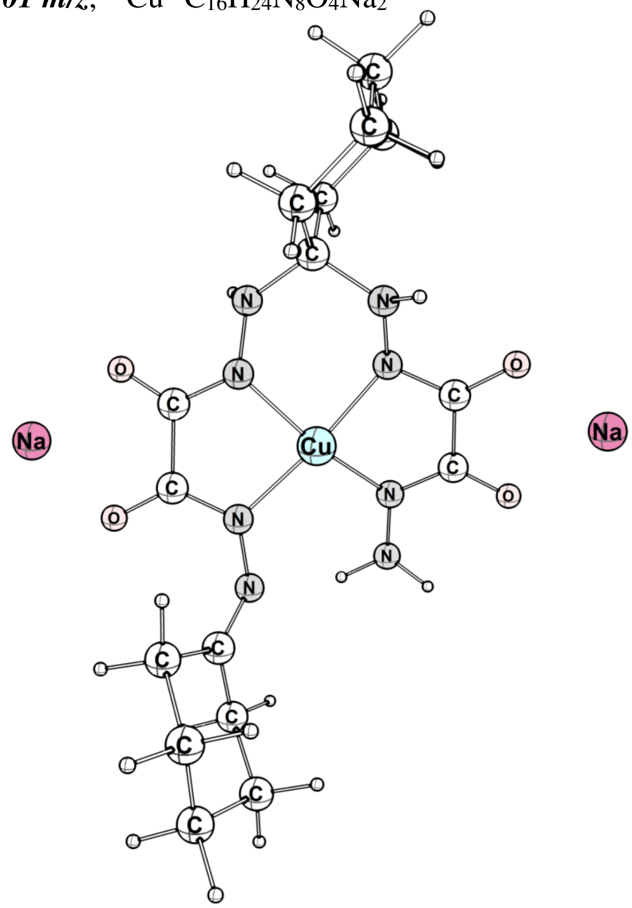
b. All paths terminate with the originating Cu atom (not indicated).

Table S3. Spin Hamiltonian g and ^{Cu}A parameters for Cu^{II} EPR, used to fit Cu^{II} in the presence of a 20-fold excess of CPZ (spectra are shown in Figure S4). Fitting was performed using qpowg, based on a $Cu^{II}N_4$ model, and rendered using gplotn.[i]

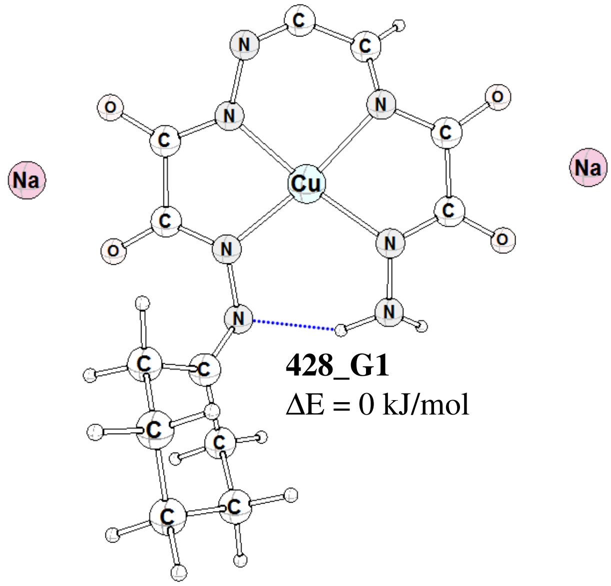
	g_1	g_2	g_3	$^{Cu}A_1$	$^{Cu}A_2$	$^{Cu}A_3$
Cu^{II}(CPZ)*xs*	2.049	2.049	2.185	–60	–60	630

Figure S1

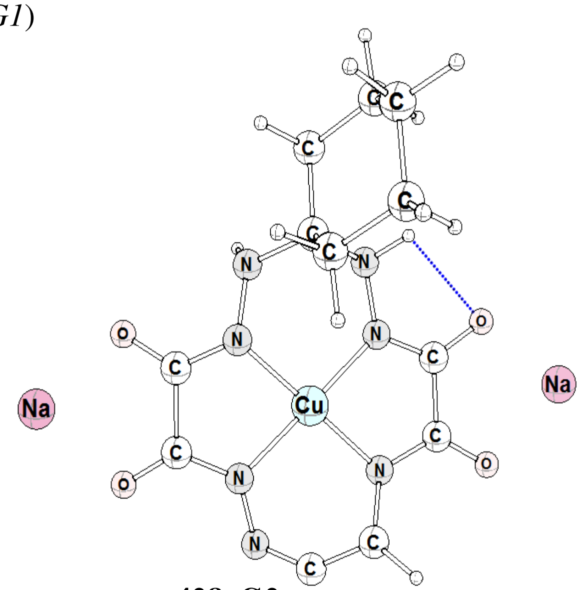
501 m/z, $^{63}Cu^{III}C_{16}H_{24}N_8O_4Na_2$



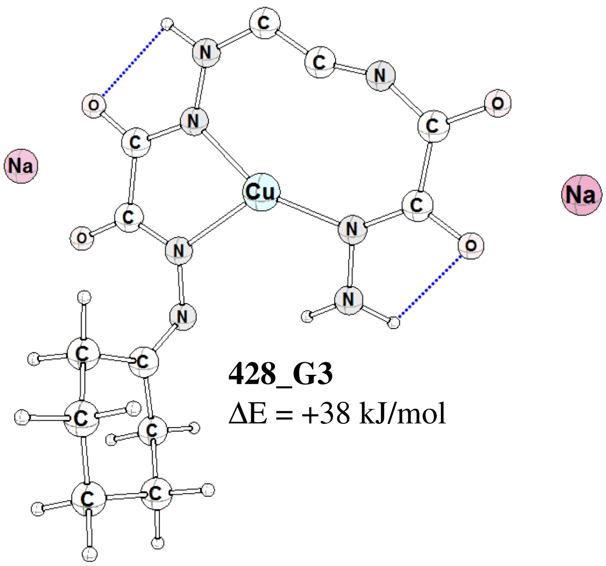
428 m/z, $^{63}Cu^{III}C_{12}H_{13}N_7O_4Na_2$ (*ΔE is relative to 428_G1*)



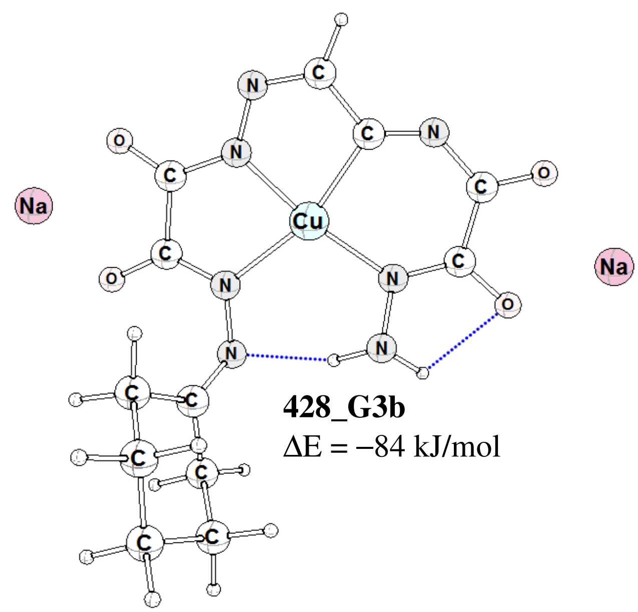
428_G1
ΔE = 0 kJ/mol



428_G2
ΔE = +12 kJ/mol



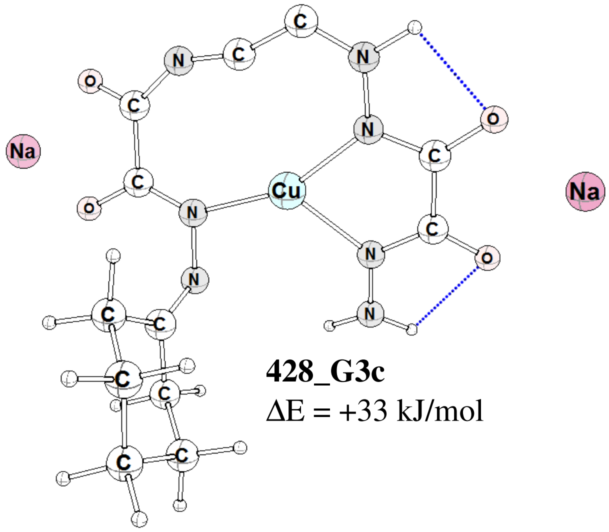
428_G3
ΔE = +38 kJ/mol



428_G3b
ΔE = −84 kJ/mol

Figure S1 (*continued*)

428 m/z, $^{63}Cu^{III}C_{12}H_{13}N_7O_4Na_2$ (*continued*)



428_G3c
ΔE = +33 kJ/mol

Stabilizing rearrangement of 428_G3 to 428_G3b ($\Delta E = E_{(428\_G3b)} - E_{(428\_G3)}$):

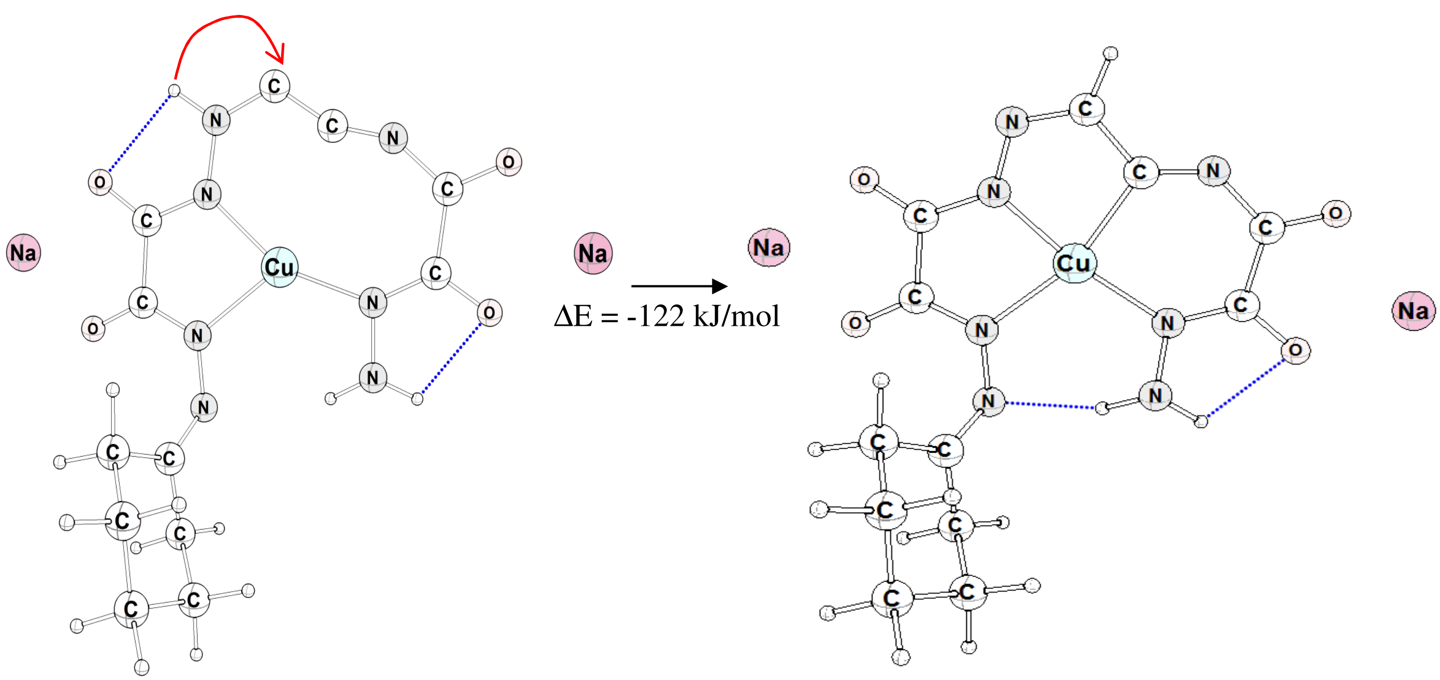
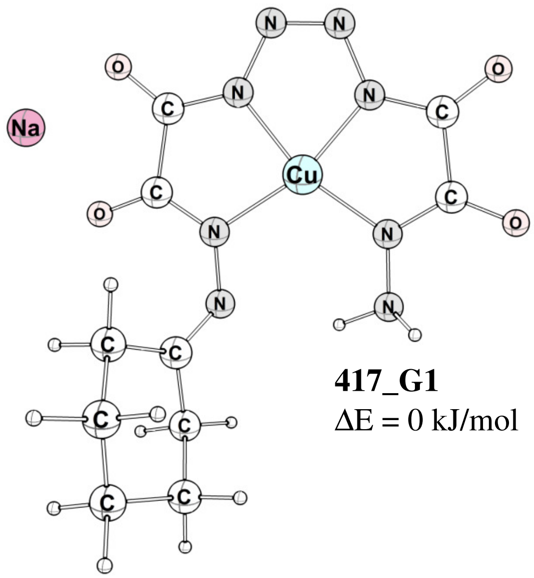
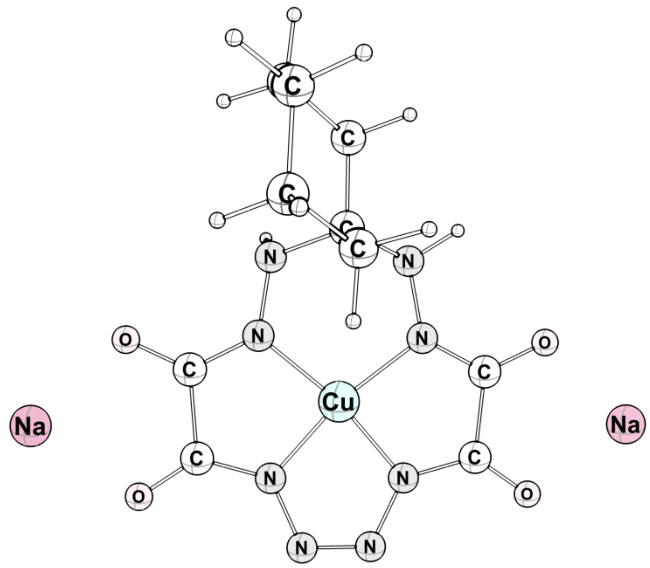


Figure S1 (*continued*)

417 m/z, $^{63}Cu^{III}C_{10}H_{12}N_8O_4Na_2$

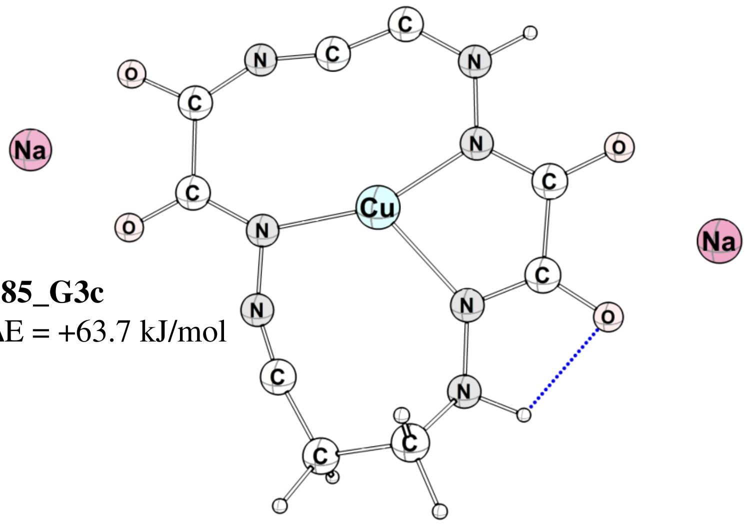


417_G1
ΔE = 0 kJ/mol

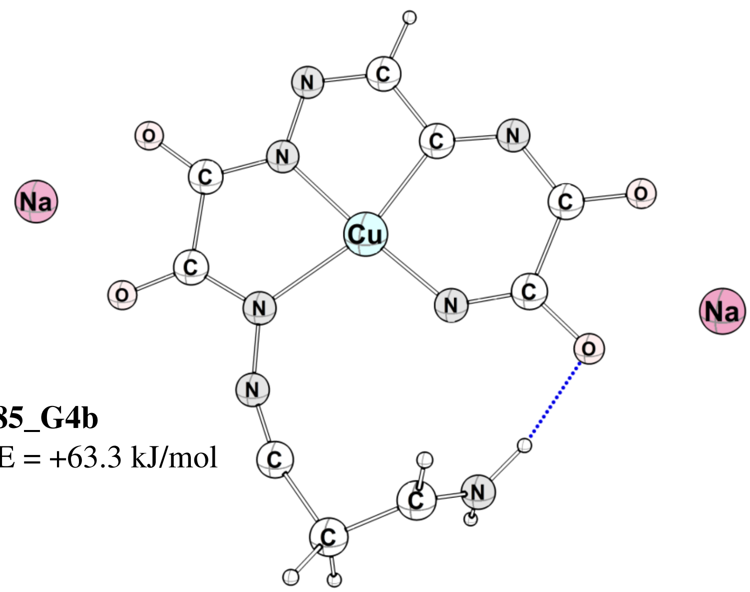


417_G2
ΔE = +22.7 kJ/mol

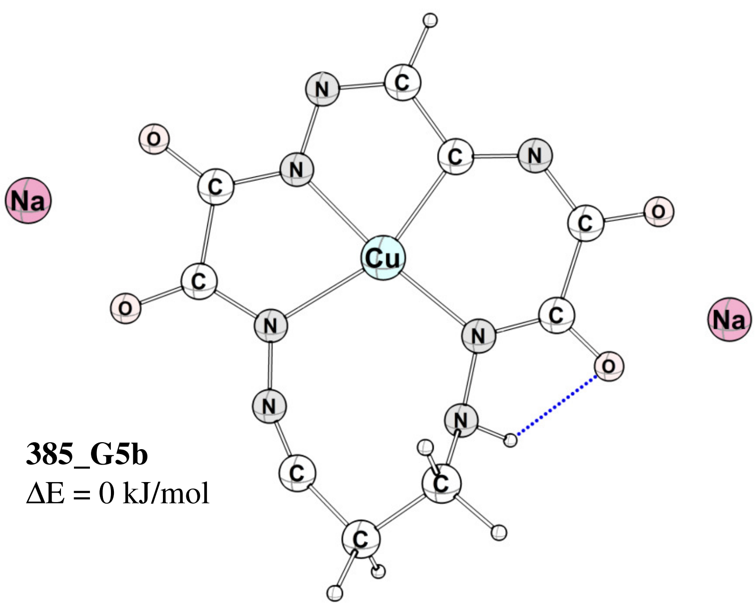
385 m/z, $^{63}Cu^{III}C_9H_6N_7O_4Na_2$



385_G3c
ΔE = +63.7 kJ/mol



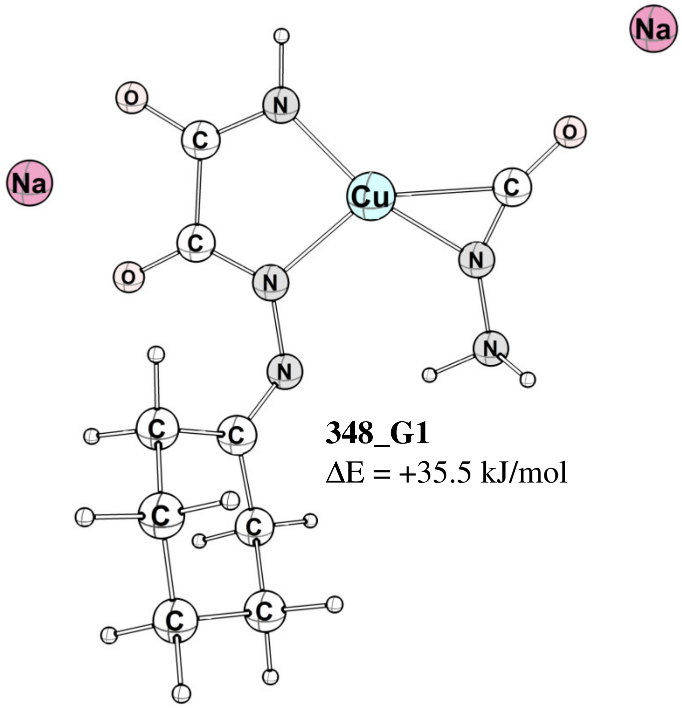
385_G4b
ΔE = +63.3 kJ/mol



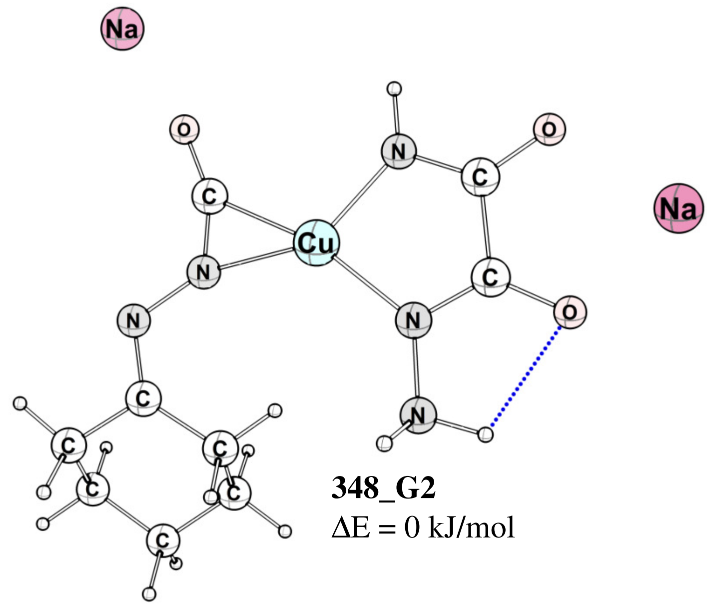
385_G5b
ΔE = 0 kJ/mol

Figure S1 (*continued*)

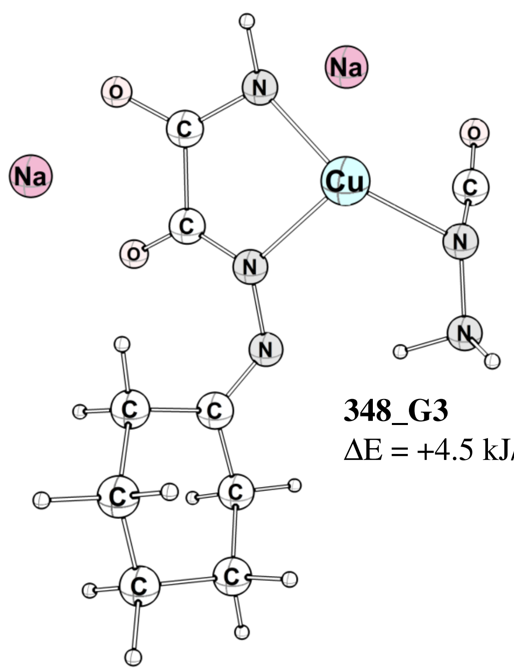
348 m/z, $^{63}Cu^{III}C_9H_{13}N_5O_3Na_2$



348_G1
ΔE = +35.5 kJ/mol



348_G2
ΔE = 0 kJ/mol



348_G3
ΔE = +4.5 kJ/mol

Figure S1 (*continued*)

305 m/z (from *417 m/z*), $^{63}Cu^{III}C_4N_6O_4Na_2$

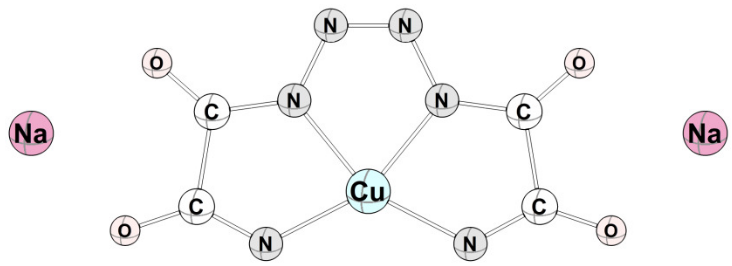
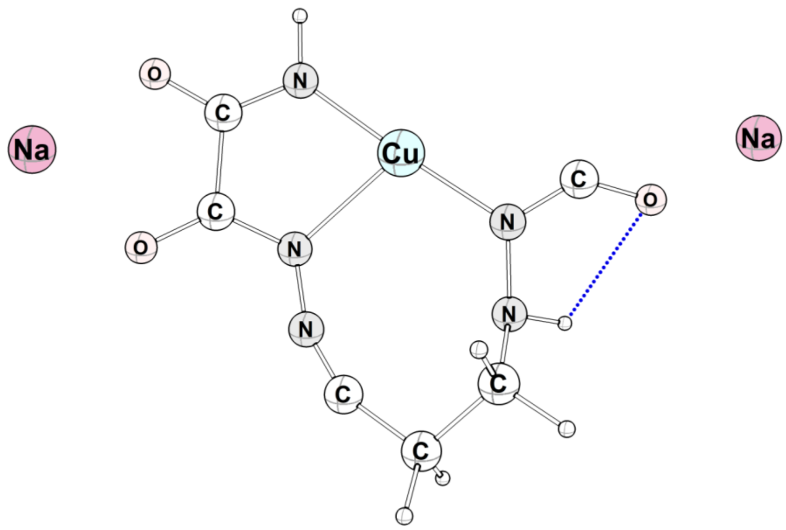


Figure S1 (*continued*)

305 m/z (from *348 m/z G1*), $^{63}Cu^{III}C_6H_6N_5O_3Na_2$



305 m/z (from *348 m/z G2*), $^{63}Cu^{III}C_6H_6N_5O_3Na_2$

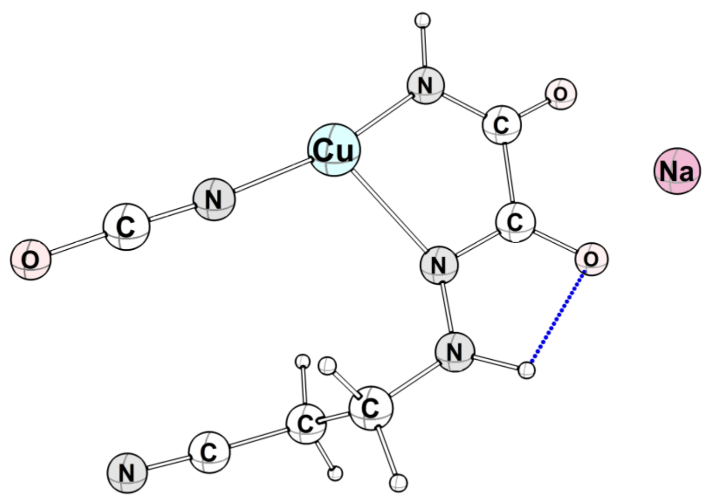


Figure S1 (*continued*)

290 m/z, $^{63}Cu^{III}C_6H_5N_4O_3Na_2$

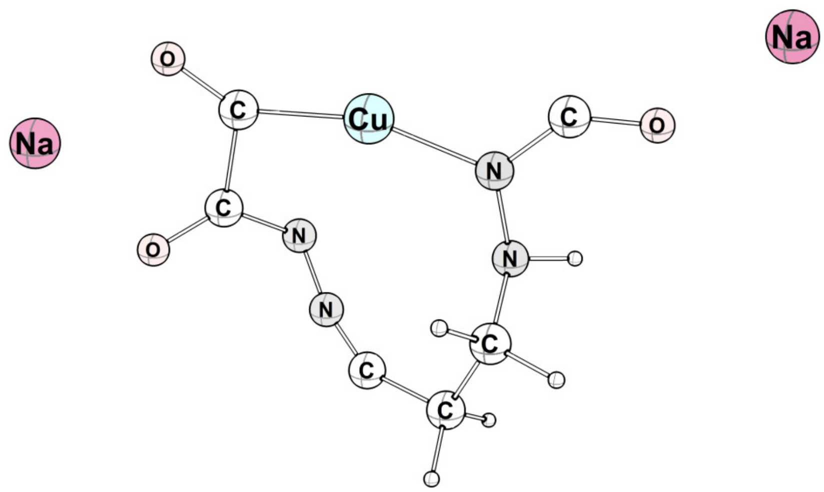
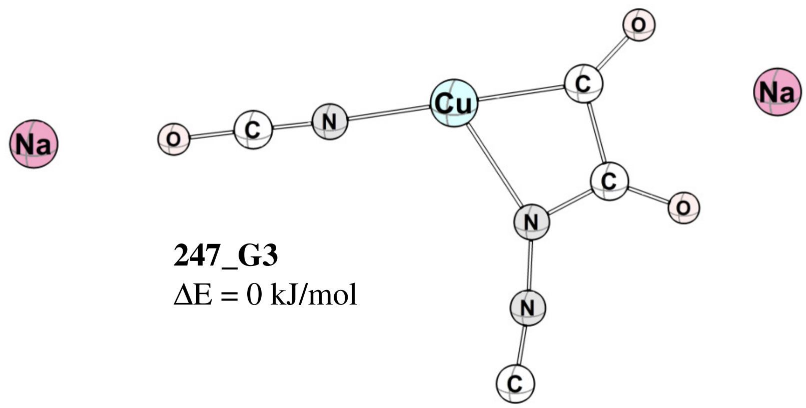
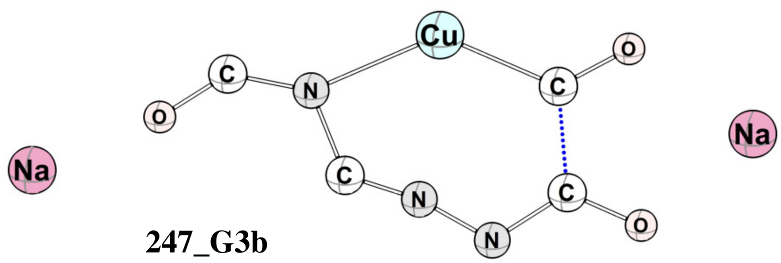


Figure S1 (*continued*)

247 m/z, $^{63}Cu^{III}C_4N_3O_3Na_2$



247_G3
ΔE = 0 kJ/mol



247_G3b
ΔE = +214.4 kJ/mol

Figure S1 (*continued*)

243 m/z, $^{63}Cu^{III}C_3H_3N_5O_3Na$

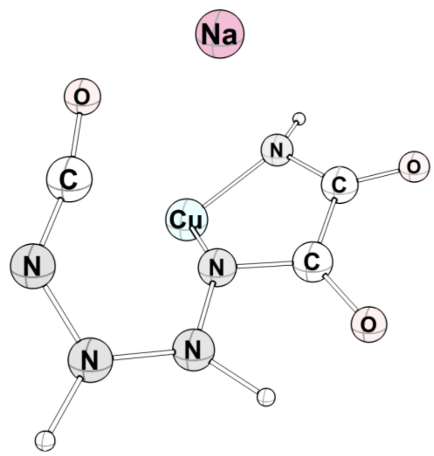
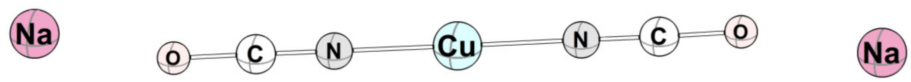


Figure S1 (*continued*)

193 m/z, $^{63}Cu^{III}C_2N_2O_2Na_2$



168 m/z, $^{63}Cu^{III}C_2N_3ONa$

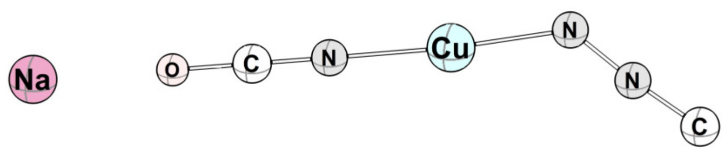


Figure S2. Summary of Positive ion mode fragmentation pattern for [$Cu^{III}(CPZmh_2)_{-4H}$]. Structural models for each of the singly positively charged ions are shown in Figure S1, while masses of the molecular ion fragments and the losses are summarized in Table S1. Each fragmentation pathway is indicated with a specific colour. The asterisk represents an alternate fragmentation pathway via a 305 *m/z* intermediate.

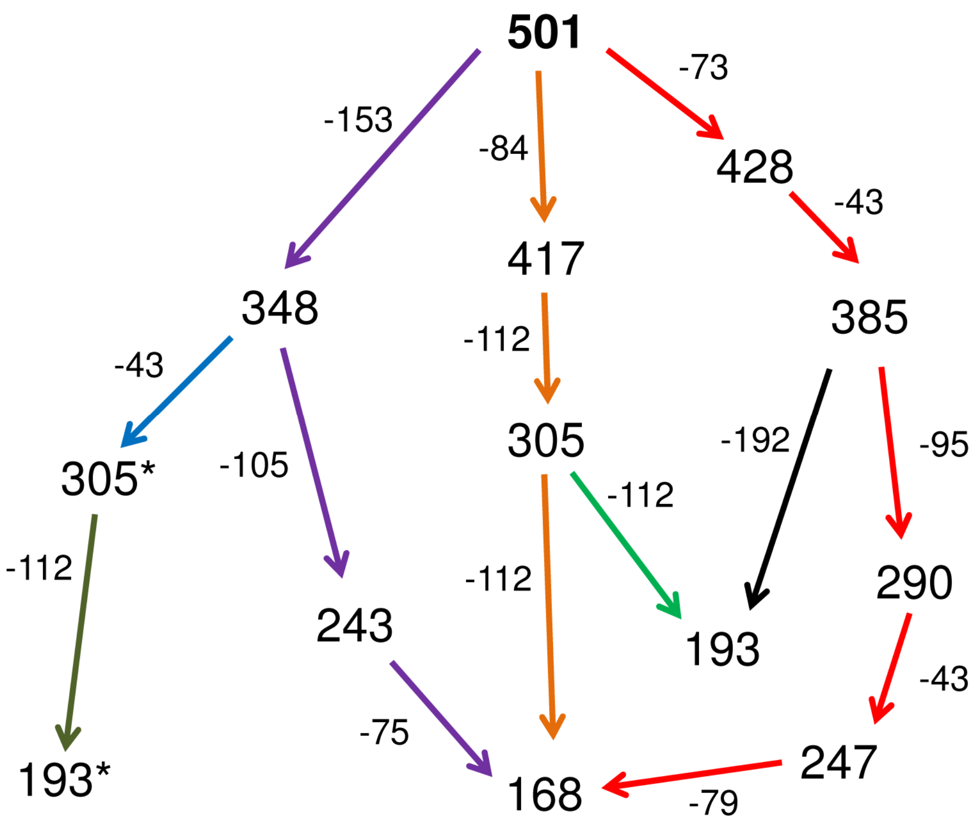


Figure S3. Cu K near edge spectrum of the crude reaction mixture, which contains both the blue and green products, demonstrating Cu(II) is present, as evidenced by the weak pre-edge peak, arising from a formally forbidden 1s→3d transition, at ~8979 eV. The rising edge obscures this same transition for Cu(III), which has a 1s→3d transition ~1 eV higher in energy.

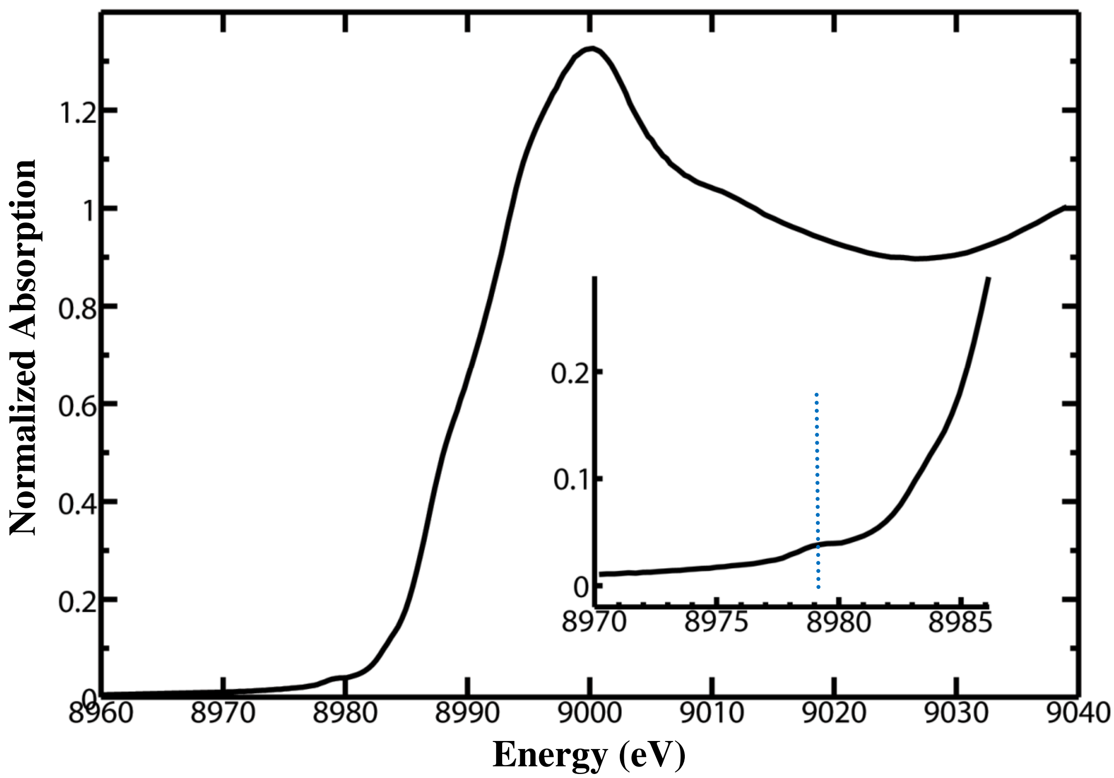


Figure S4. EPR data for Cu^{2+} in the presence of 2 equivalents of cuprizone, relative to an equivalent concentration of Cu^{II}EDTA (**A**), and 20 equivalents of cuprizone (**B**) at pH 8.5. X-band EPR spectra were recorded on a JEOL RE1X spectrometer (JEOL USA, Inc. Peabody, MA, USA) at the Stanford Synchrotron Radiation Lightsource, located near to the beamline used for all X-ray absorption spectroscopy measurements. Samples were maintained at 100 K, and data were collected with 0.1 mT modulation amplitude and integrated by reference to a 1 mM aqueous Cu(II)–EDTA standard, with field calibration using a diphenylpicrylhydrazyl standard, as previously described.[ii] Fit parameters for **B** are shown in **Table S3**.

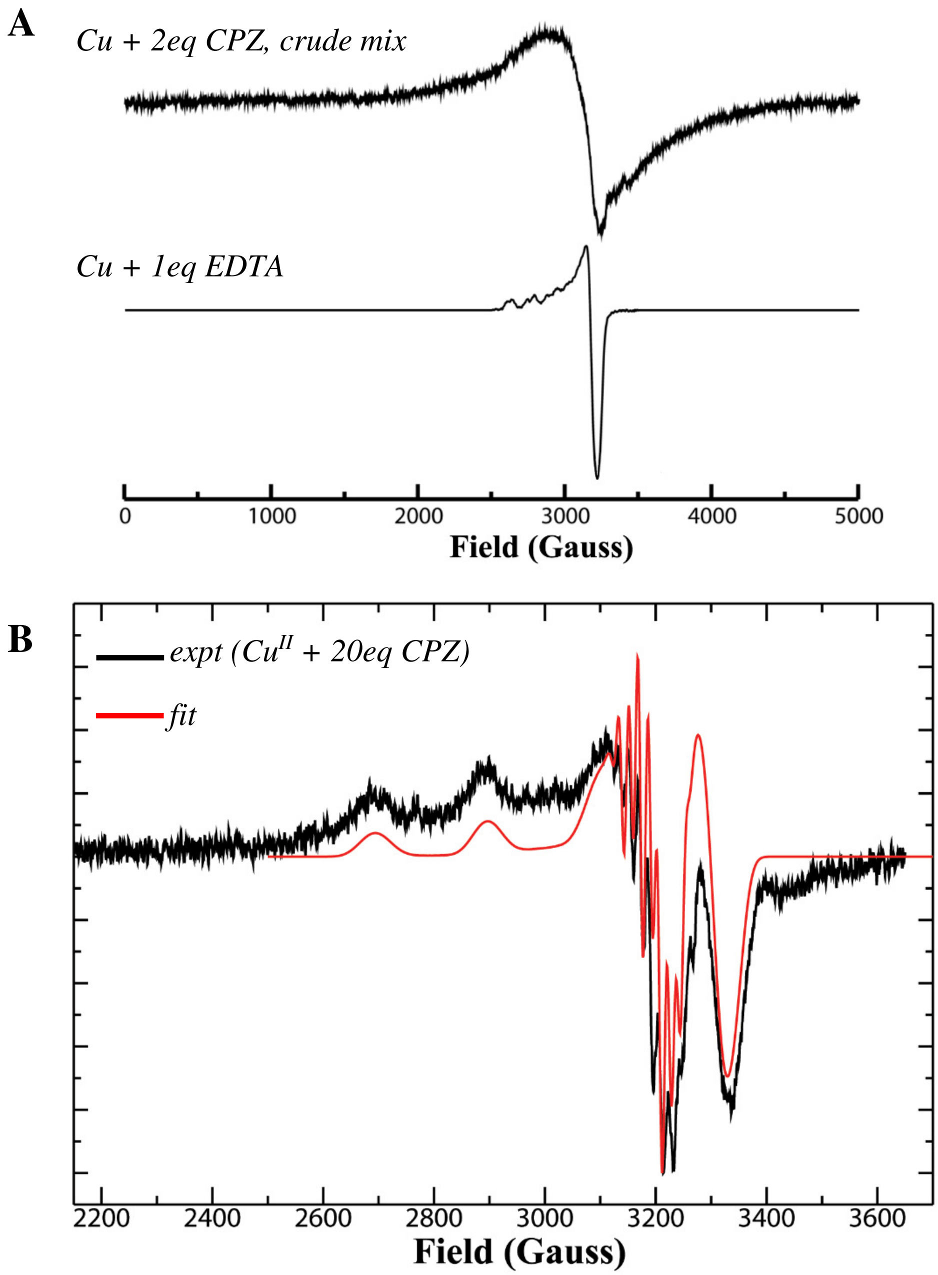


Figure S5. Structures from geometry optimizations for the multi-Cu(II) green product. Structures that indicated formation of Cu(I) and Cu(III) during geometry optimizations were omitted from consideration. Interatomic Cu···Cu and Cu–L distances are shown in Ångstroms. Only the model with a Cu···Cu close to that observed in the EXAFS Fourier transform of the green product was employed for EXAFS curve fitting. Charge and spin multiplicity are shown in the top right corner for each structure. All calculations were performed with unrestricted spin. C_6H_{10} moieties were removed for clarity.

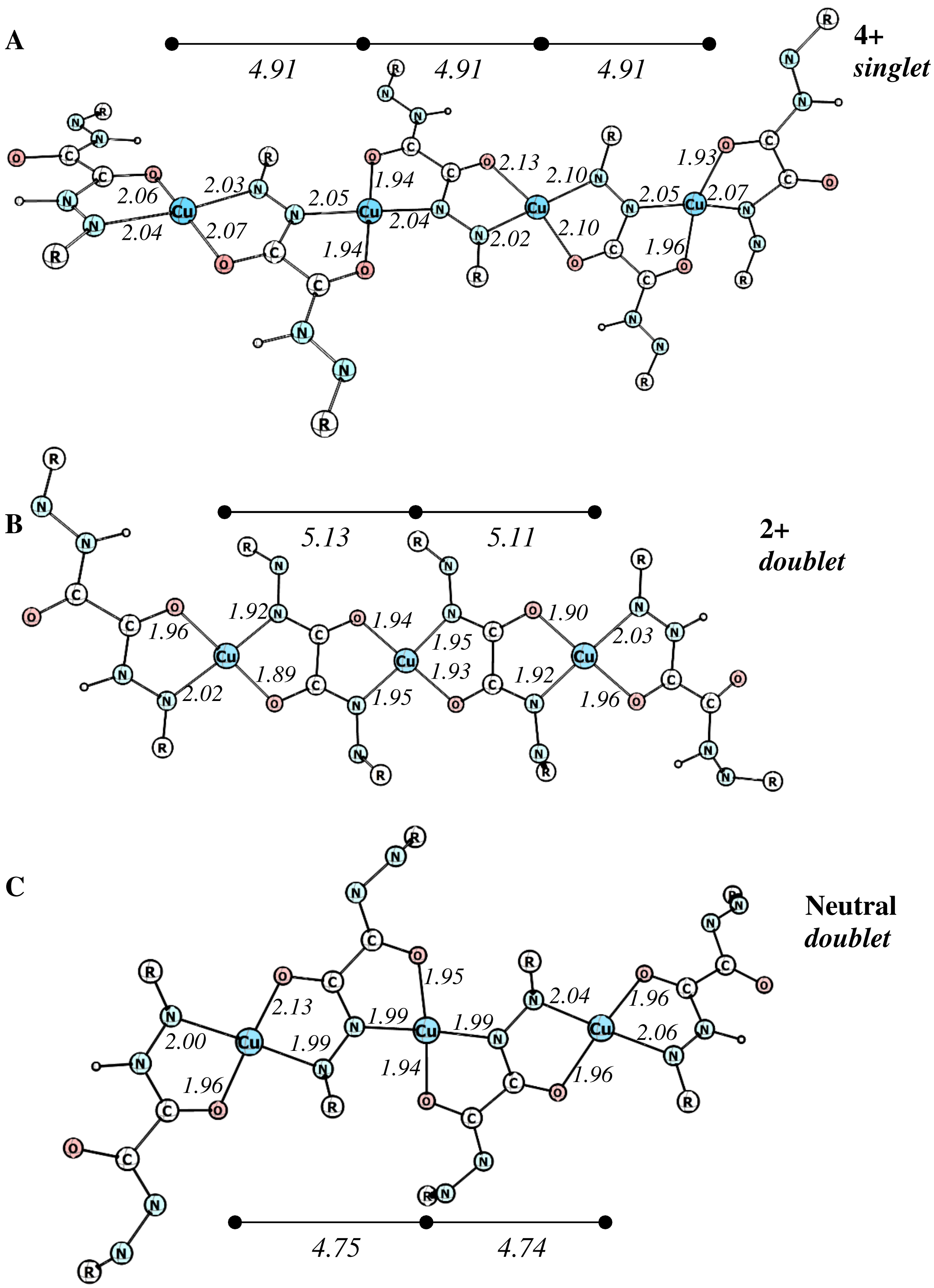
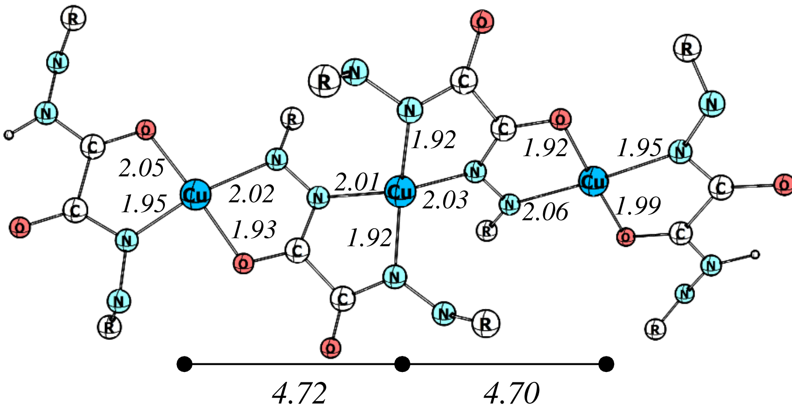


Figure S5. *(continued)*

D



Neutral
doublet

Figure S5. Gaussian output from geometry optimizations:

Tautomeric structures from Figure 5.

CuII_CPZmh2_-4H_Geom1 (unlinked structure, tautomer 1)

N	0.9908906022	1.7360187107	-0.4073767541
C	0.4109547522	2.8856842571	-0.0604752503
C	-1.1261715254	2.8437104165	-0.1871387436
O	1.0046580407	3.9251692587	0.2977451312
O	-1.8184662305	3.8360661429	0.0771277459
N	-1.5806767989	1.6382595341	-0.6264693398
N	-2.9470875061	1.4410942312	-0.7078645143
C	-3.6635757829	2.1505943217	-1.4999698026
C	-3.2098431256	3.2129777145	-2.4740525767
C	-3.950014989	4.5395330503	-2.2158085492
C	-5.4746680261	4.3426511904	-2.2076062149
C	-5.9000188592	3.2471765455	-1.2176958818
C	-5.1581384068	1.9226731606	-1.4923890705
H	-2.1330469919	3.3528405085	-2.4216781218
H	-3.4566542491	2.857058789	-3.4883803143
H	-3.670879373	5.279575045	-2.9764401379
H	-3.6078652295	4.9185214294	-1.2486182136
H	-5.8135056432	4.0625107171	-3.2167530646
H	-5.9768340572	5.287355432	-1.9617885085
H	-6.9857267463	3.0898853299	-1.2657107502
H	-5.6647310183	3.5728988086	-0.1977325433
H	-5.4794171908	1.5387378785	-2.474438085
H	-5.4023376353	1.1684921498	-0.7411819617
Cu	-0.2042304044	0.1209192844	-0.388342598
C	5.1245361958	-2.9612601904	2.6301251604
C	3.6038342719	-3.0697456486	2.7994221661
C	2.8537550276	-3.0936302338	1.4517754529
C	3.2957892903	-1.9808283622	0.5332652141
C	4.7873562742	-1.7407188807	0.434974427
C	5.4903975311	-1.7213656831	1.8036666137
N	2.5382076146	-1.2078516648	-0.1612814286
N	1.1756448801	-1.4030895331	-0.2001115366
C	0.6971553851	-2.6037656114	-0.6409917193
C	-0.8439154621	-2.6434740827	-0.6868284213
O	1.3755880265	-3.5837484929	-0.9700929327
O	-1.4574439143	-3.6869299193	-0.999394158
N	-1.4039742946	-1.4878267427	-0.3292674871
H	5.4992436813	-3.8600045019	2.1194840764
H	5.6175685234	-2.9277185093	3.6105390834
H	3.3477010649	-3.9675608155	3.3750006896
H	3.2536335264	-2.212201583	3.3885735887
H	1.7785623618	-3.012260782	1.617555742

H	3.0037295242	-4.0525951124	0.9398765015
H	4.9539539951	-0.8113474557	-0.1150948834
H	5.2264267359	-2.5517365529	-0.167352813
H	5.185180374	-0.8214462877	2.3529555334
H	6.5778711782	-1.6555640754	1.6684919032
N	-2.8160443196	-1.517168234	-0.2373303129
H	-3.1442798542	-0.5654099614	-0.3998191765
H	-3.1674689689	-2.1594419891	-0.9497954797
N	2.4052721526	1.7707278889	-0.4325087655
H	2.7266901474	0.810183952	-0.3143323668
H	2.7263632164	2.3707635888	0.3292045129

CuII_CPZmh2_-4H_GeomX1 (pseudo-macrocyclic structure, tautomer 2)

N	-2.0779561307	-2.8852752806	-0.3011394593
C	-3.3130673786	-2.6562132447	-0.7577882838
C	-3.7431572111	-1.1760511002	-0.5812727069
O	-4.065569496	-3.5045165422	-1.2838827783
O	-4.9119713553	-0.7773424747	-0.781949479
N	-2.7260458598	-0.4060440145	-0.1911788639
N	-3.0156165915	0.9452444543	0.1130686084
C	-2.0103481287	1.8883220248	-0.4383167525
C	-2.5491590849	3.3127552288	-0.1760159466
C	-3.7700967299	3.681685556	-1.032038519
C	-3.4969638572	3.4685844249	-2.5282185676
C	-2.9921069267	2.0440383252	-2.80027577
C	-1.7549906915	1.712112898	-1.955750925
H	-2.7929663633	3.3990686749	0.8887614431
H	-1.7293803787	4.0088897558	-0.3831250301
H	-4.0463216892	4.7273754645	-0.841548655
H	-4.6360272213	3.0789009287	-0.7339355358
H	-2.7363151009	4.1909974095	-2.8594997795
H	-4.4038791318	3.6748339885	-3.1113846385
H	-2.751394718	1.9289243368	-3.8643456807
H	-3.788267791	1.3230000768	-2.5824640396
H	-0.920070037	2.3680651156	-2.2297781238
H	-1.432999218	0.6876652216	-2.1421000864
Cu	-0.9571836178	-1.2353128624	-0.0234637818
C	4.217077926	-4.2930144035	-2.9746943452
C	3.6257268664	-2.8781072765	-2.9936635574
C	3.2641393111	-2.3652832976	-1.5850455075
C	2.4454144758	-3.3657861878	-0.8051365146
C	2.904508101	-4.8077740387	-0.8685862647
C	3.2515357269	-5.2719043763	-2.2943285117
N	1.3922641071	-3.1230787577	-0.1096450034
N	0.9588943419	-1.8226271688	0.0658667775

C	1.7840556841	-0.904130373	0.6375044341
C	1.0909464424	0.4770665842	0.8367993812
O	2.9532695393	-1.084872045	0.9977161305
O	1.6005051396	1.347697574	1.5594244882
N	-0.0566238053	0.5681494753	0.1431714338
H	5.1700585597	-4.2832238035	-2.4262968394
H	4.4447140355	-4.6268660769	-3.9954840636
H	4.3246947358	-2.1787454219	-3.4682222143
H	2.7211670001	-2.8840072473	-3.6156120603
H	2.7078137019	-1.4297907549	-1.6571822851
H	4.1702283407	-2.130200173	-1.0125682995
H	2.1322192149	-5.4352894319	-0.4171876798
H	3.8056857648	-4.9079052375	-0.2432765761
H	2.3298820812	-5.3354332564	-2.8867631157
H	3.6807179469	-6.2819197498	-2.2679270976
N	-0.7321611262	1.8051570405	0.2725688412
H	-0.8711266494	2.0128235998	1.2623540238
H	-3.9466981361	1.1166884398	-0.271620725
N	-1.6369862521	-4.2362143581	-0.3862203502
H	-0.6206650056	-4.2025833067	-0.4299626167
H	-2.0218796145	-4.6432418875	-1.2411843058

CuII_CPZmh2_-4H_cyc (cyclic structure, tautomer 3)

N	-0.997001045302	-1.784148120134	0.098030372816
C	-0.202283734334	-2.870672282135	0.038986051232
C	1.222579924535	-2.554479361611	0.644434780376
O	-0.471211577958	-3.988877800365	-0.422918844085
O	1.862287234676	-3.412017632281	1.269036412757
N	1.574060194693	-1.277123062470	0.392784135561
N	2.784578188658	-0.778049735165	0.954389188254
C	3.143288271205	0.577072813749	0.503343417678
C	3.273786348234	0.591888468518	-1.038525565591
C	4.379115157637	-0.339180457751	-1.552180046061
C	5.734999048599	-0.007171601784	-0.912459207113
C	5.640397456156	-0.028007966853	0.619871550996
C	4.520678492423	0.888011150214	1.132828686526
H	2.313149360461	0.325075515736	-1.477916881250
H	3.486896764260	1.626203872752	-1.338739287716
H	4.450557967660	-0.262111139935	-2.645189777250
H	4.107180185437	-1.372317609311	-1.316666775803
H	6.057387692905	0.991824750721	-1.243593625737
H	6.504115729496	-0.713391711146	-1.252307666701
H	6.598451958726	0.275092956294	1.064365578958
H	5.433578052511	-1.050355589948	0.949370478626
H	4.768791908890	1.934643234130	0.912055162083

H	4.428979617185	0.813605791024	2.222135623865
Cu	0.029455024349	-0.127276700468	0.122589931542
C	-5.711654855403	0.276058881185	0.960011591196
C	-5.591859970489	0.050343763373	-0.554350241272
C	-4.500548034305	-0.979182223397	-0.885841404611
C	-3.121009597395	-0.654848981842	-0.267850011695
C	-3.285506786431	-0.421738493414	1.253284745190
C	-4.350730781716	0.634699982486	1.574411085906
N	-2.609491606561	0.546725839558	-1.000772555352
N	-1.397835480777	1.039319188598	-0.464952743883
C	-1.186109192649	2.353877923347	-0.386714405920
C	0.264811410699	2.674508956056	0.141029555665
O	-2.004204210466	3.247407846609	-0.693318048637
O	0.700212310108	3.841433793902	0.236100066489
N	0.926033158425	1.560565899431	0.460024307857
H	-6.087454610654	-0.644536223022	1.430054135409
H	-6.449603029073	1.061527157441	1.169194064384
H	-6.551674855330	-0.291190809937	-0.964437111328
H	-5.374096851271	1.005779624296	-1.046651819885
H	-4.381122812490	-1.068889405346	-1.971336131985
H	-4.795481803272	-1.962504185801	-0.505432367185
H	-2.323048490903	-0.127109707945	1.670946544892
H	-3.553172717743	-1.382152408250	1.709183128527
H	-4.023478240306	1.611383718144	1.199513079037
H	-4.446583059187	0.738044853181	2.662192469202
N	2.227056511267	1.644825673507	1.011954015047
H	2.593381003907	2.568558488019	0.767947530901
H	2.702786664082	-0.770465982435	1.971478888509
N	-2.299824833905	-1.861357002511	-0.476300303604
H	-2.209684584382	-2.024549132618	-1.480058450968
H	-3.278783399645	1.317319590325	-0.968979407406

sCuIII_CPZmh2_-4H_Geom1 (unlinked structure, tautomer 1)

N	0.2769411212	-1.6002755011	1.0172065588
C	-0.4133340429	-2.3429862005	0.0883991682
C	-1.6539502909	-1.6355134857	-0.4344426374
O	-0.0884310618	-3.4728598078	-0.2720110313
O	-2.4238990754	-2.1755209703	-1.2209536424
N	-1.7813274622	-0.3746936287	0.0999652808
N	-2.7548859515	0.432824319	-0.4127233153
C	-4.0029788856	0.1545820039	-0.3119486902
C	-4.6327991637	-1.0208440219	0.3949385574
C	-5.5782112458	-1.7849172519	-0.5538531413
C	-6.6062965317	-0.8466488472	-1.2027218926
C	-5.9259864505	0.3350659068	-1.909154931

C	-4.9911764194	1.1006305493	-0.9499353265
H	-3.8796039291	-1.6840138727	0.812691407
H	-5.2209875849	-0.6129933509	1.2314289539
H	-6.088296607	-2.5804628202	0.00000756
H	-4.9650984393	-2.265054745	-1.3211874918
H	-7.2886083008	-0.4604050866	-0.4321998538
H	-7.2246665102	-1.4036679013	-1.9155737064
H	-6.6758643578	1.0202891523	-2.3198628885
H	-5.3352446287	-0.0381339547	-2.7536225974
H	-5.6000475345	1.5678275025	-0.1622213795
H	-4.4554542909	1.8951325328	-1.4730367865
Cu	0.0236625764	0.3636587965	0.6213739134
C	6.7123590619	-0.0784028269	-0.3825716543
C	5.5901221637	0.6807588576	-1.0990479335
C	4.590715808	1.3263772658	-0.1176329827
C	4.1072417232	0.350842079	0.9240553626
C	5.1580910453	-0.5249122492	1.568787055
C	6.1312985537	-1.1465702965	0.551438293
N	2.8944509917	0.1896222099	1.318138793
N	1.8929474883	1.0200002335	0.8466176829
C	1.9790301009	2.352048757	1.1178985534
C	0.7154525004	3.0892062761	0.6608594829
O	2.9282389039	2.9454233539	1.6208567627
O	0.7536685463	4.2530072085	0.2612933872
N	-0.4099201796	2.3238818521	0.7293971708
H	7.3163171562	0.6275071626	0.2032731081
H	7.3869017034	-0.5386282261	-1.1133868743
H	6.0056772282	1.4577566578	-1.7490904305
H	5.0512663074	-0.0164958417	-1.7529149684
H	3.7374052265	1.7351164553	-0.6595345845
H	5.0525413758	2.1747699299	0.4012497354
H	4.6654386736	-1.2887671704	2.1749464695
H	5.7320129621	0.1069188086	2.2616651152
H	5.6005909861	-1.8981614746	-0.0460969782
H	6.931619587	-1.6743857415	1.0816657484
N	-1.5127954935	2.9181573239	0.1498274346
H	-1.2362364844	3.5203115077	-0.6276135631
H	-2.1816305033	2.192755	-0.1305767073
N	1.4333496171	-2.1883873483	1.4180558748
H	2.098734777	-1.4813724719	1.7485843217
H	1.8032201393	-2.8358447439	0.7194638487

sCuIII_CPZmh2_-4H_GeomX1 (pseudo-macrocyclic structure, tautomer 2)

N	-1.8046566067	-2.732891499	0.028198347
C	-2.9695838595	-2.7787226763	-0.6666066041

C	-3.3428561804	-1.410096134	-1.2183716427
O	-3.617206507	-3.8001292729	-0.9111885313
O	-4.16875667	-1.2575627263	-2.109994072
N	-2.5952486238	-0.370934801	-0.6640852657
N	-2.7068647384	0.7768380399	-1.3797279988
C	-2.0713553801	1.9959942176	-0.9047785561
C	-2.9779018991	2.666888778	0.1548672388
C	-4.3142457821	3.1407261643	-0.4279058341
C	-4.118320155	4.0673530544	-1.6364073825
C	-3.2509277121	3.4006083781	-2.71286328
C	-1.9102399351	2.9323341934	-2.126459842
H	-3.1487205269	1.9468610369	0.9606075306
H	-2.4311452238	3.5185558352	0.5793171005
H	-4.8892742427	3.6516613285	0.3520179501
H	-4.8955105618	2.2646627483	-0.7317391663
H	-3.6330440483	4.9970215212	-1.3084899485
H	-5.0901095595	4.351100378	-2.0550227985
H	-3.0594845372	4.1000676959	-3.5342292347
H	-3.7982301758	2.5564857149	-3.1470562958
H	-1.3379268877	3.7979678442	-1.7822398641
H	-1.29387487	2.4283827464	-2.8779153489
Cu	-0.7785941205	-1.118485798	-0.3854441203
C	4.1873362206	-4.9775644378	-2.6964098281
C	3.6539059191	-3.5914982889	-3.0771441381
C	3.3627901904	-2.7101299807	-1.8449252302
C	2.5244433563	-3.4339508105	-0.8205860055
C	2.9327824194	-4.8530015558	-0.4974154263
C	3.2122881885	-5.6948843275	-1.7546705946
N	1.4918510431	-2.9716510877	-0.2140496567
N	1.1044459186	-1.6601245756	-0.3875700431
C	1.9403027691	-0.6599209355	0.0143430318
C	1.1982409085	0.6876113463	0.1004443413
O	3.1174383538	-0.7654976081	0.3437342969
O	1.6402554332	1.6216616954	0.7587022771
N	-0.0025390259	0.7020151454	-0.5820856482
H	5.1615316635	-4.8715926672	-2.1999988442
H	4.3577660941	-5.5787079349	-3.5968111569
H	4.3644695509	-3.0733132594	-3.7299026739
H	2.7303110562	-3.7138186535	-3.6568507002
H	2.8599720141	-1.7901605848	-2.1441283033
H	4.2989560773	-2.4024953714	-1.3644637495
H	2.1649131195	-5.3098016234	0.1308472055
H	3.8517417622	-4.8056785728	0.1045137588
H	2.2688675365	-5.8781892565	-2.2838528851
H	3.6060491857	-6.6752633782	-1.4643571977
N	-0.7616939628	1.7993898724	-0.2684924567

H	-0.744693207	2.0084493454	0.7283343339
H	-2.7240119956	0.6354487491	-2.3878832018
N	-1.2810192157	-3.9627598323	0.3739708012
H	-0.2634714304	-3.8854964213	0.4397412732
H	-1.5816273949	-4.6784693089	-0.2903617355

sCuIII_CPZmh2_-4H_cycGeom3 (cyclic structure, tautomer 3)

N	-0.9312151525	1.5611376731	0.5017617245
C	-0.3665345395	2.6996279645	0.0557331318
C	1.0588767353	2.4413614687	-0.4808312116
O	-0.8987149066	3.8131644205	0.0494190644
O	1.6813071255	3.2621169038	-1.1393846108
N	1.5095592829	1.1810306184	-0.1474274546
N	2.6635712168	0.7573846699	-0.7618187958
C	3.1472392652	-0.556390489	-0.3766505602
C	3.3188334189	-0.6341732425	1.1575368228
C	4.4030168983	0.3171196932	1.6809653347
C	5.7468460671	0.0736925567	0.9809218883
C	5.6016582572	0.166586956	-0.5441684911
C	4.5057401817	-0.7715614707	-1.0698294716
H	2.3645519715	-0.4288668325	1.6437535457
H	3.5860796566	-1.6692699801	1.4007404589
H	4.5111308648	0.1854040255	2.7634268349
H	4.0842208926	1.3508443807	1.5153306561
H	6.1208180252	-0.9239613812	1.2506137241
H	6.494964551	0.7935422729	1.3314372667
H	6.5518061732	-0.0766527905	-1.0332376412
H	5.3551553932	1.1968213659	-0.8195651685
H	4.8020865353	-1.814954176	-0.9100896854
H	4.3706984642	-0.6518897587	-2.1497298561
Cu	-0.005121478	-0.01347762	0.0262003662
C	-5.7568445019	-0.0999023247	-0.929575256
C	-5.6119981092	-0.1931355282	0.5955324163
C	-4.5160964559	0.7448116391	1.1215807792
C	-3.1574504599	0.5296035036	0.4287042793
C	-3.3286714767	0.6076537542	-1.1055376499
C	-4.4129044653	-0.3433571786	-1.6293973903
N	-2.6741470473	-0.7844433463	0.8136773095
N	-1.5198153469	-1.2079278844	0.1998501176
C	-1.0691831625	-2.4681414477	0.5333751551
C	0.3562616599	-2.7264508353	-0.0029730756
O	-1.6916893963	-3.2888575437	1.1919994708
O	0.8885213882	-3.8399642104	0.0038627516
N	0.9209811992	-1.5881379611	-0.4494713573
H	-6.1306240883	0.8978620222	-1.1991214644

H	-6.5049876316	-0.8195745767	-1.2804046406
H	-6.5622278089	0.0501081514	1.0844411833
H	-5.3656825659	-1.2234588147	0.8707633333
H	-4.3813026326	0.6250186657	2.2014958461
H	-4.8123161167	1.7882436444	0.9618608557
H	-2.3743038245	0.4021974075	-1.5915264244
H	-3.5956169851	1.6428363003	-1.3486991678
H	-4.0943069192	-1.3771695233	-1.4639315552
H	-4.5207981595	-0.2113710388	-2.7118484235
N	2.2491179432	-1.6430464802	-0.9122010547
H	2.6079822254	-2.5473512991	-0.5934426372
H	2.6617117666	0.9072073654	-1.7703450096
N	-2.259257979	1.6157502312	0.9647075579
H	-2.6181394437	2.5203037224	0.6467482493
H	-2.6729595057	-0.9348616428	1.8221329294

Daughter fragments shown in Figure S1 (only stable structures, failed searches are omitted).

sCuIII_CPZmh2-4H_GeomX1_Na2_Geom1 (501 *m/z*)

29	-0.04291	0.29069	-0.47331
7	0.24508	2.1015	-1.1799
6	-0.72025	2.93816	-0.79002
6	-1.92719	2.24293	-0.22684
8	-0.64889	4.19384	-0.79224
8	-2.8023	2.89452	0.37809
7	-1.94405	0.88595	-0.38675
7	-2.81723	0.23872	0.39831
6	-3.06337	-1.20692	0.25744
6	-4.27633	-1.43524	-0.67321
6	-5.58899	-0.9154	-0.07279
6	-5.8522	-1.49552	1.32314
6	-4.67209	-1.23304	2.26722
6	-3.35873	-1.76358	1.67179
1	-4.07513	-0.95085	-1.63412
1	-4.35416	-2.51428	-0.85442
1	-6.41095	-1.16515	-0.74911
1	-5.55163	0.1776	-0.01682
1	-6.01648	-2.57743	1.24472
1	-6.77005	-1.07069	1.73865
1	-4.8392	-1.7161	3.23399
1	-4.60445	-0.15818	2.47891
1	-3.42334	-2.84915	1.56748
1	-2.5043	-1.55833	2.32409
6	6.10476	0.60509	2.01279
6	4.81392	-0.09677	2.44757
6	4.12526	-0.83634	1.27972
6	3.9624	0.05671	0.07731
6	5.17677	0.84973	-0.33546
6	5.83804	1.57205	0.85392
7	2.89132	0.21819	-0.61442
7	1.74916	-0.50808	-0.32516
6	1.71284	-1.82424	-0.54016
6	0.29339	-2.40195	-0.52401
8	2.67073	-2.58516	-0.80139
8	0.09789	-3.55836	-0.94506
7	-0.65922	-1.55321	-0.0822
1	6.84424	-0.14374	1.70193
1	6.54247	1.14186	2.85934
1	5.01475	-0.81191	3.25016
1	4.11975	0.64582	2.85911
1	3.16014	-1.235	1.59307
1	4.73697	-1.69362	0.97308
1	4.90611	1.54402	-1.13336

1	5.89914	0.14049	-0.76183
1	5.1818	2.38096	1.19739
1	6.76667	2.04292	0.52016
7	-1.94101	-1.92855	-0.33488
1	-2.09578	-2.25807	-1.28469
1	-2.93368	0.63232	1.32923
7	1.4275	2.64625	-1.55815
1	2.17687	1.9507	-1.53384
1	1.63196	3.53414	-1.10349
11	2.01502	-4.60165	-1.41191
11	-2.44838	5.10014	0.10487

Na2CuC16N8H24O4_428_G1

7	1.557758	-1.370277	-0.231651
6	2.879973	-1.511389	-0.154270
6	3.601270	-0.282383	0.295540
8	3.527441	-2.549248	-0.460474
8	4.828193	-0.279380	0.427608
7	2.804563	0.837391	0.493142
6	2.434740	3.096889	0.603447
6	3.315075	2.043767	0.314535
1	4.311775	2.206996	-0.080811
29	0.837259	0.479291	-0.072056
6	-4.490044	-3.208713	1.089219
6	-3.859410	-2.001074	1.789896
6	-3.523872	-0.857680	0.806021
6	-2.738488	-1.358496	-0.377026
6	-3.257749	-2.607457	-1.043397
6	-3.582138	-3.724064	-0.032336
7	-1.662161	-0.843854	-0.861525
7	-1.139496	0.328103	-0.336991
6	-1.811716	1.477740	-0.434806
6	-0.991259	2.704189	0.006358
8	-2.987568	1.658996	-0.812244
8	-1.529149	3.806635	0.142776
7	0.302984	2.384090	0.166927
1	-5.464805	-2.926161	0.671808
1	-4.680969	-4.003731	1.815526
1	-4.524488	-1.613459	2.566530
1	-2.939657	-2.316158	2.296500
1	-2.981619	-0.062497	1.317919
1	-4.451504	-0.415406	0.422123
1	-2.546894	-2.937772	-1.803437
1	-4.180530	-2.331485	-1.571712

1	-2.649106	-4.105998	0.398666
1	-4.050508	-4.560698	-0.557615
7	1.234486	3.222919	0.674920
7	0.865403	-2.412749	-0.742911
1	-0.088631	-2.148438	-0.995327
1	1.389861	-2.979495	-1.405163
11	-3.651849	3.769264	-0.586468
11	5.675683	-2.355493	-0.020730

Na2CuC16N8H24O4_428_G2

7	0.389382	2.553199	-0.050111
6	1.745882	2.466733	0.126649
6	2.241581	1.083451	0.529949
8	2.539144	3.398005	-0.018859
8	3.459667	0.898748	0.786243
7	1.280870	0.177600	0.544879
7	1.558468	-1.127711	0.916075
6	0.755370	-2.191519	0.213148
6	1.248290	-3.540442	0.773796
6	2.659886	-3.920650	0.301096
6	2.771055	-3.880066	-1.228135
6	2.324865	-2.520780	-1.781617
6	0.905342	-2.157059	-1.323085
1	1.202669	-3.508701	1.866820
1	0.538441	-4.301503	0.437426
1	2.896836	-4.920075	0.675432
1	3.409237	-3.254300	0.746481
1	2.141688	-4.668946	-1.657790
1	3.797102	-4.097032	-1.537708
1	2.352067	-2.528296	-2.874678
1	3.032536	-1.743757	-1.466040
1	0.187748	-2.872517	-1.736546
1	0.621968	-1.174746	-1.708899
29	-0.472035	0.756021	0.030970
6	-0.204733	3.380842	-0.932171
6	-1.576883	3.450123	-0.831220
7	-2.489711	2.724958	-0.439234
7	-2.267962	1.350608	-0.388849
6	-3.248473	0.468234	-0.151510
6	-2.666558	-0.924317	0.204520
8	-4.469485	0.639210	-0.150227
8	-3.434453	-1.819726	0.583377
7	-1.328720	-0.976010	0.103770
1	0.353545	3.877804	-1.718719
7	-0.653542	-2.074478	0.582198

1	-0.809052	-2.225315	1.578215
1	2.558435	-1.290511	0.809649
11	-5.592608	-1.199811	0.456500
11	4.637297	2.760619	0.615710

Na2CuC16N8H24O4_428_G3

7	-1.965318	0.994925	-0.331073
6	-3.279039	1.169873	-0.219148
6	-4.170687	0.047595	0.219592
8	-3.848951	2.280257	-0.459915
8	-5.373017	0.257445	0.355511
7	-3.703090	-1.237931	0.468471
6	-2.175538	-3.205145	0.732211
6	-2.799444	-2.021532	0.553613
1	-0.430544	-4.240382	0.661561
29	-0.675092	-0.449403	-0.066505
6	4.297781	3.567628	1.148942
6	3.629200	2.382539	1.855406
6	3.530047	1.141492	0.942089
6	2.915855	1.485292	-0.391524
6	3.480936	2.695179	-1.090863
6	3.568600	3.915811	-0.153922
7	1.946842	0.868168	-0.962281
7	1.377783	-0.259658	-0.414943
6	2.065107	-1.399237	-0.420852
6	1.228071	-2.603365	0.004001
8	3.264109	-1.599357	-0.739946
8	1.721873	-3.742005	0.097815
7	-0.073960	-2.308090	0.237782
1	5.343824	3.320411	0.927659
1	4.317452	4.435800	1.814020
1	4.178146	2.115237	2.762791
1	2.621056	2.672690	2.174454
1	2.966157	0.345258	1.429641
1	4.536221	0.749814	0.746255
1	2.888587	2.906818	-1.982674
1	4.493732	2.436414	-1.428218
1	2.555994	4.267850	0.077568
1	4.074011	4.735150	-0.672429
7	-0.889130	-3.329310	0.563369
7	-1.304958	2.144592	-0.651433
1	-0.398865	1.994676	-1.080738
1	-1.906233	2.871233	-1.032273
11	3.888846	-3.692166	-0.592027
11	-6.001256	2.390832	-0.130082

Na2CuC16N8H24O4_428_G3b

7	1.763937	-0.931555	-0.264431
6	3.063358	-1.154068	-0.211140
6	4.016340	-0.043195	0.161388
8	3.581417	-2.289602	-0.450366
8	5.212735	-0.287475	0.211480
7	3.583901	1.256089	0.452552
6	2.050703	3.108705	0.791761
6	2.434638	1.722431	0.482249
1	2.804908	3.819039	1.106337
29	0.748092	0.706527	0.023849
6	-4.109414	-3.603911	1.107831
6	-3.565357	-2.356943	1.812788
6	-3.402047	-1.161693	0.847257
6	-2.629714	-1.551273	-0.384975
6	-3.063229	-2.823201	-1.067759
6	-3.220206	-3.994045	-0.077887
7	-1.625870	-0.930173	-0.895563
7	-1.191749	0.274533	-0.354020
6	-1.978722	1.345960	-0.436852
6	-1.286878	2.643537	-0.007061
8	-3.167451	1.413218	-0.818880
8	-1.903325	3.705295	0.028144
7	0.025998	2.456948	0.297765
1	-5.129974	-3.411269	0.753487
1	-4.177641	-4.433555	1.817173
1	-4.222645	-2.059663	2.634576
1	-2.591811	-2.589214	2.260036
1	-2.923289	-0.323513	1.353945
1	-4.389681	-0.815293	0.518616
1	-2.364714	-3.059083	-1.872674
1	-4.036613	-2.624117	-1.536268
1	-2.231253	-4.292379	0.289616
1	-3.633390	-4.858311	-0.604781
7	0.819768	3.454396	0.662652
7	1.010136	-2.059896	-0.493611
1	0.126774	-1.849442	-0.961153
1	1.578670	-2.794884	-0.909123
11	-4.005015	3.461638	-0.758603
11	5.745861	-2.458484	-0.263892

Na2CuC16N8H24O4_428_G3c

29	0.611277	0.426770	-0.236713

7	2.034763	-1.054866	-0.886697
6	3.306796	-0.820552	-0.543114
6	3.504134	0.441490	0.221497
8	4.292640	-1.566322	-0.817344
8	4.628218	0.807374	0.622035
7	2.351528	1.140524	0.428002
7	2.463135	2.290502	1.091084
6	1.464499	3.116483	1.291691
6	0.222685	2.922140	0.874397
6	-2.803689	-4.093958	1.493115
6	-2.435413	-2.741836	2.114405
6	-2.812870	-1.557891	1.197341
6	-2.276238	-1.750655	-0.198315
6	-2.550561	-3.094290	-0.826143
6	-2.165321	-4.257541	0.108662
7	-1.601131	-0.907424	-0.888432
7	-1.324167	0.366968	-0.349660
6	-2.328585	1.224448	-0.381722
6	-2.079502	2.700990	-0.000949
8	-3.514474	0.972159	-0.718076
8	-2.965581	3.512845	-0.237249
7	-0.950230	3.133847	0.656726
1	-3.894679	-4.171550	1.404029
1	-2.487203	-4.906935	2.152866
1	-2.928815	-2.615022	3.082055
1	-1.356459	-2.713834	2.308257
1	-2.463570	-0.615139	1.619220
1	-3.905420	-1.491397	1.120112
1	-2.038793	-3.156416	-1.788286
1	-3.628392	-3.147719	-1.030470
1	-1.074000	-4.292829	0.211630
1	-2.468199	-5.204443	-0.346645
1	3.405459	2.509129	1.429834
7	1.827409	-2.208390	-1.528682
1	0.937727	-2.277267	-1.999648
1	2.644134	-2.679739	-1.907250
11	-4.884182	2.621870	-1.073600
11	6.167818	-0.738481	-0.012538

Na2CuC16N8H24O4_417_G1

29	0.868236	0.338862	-0.096016
7	1.654435	-1.359375	-0.572495
6	2.945007	-1.454951	-0.216832
6	3.581724	-0.104043	0.180653
8	3.638284	-2.484432	-0.172971
8	4.784839	-0.027985	0.412730
7	2.641306	0.859985	0.233947
7	2.834313	2.180111	0.570390
6	-4.777348	-2.868838	0.999665
6	-4.019884	-1.773315	1.756251
6	-3.537691	-0.638546	0.824617
6	-2.804139	-1.178374	-0.373968
6	-3.450252	-2.333723	-1.094384
6	-3.919607	-3.442542	-0.132914
7	-1.678455	-0.761163	-0.841875
7	-1.050141	0.335208	-0.273404
6	-1.572247	1.570998	-0.310839
6	-0.569389	2.684559	0.104190
8	-2.720532	1.908851	-0.644515
8	-0.936818	3.853791	0.176987
7	0.653080	2.163413	0.322803
1	-5.705580	-2.456789	0.584399
1	-5.071623	-3.663911	1.690338
1	-4.645847	-1.340945	2.541416
1	-3.151493	-2.214778	2.259590
1	-2.911937	0.065550	1.373585
1	-4.401431	-0.072804	0.453969
1	-2.768695	-2.713433	-1.857829
1	-4.326374	-1.932941	-1.622197
1	-3.045312	-3.950456	0.292042
1	-4.474227	-4.196428	-0.697503
7	1.810774	2.867028	0.564640
7	0.965315	-2.500111	-0.891905
1	0.023442	-2.263590	-1.198058
1	0.987524	-3.210773	-0.164126
11	-3.062115	4.120222	-0.520543
11	5.799851	-2.042086	0.224875

Na2CuC16N8H24O4_417_G2

29	-0.391331	-0.735432	0.106187
7	0.259390	-2.412583	-0.213960
6	1.594543	-2.539252	-0.092654
6	2.245538	-1.160018	0.325918
8	2.307769	-3.527790	-0.224471

8	3.444337	-1.139724	0.618302
7	1.358393	-0.149382	0.331277
7	1.617567	1.128044	0.788597
6	0.673964	2.174810	0.317060
6	0.703268	2.268327	-1.220370
6	2.058647	2.746821	-1.760434
6	2.478527	4.078781	-1.126736
6	2.489931	3.984563	0.403762
6	1.139474	3.499034	0.950427
1	0.432767	1.308030	-1.665611
1	-0.080930	2.975999	-1.511693
1	1.992856	2.846053	-2.847681
1	2.821327	1.988077	-1.557248
1	1.782342	4.867249	-1.440037
1	3.466122	4.374913	-1.490686
1	2.718380	4.958193	0.845823
1	3.282027	3.300270	0.722705
1	0.373159	4.253678	0.739265
1	1.172362	3.386224	2.039199
7	-1.864112	-2.918010	-0.585271
7	-1.985761	-1.589050	-0.239832
6	-3.080371	-0.792066	-0.168783
6	-2.673831	0.667972	0.236911
8	-4.260159	-1.076274	-0.340582
8	-3.566469	1.513034	0.456414
7	-1.358328	0.833369	0.316797
7	-0.698901	1.917907	0.868600
1	-1.287497	2.746386	0.868202
1	1.695156	1.144430	1.804888
7	-0.705440	-3.357349	-0.568445
11	-5.611045	0.689296	0.102707
11	4.469128	-3.118423	0.284675

Na2CuC16N8H24O4_385_G3c

29	-0.091832	-0.169682	0.025177
7	-1.869245	1.067393	0.001323
6	-2.946673	0.301463	-0.082049
6	-2.717369	-1.212204	0.039319
8	-4.135169	0.707221	-0.264190
8	-3.683741	-2.006217	0.059854
7	-1.427186	-1.555561	0.092548
7	-1.091710	-2.881934	0.173944
6	0.164970	-3.265325	0.185934
6	1.242265	-2.528260	0.125958
6	-1.467324	3.366083	0.639954
6	-0.143649	3.963067	0.029096
6	0.848212	2.914654	-0.075149
7	1.455836	1.935546	-0.080753
7	1.692885	0.629247	-0.051674
6	3.007257	0.270878	-0.068047
6	3.350269	-1.233193	-0.005904
8	3.936160	1.085040	-0.124435
8	4.571524	-1.496814	-0.031089
7	2.423002	-2.182044	0.074584
1	-1.244401	2.941000	1.625116
1	0.237500	4.762532	0.671681
1	-0.342591	4.375524	-0.963386
1	-1.867684	-3.540131	0.210062
7	-2.141477	2.430646	-0.233139
1	-2.120938	4.228672	0.787044
1	-3.151052	2.569148	-0.253055
11	6.000865	0.162717	-0.155819
11	-5.608173	-0.916887	-0.253385

Na2CuC16N8H24O4_385_G4b

29	-0.295365	-0.272807	-0.826949
7	-0.094692	1.539430	-0.792079
6	-0.976001	2.454490	-0.778740
6	-2.542179	2.146411	-0.794571
8	-0.727765	3.728740	-0.758600
8	-3.322570	3.078385	-0.795801
7	-3.013189	0.830561	-0.809020
6	-2.250952	-0.171249	-0.833377
6	-2.732186	-1.566581	-0.847929
7	-1.911815	-2.564085	-0.860612
6	2.715704	2.743384	-0.014939
6	3.945463	1.969240	-0.299143
6	3.523271	0.588461	-0.740786

7	2.834325	-0.360238	-0.843034
7	1.685095	-1.026482	-0.819585
6	1.769743	-2.377016	-0.859875
6	0.382361	-3.070441	-0.866238
8	2.790647	-3.072647	-0.882337
8	0.334745	-4.303845	-0.879931
7	-0.620400	-2.179878	-0.859367
1	2.124664	2.479924	0.852202
1	4.564004	1.836520	0.591826
1	4.567166	2.417907	-1.077760
1	-3.799274	-1.757803	-0.853335
7	2.126130	3.525690	-0.910665
1	2.593628	3.756835	-1.776114
1	1.109901	3.720853	-0.849292
11	2.334647	-5.276996	-0.929200
11	-2.388072	5.128863	-0.741468

Na2CuC16N8H24O4_385_G5b

29	0.100260	-0.350393	-0.155024
7	-1.598794	0.668994	0.095810
6	-2.810756	0.130444	-0.005971
6	-3.020339	-1.396028	0.182065
8	-3.850545	0.794179	-0.282441
8	-4.185512	-1.791636	0.129731
7	-2.008123	-2.285660	0.423041
6	-0.793048	-2.142699	0.070380
6	0.252269	-3.148037	0.245108
7	1.507571	-2.848390	0.147011
6	-1.279991	2.979587	0.823994
6	-0.244997	4.052034	0.351445
6	0.896965	3.273573	-0.112799
7	1.521191	2.310658	-0.247074
7	1.725438	1.026612	-0.370753
6	2.969962	0.511741	-0.193939
6	2.950878	-1.030222	-0.061782
8	4.028806	1.134448	-0.108877
8	4.040152	-1.615153	0.024684
7	1.708286	-1.513622	0.005287
1	-0.868728	2.427274	1.669906
1	0.046191	4.720651	1.166373
1	-0.642495	4.660931	-0.463573
1	-0.020528	-4.192501	0.362251
7	-1.577088	2.046847	-0.269866
1	-2.172748	3.509259	1.174632
1	-2.490595	2.257814	-0.669887

11	5.804616	-0.298794	0.058990
11	-5.758877	-0.302766	-0.342988

Na2CuC16N8H24O4_348_G1

29	0.081953	0.670131	-0.430770
7	0.425107	2.458745	-0.890375
6	-0.786607	2.580528	-0.912324
8	-1.876352	3.104828	-1.068606
6	6.324629	0.437984	1.908676
6	4.980956	-0.118296	2.391202
6	4.185557	-0.804244	1.259558
6	4.080800	0.073800	0.038921
6	5.359419	0.734805	-0.417050
6	6.125012	1.406692	0.737764
7	3.018614	0.329858	-0.638737
7	1.809564	-0.288424	-0.305769
6	1.635012	-1.600506	-0.403669
6	0.144389	-2.028369	-0.233424
8	2.499822	-2.482385	-0.622765
8	-0.110803	-3.252030	-0.171951
7	-0.736371	-1.036519	-0.182246
1	6.972779	-0.388986	1.591818
1	6.840910	0.940374	2.732035
1	5.130112	-0.833640	3.205102
1	4.379908	0.700718	2.805198
1	3.192834	-1.088445	1.608123
1	4.690507	-1.730258	0.958657
1	5.135576	1.437872	-1.222155
1	5.995402	-0.049630	-0.849611
1	5.564983	2.284388	1.084465
1	7.087231	1.775357	0.371214
1	-1.689670	-1.358977	-0.065695
7	1.617271	3.128672	-1.242887
1	2.333288	2.390781	-1.267615
1	1.849099	3.754334	-0.471746
11	1.649192	-4.509274	-0.574060
11	-3.844751	3.757458	-1.458647

Na2CuC16N8H24O4_348_G2

29	0.661927	0.546902	0.179713
7	1.509006	-1.231866	0.456771
6	2.790074	-1.210535	0.144557
6	3.345824	0.199497	-0.145002
8	3.554922	-2.212677	0.062620
8	4.568797	0.330295	-0.370340
7	2.441682	1.171384	-0.125843
6	-4.613537	-2.542425	-0.668305
6	-3.110424	-2.389645	-0.925737

6	-2.409952	-1.580520	0.190891
6	-3.115706	-0.274542	0.418465
6	-4.605609	-0.362379	0.641258
6	-5.286140	-1.178072	-0.478199
7	-2.629781	0.913094	0.420046
7	-1.233459	1.047395	0.210827
6	-0.598270	2.092848	0.036130
8	-0.505024	3.298931	-0.123298
1	-4.771346	-3.156547	0.227094
1	-5.081681	-3.078128	-1.498854
1	-2.625280	-3.365593	-1.001791
1	-2.949998	-1.884654	-1.885263
1	-1.353244	-1.453307	-0.032037
1	-2.475299	-2.150143	1.127337
1	-5.026030	0.640776	0.723781
1	-4.766211	-0.869978	1.601492
1	-5.238640	-0.609862	-1.414514
1	-6.345735	-1.297648	-0.237345
1	2.818934	2.090718	-0.320759
7	0.919700	-2.507485	0.619500
1	0.553147	-2.569261	1.566142
1	1.657600	-3.206853	0.523951
11	-0.703670	5.388045	-0.292334
11	5.615556	-1.620327	-0.389140

Na2CuC16N8H24O4_348_G3

29	-1.501535	0.687656	0.964940
7	-1.622832	2.620848	0.138050
6	-2.687612	2.438410	-0.417227
8	-3.742173	2.136974	-0.858192
6	5.104666	0.528874	0.431737
6	4.053118	-0.208588	1.267859
6	2.897054	-0.758302	0.403550
6	2.323345	0.305889	-0.496397
6	3.323661	1.125293	-1.273842
6	4.463974	1.656912	-0.384612
7	1.081318	0.597638	-0.644556
7	0.093277	-0.134349	0.027573
6	-0.144978	-1.392865	-0.304735
6	-1.410626	-1.991574	0.377185
8	0.520890	-2.146284	-1.063136
8	-1.482179	-3.231060	0.466301
7	-2.359888	-1.128378	0.818084
1	5.597632	-0.178794	-0.246838
1	5.885942	0.930679	1.083151

1	4.509756	-1.035165	1.819575
1	3.642813	0.476622	2.019397
1	2.116377	-1.186200	1.032963
1	3.270819	-1.564559	-0.239918
1	2.805678	1.931607	-1.796948
1	3.754216	0.470296	-2.043399
1	4.068483	2.420394	0.296646
1	5.210171	2.154091	-1.010226
1	-2.991880	-1.633168	1.439674
7	-0.444646	3.289759	-0.329291
1	0.198476	2.530633	-0.610166
1	-0.048793	3.732619	0.497047
11	0.116474	-4.271241	-0.707177
11	-3.899539	-0.275216	-0.772289

Na2CuC16N8H24O4_305 (*from 417 m/z*)

7	-1.682945	-1.562371	-0.000890
6	-2.824517	-0.948964	0.000003
6	-2.569820	0.610636	0.000741
8	-4.001993	-1.344088	-0.000197
8	-3.477951	1.407940	-0.000297
7	-1.216747	0.795235	0.002479
7	-0.614100	2.026515	0.001039
29	0.000111	-0.697797	0.000770
7	1.682875	-1.562144	0.001492
6	2.824479	-0.948849	-0.000311
6	2.569786	0.610878	-0.000730
8	4.001975	-1.343928	-0.001278
8	3.477932	1.408152	-0.000511
7	1.216708	0.795458	-0.001213
7	0.613928	2.026553	-0.000192
11	5.547845	0.255976	-0.000335
11	-5.547891	0.256258	-0.001600

Na2CuC16N8H24O4_305_G1

29	-0.220480	0.946330	-0.098307
7	-1.944722	0.030080	-0.160679
6	-2.976051	0.797036	-0.206262
8	-4.186650	0.657290	0.074575
7	1.311492	-0.638888	0.466356
6	2.558968	-0.216176	0.166724
6	2.617795	1.329655	0.024588
8	3.568966	-0.910723	0.006386
8	3.765949	1.841215	0.014161
7	1.455216	1.930621	-0.113739
1	1.575070	2.933382	-0.225382
11	5.401665	0.405061	-0.108267
11	-5.904757	1.872370	0.185154
7	0.969081	-1.881908	0.358849
6	0.276629	-2.806223	0.268502
1	-1.388693	-3.972092	0.778203
1	-0.780151	-4.245125	-0.856185
6	-0.967854	-3.476869	-0.100537
1	-1.508119	-1.941196	-1.548630
1	-2.868580	-2.881022	-0.933894
6	-1.937216	-2.380384	-0.646476
7	-2.163001	-1.327202	0.348740
1	-3.117809	-1.362674	0.694127

Na2CuC16N8H24O4_305_G2

29	-0.225464	-1.407039	0.037542
7	-1.052028	0.663637	0.058569
6	-2.407399	0.548131	0.071300
6	-2.954574	-0.825261	-0.342892
8	-3.179938	1.463429	0.413578
8	-4.188414	-0.910947	-0.538585
7	-2.049616	-1.780527	-0.398773
6	0.848875	1.943801	0.726984
6	1.468090	2.134781	-0.682903
6	2.902746	1.888244	-0.663527
7	4.026988	1.642467	-0.608410
7	1.637158	-1.397293	0.340860
6	2.811676	-1.464758	0.387991
8	4.021061	-1.501340	0.433928
1	1.042787	2.815721	1.351759
1	1.299391	1.063374	1.197886
1	1.273084	3.137096	-1.072489
1	1.018632	1.412963	-1.370585
1	-2.455715	-2.689523	-0.600424
7	-0.582846	1.768695	0.641899
1	-1.204879	2.263493	1.277803
11	5.565446	-0.069549	-0.140765
11	-5.340954	0.866220	-0.001485

Na2CuC16N8H24O4_290

29	0.085742	-1.049626	-0.072893
7	-1.665096	-0.186600	0.151712
6	-2.748936	-0.877286	0.208366
8	-3.960841	-0.628528	0.039620
6	-1.439891	2.147564	0.882039
6	-0.677586	3.386913	0.334171
6	0.566396	2.944222	-0.323911
7	1.168377	2.003055	-0.655339
7	1.544227	0.853559	-1.047760
6	2.508812	0.162496	-0.367747
6	2.016218	-1.328876	-0.191649
8	3.508258	0.603268	0.208277
8	2.891914	-2.167481	0.010503
1	-0.796845	1.613853	1.583763
1	-0.448059	4.089376	1.139925
1	-1.280264	3.932335	-0.397804
7	-1.801920	1.229531	-0.204283
1	-2.310099	2.505405	1.447512
1	-2.767955	1.375387	-0.485195
11	4.839606	-1.190623	0.593920
11	-5.791164	-1.667767	-0.066597

Na2CuC16N8H24O4_247_G3

29	0.145982	-0.690451	-0.007763
7	2.033366	-0.405059	-0.023421
6	3.198855	-0.279162	-0.027946
8	4.405554	-0.132619	-0.038423
6	-0.804906	3.595146	0.055605
7	-0.996156	2.436273	0.009427
7	-1.044380	1.119143	0.016334
6	-2.236099	0.494714	-0.018945
6	-1.822392	-0.988088	0.008567
8	-3.398192	0.902067	-0.076902
8	-2.641760	-1.869257	0.068301
11	-4.783330	-0.871658	0.009871
11	6.499618	-0.052580	0.033879

Na2CuC16N8H24O4_247_G3b

29	0.150481	-1.292635	-0.000469
7	-1.807062	-0.441424	-0.002141
6	-3.075253	-0.690628	-0.002580
8	-4.107977	-0.033502	-0.004024
6	-1.288280	0.851395	-0.002767
7	-0.156683	1.213348	-0.002041
7	0.953327	1.835974	-0.002218
6	2.091871	1.107407	-0.000582
6	1.954481	-0.515204	0.000995
8	3.218682	1.605310	-0.000340
8	3.026920	-1.089151	0.002930
11	4.915046	0.204881	0.002666
11	-6.050405	0.781667	0.006377

Na2CuC16N8H24O4_243

29	0.324141	0.598095	-1.480384
7	-2.860000	0.269500	0.399180
6	-1.967765	1.046321	0.690018
8	-1.300272	1.966761	1.008230
7	-1.530471	-1.580937	0.004956
7	-0.493765	-0.740334	-0.078819
6	0.652377	-1.439014	0.300001
6	1.956186	-0.609607	0.340698
8	0.571878	-2.626393	0.598282
8	2.923523	-1.067586	0.912673
7	1.869302	0.615609	-0.267740
1	2.809568	1.036335	-0.373108
7	-2.737836	-1.019009	-0.007599
1	-1.157610	-2.608913	0.238616
1	-3.622062	-1.558008	-0.127901
11	1.039417	2.073052	1.336899

Na2CuC16N8H24O4_193

29	-0.003747	-0.013712	-0.048872
6	-3.019869	-0.136309	-0.001270
8	-4.240654	-0.194148	0.022380
7	-1.851431	-0.090298	-0.022105
6	3.021394	0.123879	-0.014525
8	4.239189	0.194847	0.002635
7	1.854146	0.075349	-0.026347
11	6.294434	-0.119006	0.081939
11	-6.286048	0.170940	0.068160

Na2CuC16N8H24O4_193

29	0.983351	-0.236953	0.000000
7	-0.854671	-0.083905	0.000000
6	-2.026802	0.007655	0.000001
8	-3.229470	0.101516	0.000001
6	4.757121	0.943849	0.000000
7	3.737767	0.250917	0.000000
7	2.790335	-0.507729	0.000001
11	-5.343397	0.248683	-0.000001

Structures shown in Figure 9, used for EXAFS multiple scattering calculations.

sCuIII_CPZmh2_-4H_GeomX1b

7	0.406729000	2.132321000	-1.118510000
6	-0.294260000	3.048534000	-0.405367000
6	-1.517172000	2.427210000	0.239074000
8	0.041922000	4.219803000	-0.222641000
8	-2.147477000	2.972920000	1.133757000
7	-1.780507000	1.151320000	-0.244729000
7	-2.637116000	0.462488000	0.555380000
6	-3.133722000	-0.818338000	0.084362000
6	-4.328898000	-0.580883000	-0.845532000
6	-5.507594000	0.051273000	-0.116800000
6	-5.923494000	-0.772968000	1.097110000
6	-4.748610000	-0.975941000	2.049102000
6	-3.574451000	-1.616587000	1.315974000
1	-3.995382000	0.061271000	-1.673160000
1	-4.623377000	-1.553771000	-1.272954000
1	-6.351038000	0.165320000	-0.810924000
1	-5.221032000	1.061740000	0.208310000
1	-6.287326000	-1.759141000	0.760908000
1	-6.761055000	-0.289116000	1.618001000
1	-5.043595000	-1.609898000	2.896500000
1	-4.456991000	-0.004195000	2.475255000
1	-3.861864000	-2.613793000	0.954856000
1	-2.702503000	-1.761926000	1.970006000
29	-0.059240000	0.345840000	-0.610444000
6	5.963384000	-0.337852000	1.860911000
6	4.574593000	-0.845043000	2.227396000
6	3.811659000	-1.373514000	1.009061000
6	3.825238000	-0.385719000	-0.119079000
6	5.149326000	0.246066000	-0.440322000
6	5.865858000	0.759343000	0.808046000
7	2.815837000	-0.012307000	-0.820186000
7	1.597573000	-0.615135000	-0.615561000
6	1.468021000	-1.937319000	-0.912611000
6	-0.008378000	-2.339754000	-0.975965000
8	2.371840000	-2.729837000	-1.155786000
8	-0.374044000	-3.357241000	-1.546098000
7	-0.830873000	-1.416701000	-0.369258000
1	6.564862000	-1.172021000	1.461703000
1	6.486890000	0.029441000	2.754472000
1	4.635921000	-1.633238000	2.989517000
1	4.003068000	-0.018635000	2.679231000
1	2.777836000	-1.617354000	1.274018000
1	4.263597000	-2.310576000	0.647690000
1	4.992552000	1.038043000	-1.182595000

1	5.780963000	-0.522939000	-0.916959000
1	5.305165000	1.611220000	1.224481000
1	6.861654000	1.137947000	0.540245000
7	-2.157305000	-1.599090000	-0.668263000
1	-2.325318000	-1.605702000	-1.675719000
1	-2.386534000	0.502075000	1.544923000
7	1.633067000	2.579595000	-1.567338000
1	2.266089000	1.781215000	-1.651746000
1	1.996736000	3.290656000	-0.927661000

CuII_CPZ-Dec2019-green-Jul2020

8	0.044855000	-6.443178000	0.532004000
8	1.966763000	-3.497605000	0.416796000
7	-0.406381000	-4.272086000	1.141811000
7	2.393194000	-5.476014000	-0.634167000
7	-1.595830000	-4.783343000	1.656626000
7	3.537391000	-4.980958000	-1.228992000
6	0.348625000	-5.216691000	0.617969000
6	1.658496000	-4.681393000	0.116160000
6	4.284959000	-5.832898000	-1.856457000
6	5.497114000	-5.274656000	-2.523143000
6	6.763662000	-5.999163000	-2.041594000
6	6.628190000	-7.504736000	-2.216867000
6	5.399020000	-8.027732000	-1.487244000
6	4.118150000	-7.315842000	-1.968229000
1	5.544666000	-4.194581000	-2.348492000
1	5.390106000	-5.435246000	-3.607996000
1	7.626720000	-5.613860000	-2.594439000
1	6.936060000	-5.760374000	-0.981506000
1	7.524471000	-8.012755000	-1.844840000
1	6.556459000	-7.750654000	-3.287255000
1	5.277494000	-9.105701000	-1.638234000
1	5.512660000	-7.870211000	-0.404418000
1	3.248121000	-7.712363000	-1.429030000
1	3.965605000	-7.549194000	-3.033583000
6	-2.656100000	-4.026983000	1.686289000
6	-2.788611000	-2.697563000	1.028772000
6	-3.880754000	-2.811007000	-0.059924000
6	-5.194713000	-3.324209000	0.509065000
6	-4.999187000	-4.662662000	1.203818000
6	-3.907596000	-4.562462000	2.286479000
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1	-3.206206000	-7.470701000	5.603386000

References used in Supporting Information.

[i] QPOWG and GPLOTN are © GN George.

[ii] Pushie MJ, Nienaber KH, Summers KL, Cotelesage JJ, Ponomarenko O, Nichol HK, Pickering IJ, George GN. (**2014**) The solution structure of the copper clioquinol complex. J Inorg Biochem. 133:50-56.