A new chiral, poly-imidazole N_8-ligand and the related di- and tri-copper(II) complexes: synthesis, theoretical modelling, spectroscopic properties, and biomimetic stereoselective oxidations

Francesco G. Mutti,[‡] *Michele Gullotti,*[‡*] *Luigi Casella,*[#] *Laura Santagostini,*[‡] *Roberto Pagliarin,*[§] *K. Kristoffer Andersson,*[¶] *Maria F. Iozzi,*[¥] *Giorgio Zoppellaro*[¶*]

SUPPORTING INFORMATION

CONTENTS

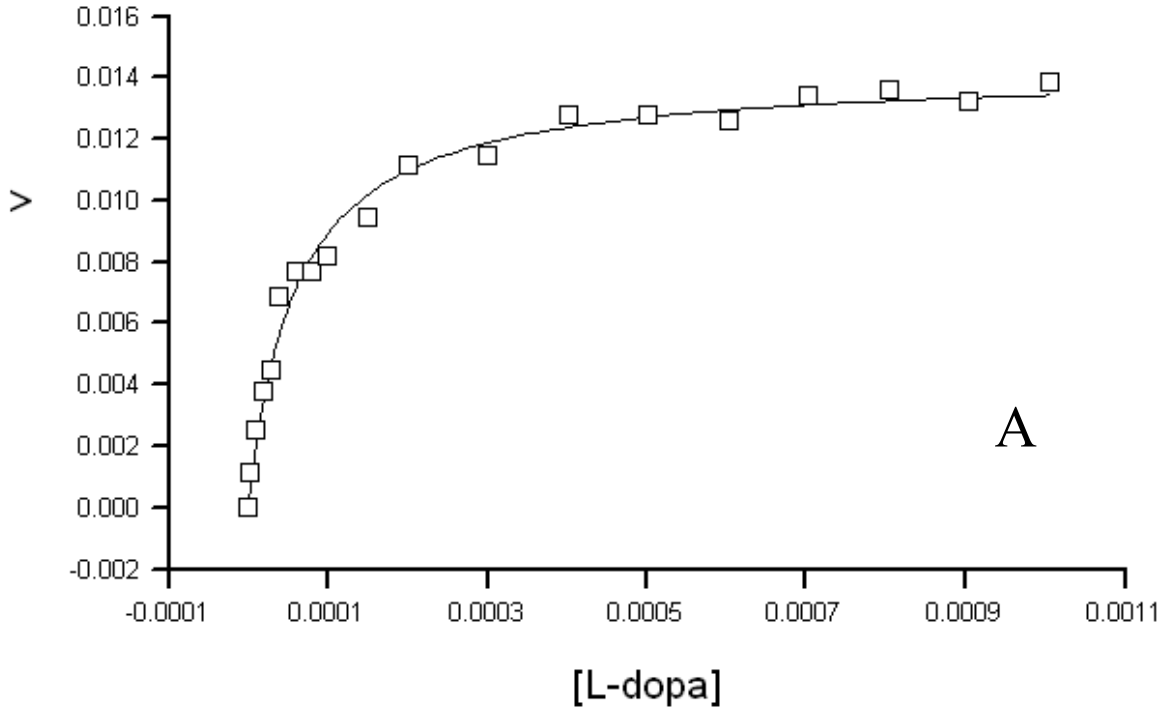
Part 1: Catalytic Oxidations

The kinetics of catalytic oxidation of *o*-catechols and flavonoids were performed as described in the general procedure. The plots of reaction rate versus substrate concentration were obtained according to the steady-state theory. Hence, for every substrate concentration, the initial reaction rate was determined in an independent experiment, fitting the absorbance versus time in the first few seconds. Furthermore, every single point was obtained as avarage of three determinations to avoid reproducibility mistakes. The collected data as ΔA / s unit were converted into mols of substrate reacted / s using the Lambert-Beer equation. Finally, the data were normalized dividing for the concentration of the catalyst and fitted using either the Michaelis-Menten equation or the modified one with inhibition effect, implemented in the software FigSys®.[1] A mixture of aqueous buffer (50 mM, pH 8.6) and methanol (9:1, v.v) was used as solvent for the catalytic oxidation of the *o*-catechols, whereas a mixture of aqueous buffer (50 mM, pH 7.0) and methanol (9:1, v.v) was used for the catalytic oxidation of the flavonoids. In all the kinetics, the temperature was kept constant at 20±0.1 °C. The substrate concentration was varied from 4.0×10^{-6} M to 1.0×10^{-3} M and an excess of methyl-2-benzothiazolinone hydrazone (MBTH, 1.0×10^{-3} M) was added to generate an adduct with the formed *o*-quinone, which is stable and detectable by UV-Vis spectroscopy.

1) Biosoft, Great Shelford, Cambridge, CB22, United Kingdom.
http://www.biosoft.com/w/figsys.htm

Figure S1: Complex: $[Cu_2(L)][ClO_4]_4$

- Substrate: L-Dopa



- Substrate: D-Dopa

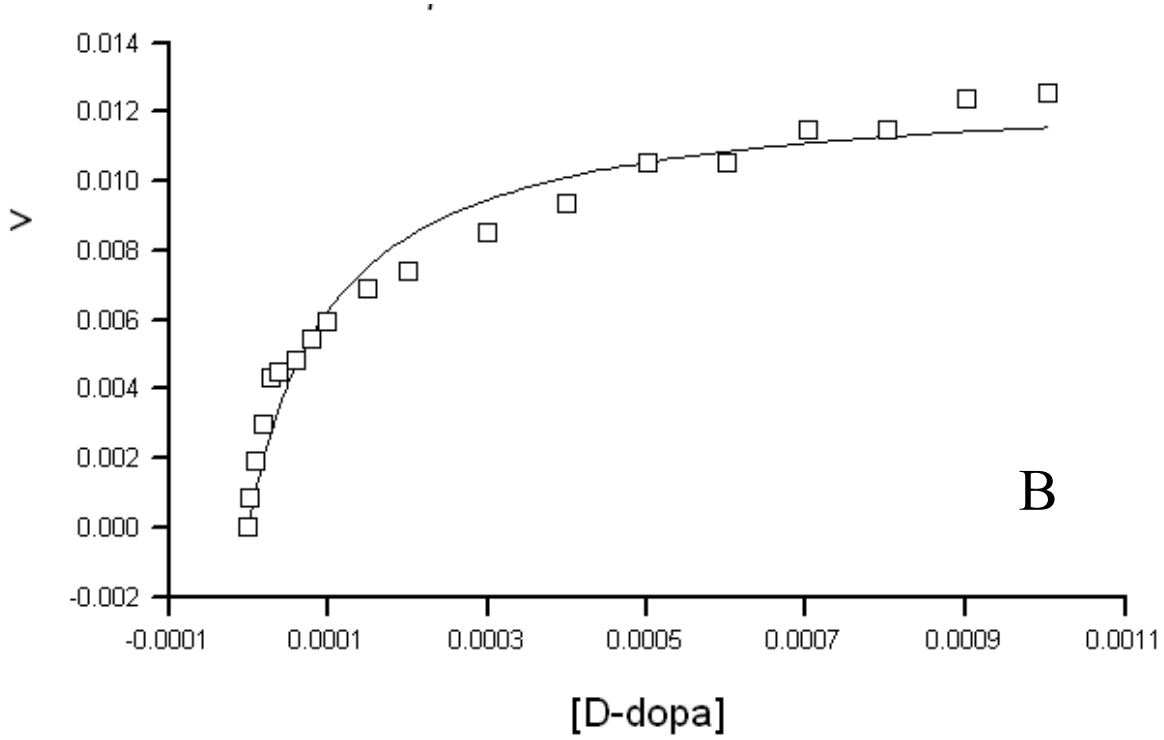
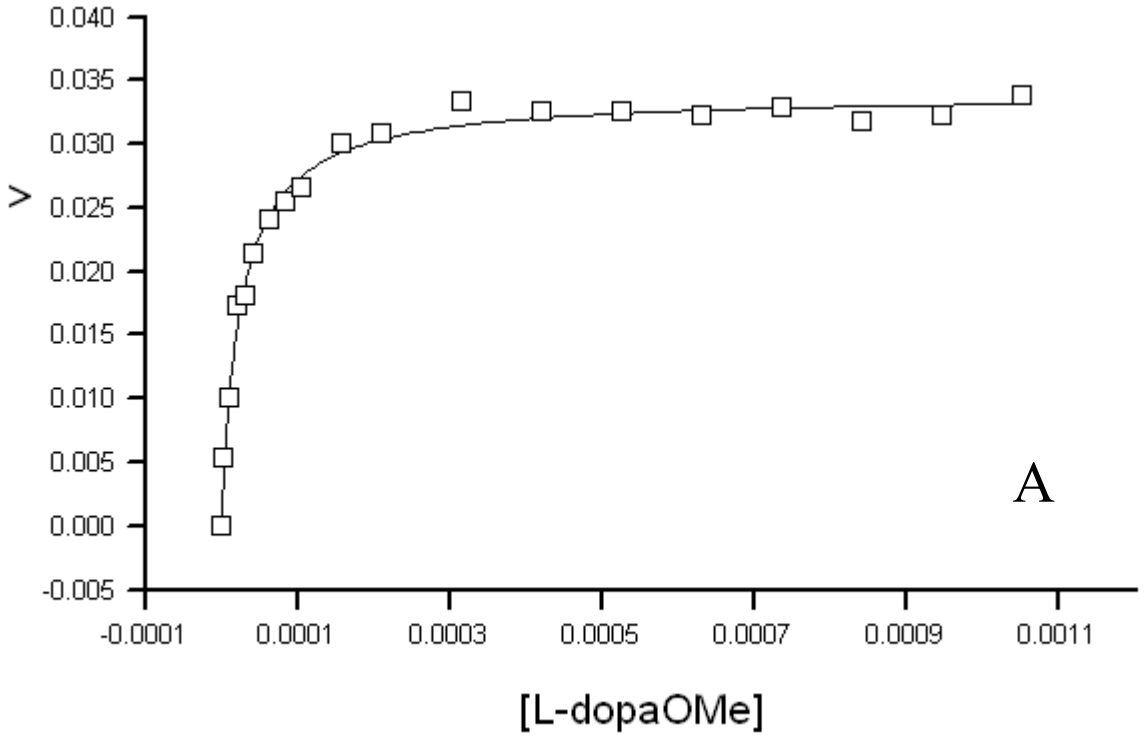


Figure S2: Complex: $[Cu_2(L)][ClO_4]_4$

- Substrate: L-DopaOMe



- Substrate: D-DopaOMe

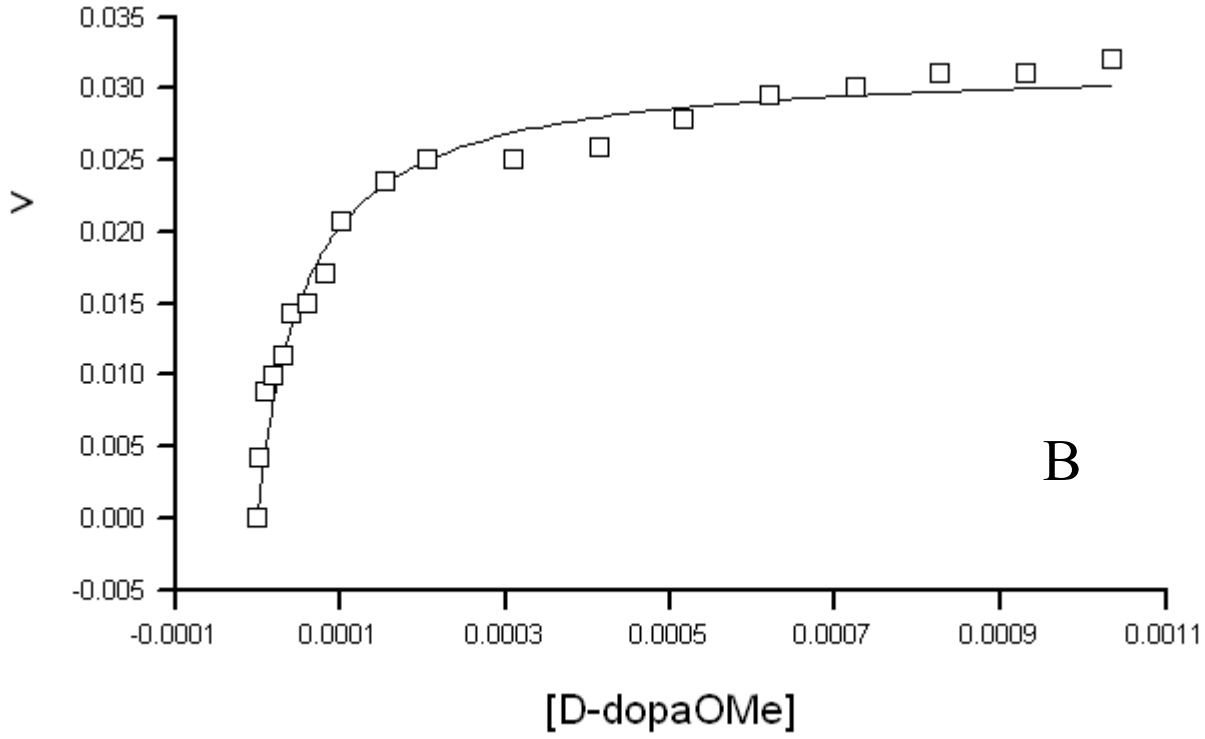
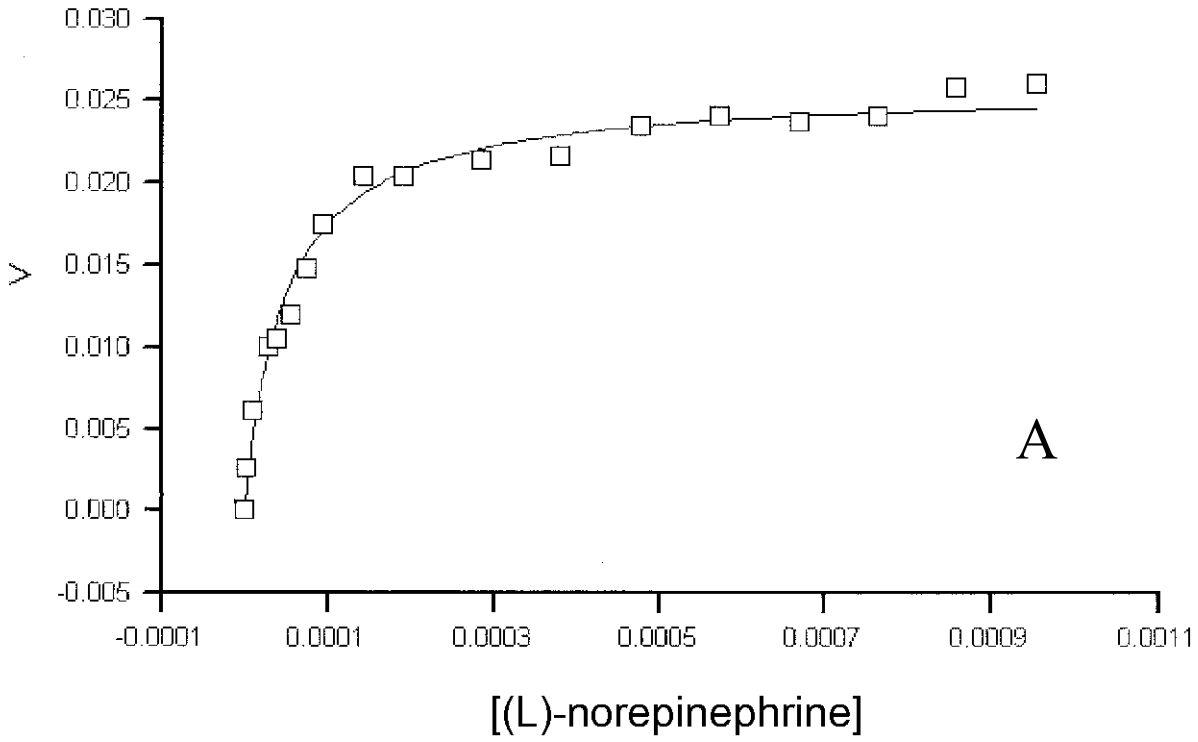


Figure S3: Complex: $[Cu_2(L)][ClO_4]_4$

- Substrate: L-norepinephrine



- Substrate: D-norepinephrine

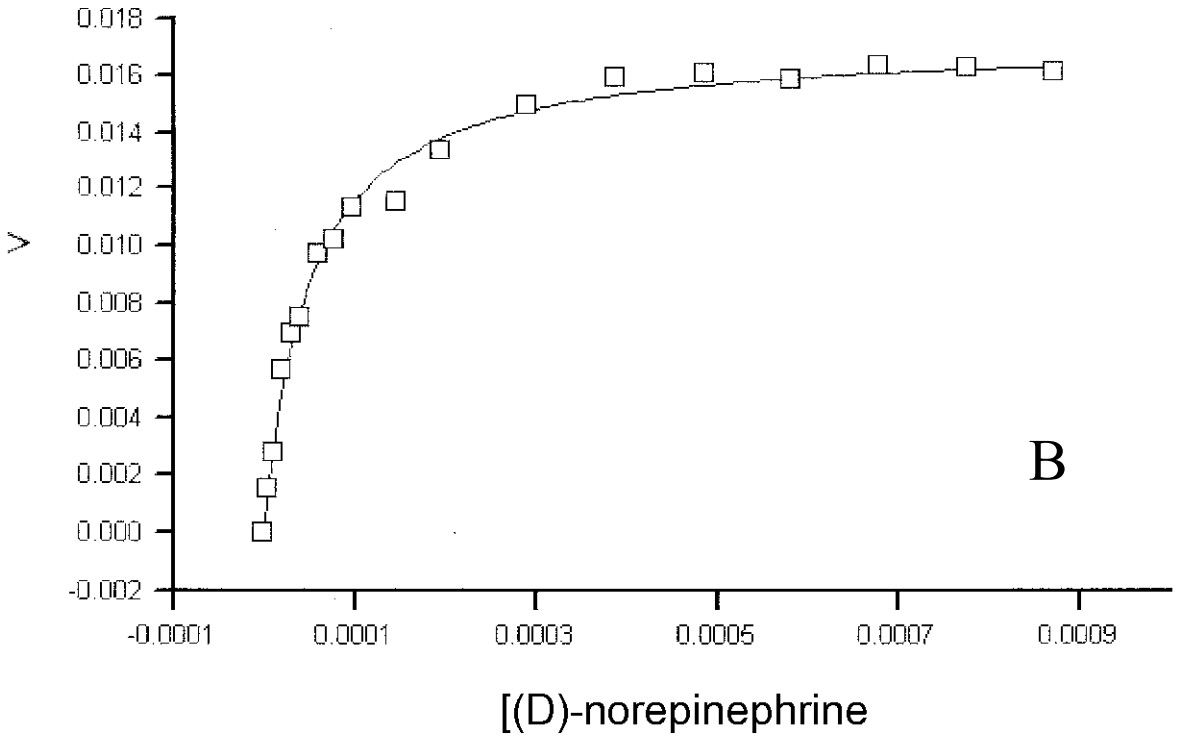
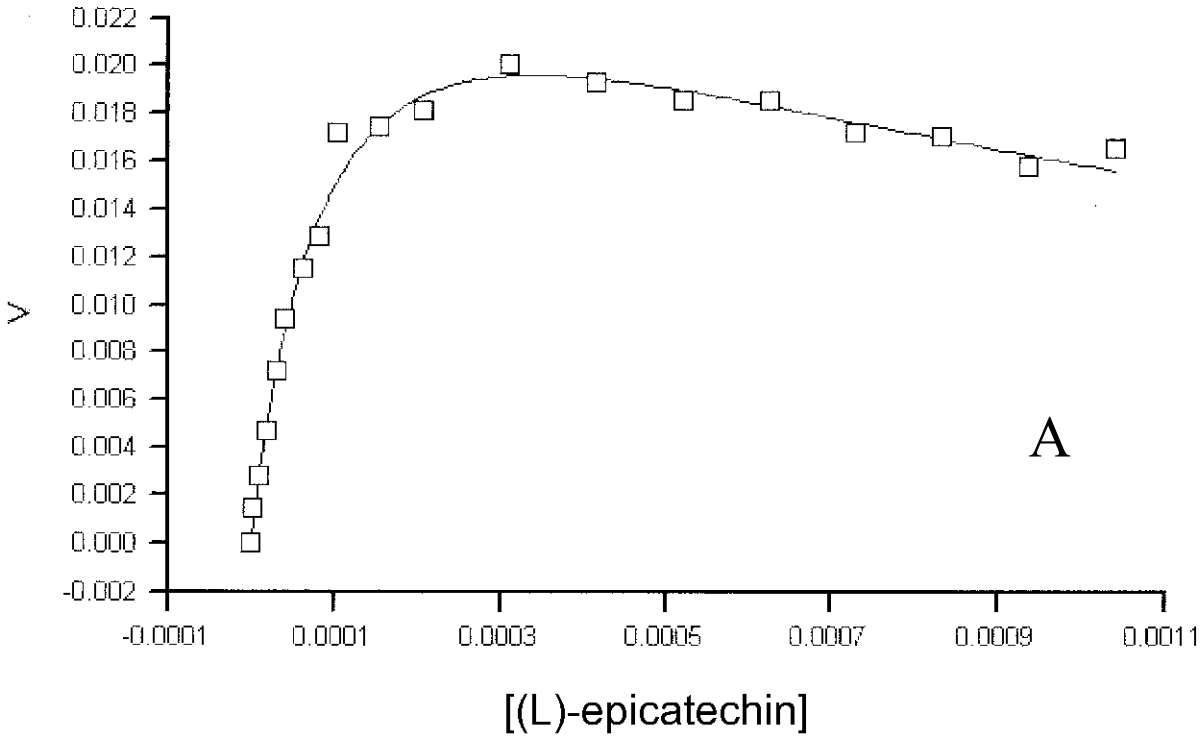


Figure S4: Complex: $[Cu_2(L)][ClO_4]_4$

- Substrate: L-epicatechin



- Substrate: D-catechin

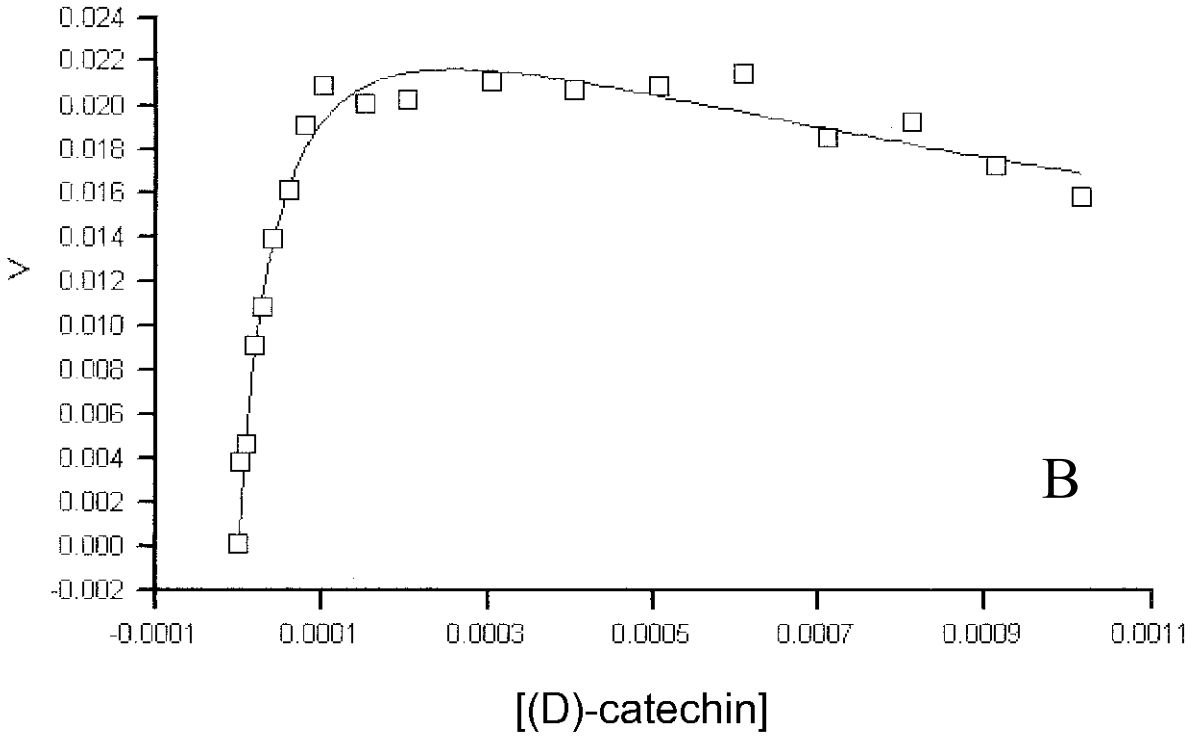
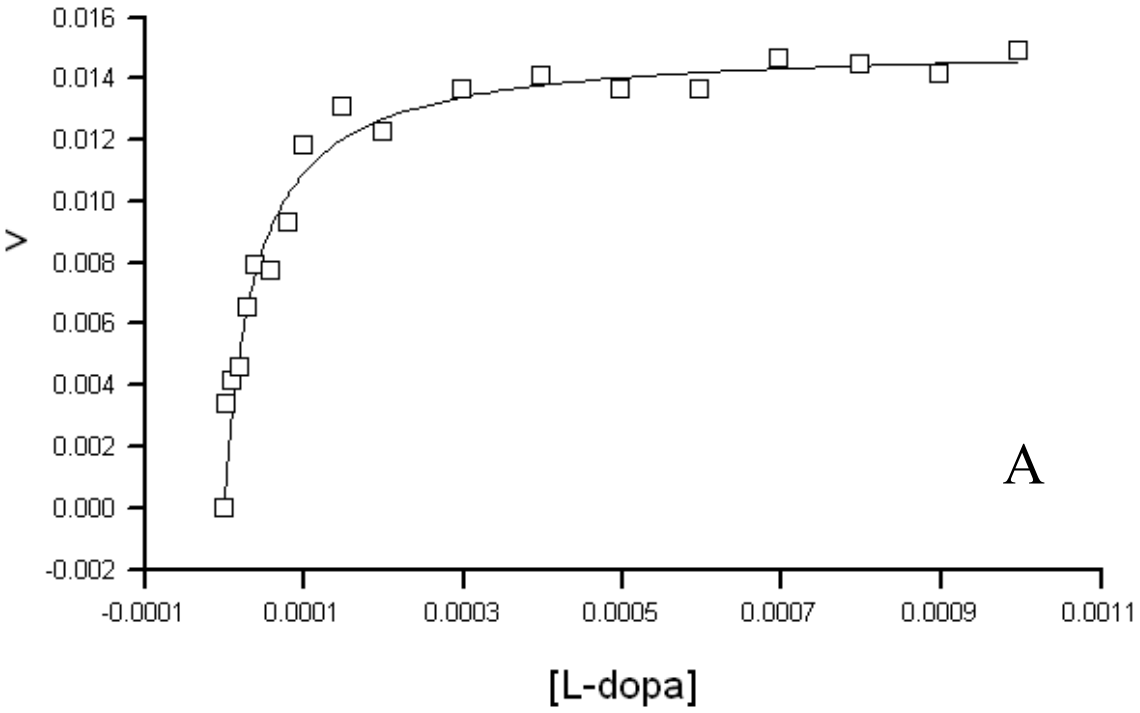


Figure S5: Complex: $[Cu_3(L)][ClO_4]_6$

- Substrate: L-dopa



- Substrate: D-dopa

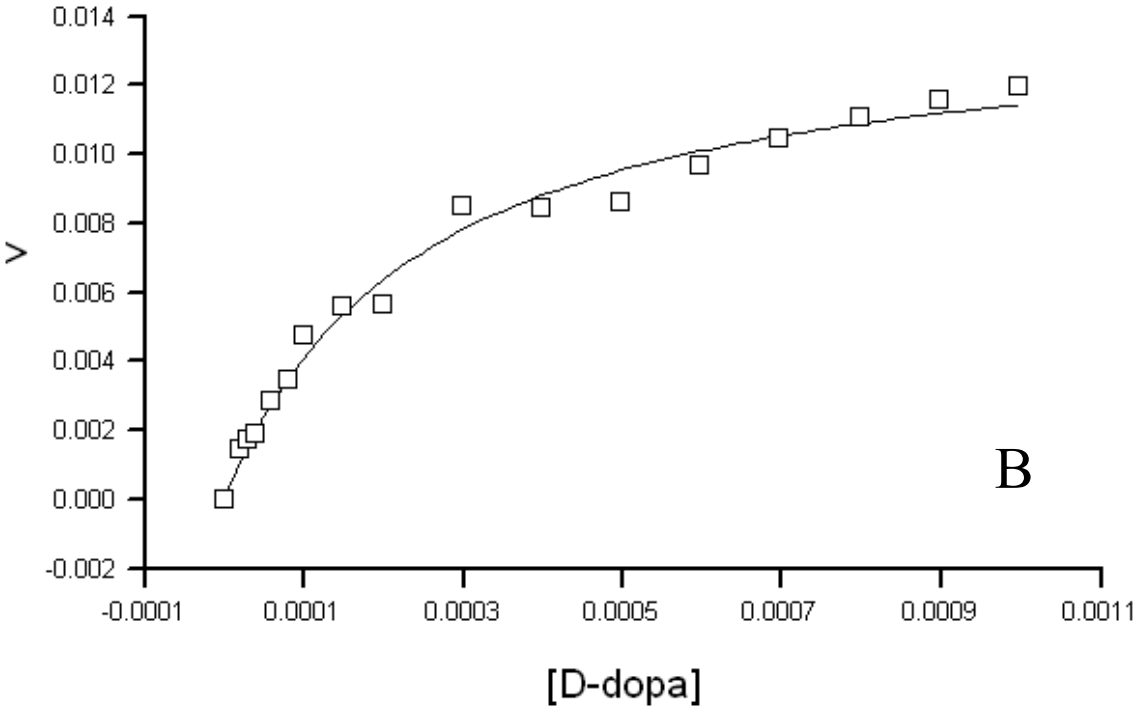
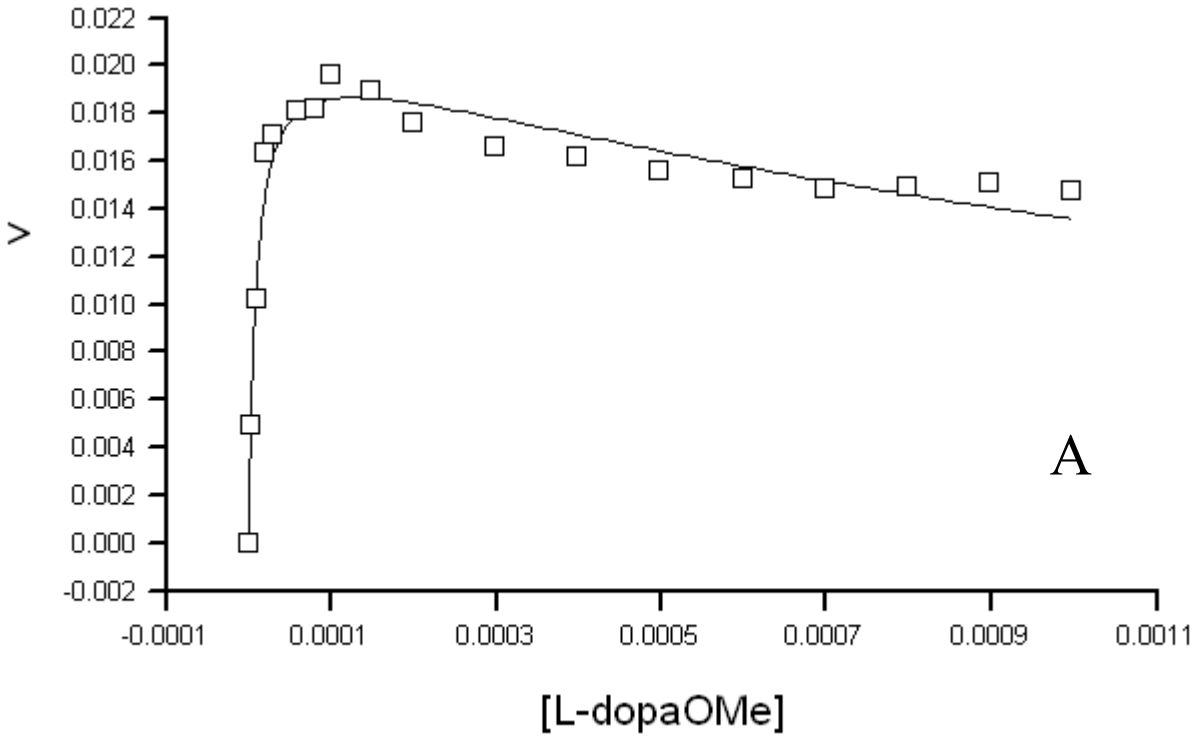


Figure S6: Complex: $[Cu_3(L)][ClO_4]_6$

- Substrate: L-dopaOMe



- Substrate: D-dopaOMe

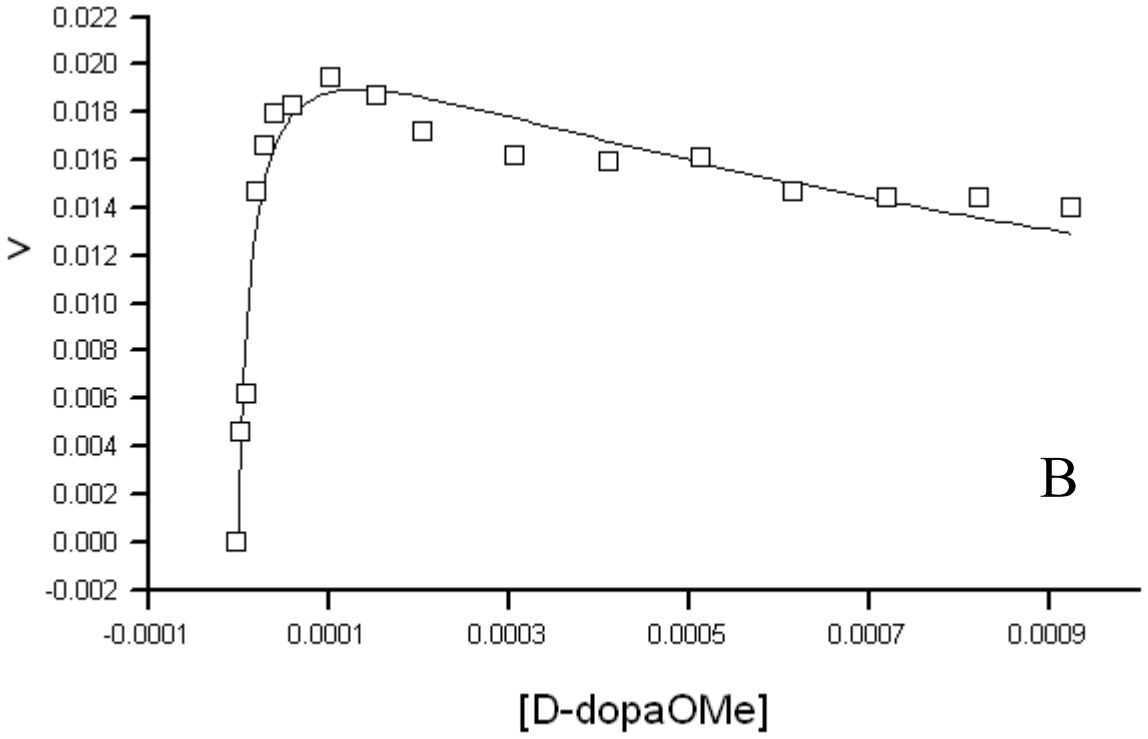
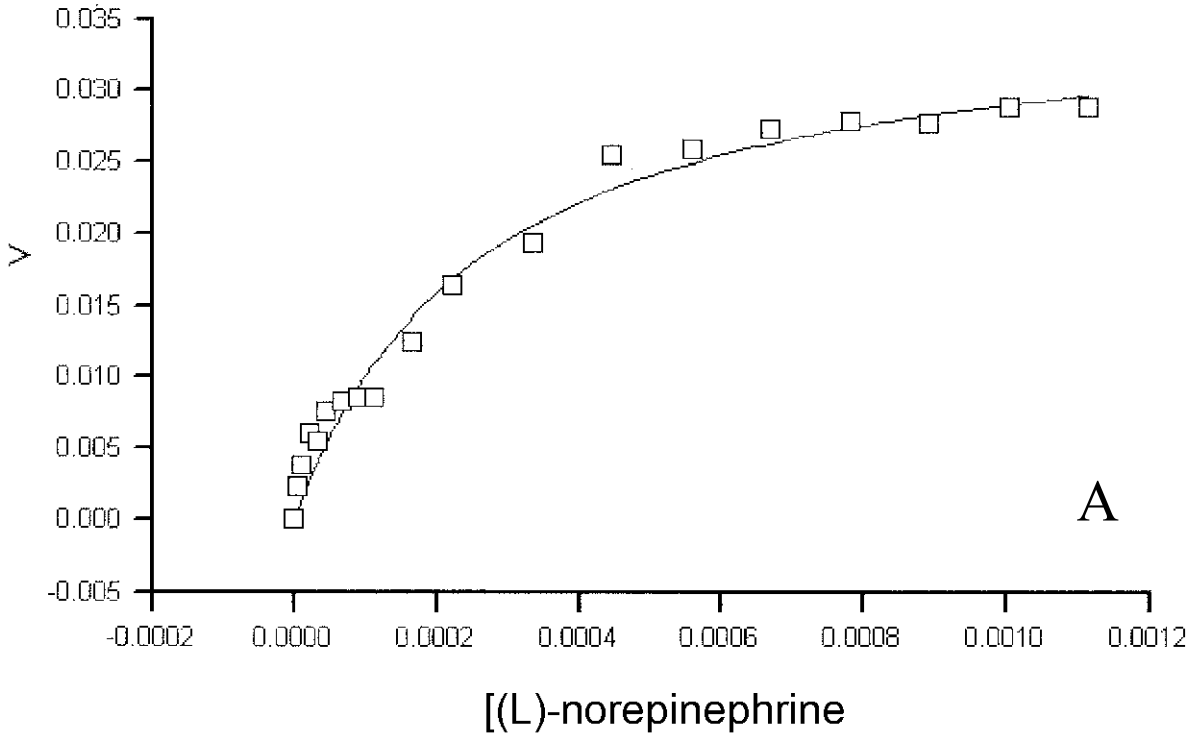


Figure S7: Complex: $[Cu_3(L)][ClO_4]_6$

- Substrate: L-norepinephrine



- Substrate: D-norepinephrine

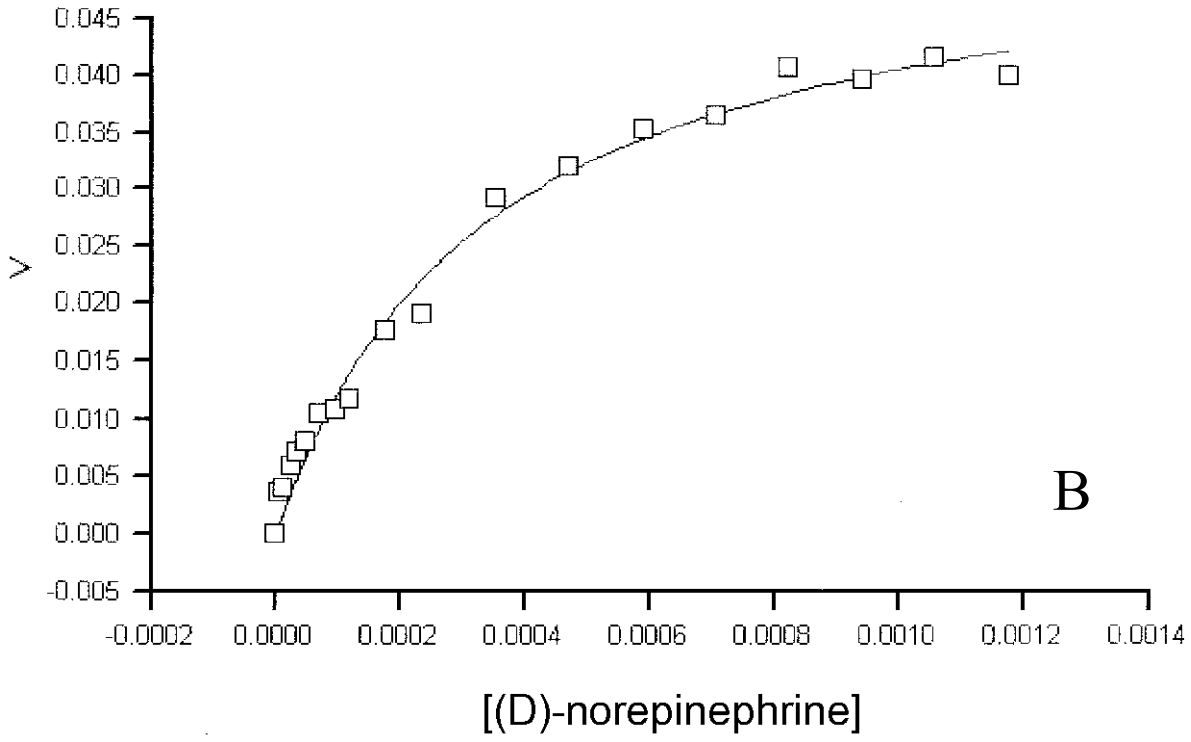
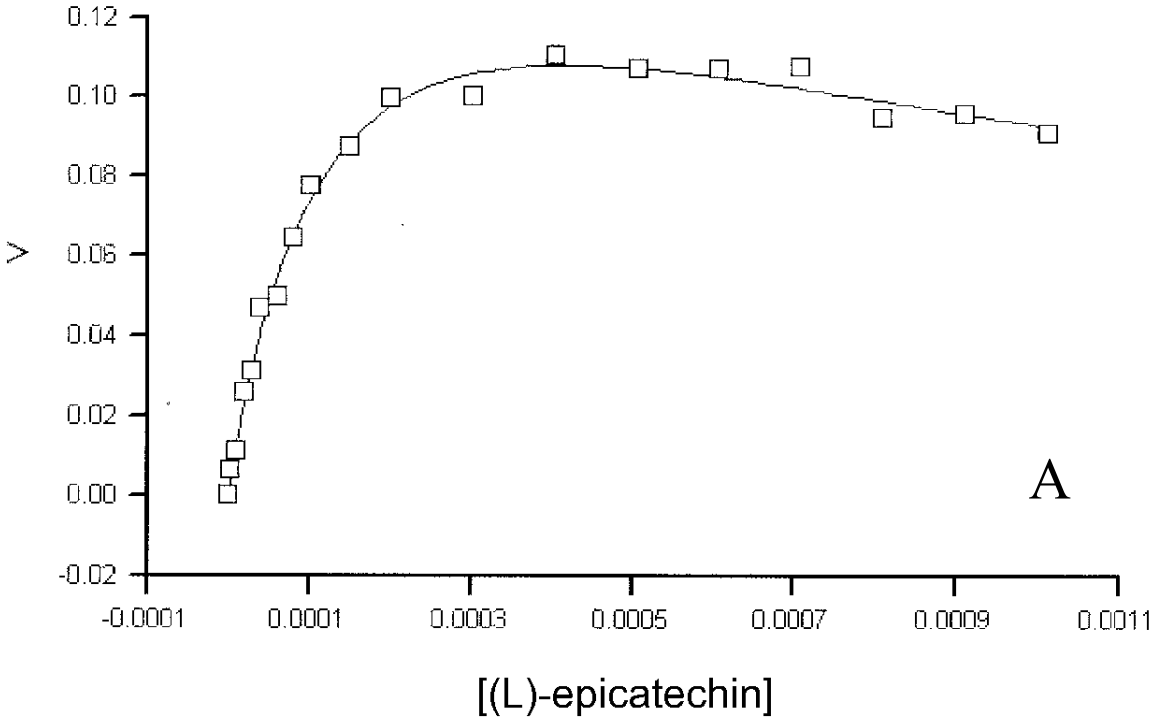


Figure S8: Complex: $[Cu_3(L)][ClO_4]_6$

- Substrate: L-epicatechin



- Substrate: D-catechin

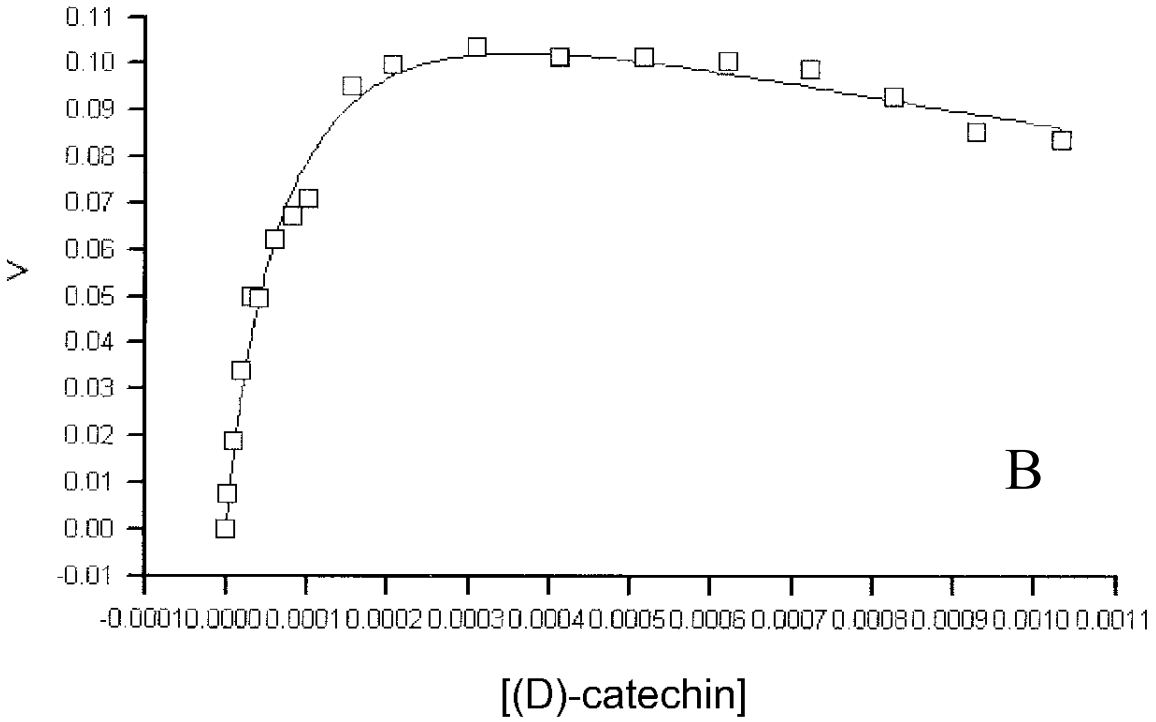


Figure S9: The low energy conformer of $[Cu_2(L)$-D-catechin$](OH)_2$ from MC/MMFF94 showing the angles between ring planes. In violet is drawn the plane containing the phenyl ring located at the phenylmethyl-*N*-acetoxy residue, in red (almost perpendicular to the viewer) the plane containing the phenyl ring of the 3,5,7 chroman residue of the substrate, and in light grey-blue the plane containing the N-methylimidazole (at the CuA2 site).

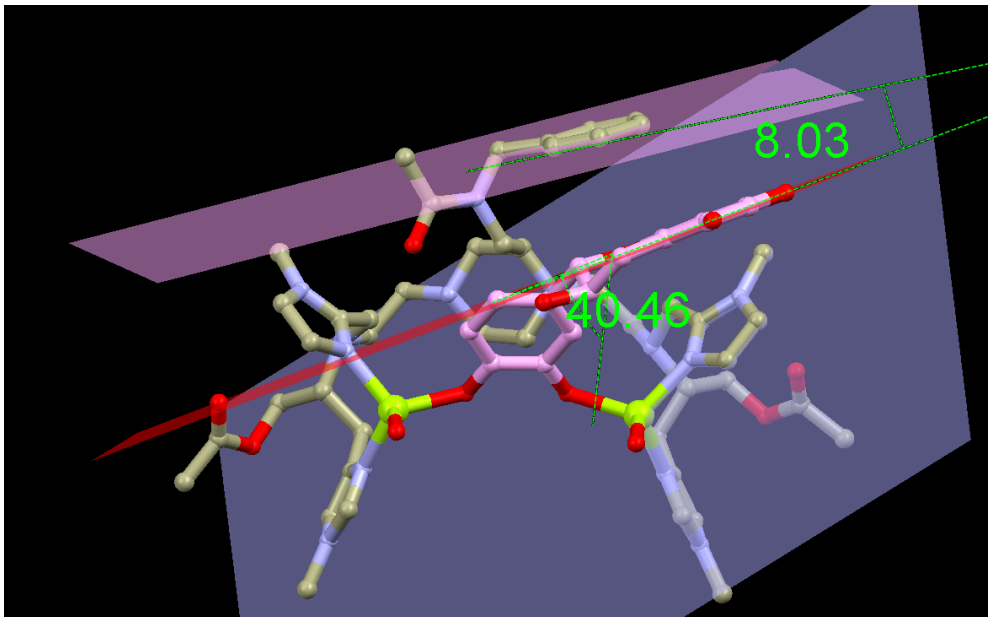


Figure S10: The low energy conformer of $[Cu_3(L)$-D-catechin$](OH)_4$ from MC/MMFF94 showing the angles between ring planes. In light grey-blue (almost perpendicular to the viewer) the plane containing the phenyl ring of the 3,5,7 chroman residue of the substrate, and in light tan the plane containing the *N*-methylimidazole ligand (at the CuA2 site). The distance between 3-OH in the 3,5,7 chroman residue with the methyl group of the same as above imidazole ligand is also shown.

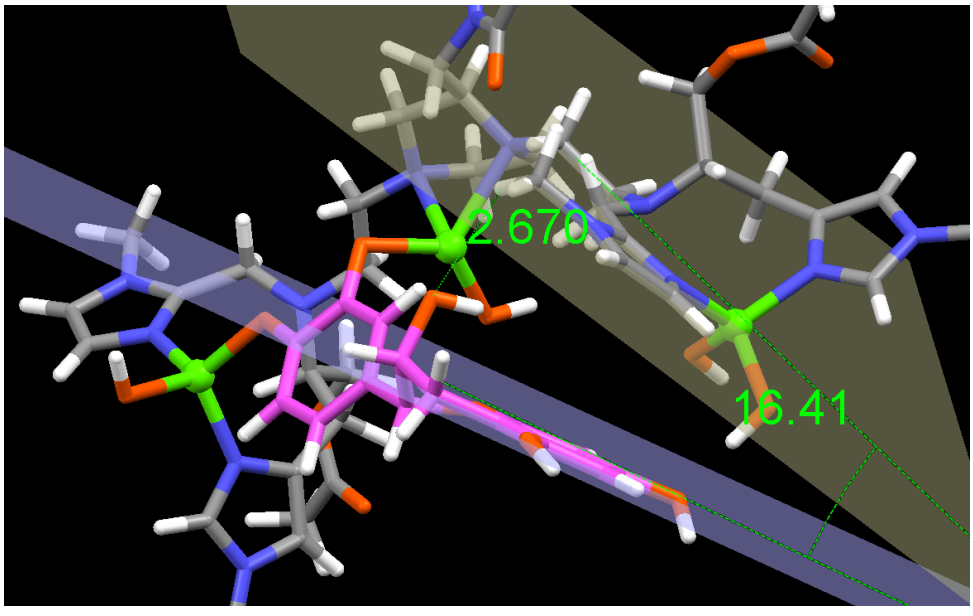
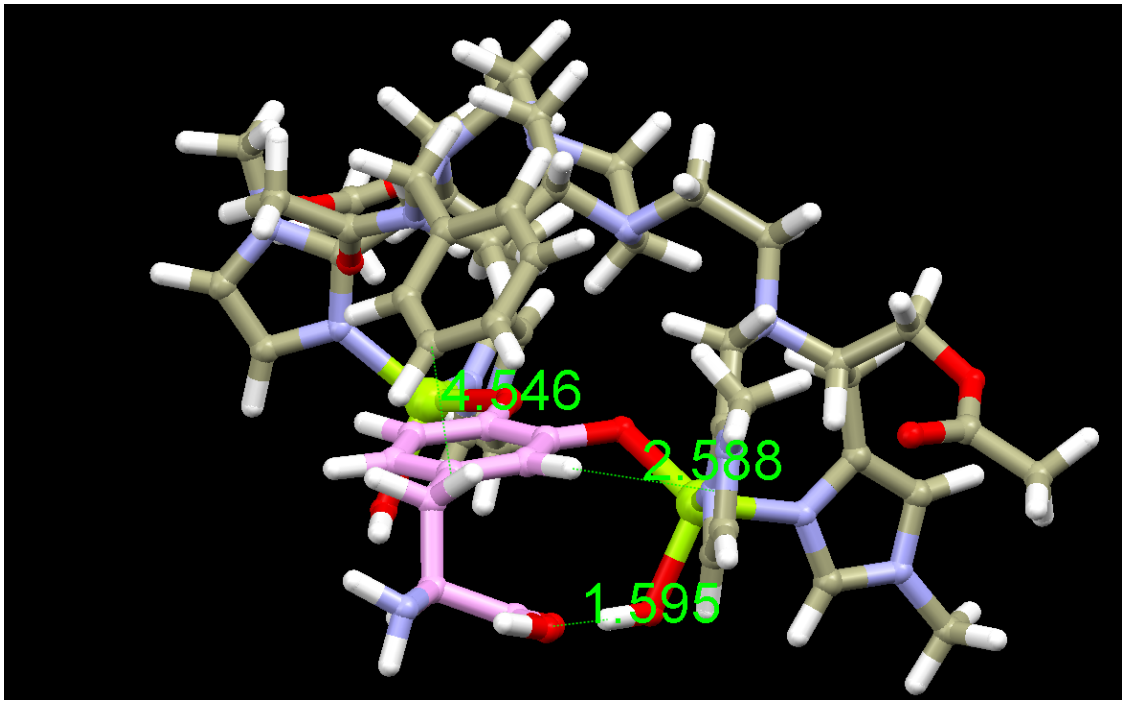


Figure S11: The low energy conformer of $[Cu_2(L)\text{-D-Dopa}](OH)_2$ from MC/MMFF94 showing the close distances between the phenyl ring of the substrate with the phenyl ring of the chiral residue located at the piperazine ring. Other close contacts are shown as well.



Part 2. Cartesian Coordinates Output (pdb or x,y,z format)

Table 1: The optimized geometry (RI−PB86/TZVP) of the dinuclear copper complex $[Cu_2(L)]^{4+}[H_2O]_4$ in pdb format

Binuclear Copper Complex charged form

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HEADER    CSD ENTRY Energy =   -6464.6831352420
CRYST1   1.0000   1.0000   1.0000  90.00  90.00  90.00
SCALE1      1.000000  0.000000  0.000000       0.000000
SCALE2      0.000000  1.000000  0.000000       0.000000
SCALE3      0.000000  0.000000  1.000000       0.000000
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HETATM    2  N   UNK     1      -3.076  -6.835   1.109  1.00  0.00           N
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HETATM   13  N   UNK     1      -0.374   1.313   0.634  1.00  0.00           N
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HETATM   22  C   UNK     1      -6.125   0.629  -2.468  1.00  0.00           C
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HETATM  107  H   UNK     1      -2.840   7.188  -4.657  1.00  0.00           H
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HETATM  111  H   UNK     1       -5.114    4.888    1.903  1.00  0.00           H
HETATM  112  H   UNK     1       -5.793    3.486    2.797  1.00  0.00           H
HETATM  113  H   UNK     1       -5.692    3.426    1.007  1.00  0.00           H
HETATM  114  H   UNK     1       -5.579    1.242    2.271  1.00  0.00           H
HETATM  115  H   UNK     1       -4.406   -0.050    2.006  1.00  0.00           H
HETATM  116  H   UNK     1       -3.700    2.235   -0.653  1.00  0.00           H
HETATM  117  H   UNK     1       -6.773   -0.531    0.698  1.00  0.00           H
HETATM  118  H   UNK     1       -7.615   -0.733   -1.640  1.00  0.00           H
HETATM  119  H   UNK     1       -4.550    2.052   -2.982  1.00  0.00           H
HETATM  120  H   UNK     1       -6.513    0.554   -3.497  1.00  0.00           H
HETATM  121  H   UNK     1        4.745    6.797   -1.525  1.00  0.00           H
HETATM  122  H   UNK     1        2.266    5.728   -4.823  1.00  0.00           H
HETATM  123  H   UNK     1        4.452    7.657   -5.006  1.00  0.00           H
HETATM  124  H   UNK     1        5.152    5.986   -5.041  1.00  0.00           H
HETATM  125  H   UNK     1        5.725    7.183   -3.815  1.00  0.00           H
HETATM  126  H   UNK     1        5.317   -5.722   -1.334  1.00  0.00           H
HETATM  127  H   UNK     1        2.086   -7.249   -3.657  1.00  0.00           H
HETATM  128  H   UNK     1        5.688   -7.662   -3.418  1.00  0.00           H
HETATM  129  H   UNK     1        5.430   -6.083   -4.268  1.00  0.00           H
HETATM  130  H   UNK     1        4.384   -7.503   -4.659  1.00  0.00           H
HETATM  131  H   UNK     1       -4.748   -6.700    2.383  1.00  0.00           H
HETATM  132  H   UNK     1       -3.273   -5.862    2.984  1.00  0.00           H
HETATM  133  H   UNK     1       -3.377   -7.670    3.045  1.00  0.00           H
HETATM  134  H   UNK     1       -2.944   -7.625   -2.087  1.00  0.00           H
HETATM  135  H   UNK     1       -4.763   -7.695    0.033  1.00  0.00           H
HETATM  136  H   UNK     1        4.874    6.354    1.333  1.00  0.00           H
HETATM  137  H   UNK     1       -0.331   -8.620   -2.987  1.00  0.00           H
HETATM  138  H   UNK     1        4.228    7.840    1.110  1.00  0.00           H
HETATM  139  H   UNK     1       -0.796   -7.222   -3.702  1.00  0.00           H
HETATM  140  O   UNK     1       -0.449  -10.151   -2.871  1.00  0.00           O
HETATM  141  H   UNK     1        0.204  -10.742   -3.308  1.00  0.00           H
HETATM  142  H   UNK     1       -1.295  -10.651   -2.840  1.00  0.00           H
HETATM  143  O   UNK     1        4.181    9.336    1.461  1.00  0.00           O
HETATM  144  H   UNK     1        4.723    9.983    0.956  1.00  0.00           H
HETATM  145  H   UNK     1        4.098    9.699    2.371  1.00  0.00           H
CONECT    1    2    5  135
CONECT    2    1    3   39
CONECT    3    2    4    6
CONECT    4    3    5   37
CONECT    5    1    4  134
CONECT    6    3    7   69   70
CONECT    7    6    8   37   40
CONECT    8    7    9   74   75
CONECT    9    8   10   76   77
CONECT   10    9   11   15
CONECT   11   10   12   80   83
CONECT   12   11   13   79   82
CONECT   13   12   14   25
CONECT   14   13   15   16   78
CONECT   15   10   14   81   84
CONECT   16   14   17  109  110
CONECT   17   16   18   66
CONECT   18   17   19  114  115
CONECT   19   18   20   24
CONECT   20   19   21  116
CONECT   21   20   22  119
CONECT   22   21   23  120
CONECT   23   22   24  118
CONECT   24   19   23  117
CONECT   25   13   26   85   86
CONECT   26   25   27   87   88
CONECT   27   26   28   34   52
CONECT   28   27   29   92   93
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CONECT   29   28   30   33
CONECT   30   29   31   34
CONECT   31   30   32   94
CONECT   32   31   33   95
CONECT   33   29   32   36
CONECT   34   27   30   35   59
CONECT   35   34  136  138
CONECT   36   33   96   97   98
CONECT   37    4    7   38   50
CONECT   38   37  137  139
CONECT   39    2  131  132  133
CONECT   40    7   41   45   73
CONECT   41   40   42   99  100
CONECT   42   41   43
CONECT   43   42   44   64
CONECT   44   43  101  102  103
CONECT   45   40   46   71   72
CONECT   46   45   47   50
CONECT   47   46   48  126
CONECT   48   47   49   51
CONECT   49   48   50  127
CONECT   50   37   46   49
CONECT   51   48  128  129  130
CONECT   52   27   53   57   89
CONECT   53   52   54  104  105
CONECT   54   53   55
CONECT   55   54   56   65
CONECT   56   55  106  107  108
CONECT   57   52   58   90   91
CONECT   58   57   59   62
CONECT   59   34   58   60
CONECT   60   59   61  121
CONECT   61   60   62   63
CONECT   62   58   61  122
CONECT   63   61  123  124  125
CONECT   64   43
CONECT   65   55
CONECT   66   17   67   68
CONECT   67   66  111  112  113
CONECT   68   66
CONECT   69    6
CONECT   70    6
CONECT   71   45
CONECT   72   45
CONECT   73   40
CONECT   74    8
CONECT   75    8
CONECT   76    9
CONECT   77    9
CONECT   78   14
CONECT   79   12
CONECT   80   11
CONECT   81   15
CONECT   82   12
CONECT   83   11
CONECT   84   15
CONECT   85   25
CONECT   86   25
CONECT   87   26
CONECT   88   26
CONECT   89   52
CONECT   90   57
CONECT   91   57
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CONECT   92   28
CONECT   93   28
CONECT   94   31
CONECT   95   32
CONECT   96   36
CONECT   97   36
CONECT   98   36
CONECT   99   41
CONECT  100   41
CONECT  101   44
CONECT  102   44
CONECT  103   44
CONECT  104   53
CONECT  105   53
CONECT  106   56
CONECT  107   56
CONECT  108   56
CONECT  109   16
CONECT  110   16
CONECT  111   67
CONECT  112   67
CONECT  113   67
CONECT  114   18
CONECT  115   18
CONECT  116   20
CONECT  117   24
CONECT  118   23
CONECT  119   21
CONECT  120   22
CONECT  121   60
CONECT  122   62
CONECT  123   63
CONECT  124   63
CONECT  125   63
CONECT  126   47
CONECT  127   49
CONECT  128   51
CONECT  129   51
CONECT  130   51
CONECT  131   39
CONECT  132   39
CONECT  133   39
CONECT  134    5
CONECT  135    1
CONECT  136   35
CONECT  137   38
CONECT  138   35
CONECT  139   38
CONECT  140  141  142
CONECT  141  140
CONECT  142  140
CONECT  143  144  145
CONECT  144  143
CONECT  145  143
MASTER        0    0    0    0    0    0    0    3  145    0  145    0
END
```

Table 2: The optimized geometry (RI−PB86/TZVP) of the dinuclear copper complex $[Cu_2(L)][OH_4]_4$ in cartesian coordinates format (x, y, z)

Binuclear Copper Complex neutral form

C	-6.428071	-1.842239	-0.713840
C	-6.153971	-0.700747	-1.657508
H	-5.841606	-1.107928	-2.642112
H	-7.112290	-0.186157	-1.830394
C	-4.635047	2.695715	-0.715417
H	-3.698427	2.685359	-1.298666
H	-5.097559	3.680097	-0.894787
C	-5.631267	1.677841	-1.295189
H	-6.577030	1.766475	-0.725641
N	-5.225933	0.274896	-1.114450
C	-3.823584	-0.101806	-1.018321
H	-3.798944	-1.119873	-0.603074
H	-3.364545	0.539136	-0.253273
Cu	-5.900602	0.024988	1.512228
C	-2.906963	-0.016506	-2.271697
H	-3.305046	0.723173	-2.984291
H	-2.866706	-0.994015	-2.806547
N	-1.574547	0.444787	-1.870451
C	0.312563	0.253315	-0.306575
C	0.613273	1.340107	-2.451570
N	1.276798	0.556960	-1.391114
C	-0.653885	0.671272	-2.978746
C	-0.920228	-0.430081	-0.897492
H	-0.020457	1.190002	0.183746
H	0.339680	2.356171	-2.088668
H	-0.389212	-0.279570	-3.497544
H	-0.620875	-1.399403	-1.359228
H	1.327555	1.461076	-3.280489
H	-1.128390	1.337695	-3.716915
H	-1.611411	-0.652446	-0.078398
C	2.498309	1.260008	-0.935701
H	2.730400	2.048002	-1.668187
H	2.312312	1.784562	0.022663
C	3.724973	0.321708	-0.824538
H	3.839259	-0.200216	-1.785056
H	3.508982	-0.467806	-0.085451
N	4.997956	0.928779	-0.467039
C	5.916444	1.457534	-1.475487
H	6.892210	1.479470	-0.954529
C	6.090908	0.560822	-2.714104
H	6.915760	1.017230	-3.287341
H	5.206486	0.625793	-3.371998
C	5.099766	1.567226	0.840393
H	4.375993	2.391806	0.991768
H	6.112213	1.996031	0.897320
C	5.003169	0.591908	1.980440
N	5.753824	-0.505763	2.075389
C	5.479955	-1.083771	3.293570
C	4.550461	-0.320696	3.957900
N	4.254943	0.745213	3.120508
H	5.992058	-1.984150	3.616709
H	4.087460	-0.420556	4.933094
C	3.296770	1.807952	3.433179
H	2.290593	1.572785	3.054416
H	3.639593	2.755696	3.003202
H	3.250105	1.923339	4.522646

Cu	7.187005	-1.022203	0.642791
C	-5.932543	2.080402	-2.767870
H	-5.381479	1.457768	-3.483376
H	-5.698862	3.138845	-2.945194
O	-7.335750	1.861761	-3.105454
C	-8.188729	2.867810	-2.733115
O	-7.817172	3.924096	-2.257798
C	-9.624124	2.471487	-2.969207
H	-10.235071	3.370878	-3.100464
H	-9.981326	1.934584	-2.077228
H	-9.723972	1.803816	-3.833135
C	5.628168	2.897335	-1.972623
H	4.554318	3.082285	-2.103947
H	6.157294	3.097797	-2.915260
O	6.057360	3.885524	-0.991328
C	7.359363	4.296399	-1.100210
O	8.097567	3.974826	-2.012659
C	7.749137	5.166607	0.068188
H	8.546526	5.853221	-0.236344
H	8.140514	4.511718	0.861721
H	6.891148	5.718789	0.469184
C	0.958806	-0.643405	0.771116
H	1.808458	-0.115879	1.226502
H	1.337964	-1.555449	0.289895
N	0.040060	-1.063773	1.849977
C	-0.382730	-0.108842	2.750989
O	0.007959	1.068952	2.645352
C	-1.390281	-0.491616	3.819051
H	-1.428393	0.332237	4.540063
H	-1.144397	-1.411077	4.366871
H	-2.398561	-0.617486	3.371214
C	-0.052871	-2.515240	2.099267
H	-0.467770	-2.659716	3.102180
H	0.973490	-2.919562	2.120856
C	-0.875127	-3.318054	1.108015
C	-2.387865	-4.913139	-0.647200
C	-2.270183	-3.167784	1.037235
C	-0.251969	-4.270190	0.289020
C	-1.000425	-5.062951	-0.587745
C	-3.018637	-3.963511	0.166073
H	-2.782588	-2.420067	1.652783
H	0.832256	-4.398678	0.344052
H	-0.498833	-5.800194	-1.217224
H	-4.104241	-3.848503	0.136307
H	-2.977009	-5.538335	-1.320885
C	6.404888	-0.897133	-2.513557
N	7.007550	-1.471745	-1.402239
C	7.174312	-2.764300	-1.679902
H	7.525127	-3.484418	-0.942185
N	6.710523	-3.057493	-2.922301
C	6.213235	-1.882698	-3.462654
H	5.782734	-1.846291	-4.457697
C	6.724084	-4.368069	-3.556944
H	7.337257	-4.351472	-4.468629
H	5.702909	-4.682404	-3.813500
H	7.152157	-5.092394	-2.854997
C	-4.266398	2.607554	0.741998
C	-3.271366	3.339962	1.358646
H	-2.566222	4.064751	0.967730
N	-4.866608	1.801269	1.697158
C	-4.244551	2.041490	2.850556
H	-4.429202	1.502304	3.772438
N	-3.275720	2.977451	2.692556

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C      -2.312595    3.408550    3.701729
H      -2.201728    4.500126    3.666819
H      -1.343685    2.918416    3.524450
H      -2.689687    3.125918    4.691457
N      -6.431171   -1.758611    0.612843
N      -6.827278   -3.096058   -1.104638
C      -7.008236   -3.575154   -2.471366
H      -7.136878   -4.663010   -2.446214
H      -6.125305   -3.341688   -3.079771
H      -7.895570   -3.122311   -2.935324
C      -6.843940   -2.979287    1.098070
H      -6.939276   -3.168175    2.161641
C      -7.101319   -3.823070    0.045505
H      -7.444304   -4.850558    0.001992
O       8.037405    0.693406    0.649623
H       8.760222    0.685536   -0.002352
O       7.194083   -2.886916    1.086731
H       6.399590   -3.141478    1.583794
O      -7.580641    0.791032    0.979230
H      -7.620506    1.689914    1.351919
O      -4.490181   -0.793176    2.593693
H      -4.758857   -1.709725    2.780816
```

Table 3: The optimized geometry (RI−PB86/TZVP) of the charged trinuclear copper complex $[Cu_3(L)]^{6+}[H_2O]_6$ in pdb format

```
Trinuclear Copper Complex charged form

HEADER    CSD ENTRY Energy =   -8256.9059604390
CRYST1   1.0000   1.0000   1.0000  90.00  90.00  90.00
SCALE1      1.000000  0.000000  0.000000       0.000000
SCALE2      0.000000  1.000000  0.000000       0.000000
SCALE3      0.000000  0.000000  1.000000       0.000000
HETATM    1  C   UNK     1      -0.387  -1.857   0.483  1.00  0.00           C
HETATM    2  C   UNK     1      -0.362  -1.687  -1.041  1.00  0.00           C
HETATM    3  H   UNK     1       0.154  -2.798   0.710  1.00  0.00           H
HETATM    4  H   UNK     1      -1.437  -1.966   0.871  1.00  0.00           H
HETATM    5  H   UNK     1       0.401  -2.365  -1.467  1.00  0.00           H
HETATM    6  H   UNK     1      -1.310  -2.012  -1.499  1.00  0.00           H
HETATM    7  C   UNK     1       1.636  -0.506   0.465  1.00  0.00           C
HETATM    8  H   UNK     1       2.059  -1.521   0.430  1.00  0.00           H
HETATM    9  C   UNK     1       1.373  -0.025  -1.015  1.00  0.00           C
HETATM   10  H   UNK     1       1.515   1.054  -1.163  1.00  0.00           H
HETATM   11  H   UNK     1       2.091  -0.544  -1.678  1.00  0.00           H
HETATM   12  N   UNK     1      -0.039  -0.287  -1.400  1.00  0.00           N
HETATM   13  N   UNK     1       0.294  -0.683   1.151  1.00  0.00           N
HETATM   14  C   UNK     1       0.428  -1.043   2.620  1.00  0.00           C
HETATM   15  H   UNK     1       1.423  -1.555   2.749  1.00  0.00           H
HETATM   16  H   UNK     1      -0.360  -1.777   2.822  1.00  0.00           H
HETATM   17  C   UNK     1      -0.420   0.120  -2.794  1.00  0.00           C
HETATM   18  H   UNK     1      -1.520   0.233  -2.771  1.00  0.00           H
HETATM   19  H   UNK     1      -0.038   1.151  -2.917  1.00  0.00           H
HETATM   20 Cu   UNK     1      -0.866   0.824   0.302  1.00  0.00          Cu
HETATM   21  O   UNK     1      -2.704   0.974   1.216  1.00  0.00           O
HETATM   22  H   UNK     1      -3.021   1.794   1.634  1.00  0.00           H
HETATM   23  O   UNK     1      -1.072   2.809  -0.237  1.00  0.00           O
HETATM   24  H   UNK     1      -1.934   3.201  -0.455  1.00  0.00           H
HETATM   25  C   UNK     1       2.629   0.411   1.217  1.00  0.00           C
HETATM   26  H   UNK     1       2.641   1.424   0.782  1.00  0.00           H
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HETATM   27  H   UNK     1       2.307   0.500   2.280  1.00  0.00           H
HETATM   28  N   UNK     1       4.016  -0.073   1.249  1.00  0.00           N
HETATM   29  C   UNK     1       4.217  -1.310   1.883  1.00  0.00           C
HETATM   30  O   UNK     1       3.256  -1.924   2.352  1.00  0.00           O
HETATM   31  C   UNK     1       5.597  -1.920   2.031  1.00  0.00           C
HETATM   32  H   UNK     1       6.101  -1.525   2.932  1.00  0.00           H
HETATM   33  H   UNK     1       5.486  -3.000   2.172  1.00  0.00           H
HETATM   34  H   UNK     1       6.219  -1.719   1.118  1.00  0.00           H
HETATM   35  C   UNK     1       5.081   0.982   1.186  1.00  0.00           C
HETATM   36  H   UNK     1       4.735   1.805   1.832  1.00  0.00           H
HETATM   37  H   UNK     1       5.975   0.522   1.682  1.00  0.00           H
HETATM   38  C   UNK     1       5.482   1.509  -0.170  1.00  0.00           C
HETATM   39  C   UNK     1       5.215   2.841  -0.533  1.00  0.00           C
HETATM   40  C   UNK     1       6.316   0.691  -0.997  1.00  0.00           C
HETATM   41  C   UNK     1       5.800   3.334  -1.699  1.00  0.00           C
HETATM   42  H   UNK     1       4.619   3.491   0.108  1.00  0.00           H
HETATM   43  C   UNK     1       6.877   1.201  -2.168  1.00  0.00           C
HETATM   44  H   UNK     1       6.553  -0.342  -0.659  1.00  0.00           H
HETATM   45  C   UNK     1       6.640   2.535  -2.538  1.00  0.00           C
HETATM   46  H   UNK     1       5.681   4.385  -1.960  1.00  0.00           H
HETATM   47  H   UNK     1       7.542   0.580  -2.766  1.00  0.00           H
HETATM   48  H   UNK     1       7.134   2.959  -3.423  1.00  0.00           H
HETATM   49  C   UNK     1       0.196   0.046   3.723  1.00  0.00           C
HETATM   50  N   UNK     1      -0.412  -0.504   4.975  1.00  0.00           N
HETATM   51  H   UNK     1       1.131   0.585   4.020  1.00  0.00           H
HETATM   52  H   UNK     1      -0.525   0.792   3.352  1.00  0.00           H
HETATM   53  C   UNK     1       0.138  -1.830   5.438  1.00  0.00           C
HETATM   54  C   UNK     1      -1.905  -0.531   5.122  1.00  0.00           C
HETATM   55  C   UNK     1       1.503  -1.701   6.049  1.00  0.00           C
HETATM   56  H   UNK     1       0.101  -2.565   4.608  1.00  0.00           H
HETATM   57  H   UNK     1      -0.560  -2.222   6.212  1.00  0.00           H
HETATM   58  C   UNK     1      -2.529   0.876   5.188  1.00  0.00           C
HETATM   59  C   UNK     1      -2.596  -1.369   4.011  1.00  0.00           C
HETATM   60  H   UNK     1      -2.080  -1.046   6.072  1.00  0.00           H
HETATM   61  N   UNK     1       1.800  -0.623   6.791  1.00  0.00           N
HETATM   62  N   UNK     1       2.531  -2.581   6.097  1.00  0.00           N
HETATM   63  C   UNK     1      -2.424   1.589   6.501  1.00  0.00           C
HETATM   64  H   UNK     1      -2.107   1.465   4.338  1.00  0.00           H
HETATM   65  H   UNK     1      -3.599   0.794   4.941  1.00  0.00           H
HETATM   66  O   UNK     1      -3.977  -1.613   4.312  1.00  0.00           O
HETATM   67  H   UNK     1      -2.041  -2.324   3.879  1.00  0.00           H
HETATM   68  H   UNK     1      -2.538  -0.813   3.036  1.00  0.00           H
HETATM   69  C   UNK     1       3.059  -0.789   7.302  1.00  0.00           C
HETATM   70  C   UNK     1       2.565  -3.900   5.442  1.00  0.00           C
HETATM   71  C   UNK     1       3.535  -2.015   6.873  1.00  0.00           C
HETATM   72  C   UNK     1      -3.386   2.386   7.111  1.00  0.00           C
HETATM   73  N   UNK     1      -1.291   1.670   7.284  1.00  0.00           N
HETATM   74  C   UNK     1      -4.940  -1.150   3.445  1.00  0.00           C
HETATM   75  H   UNK     1       3.551  -0.041   7.910  1.00  0.00           H
HETATM   76  H   UNK     1       3.392  -4.470   5.876  1.00  0.00           H
HETATM   77  H   UNK     1       2.661  -3.842   4.335  1.00  0.00           H
HETATM   78  H   UNK     1       1.634  -4.422   5.693  1.00  0.00           H
HETATM   79  H   UNK     1       4.488  -2.502   7.049  1.00  0.00           H
HETATM   80  N   UNK     1      -2.837   2.928   8.242  1.00  0.00           N
HETATM   81  H   UNK     1      -4.408   2.583   6.798  1.00  0.00           H
HETATM   82  C   UNK     1      -1.566   2.493   8.310  1.00  0.00           C
HETATM   83  O   UNK     1      -4.673  -0.432   2.487  1.00  0.00           O
HETATM   84  C   UNK     1      -6.328  -1.596   3.821  1.00  0.00           C
HETATM   85  C   UNK     1      -3.514   3.828   9.191  1.00  0.00           C
HETATM   86  H   UNK     1      -0.873   2.744   9.105  1.00  0.00           H
HETATM   87  H   UNK     1      -6.998  -1.179   3.060  1.00  0.00           H
HETATM   88  H   UNK     1      -6.564  -1.238   4.832  1.00  0.00           H
HETATM   89  H   UNK     1      -6.397  -2.693   3.812  1.00  0.00           H
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HETATM   90  H   UNK     1      -3.814   4.760   8.699  1.00  0.00           H
HETATM   91  H   UNK     1      -2.818   4.033  10.009  1.00  0.00           H
HETATM   92  H   UNK     1      -4.364   3.306   9.645  1.00  0.00           H
HETATM   93  O   UNK     1      -0.615  -0.874   8.706  1.00  0.00           O
HETATM   94  H   UNK     1      -0.169  -1.587   9.198  1.00  0.00           H
HETATM   95 Cu   UNK     1       0.288   0.530   7.190  1.00  0.00          Cu
HETATM   96  O   UNK     1       1.283   1.587   8.800  1.00  0.00           O
HETATM   97  H   UNK     1       1.470   1.121   9.633  1.00  0.00           H
HETATM   98  C   UNK     1       0.089  -0.851  -3.902  1.00  0.00           C
HETATM   99  N   UNK     1      -0.522  -0.801  -5.285  1.00  0.00           N
HETATM  100  H   UNK     1      -0.077  -1.875  -3.512  1.00  0.00           H
HETATM  101  H   UNK     1       1.173  -0.703  -4.037  1.00  0.00           H
HETATM  102  C   UNK     1       0.084  -1.916  -6.093  1.00  0.00           C
HETATM  103  C   UNK     1      -2.026  -0.855  -5.375  1.00  0.00           C
HETATM  104  C   UNK     1       1.485  -1.623  -6.530  1.00  0.00           C
HETATM  105  H   UNK     1      -0.022  -2.858  -5.531  1.00  0.00           H
HETATM  106  H   UNK     1      -0.557  -2.042  -6.991  1.00  0.00           H
HETATM  107  C   UNK     1      -2.716   0.512  -5.205  1.00  0.00           C
HETATM  108  C   UNK     1      -2.596  -1.921  -4.412  1.00  0.00           C
HETATM  109  H   UNK     1      -2.242  -1.211  -6.390  1.00  0.00           H
HETATM  110  N   UNK     1       1.826  -0.363  -6.857  1.00  0.00           N
HETATM  111  N   UNK     1       2.494  -2.500  -6.807  1.00  0.00           N
HETATM  112  C   UNK     1      -2.597   1.456  -6.354  1.00  0.00           C
HETATM  113  H   UNK     1      -2.296   1.014  -4.306  1.00  0.00           H
HETATM  114  H   UNK     1      -3.766   0.264  -5.009  1.00  0.00           H
HETATM  115  O   UNK     1      -3.919  -2.239  -4.826  1.00  0.00           O
HETATM  116  H   UNK     1      -1.966  -2.824  -4.418  1.00  0.00           H
HETATM  117  H   UNK     1      -2.608  -1.595  -3.352  1.00  0.00           H
HETATM  118  C   UNK     1       3.091  -0.412  -7.373  1.00  0.00           C
HETATM  119  C   UNK     1       2.545  -3.953  -6.677  1.00  0.00           C
HETATM  120  C   UNK     1       3.503  -1.736  -7.363  1.00  0.00           C
HETATM  121  C   UNK     1      -3.624   2.182  -6.946  1.00  0.00           C
HETATM  122  N   UNK     1      -1.435   1.828  -6.991  1.00  0.00           N
HETATM  123  C   UNK     1      -4.614  -3.062  -3.949  1.00  0.00           C
HETATM  124  H   UNK     1       3.618   0.471  -7.713  1.00  0.00           H
HETATM  125  H   UNK     1       3.577  -4.274  -6.511  1.00  0.00           H
HETATM  126  H   UNK     1       1.947  -4.272  -5.812  1.00  0.00           H
HETATM  127  H   UNK     1       2.189  -4.454  -7.586  1.00  0.00           H
HETATM  128  H   UNK     1       4.435  -2.187  -7.689  1.00  0.00           H
HETATM  129  N   UNK     1      -3.055   3.012  -7.880  1.00  0.00           N
HETATM  130  H   UNK     1      -4.689   2.220  -6.749  1.00  0.00           H
HETATM  131  C   UNK     1      -1.728   2.776  -7.905  1.00  0.00           C
HETATM  132  O   UNK     1      -4.108  -3.356  -2.882  1.00  0.00           O
HETATM  133  C   UNK     1      -5.953  -3.448  -4.495  1.00  0.00           C
HETATM  134  C   UNK     1      -3.772   3.997  -8.693  1.00  0.00           C
HETATM  135  H   UNK     1      -1.028   3.262  -8.572  1.00  0.00           H
HETATM  136  H   UNK     1      -6.464  -4.134  -3.815  1.00  0.00           H
HETATM  137  H   UNK     1      -6.605  -2.602  -4.753  1.00  0.00           H
HETATM  138  H   UNK     1      -5.812  -3.962  -5.458  1.00  0.00           H
HETATM  139  H   UNK     1      -4.209   4.752  -8.028  1.00  0.00           H
HETATM  140  H   UNK     1      -3.138   4.498  -9.430  1.00  0.00           H
HETATM  141  H   UNK     1      -4.581   3.501  -9.246  1.00  0.00           H
HETATM  142  O   UNK     1      -0.380  -0.160  -8.967  1.00  0.00           O
HETATM  143  H   UNK     1       0.086  -0.806  -9.523  1.00  0.00           H
HETATM  144 Cu   UNK     1       0.244   0.820  -6.933  1.00  0.00          Cu
HETATM  145  O   UNK     1       1.129   2.179  -8.288  1.00  0.00           O
HETATM  146  H   UNK     1       1.228   1.808  -9.190  1.00  0.00           H
HETATM  147  H   UNK     1       1.902   2.337   8.722  1.00  0.00           H
HETATM  148  H   UNK     1      -0.399   3.516  -0.240  1.00  0.00           H
HETATM  149  H   UNK     1      -3.364   0.267   1.531  1.00  0.00           H
HETATM  150  H   UNK     1       1.850   2.826  -8.119  1.00  0.00           H
HETATM  151  H   UNK     1      -1.230  -0.001  -9.411  1.00  0.00           H
HETATM  152  H   UNK     1      -1.433  -0.714   9.214  1.00  0.00           H
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CONECT    1    2    3    4   13
CONECT    2    1    5    6   12
CONECT    3    1
CONECT    4    1
CONECT    5    2
CONECT    6    2
CONECT    7    8    9   13   25
CONECT    8    7
CONECT    9    7   10   11   12
CONECT   10    9
CONECT   11    9
CONECT   12    2    9   17   20
CONECT   13    1    7   14   20
CONECT   14   13   15   16   49
CONECT   15   14
CONECT   16   14
CONECT   17   12   18   19   98
CONECT   18   17
CONECT   19   17
CONECT   20   12   13   21   23
CONECT   21   20   22  149
CONECT   22   21
CONECT   23   20   24  148
CONECT   24   23
CONECT   25    7   26   27   28
CONECT   26   25
CONECT   27   25
CONECT   28   25   29   35
CONECT   29   28   30   31
CONECT   30   29
CONECT   31   29   32   33   34
CONECT   32   31
CONECT   33   31
CONECT   34   31
CONECT   35   28   36   37   38
CONECT   36   35
CONECT   37   35
CONECT   38   35   39   40
CONECT   39   38   41   42
CONECT   40   38   43   44
CONECT   41   39   45   46
CONECT   42   39
CONECT   43   40   45   47
CONECT   44   40
CONECT   45   41   43   48
CONECT   46   41
CONECT   47   43
CONECT   48   45
CONECT   49   14   50   51   52
CONECT   50   49   53   54   95
CONECT   51   49
CONECT   52   49
CONECT   53   50   55   56   57
CONECT   54   50   58   59   60
CONECT   55   53   61   62
CONECT   56   53
CONECT   57   53
CONECT   58   54   63   64   65
CONECT   59   54   66   67   68
CONECT   60   54
CONECT   61   55   69   95
CONECT   62   55   70   71
CONECT   63   58   72   73
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CONECT   64   58
CONECT   65   58
CONECT   66   59   74
CONECT   67   59
CONECT   68   59
CONECT   69   61   71   75
CONECT   70   62   76   77   78
CONECT   71   62   69   79
CONECT   72   63   80   81
CONECT   73   63   82   95
CONECT   74   66   83   84
CONECT   75   69
CONECT   76   70
CONECT   77   70
CONECT   78   70
CONECT   79   71
CONECT   80   72   82   85
CONECT   81   72
CONECT   82   73   80   86
CONECT   83   74
CONECT   84   74   87   88   89
CONECT   85   80   90   91   92
CONECT   86   82
CONECT   87   84
CONECT   88   84
CONECT   89   84
CONECT   90   85
CONECT   91   85
CONECT   92   85
CONECT   93   94   95  152
CONECT   94   93
CONECT   95   50   61   73   93
CONECT   95   96
CONECT   96   95   97  147
CONECT   97   96
CONECT   98   17   99  100  101
CONECT   99   98  102  103  144
CONECT  100   98
CONECT  101   98
CONECT  102   99  104  105  106
CONECT  103   99  107  108  109
CONECT  104  102  110  111
CONECT  105  102
CONECT  106  102
CONECT  107  103  112  113  114
CONECT  108  103  115  116  117
CONECT  109  103
CONECT  110  104  118  144
CONECT  111  104  119  120
CONECT  112  107  121  122
CONECT  113  107
CONECT  114  107
CONECT  115  108  123
CONECT  116  108
CONECT  117  108
CONECT  118  110  120  124
CONECT  119  111  125  126  127
CONECT  120  111  118  128
CONECT  121  112  129  130
CONECT  122  112  131  144
CONECT  123  115  132  133
CONECT  124  118
CONECT  125  119
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CONECT  126  119
CONECT  127  119
CONECT  128  120
CONECT  129  121  131  134
CONECT  130  121
CONECT  131  122  129  135
CONECT  132  123
CONECT  133  123  136  137  138
CONECT  134  129  139  140  141
CONECT  135  131
CONECT  136  133
CONECT  137  133
CONECT  138  133
CONECT  139  134
CONECT  140  134
CONECT  141  134
CONECT  142  143  144  151
CONECT  143  142
CONECT  144   99  110  122  142
CONECT  144  145
CONECT  145  144  146  150
CONECT  146  145
CONECT  147   96
CONECT  148   23
CONECT  149   21
CONECT  150  145
CONECT  151  142
CONECT  152   93
MASTER        0    0    0    0    0    0    0    3  152    0  154    0
END
```

Table 4: The optimized geometry (RI−PB86/TZVP) of the neutral trinuclear copper complex $[Cu_3(L)][OH_4]_6$ in cartesian coordinates format (x, y, z)

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Trinuclear Copper Complex neutral form

C      -1.429848   -2.164520    0.510590
C      -1.508498   -1.830093   -0.995361
H      -1.147640   -3.224270    0.666638
H      -2.410688   -2.011693    0.978496
H      -1.417487   -2.758869   -1.588372
H      -2.469258   -1.354988   -1.240399
C       0.907951   -1.596623    0.637766
H       1.136399   -2.654311    0.855209
C       0.871489   -1.390067   -0.910432
H       1.635958   -0.663025   -1.213953
H       1.100105   -2.347086   -1.417493
N      -0.446381   -0.863735   -1.323981
N      -0.450273   -1.277888    1.196253
C      -0.555988   -1.531864    2.670290
H       0.085816   -2.399076    2.918596
H      -1.591102   -1.854005    2.847846
C      -0.522176   -0.324049   -2.708884
H      -1.316093    0.436120   -2.695053
H       0.418876    0.202235   -2.913824
Cu     -0.840365    0.651058    0.176299
O      -1.876331    1.739892   -1.015977
H      -2.251703    2.501451   -0.540910
```

O	-0.261783	1.865245	1.540652
H	-0.401501	2.784503	1.252891
C	1.962130	-0.719897	1.350208
H	1.589722	0.315169	1.375608
H	2.059151	-1.074537	2.387269
N	3.305138	-0.702972	0.751705
C	4.018219	-1.878249	0.769494
O	3.508732	-2.930367	1.189112
C	5.443776	-1.865950	0.239020
H	6.136645	-1.439040	0.980897
H	5.737166	-2.905786	0.059837
H	5.542984	-1.289753	-0.689807
C	3.946595	0.634681	0.620182
H	3.600830	1.236324	1.474844
H	5.029111	0.510604	0.738576
C	3.653790	1.353099	-0.680423
C	2.415446	1.980890	-0.898212
C	4.622956	1.401746	-1.694314
C	2.133760	2.574821	-2.132603
H	1.666779	2.018822	-0.098116
C	4.346868	2.020466	-2.917383
H	5.607481	0.957456	-1.522303
C	3.090216	2.586889	-3.154437
H	1.149446	3.018780	-2.294929
H	5.111880	2.054375	-3.696373
H	2.852313	2.992551	-4.142438
C	-0.267149	-0.347483	3.617752
N	-0.367319	-0.692778	5.047258
H	0.740714	0.050829	3.465768
H	-0.926156	0.494563	3.379813
C	0.621773	-1.678340	5.521276
C	-1.705789	-0.835021	5.680208
C	2.008953	-1.144788	5.315226
H	0.517173	-2.681024	5.065492
H	0.461411	-1.741184	6.618753
C	-2.698464	0.250670	5.223350
C	-2.342896	-2.221989	5.470889
H	-1.514500	-0.728276	6.763882
N	2.304009	0.138649	5.507883
N	3.139194	-1.864858	5.021362
C	-2.398037	1.666812	5.624755
H	-2.820656	0.190662	4.126868
H	-3.675924	-0.024371	5.646946
O	-3.386353	-2.374510	6.474466
H	-1.612653	-3.031239	5.605118
H	-2.800845	-2.337943	4.475438
C	3.662932	0.260922	5.331744
C	3.246506	-3.284315	4.682724
C	4.200467	-0.968555	5.027075
C	-3.303821	2.687223	5.842476
N	-1.120746	2.155903	5.822439
C	-3.998689	-3.592881	6.511522
H	4.162811	1.215875	5.455621
H	4.174480	-3.684618	5.110232
H	3.257253	-3.424623	3.591472
H	2.405018	-3.831902	5.120996
H	5.215288	-1.295732	4.828858
N	-2.556177	3.805534	6.178505
H	-4.387392	2.717970	5.798508
C	-1.245626	3.432505	6.159760
O	-3.726824	-4.506249	5.753757
C	-5.041681	-3.632349	7.603155
C	-3.073477	5.125094	6.511735

H	-0.414630	4.064197	6.463020
H	-5.442809	-4.647086	7.686801
H	-5.856833	-2.933560	7.365842
H	-4.607004	-3.314123	8.560193
H	-3.621846	5.554558	5.661427
H	-2.230215	5.781475	6.755637
H	-3.741297	5.069902	7.382873
O	0.138357	-0.161937	8.021300
H	0.823030	-0.135742	8.711114
Cu	0.582606	1.079461	6.531688
O	1.363994	2.567590	7.505501
H	1.096573	2.466582	8.436975
C	-0.745978	-1.398230	-3.792568
N	-0.645605	-0.899926	-5.191221
H	-1.720848	-1.895103	-3.641087
H	0.022748	-2.176634	-3.670046
C	0.140057	-1.825963	-6.035273
C	-1.927312	-0.494640	-5.842053
C	1.570637	-1.782474	-5.598644
H	-0.244232	-2.865620	-6.018543
H	0.091176	-1.410301	-7.063818
C	-2.709347	0.549970	-5.024496
C	-2.839059	-1.702409	-6.127727
H	-1.623213	-0.057288	-6.808304
N	2.150272	-0.664552	-5.167961
N	2.477700	-2.809619	-5.661988
C	-2.118160	1.926001	-4.937495
H	-2.895578	0.154156	-4.010719
H	-3.700928	0.636070	-5.492728
O	-3.903928	-1.247181	-7.007174
H	-2.296372	-2.511591	-6.634520
H	-3.291501	-2.118307	-5.213323
C	3.475610	-0.971016	-4.951944
C	2.255061	-4.162451	-6.159297
C	3.702110	-2.292615	-5.255634
C	-2.796394	3.122593	-4.816049
N	-0.761005	2.184418	-4.961440
C	-4.778840	-2.210855	-7.422175
H	4.171077	-0.222353	-4.589814
H	3.005024	-4.831760	-5.721275
H	1.259399	-4.513783	-5.862113
H	2.335037	-4.202579	-7.255462
H	4.592199	-2.911170	-5.216304
N	-1.831429	4.114450	-4.765613
H	-3.854838	3.352506	-4.757459
C	-0.619655	3.499793	-4.863749
O	-4.705952	-3.375857	-7.078857
C	-5.820494	-1.623220	-8.343979
C	-2.066339	5.545231	-4.631308
H	0.332626	4.018953	-4.928081
H	-6.472296	-2.421488	-8.711865
H	-6.419566	-0.874893	-7.805927
H	-5.337632	-1.110166	-9.186906
H	-2.545934	5.770897	-3.668459
H	-1.103115	6.066061	-4.676691
H	-2.704317	5.909179	-5.448538
O	0.300708	0.573279	-7.701727
H	1.065410	0.665424	-8.295227
Cu	0.808624	1.000757	-5.821723
O	2.027305	2.479801	-6.160014
H	1.829303	2.803837	-7.057155

Table 5: The optimized geometry (RI-BP86/def2-SV(P)) of the $[Cu_2(L)\text{-}L\text{-}Dopa](OH)_2$ adduct with bound L-Dopa in cartesian coordinate format (x,y,z).

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160
 C     1.952032    -1.487698     0.671922
 C     2.614226    -2.129836    -0.556189
 H     1.445038    -2.252426     1.293087
 H     1.143261    -0.796403     0.345480
 H     3.327841    -2.952185    -0.250580
 H     1.817878    -2.606885    -1.165422
 C     3.621603     0.257541     0.698162
 H     4.441343     0.657449     1.338386
 C     4.281737    -0.382008    -0.549860
 H     5.123558    -1.058858    -0.220175
 H     4.730088     0.414104    -1.181709
 N     3.304035    -1.113398    -1.353105
 N     2.897160    -0.735320     1.510593
 C     3.787497    -1.526398     2.352883
 H     4.347579    -0.810355     2.998881
 H     4.580771    -2.092397     1.789580
 C     3.888036    -1.609334    -2.596451
 H     4.461322    -0.775672    -3.062101
 H     4.633664    -2.430408    -2.385096
 C     2.699264     1.451408     0.325378
 H     2.146549     1.243666    -0.610099
 H     1.954784     1.590602     1.136695
 N     3.449063     2.702335     0.137873
 C     3.815945     3.097819    -1.131999
 O     3.550546     2.417162    -2.132625
 C     4.589740     4.408460    -1.253732
 H     4.652700     4.667779    -2.328437
 H     4.108420     5.242447    -0.699723
 H     5.626000     4.296315    -0.861043
 C     3.814345     3.461326     1.333981
 H     3.740311     2.757308     2.192962
 H     4.884927     3.759778     1.289556
 C     2.964481     4.694077     1.636156
 C     3.484288     5.694622     2.485088
 C     1.661664     4.846404     1.123938
 C     2.717678     6.820925     2.823904
 H     4.507812     5.590626     2.887862
 C     0.896230     5.977879     1.456490
 H     1.234377     4.077922     0.459736
 C     1.417665     6.965843     2.308132
 H     3.140278     7.592625     3.488971
 H    -0.121142     6.077138     1.044930
 H     0.812995     7.850389     2.569122
 C     3.097464    -2.581627     3.236475
 N     1.888571    -2.154324     3.933988
 H     2.830598    -3.460619     2.610633
 H     3.903145    -2.940497     3.938844
 C     2.080519    -0.930011     4.714428
 C     1.150310    -3.245387     4.590330
 C     0.822322    -0.375939     5.324263
 H     2.464889    -0.169713     3.998756
 H     2.853161    -1.044307     5.523788
 C     0.390929    -4.145791     3.567671
 C     2.042369    -4.100523     5.528107
 H     0.389178    -2.756570     5.235898
 N    -0.287932    -0.046800     4.653772
 N     0.673123    -0.064544     6.658345
 C    -1.046320    -3.768367     3.342271
```

H	0.945789	-4.140138	2.602204
H	0.406988	-5.195924	3.930710
O	1.231941	-4.986347	6.333145
H	2.647092	-3.457846	6.201392
H	2.712356	-4.771659	4.952120
C	-1.184356	0.473422	5.564429
C	1.632435	-0.278729	7.737508
C	-0.597228	0.474371	6.814653
C	-2.158242	-4.588406	3.497401
N	-1.467032	-2.498642	2.985381
C	0.931126	-4.594060	7.599241
H	-2.179481	0.767138	5.188243
H	2.598727	0.224878	7.518017
H	1.797261	-1.363960	7.909122
H	1.215393	0.164260	8.663783
H	-0.958933	0.802491	7.796313
N	-3.263962	-3.792280	3.232721
H	-2.254958	-5.647696	3.766606
C	-2.796878	-2.542777	2.934087
O	1.357340	-3.577645	8.120790
C	-0.012284	-5.579233	8.255537
C	-4.658640	-4.197173	3.269305
H	-3.398111	-1.616173	2.807393
H	-0.009694	-5.422194	9.351656
H	0.265017	-6.624901	8.007882
H	-1.042334	-5.406583	7.870867
H	-4.873749	-4.964450	2.492785
H	-5.290173	-3.307175	3.074730
H	-4.924577	-4.610814	4.266920
O	-2.831459	0.240779	3.230300
H	-3.232884	0.886220	2.605528
Cu	-1.012397	-0.250236	2.749378
O	-0.785718	0.297388	0.914736
C	2.901178	-2.166816	-3.636050
N	2.151488	-1.177170	-4.422633
H	2.223838	-2.900635	-3.125073
H	3.512330	-2.765856	-4.346035
C	1.483203	-0.139309	-3.606548
C	1.248140	-1.783561	-5.419887
C	0.841069	0.924304	-4.439815
H	0.679800	-0.538150	-2.935505
H	2.240115	0.315936	-2.936199
C	0.186726	-2.778630	-4.827830
C	2.067350	-2.411131	-6.563023
H	0.695403	-0.935353	-5.876362
N	-0.479882	1.110616	-4.549110
N	1.513509	1.838863	-5.208937
C	-1.208956	-2.655791	-5.365749
H	0.115583	-2.595697	-3.732345
H	0.534732	-3.827450	-4.950066
O	1.207391	-2.854340	-7.635020
H	2.791836	-1.666820	-6.952503
H	2.601373	-3.329337	-6.240136
C	-0.665057	2.179713	-5.397670
C	2.964944	1.954740	-5.319467
C	0.568416	2.643547	-5.820187
C	-1.904244	-3.471545	-6.248585
N	-2.068037	-1.658995	-4.926687
C	0.970329	-1.960030	-8.639765
H	-1.667804	2.545822	-5.649689
H	3.390156	0.950076	-5.522020
H	3.205690	2.635427	-6.160467
H	3.386723	2.346482	-4.368136

H	0.856229	3.459561	-6.493050
N	-3.194599	-2.958427	-6.326777
H	-1.599761	-4.368953	-6.799848
C	-3.245858	-1.867354	-5.508957
O	1.464888	-0.850902	-8.693334
C	0.006650	-2.545627	-9.651068
C	-4.294249	-3.495389	-7.111885
H	-4.130984	-1.251415	-5.276472
H	0.304591	-3.578149	-9.931065
H	-1.007773	-2.602328	-9.197557
H	-0.028833	-1.896760	-10.547434
H	-5.196753	-2.878843	-6.928162
H	-4.058323	-3.466513	-8.198121
H	-4.512539	-4.545041	-6.818392
O	-3.891178	0.181391	-3.710724
H	-4.221922	0.350696	-2.802756
C	-1.407840	1.322142	0.376130
C	-2.835361	3.501611	-0.795694
C	-1.734182	2.497350	1.118370
C	-1.788456	1.273907	-1.041814
C	-2.501495	2.394133	-1.576252
C	-2.455061	3.570273	0.570574
H	-1.454610	2.504533	2.186484
H	-2.852060	2.312778	-2.620002
H	-3.415640	4.327110	-1.247347
C	-2.871331	4.754421	1.415868
H	-2.276396	4.791733	2.355951
Cu	-2.002179	-0.010628	-3.648817
H	-2.666251	5.703776	0.860025
C	-4.379587	4.802198	1.794727
H	-4.978275	4.662199	0.867015
C	-4.738185	3.643670	2.762283
O	-4.938648	2.501299	2.405599
O	-4.762453	4.053376	4.046256
H	-4.637246	5.062486	3.956141
N	-4.672305	6.073020	2.495490
H	-4.055690	6.835252	2.177944
H	-5.646925	6.373203	2.347643
O	-1.475117	0.229693	-1.761192

Table 6: The optimized geometry (RI-BP86/def2-SV(P)) of the $[Cu_2(L)$-D-Catechin$](OH)_2$ adduct with bound D-Catechin in cartesian coordinate format (x,y,z).

170			
C	1.811606	-2.039596	-0.108083
C	2.196658	-2.505153	-1.516102
H	1.112514	-2.752507	0.371951
H	1.240707	-1.089261	-0.183568
H	2.649847	-3.540608	-1.490068
H	1.267294	-2.569384	-2.119095
C	3.953839	-0.933973	0.153533
H	4.889201	-1.033559	0.748839
C	4.306082	-1.360543	-1.294975
H	4.916957	-2.309469	-1.253006
H	4.949669	-0.583831	-1.763403
N	3.121868	-1.550560	-2.131332
N	2.964495	-1.830057	0.776080
C	3.576589	-3.013521	1.373344
H	4.246086	-2.657023	2.192020
H	4.248350	-3.584553	0.672821
C	3.503011	-1.893322	-3.502033

H	4.244360	-1.139618	-3.850504
H	4.027927	-2.893480	-3.520602
C	3.498465	0.544326	0.267612
H	2.776342	0.800739	-0.530358
H	2.998379	0.675277	1.251426
N	4.610809	1.502152	0.181119
C	4.808528	2.208042	-0.989624
O	4.126785	1.987799	-1.997926
C	5.903288	3.276027	-1.004537
H	5.797915	3.844490	-1.949035
H	5.830633	3.982139	-0.149600
H	6.918896	2.820957	-0.987687
C	5.430312	1.667936	1.377612
H	5.724075	0.658790	1.748567
H	6.383063	2.159319	1.091142
C	4.782316	2.438492	2.526119
C	5.234824	2.218445	3.844389
C	3.765524	3.388024	2.308690
C	4.687163	2.934317	4.920744
H	6.024892	1.469273	4.031382
C	3.213290	4.103501	3.385767
H	3.381612	3.554437	1.288460
C	3.670349	3.879779	4.695841
H	5.047322	2.743120	5.945592
H	2.405459	4.829260	3.198294
H	3.216620	4.421863	5.541635
C	2.609156	-4.069437	1.937757
N	1.472068	-3.582397	2.717241
H	2.202204	-4.672482	1.095695
H	3.267775	-4.771130	2.522472
C	1.830439	-2.585614	3.730931
C	0.543506	-4.640309	3.148090
C	0.649560	-1.963003	4.428024
H	2.372550	-1.778006	3.187564
H	2.531960	-2.987095	4.512126
C	-0.293424	-5.216335	1.959630
C	1.234127	-5.772823	3.952129
H	-0.165729	-4.149714	3.848562
N	-0.428703	-1.432421	3.838015
N	0.567617	-1.791518	5.792647
C	-1.701634	-4.699905	1.887221
H	0.233570	-4.991178	1.005976
H	-0.339441	-6.323690	2.038432
O	0.246077	-6.598629	4.606864
H	1.917738	-5.355568	4.721008
H	1.795252	-6.466877	3.292867
C	-1.233040	-0.917980	4.834848
C	1.511973	-2.252168	6.805705
C	-0.623190	-1.128793	6.054941
C	-2.882356	-5.429301	1.952018
N	-2.009717	-3.354689	1.783457
C	-0.060759	-6.301171	5.898676
H	-2.188316	-0.454115	4.539308
H	2.530099	-1.851148	6.613871
H	1.534569	-3.362021	6.838386
H	1.173414	-1.876657	7.791843
H	-0.918276	-0.868456	7.078060
N	-3.914080	-4.501417	1.890773
H	-3.073132	-6.506665	2.032313
C	-3.338461	-3.265846	1.793821
O	0.498406	-5.436957	6.550970
C	-1.184890	-7.183811	6.397043
C	-5.339006	-4.783405	1.927888

H	-3.850010	-2.281590	1.844051
H	-1.316893	-7.037888	7.486363
H	-0.976640	-8.251173	6.171212
H	-2.127422	-6.913409	5.871926
H	-5.645821	-5.401922	1.055754
H	-5.891577	-3.823372	1.895507
H	-5.611696	-5.320265	2.862890
O	-2.992992	-0.549163	2.515196
H	-3.131272	0.220210	1.918735
Cu	-1.250360	-1.280051	1.959890
O	-0.966927	-0.355267	0.269435
C	2.368486	-1.975412	-4.540268
N	1.856634	-0.695709	-5.046441
H	1.549572	-2.627169	-4.135870
H	2.793594	-2.529076	-5.404117
C	1.306006	0.170394	-3.980528
C	0.944356	-0.829989	-6.200044
C	0.899701	1.520005	-4.483273
H	0.400105	-0.258420	-3.478814
H	2.080538	0.264339	-3.189640
C	-0.298206	-1.756104	-5.954474
C	1.742653	-1.228655	-7.455803
H	0.563982	0.194221	-6.398464
N	-0.365906	1.955510	-4.545662
N	1.750833	2.480455	-4.965054
C	-1.608171	-1.257679	-6.493663
H	-0.433479	-1.868392	-4.855738
H	-0.099792	-2.775096	-6.352387
O	0.902837	-1.236857	-8.629416
H	2.579380	-0.516072	-7.603666
H	2.134223	-2.265385	-7.390518
C	-0.328984	3.232830	-5.062132
C	3.204534	2.366805	-5.062280
C	0.984439	3.572038	-5.331359
C	-2.358731	-1.702300	-7.573911
N	-2.319513	-0.251875	-5.855046
C	0.835031	-0.073796	-9.342108
H	-1.244049	3.819635	-5.209427
H	3.454725	1.377117	-5.496518
H	3.578740	3.168740	-5.729580
H	3.669016	2.450296	-4.055807
H	1.437399	4.479102	-5.747625
N	-3.534073	-0.958496	-7.570638
H	-2.166963	-2.484874	-8.316894
C	-3.465936	-0.099721	-6.512645
O	1.456849	0.931598	-9.059988
C	-0.123131	-0.222239	-10.505800
C	-4.642792	-1.088087	-8.502343
H	-4.254732	0.588814	-6.164777
H	0.069312	-1.164192	-11.061632
H	-1.164116	-0.272365	-10.115899
H	-0.026842	0.651487	-11.178767
H	-5.436186	-0.369974	-8.214517
H	-4.316713	-0.861613	-9.541115
H	-5.063625	-2.116693	-8.473645
O	-3.944577	1.468525	-4.227272
H	-4.348395	1.388366	-3.337288
C	-1.409914	0.861050	0.078765
C	-2.550057	3.465975	-0.276126
C	-1.482575	1.808753	1.142875
C	-1.911452	1.275385	-1.249432
C	-2.486466	2.580465	-1.357102
C	-2.045399	3.084045	0.996218

H	-1.091234	1.491643	2.122718
H	-2.898637	2.855875	-2.344024
H	-2.982116	4.472262	-0.418132
Cu	-2.109336	0.954947	-4.154470
O	-1.841726	0.456725	-2.258528
C	-2.641004	4.723630	4.888510
C	-0.323740	4.815864	6.522976
C	-1.386562	4.270096	4.411523
C	-2.689459	5.246564	6.203279
C	-1.546757	5.301933	7.022668
C	-0.235566	4.299064	5.221686
H	-1.637068	5.721336	8.037745
H	0.714489	3.913565	4.828675
O	-1.218216	3.768327	3.153492
C	-3.885659	4.601304	4.035177
H	-4.203402	5.582036	3.604202
H	-4.751193	4.217877	4.628962
C	-3.648746	3.649100	2.862267
C	-2.278936	3.966699	2.200213
H	-2.291478	5.042028	1.894556
O	0.826655	4.838313	7.273954
H	0.618626	5.242857	8.143813
O	-3.859298	5.717785	6.736894
H	-4.566809	5.632281	6.060240
O	-4.716134	3.812101	1.946297
H	-4.484765	3.281421	1.145584
H	-3.585455	2.594540	3.234313

Table 7: The optimized geometry (RI-BP86/def2-SV(P)) of the $[Cu_3(L)\text{-L-Dopa}](OH)_3$ adduct with bound L-Dopa in cartesian coordinate format (x,y,z).

C	-2.860580	0.325245	0.239876
C	-2.616085	-1.214060	0.140267
H	-3.861224	0.523946	0.644925
H	-2.860402	0.727447	-0.778948
H	-3.495447	-1.763395	0.499620
H	-2.502722	-1.466183	-0.920235
C	-1.949229	0.356215	2.427059
H	-2.997912	0.492323	2.726458
C	-1.689996	-1.192770	2.290515
H	-0.843782	-1.513663	2.910849
H	-2.562926	-1.741837	2.667264
N	-1.436797	-1.532997	0.902013
N	-1.819592	0.924682	1.060893
C	-1.775273	2.364561	1.015399
H	-0.984830	2.736514	1.663555
H	-2.714701	2.730953	1.448692
C	-0.883523	-2.848553	0.760319
H	0.127009	-2.833204	1.191023
H	-1.471776	-3.542743	1.378347
Cu	-0.003441	-0.006723	0.295059
C	-1.067256	0.919439	3.584064
H	-0.393792	0.158858	3.994493
H	-0.395201	1.706123	3.235515
N	-1.841841	1.455798	4.721254
C	-2.182954	2.799796	4.731686
O	-1.809661	3.591659	3.860852
C	-3.025506	3.309291	5.875408
H	-2.433175	3.336607	6.793461
H	-3.356608	4.328202	5.650089
H	-3.918854	2.694902	6.006561

C	-2.095180	0.546808	5.852340
H	-1.115738	0.165171	6.167344
H	-2.491228	1.080802	6.719878
C	-3.030816	-0.594075	5.541182
C	-2.639378	-1.916422	5.803168
C	-4.326416	-0.359665	5.057423
C	-3.514909	-2.977737	5.565329
H	-1.656615	-2.132620	6.216422
C	-5.198547	-1.422517	4.815694
H	-4.673274	0.653010	4.868797
C	-4.792333	-2.730479	5.068515
H	-3.211553	-3.997434	5.789816
H	-6.204241	-1.230259	4.448320
H	-5.481701	-3.554882	4.900284
C	-1.561682	3.053148	-0.356047
N	-1.332844	4.497630	-0.398615
H	-0.753903	2.550983	-0.888521
H	-2.457863	2.833871	-0.945841
C	-2.175822	5.264271	0.507083
C	-1.283874	5.096185	-1.735201
C	-1.481663	5.774794	1.730686
H	-3.054575	4.715128	0.853002
H	-2.556442	6.182894	0.044783
C	-0.050505	4.666265	-2.556574
C	-2.589818	4.928371	-2.567482
H	-1.188148	6.181138	-1.564302
N	-0.157347	5.705109	1.901582
N	-1.983899	6.429803	2.799997
C	1.014143	5.650016	-2.292001
H	0.317373	3.668292	-2.307832
H	-0.247345	4.666209	-3.633450
O	-3.204948	6.198888	-2.877143
H	-3.354942	4.387809	-2.004418
H	-2.434509	4.372250	-3.499126
C	0.200975	6.194451	3.127911
C	-3.397786	6.711779	3.024375
C	-0.951439	6.663998	3.700336
C	1.639381	6.569505	-3.104893
N	1.463391	5.924929	-1.017241
C	-2.548280	6.999917	-3.761002
H	1.223666	6.156183	3.449734
H	-3.520808	7.337765	3.912049
H	-3.928869	5.766944	3.166446
H	-3.798846	7.238286	2.154475
H	-1.178408	7.129467	4.645233
N	2.440258	7.366650	-2.298583
H	1.575821	6.788162	-4.159789
C	2.289354	6.980416	-1.020211
O	-1.410677	6.796816	-4.166908
C	-3.388804	8.185814	-4.120474
C	3.248132	8.497839	-2.751879
H	2.759073	7.433366	-0.156860
H	-2.890076	8.756849	-4.908732
H	-3.517246	8.826495	-3.244808
H	-4.358452	7.852702	-4.499308
H	3.774585	8.222479	-3.669563
H	3.977776	8.758132	-1.980626
H	2.588603	9.349128	-2.938814
O	2.702812	5.245125	1.433937
H	2.954709	4.447350	1.938110
C	-0.800708	-3.460047	-0.651323
N	-0.035266	-4.681223	-0.850428
H	-0.436909	-2.694173	-1.338434

H	-1.835804	-3.644375	-0.966052
C	0.224427	-5.509714	0.318343
C	-0.393926	-5.476685	-2.039643
C	1.568309	-6.187705	0.261352
H	0.299073	-4.953946	1.253940
H	-0.519367	-6.299195	0.450703
C	-0.287530	-4.716008	-3.381936
C	-1.800794	-6.142844	-1.921271
H	0.334156	-6.300665	-2.079634
N	2.591229	-5.651888	-0.412210
N	2.015072	-7.347577	0.783924
C	1.049953	-4.885945	-3.994571
H	-0.488896	-3.646250	-3.282644
H	-1.011842	-5.094342	-4.112443
O	-1.696764	-7.578882	-1.806211
H	-2.324539	-5.813985	-1.018328
H	-2.463621	-5.906454	-2.761775
C	3.698098	-6.445406	-0.366672
C	1.220293	-8.269374	1.593374
C	3.344207	-7.526230	0.399849
C	1.436260	-5.361863	-5.227940
N	2.232899	-4.593623	-3.347062
C	-1.312785	-8.231027	-2.941867
H	4.591421	-6.148682	-0.882377
H	1.860340	-9.050393	2.011853
H	0.749444	-7.712713	2.407845
H	0.454524	-8.723074	0.958754
H	3.864610	-8.413954	0.722028
N	2.822916	-5.289360	-5.296747
H	0.891349	-5.743899	-6.077060
C	3.293043	-4.799826	-4.135709
O	-0.864038	-7.677817	-3.938144
C	-1.456421	-9.711483	-2.771493
C	3.638461	-5.684546	-6.442080
H	4.331119	-4.626128	-3.888647
H	-1.258384	-10.206267	-3.726514
H	-0.738362	-10.068828	-2.029526
H	-2.477722	-9.952888	-2.465890
H	3.331167	-5.104385	-7.316130
H	4.693021	-5.491162	-6.229019
H	3.493820	-6.751577	-6.630376
C	2.493400	1.058740	0.765782
C	4.431995	1.987714	-0.934102
C	3.613169	0.263079	0.514584
C	2.351081	2.350133	0.240239
C	3.337946	2.816402	-0.615147
C	4.577613	0.693102	-0.389723
H	3.677593	-0.693316	1.021648
H	3.276188	3.790628	-1.086611
H	5.187498	2.364304	-1.627629
C	5.776652	-0.144360	-0.802200
H	6.657604	0.380593	-0.406138
H	5.844190	-0.102614	-1.898502
C	5.857598	-1.628082	-0.365209
C	4.876262	-2.522867	-1.149658
Cu	2.289611	-3.917770	-1.414262
Cu	0.977684	4.895212	0.556978
O	0.018313	0.139295	-1.646542
H	-0.866204	0.356893	-1.995012
O	1.478156	0.477825	1.478371
O	5.077496	-2.976693	-2.272056
N	7.235904	-2.106728	-0.591074
H	7.377125	-3.065366	-0.274254

H	7.476757	-2.090835	-1.585703
H	5.664254	-1.733547	0.707456
O	1.189686	2.995782	0.565215
O	1.905068	-2.065118	-2.286809
H	1.286017	-1.553288	-1.734647
O	3.755590	-2.772445	-0.401140