

Supporting Information

Mono-nuclear copper complexes mimicking the intermediates for binuclear copper center of the subunit II of cytochrome oxidase: a peptide based approach

Dwaipayan Dutta Gupta,^a Dandamudi Usharani^b and Shyamalava Mazumdar^{a,*}

^aTata Institute of Fundamental Research, Homi Bhabha Road, Colaba, Mumbai- 400 005, INDIA

^bDepartment of Lipid Science, CSIR- Central Food Technological Research Institute, Mysore- 570020, INDIA

*Email: shyamal@tifr.res.in

Matrix assisted Laser Desorption/ Ionisation time-of-flight (MALDI-TOF) mass spectrometry

Successful synthesis of the peptides were confirmed by MALDI-TOF using Bruker ultrafleXtreme (Bruker Daltonics) mass spectrometer. All spectra were recorded in reflector positive mode. A pinch of ether precipitated peptide post cleavage is dissolved in water and 1ul of this solution is mixed with 1 ul of the matrix α -cyano-4-hydroxycinnamic acid (HCCA). 0.5ul of this mixture is spotted on a well of the MALDI target plate and after complete solvent evaporation the sample is irradiated with a 337nm laser for detection. For each peptide, a sum of 20 spectra was taken by irradiating each sample 20 times over different regions of the well containing the dried sample. Expected protonated monoisotopic mass ($M+H^+$) of nine amino acid peptide (9AA) =1021.4, eleven amino acid peptide (11AA) =1147.4, twelve amino acid peptide (12AA) =1366.5.

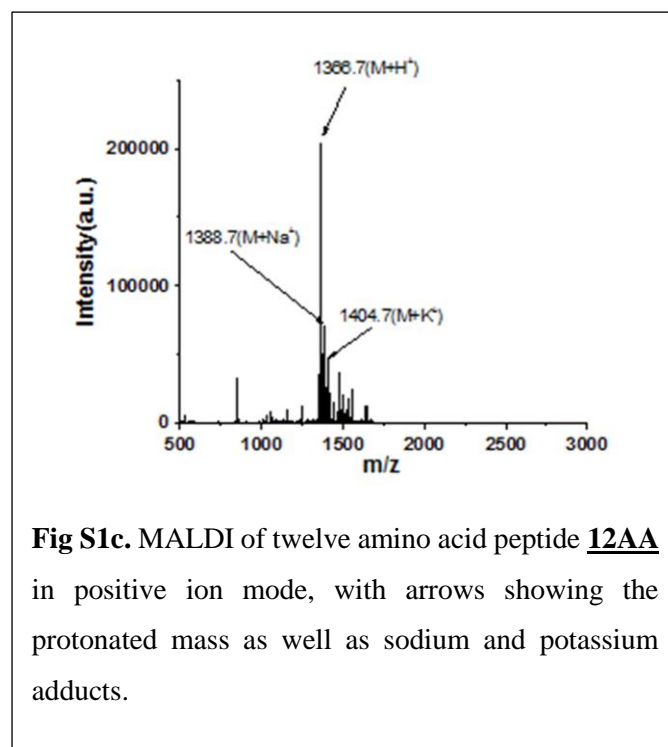
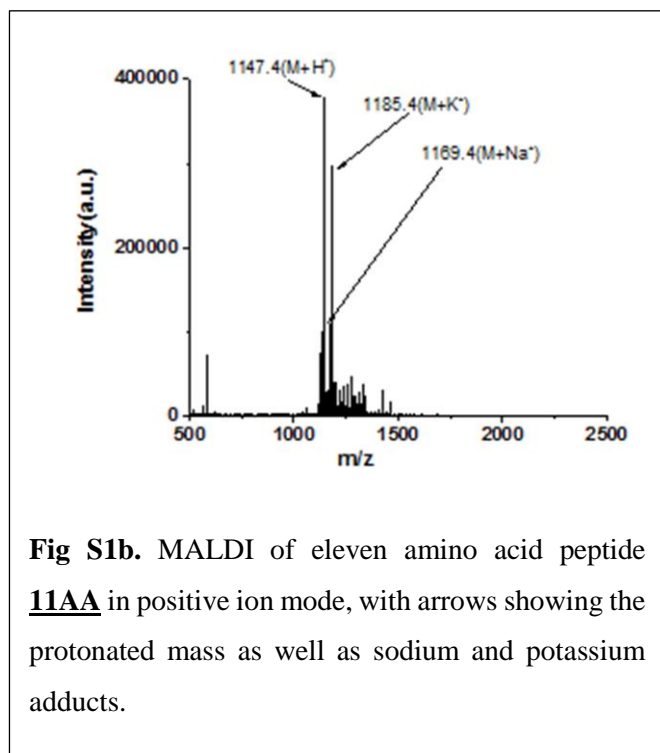
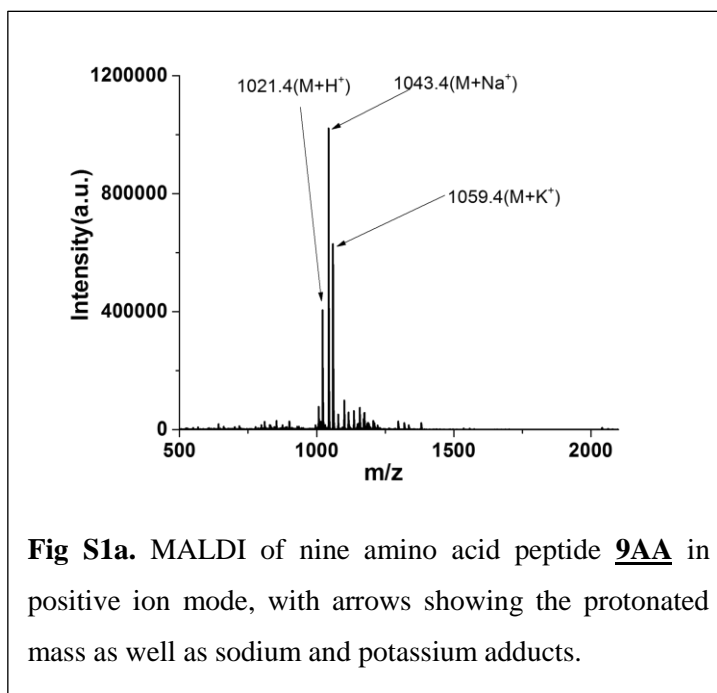


Table S1: EPR simulation results for peptide copper complexes

Sample	gx(Ax)	gy (Ay)	gz(Az)
Cu- <u>9AA</u>	2.055 (5)	2.055 (5)	2.225 (155)
Cu- <u>11AA</u>	2.060 (10)	2.060 (10)	2.23 (160)
Cu- <u>12AA</u>	2.052 (20)	2.052 (20)	2.235 (170)
Ax, Ay, Az values are in 10 ⁻⁴ cm ⁻¹			

Table S2: Computed spin densities and NBO charges of first coordination sphere of Cu-9AA, Cu-11AA and Cu-12AA peptide complexes at UB3LYP/def-SV(P) level of theory.

Cu- <u>9AA</u>	Spin	Charge	Cu- <u>11AA</u>	Spin	Charge	Cu- <u>12AA</u>	Spin	Charge
Cu	0.43	1.16	Cu	0.46	1.12	Cu	0.45	1.12
S(Cys)	0.24	-0.44	S(Cys ₁)	0.27	-0.38	S(Cys ₁)	0.16	-0.50
S(Met)	0.00	0.10	S(Cys ₂)	0.20	-0.53	S(Cys ₂)	0.22	-0.46
N(His)	0.05	-0.63	N(His)	0.00	-0.69	S(Met)	0.03	0.15
NH(Cys)	0.25	-0.67	NH ₂ (Cys ₁)	0.00	-0.17	N(His)	0.09	-0.63
H ₂ O _e	0.02	-0.02	H ₂ O _{e1}	0.02	0.03	NH ₂ (Cys ₁)	0.02	-1.06
H ₂ O _a	0.00	0.00	H ₂ O _{e2}	0.02	0.03	H ₂ O _a	0.01	0.01

Cartesian Coordinates of Model Cu-Peptide Complexes at UB3LYP/def-SV(P) level of Theory

Cu-9AA

O	-0.332761000	-0.588342000	0.747260000	H	-1.537150000	-1.843565000	-4.262374000
O	0.965182000	-0.263775000	-1.454187000	H	-2.672166000	0.015154000	-4.458465000
O	-5.626811000	-3.800680000	3.605432000	H	-2.549004000	1.187723000	-2.394281000
N	-0.040804000	-3.083090000	-2.369595000	H	-0.786964000	0.933616000	-2.226122000
C	0.666385000	-2.785985000	-3.599041000	N	0.078370000	1.848671000	-4.724496000
C	0.372837000	-1.350249000	-4.098225000	C	0.599315000	3.114247000	-5.183487000
O	1.278903000	-0.498160000	-4.085546000	C	1.004029000	4.097933000	-4.072724000
C	0.402421000	-3.861712000	-4.690281000	O	1.943811000	4.875543000	-4.227717000
C	1.233757000	-3.721101000	-5.947525000	H	0.732636000	1.094664000	-4.463095000
C	2.506517000	-4.313560000	-6.039001000	H	1.494471000	2.966322000	-5.808610000
C	0.786162000	-2.977893000	-7.050309000	H	-0.175976000	3.605903000	-5.797542000
C	3.301863000	-4.175020000	-7.175785000	N	0.233461000	4.098892000	-2.953684000
C	1.571187000	-2.829437000	-8.198177000	C	0.378606000	5.097785000	-1.892464000
C	2.836421000	-3.427247000	-8.267344000	C	1.487462000	4.665059000	-0.898015000
O	3.645278000	-3.320972000	-9.359293000	O	1.262144000	4.301939000	0.248407000
H	-1.018676000	-3.260216000	-2.628006000	C	-0.936323000	5.369890000	-1.153042000
H	1.754148000	-2.770360000	-3.408610000	C	-2.111311000	5.985855000	-1.953184000
H	0.600634000	-4.833532000	-4.206391000	C	-1.694913000	7.215252000	-2.775237000
H	-0.674715000	-3.857086000	-4.946383000	C	-2.894245000	4.976180000	-2.810122000
H	2.882603000	-4.905163000	-5.196888000	H	-0.452986000	3.359703000	-2.835655000
H	-0.198082000	-2.499420000	-7.017331000	H	0.734917000	6.014297000	-2.389923000
H	4.288024000	-4.642848000	-7.240232000	H	-1.267875000	4.437218000	-0.660268000
H	1.195958000	-2.245095000	-9.046929000	H	-0.681350000	6.055252000	-0.325601000
H	3.207938000	-2.775832000	-10.034743000	H	-2.815486000	6.341881000	-1.175983000
N	-0.917279000	-1.049436000	-4.406038000	H	-2.582762000	7.724180000	-3.192429000
C	-1.653313000	0.196595000	-4.091267000	H	-1.047355000	6.937726000	-3.627431000
C	-1.242156000	1.521983000	-4.776712000	H	-1.146153000	7.951831000	-2.158698000
O	-2.113408000	2.278947000	-5.186320000	H	-2.323602000	4.606994000	-3.678794000
C	-1.726656000	0.469527000	-2.557920000	H	-3.817413000	5.440262000	-3.203176000
S	-2.029765000	-1.015350000	-1.522455000	H	-3.199422000	4.096453000	-2.212876000

N	2.750716000	4.706899000	-1.414460000	N	-3.532986000	1.690233000	5.355814000
C	3.819761000	4.056188000	-0.693851000	H	0.951880000	0.654107000	1.649196000
C	3.472820000	2.580373000	-0.428153000	H	1.137545000	1.758379000	4.395118000
O	2.754199000	1.967308000	-1.205607000	H	-0.053357000	3.081118000	2.692675000
H	2.836255000	4.861897000	-2.423389000	H	-1.068165000	1.701768000	2.243058000
H	4.021229000	4.572323000	0.261877000	H	-1.262383000	2.909486000	5.065274000
H	4.735831000	4.105233000	-1.306358000	H	-2.138738000	3.549878000	3.678802000
N	4.000601000	2.006974000	0.697789000	H	-3.117408000	2.124071000	6.177975000
C	3.420433000	0.753491000	1.163933000	H	-4.149750000	0.900953000	5.546065000
C	2.775027000	1.004700000	2.540383000	N	-0.463116000	-0.058279000	5.464164000
O	3.444376000	1.257713000	3.533054000	C	-1.035024000	-1.241312000	6.120118000
C	4.324371000	-0.518993000	1.123409000	C	-2.450248000	-1.582854000	5.570719000
C	3.388134000	-1.675073000	0.886012000	O	-3.467323000	-1.299240000	6.194468000
N	2.612484000	-2.235623000	1.891734000	C	-1.073938000	-1.048042000	7.642527000
C	2.684581000	-1.945951000	-0.267889000	C	-1.838564000	0.194291000	8.093620000
C	1.497516000	-2.751186000	1.325736000	O	-1.582711000	1.304350000	7.623141000
N	1.469359000	-2.538564000	0.017303000	N	-2.737261000	0.022241000	9.090424000
H	4.466399000	2.594811000	1.384529000	H	-0.545429000	0.812327000	5.995536000
H	2.629805000	0.553567000	0.439545000	H	-0.370335000	-2.091578000	5.895015000
H	5.022533000	-0.423240000	0.276294000	H	-1.482639000	-1.960928000	8.102495000
H	4.920649000	-0.616144000	2.047569000	H	-0.037304000	-0.929542000	8.007461000
H	2.785698000	-2.178345000	2.889540000	H	-3.105325000	-0.898358000	9.304875000
H	2.942259000	-1.637628000	-1.276070000	H	-3.278582000	0.831319000	9.384890000
H	0.701672000	-3.208899000	1.906679000	N	-2.428061000	-2.193561000	4.367914000
N	1.419450000	0.970828000	2.503291000	C	-3.613513000	-2.435419000	3.573946000
C	0.540752000	1.250295000	3.619792000	C	-4.354237000	-3.695397000	4.057038000
C	0.016786000	-0.081839000	4.205736000	O	-3.867050000	-4.554810000	4.734255000
O	0.041182000	-1.127108000	3.538655000	C	-3.227716000	-2.545826000	2.077817000
C	-0.575167000	2.197359000	3.095281000	C	-2.362891000	-3.768879000	1.733225000
C	-1.668078000	2.630440000	4.074934000	S	-1.418263000	-3.486737000	0.156939000
C	-2.795999000	1.600465000	4.214819000	H	-1.518968000	-2.230351000	3.905813000
O	-3.037012000	0.787285000	3.330409000	H	-4.279304000	-1.561321000	3.685896000

H	-4.140657000	-2.553289000	1.459088000	N	-6.417522000	-2.492449000	4.922687000
H	-2.711070000	-1.605697000	1.822865000	H	-5.659008000	-2.906514000	5.451910000
H	-1.642472000	-3.990797000	2.541080000	H	-7.319465000	-2.364110000	5.371792000
H	-2.991353000	-4.668258000	1.612139000	N	-2.593878000	-4.271088000	0.378856000
H	-5.889974000	-3.008157000	3.103072000	H	-3.170522000	-4.068014000	-0.432638000
Cu	-0.117800000	-1.966002000	-0.836389000	C	-1.434676000	-5.062481000	-0.064469000
H	-0.481750000	-0.903246000	1.665393000	H	-1.861227000	-5.959354000	-0.554189000
H	-1.200046000	-0.311763000	0.333698000	C	-0.492763000	-5.702331000	0.982533000
H	1.331175000	-0.258849000	-2.368081000	O	0.552738000	-6.202084000	0.568484000
H	1.345126000	0.541601000	-1.050581000	C	-0.634068000	-4.284900000	-1.142435000
C	-0.659450000	-5.133068000	-0.018410000	H	-1.209155000	-4.311951000	-2.087377000
H	-0.059807000	-5.053562000	-0.939655000	H	0.302480000	-4.835790000	-1.323536000
H	-0.010743000	-5.377158000	0.841344000	S	-0.248348000	-2.561403000	-0.673258000
H	-1.439960000	-5.904876000	-0.130359000	N	-0.915958000	-5.801044000	2.264289000
				H	-1.557223000	-5.058128000	2.563151000
				C	-0.157980000	-6.465641000	3.330295000
Cu-11AA				H	-0.840583000	-6.550834000	4.188098000
O	-2.512197000	-2.390215000	-3.150948000	C	0.999244000	-5.584276000	3.857008000
O	-3.062287000	0.185852000	-2.486457000	O	0.993441000	-5.166001000	5.010613000
Cu	-1.661182000	-1.159840000	-1.662978000	C	0.268392000	-7.897096000	2.976638000
N	-3.478995000	-1.697873000	-0.527000000	H	-0.609555000	-8.417624000	2.537905000
C	-3.421734000	-1.989206000	0.919012000	H	1.068828000	-7.893320000	2.218109000
H	-2.875375000	-1.146283000	1.368973000	O	0.684582000	-8.497831000	4.186038000
C	-2.551349000	-3.206831000	1.257807000	H	1.228050000	-9.274305000	3.981508000
O	-1.994054000	-3.260468000	2.351420000	N	1.967126000	-5.278927000	2.952607000
C	-4.821662000	-2.094522000	1.564565000	H	1.820696000	-5.569411000	1.981993000
H	-5.411401000	-1.212944000	1.258298000	C	3.011018000	-4.285255000	3.224971000
H	-5.354354000	-2.973746000	1.151587000	H	3.352089000	-4.448915000	4.260834000
C	-4.833958000	-2.159913000	3.093137000	C	2.378962000	-2.870515000	3.116765000
H	-4.367989000	-3.088728000	3.462836000	O	2.478275000	-2.192160000	2.105230000
H	-4.220538000	-1.334602000	3.505741000	C	4.169769000	-4.472086000	2.244240000
C	-6.250123000	-2.007642000	3.655958000	H	4.488548000	-5.529090000	2.288774000
O	-7.154686000	-1.480488000	3.033638000				

H	3.807958000	-4.269901000	1.222901000	C	0.661522000	0.786797000	0.070905000
C	5.357906000	-3.547627000	2.546851000	H	1.233728000	-0.145475000	-0.072586000
H	5.037537000	-2.498739000	2.406189000	H	1.027535000	1.553796000	-0.629659000
H	5.705958000	-3.657095000	3.586779000	S	-1.127112000	0.459249000	-0.241621000
C	6.562593000	-3.772679000	1.660503000	N	-0.790879000	2.666199000	2.646448000
O	6.227869000	-3.887538000	0.352919000	H	-0.972131000	1.813373000	3.168068000
O	7.708358000	-3.833384000	2.031775000	C	-1.623842000	3.840814000	2.793903000
N	1.676063000	-2.500311000	4.222434000	H	-2.316007000	3.680638000	3.637179000
H	1.513261000	-3.241056000	4.909024000	H	-1.016221000	4.731560000	3.018976000
C	0.688692000	-1.427225000	4.203941000	C	-2.450170000	4.208656000	1.536733000
H	-0.191232000	-1.778607000	3.632241000	O	-2.808829000	5.360461000	1.359746000
C	1.236916000	-0.164836000	3.506499000	N	-2.725256000	3.148468000	0.722992000
O	2.204719000	0.456600000	3.903217000	H	-2.240885000	2.269131000	0.924081000
C	0.198382000	-1.138327000	5.651376000	C	-3.289965000	3.162476000	-0.618464000
H	-0.215575000	-2.104586000	6.005751000	H	-3.692673000	2.152162000	-0.786078000
C	-0.968903000	-0.128773000	5.636283000	C	-2.244606000	3.360039000	-1.740320000
H	-0.577645000	0.871717000	5.365521000	O	-2.501035000	2.979631000	-2.890944000
H	-1.676773000	-0.419261000	4.835184000	C	-4.442020000	4.161014000	-0.823579000
C	1.325140000	-0.726847000	6.611602000	H	-4.861458000	4.017681000	-1.833657000
H	0.958773000	-0.694127000	7.652680000	H	-5.234412000	3.972435000	-0.079019000
H	2.159678000	-1.447178000	6.574347000	H	-4.103763000	5.199642000	-0.703522000
H	1.735951000	0.260096000	6.344116000	N	-1.135108000	4.053345000	-1.419116000
C	-1.740364000	-0.023661000	6.956828000	H	-0.847141000	4.095490000	-0.438425000
H	-2.599849000	0.664455000	6.858838000	C	-0.241101000	4.667394000	-2.388357000
H	-2.133893000	-1.009383000	7.268663000	H	-0.860295000	5.184807000	-3.139379000
H	-1.107268000	0.356371000	7.777230000	C	0.700423000	3.676692000	-3.117770000
N	0.453903000	0.248062000	2.454317000	O	1.620317000	3.120200000	-2.541327000
H	-0.187370000	-0.432951000	2.045744000	C	0.607057000	5.688209000	-1.613637000
C	0.894123000	1.269198000	1.519348000	H	-0.062125000	6.280998000	-0.964401000
H	1.973451000	1.438598000	1.675685000	H	1.286980000	5.129357000	-0.944770000
C	0.204206000	2.628450000	1.724168000	C	1.412991000	6.635125000	-2.489527000
O	0.485118000	3.609309000	1.036047000	O	1.471549000	6.542143000	-3.712875000

N	2.068141000	7.615372000	-1.819274000	H	-3.512848000	-0.168252000	-3.273861000
H	2.035746000	7.692837000	-0.808706000	H	-1.688374000	-2.224362000	-3.664270000
H	2.632801000	8.273198000	-2.348997000	H	-2.619776000	-3.356261000	-3.086245000
N	0.480636000	3.557098000	-4.461270000	C	3.890137000	6.629358000	-6.362867000
H	-0.367581000	3.958675000	-4.847396000	O	4.554695000	5.689235000	-5.677429000
C	1.404109000	2.882251000	-5.349398000	H	5.375035000	6.102154000	-5.337684000
H	2.270392000	2.632181000	-4.712094000	H	7.065366000	-4.013464000	-0.137007000
C	1.956167000	3.802797000	-6.464536000	H	-4.171146000	-2.301570000	-0.989073000
O	2.389003000	3.333960000	-7.505311000				
C	0.839718000	1.577464000	-5.952870000				
H	-0.078018000	1.803042000	-6.522610000	Cu-<u>12AA</u>			
H	1.575756000	1.205302000	-6.684648000	symmetry c1			
C	0.521272000	0.554041000	-4.914386000	O	0.152818000	-0.977753000	0.733620000
N	1.480436000	-0.141566000	-4.196723000	O	-3.428193000	-2.472404000	3.419781000
H	2.485811000	-0.035613000	-4.286434000	N	0.763392000	-0.940849000	-1.833101000
C	-0.671422000	0.134905000	-4.379957000	C	1.181848000	-1.252793000	-3.230838000
H	-1.667068000	0.466831000	-4.663032000	C	0.483267000	-0.379208000	-4.301754000
C	0.855447000	-0.923557000	-3.285685000	O	0.266982000	-0.784024000	-5.437137000
H	1.360998000	-1.571235000	-2.568506000	C	0.977401000	-2.751014000	-3.544527000
N	-0.460599000	-0.779391000	-3.360357000	S	-0.571177000	-3.362218000	-2.793249000
N	1.947563000	5.127781000	-6.162515000	H	2.259831000	-1.015850000	-3.327786000
H	1.647602000	5.432211000	-5.232823000	H	1.852128000	-3.312153000	-3.166015000
C	2.596579000	6.113724000	-6.996468000	H	0.944103000	-2.880514000	-4.636331000
H	2.887167000	5.605289000	-7.933020000	H	1.534394000	-0.469677000	-1.348684000
O	4.304592000	7.763886000	-6.471736000	N	0.123456000	0.872769000	-3.889828000
C	1.656006000	7.289079000	-7.344158000	C	-0.590610000	1.828635000	-4.721349000
H	0.749301000	6.867881000	-7.808570000	C	-2.005887000	1.412896000	-5.174844000
H	1.351277000	7.788984000	-6.399749000	O	-2.601082000	2.156003000	-5.955158000
O	2.224456000	8.180489000	-8.264616000	C	0.229362000	2.400300000	-5.883500000
H	3.031948000	8.534458000	-7.845275000	C	1.205164000	3.467124000	-5.387011000
H	-3.857245000	-0.754640000	-0.654947000	O	0.990561000	4.141450000	-4.389897000
H	-2.828683000	1.135250000	-2.670352000	N	2.316040000	3.640498000	-6.155355000
				H	0.606419000	1.259359000	-3.075586000

H	-0.785885000	2.696439000	-4.069599000	C	-9.389682000	3.713796000	-5.663764000
H	0.737383000	1.591375000	-6.433273000	O	-10.214038000	3.982312000	-6.714539000
H	-0.476051000	2.893407000	-6.576237000	H	-4.271386000	2.415662000	-4.595564000
H	2.477792000	3.100302000	-6.997106000	H	-5.078033000	3.848240000	-3.058658000
H	2.961477000	4.386331000	-5.913254000	H	-6.947854000	1.663784000	-2.017029000
N	-2.582524000	0.326929000	-4.615814000	H	-6.915194000	3.376299000	-1.518418000
C	-3.964848000	-0.047628000	-4.947878000	H	-7.936087000	1.005339000	-4.186518000
C	-4.890491000	0.609553000	-3.896688000	H	-7.676858000	5.169910000	-3.098253000
O	-5.535726000	-0.049191000	-3.087216000	H	-9.435922000	1.603643000	-6.091879000
C	-4.166988000	-1.565936000	-5.010122000	H	-9.164810000	5.761782000	-4.988393000
C	-3.116905000	-2.307088000	-5.852068000	H	-10.368694000	4.940175000	-6.769813000
C	-3.009142000	-1.756738000	-7.273103000	N	-3.825339000	1.439581000	-1.224097000
O	-3.972905000	-1.704312000	-8.022982000	C	-3.063184000	1.142968000	-0.021998000
N	-1.764786000	-1.328957000	-7.633152000	C	-1.719504000	1.885659000	0.048571000
H	-2.120927000	-0.192476000	-3.866514000	O	-1.145898000	2.087229000	1.122986000
H	-4.168164000	0.402165000	-5.932142000	C	-2.911705000	-0.384525000	0.131769000
H	-4.167512000	-1.975379000	-3.986984000	S	-2.178641000	-1.302028000	-1.306747000
H	-5.170290000	-1.741067000	-5.433138000	H	-4.180921000	0.634074000	-1.739419000
H	-2.143550000	-2.313039000	-5.336186000	H	-3.604388000	1.526654000	0.863317000
H	-3.434387000	-3.361587000	-5.937264000	H	-3.927010000	-0.792843000	0.297743000
H	-1.009533000	-1.235279000	-6.954592000	H	-2.334470000	-0.570156000	1.044610000
H	-1.670343000	-0.891471000	-8.545214000	N	-1.206790000	2.325043000	-1.124233000
N	-4.820018000	1.970539000	-3.858817000	C	-0.159095000	3.328776000	-1.157822000
C	-5.250079000	2.809416000	-2.739371000	C	1.246335000	2.789810000	-0.845380000
C	-4.374116000	2.668906000	-1.464161000	O	1.942057000	2.257258000	-1.703692000
O	-4.180223000	3.629429000	-0.734882000	H	-1.768511000	2.157330000	-1.953458000
C	-6.754216000	2.688445000	-2.366629000	H	-0.093659000	3.747371000	-2.174203000
C	-7.687100000	3.042205000	-3.503823000	H	-0.416204000	4.142811000	-0.457358000
C	-8.199708000	2.053111000	-4.362313000	N	1.672414000	3.011951000	0.427986000
C	-8.050545000	4.373999000	-3.752720000	C	3.030971000	2.782205000	0.861855000
C	-9.039485000	2.376484000	-5.427952000	C	3.466137000	1.315377000	0.669246000
C	-8.890381000	4.713772000	-4.817471000	O	2.672948000	0.381444000	0.563786000

C	3.232538000	3.186132000	2.341953000	H	3.608793000	-0.854823000	1.879033000
C	3.057453000	4.676458000	2.728335000	H	2.947322000	-2.670180000	2.871790000
C	3.936205000	5.613677000	1.887101000	H	5.231404000	-3.963399000	1.326476000
C	1.598760000	5.164323000	2.770606000	H	4.102406000	-4.870471000	2.351858000
H	0.945900000	3.166923000	1.122862000	H	3.162011000	-5.870357000	-0.190084000
H	3.697475000	3.387714000	0.220875000	H	2.220037000	-1.899419000	0.807607000
H	2.571161000	2.551944000	2.959203000	H	1.093911000	-5.144184000	-1.565749000
H	4.262205000	2.894945000	2.615011000	N	4.728694000	-1.897199000	4.856632000
H	3.431879000	4.725372000	3.769163000	C	4.633713000	-1.904120000	6.305539000
H	3.903999000	6.642675000	2.287369000	C	3.169148000	-1.849876000	6.809571000
H	3.593531000	5.662172000	0.836745000	O	2.907181000	-2.069968000	7.979646000
H	4.994673000	5.291585000	1.887920000	C	5.456235000	-0.734822000	6.887574000
H	1.180530000	5.318400000	1.760492000	C	5.694877000	-0.801915000	8.395960000
H	1.535488000	6.133641000	3.296897000	C	6.311447000	0.491936000	8.930739000
H	0.949392000	4.450353000	3.310441000	O	6.277278000	1.544885000	8.317657000
N	4.809960000	1.118214000	0.673349000	N	6.891125000	0.382897000	10.163602000
C	5.467244000	-0.137617000	0.330365000	H	4.745302000	-1.010657000	4.359788000
C	5.536732000	-1.262943000	1.384231000	H	5.038010000	-2.864984000	6.658104000
O	6.519247000	-1.976329000	1.450806000	H	6.427112000	-0.724091000	6.361529000
H	5.407549000	1.933190000	0.763048000	H	4.966507000	0.226744000	6.650360000
H	4.957202000	-0.576697000	-0.547705000	H	4.738114000	-0.972773000	8.921436000
H	6.504734000	0.080864000	0.041915000	H	6.340330000	-1.663650000	8.648563000
N	4.394717000	-1.459951000	2.117847000	H	6.867158000	-0.476623000	10.699832000
C	4.032290000	-2.759993000	2.688091000	H	7.248266000	1.226478000	10.601975000
C	4.529545000	-3.026815000	4.119445000	N	2.213731000	-1.494140000	5.883140000
O	4.535583000	-4.152087000	4.585647000	C	0.917076000	-0.996641000	6.317207000
C	4.207881000	-3.959593000	1.738035000	C	-0.330665000	-1.760659000	5.835748000
C	3.147646000	-3.907010000	0.677823000	O	-1.430445000	-1.409124000	6.236870000
N	2.732149000	-4.953304000	-0.129081000	C	0.732109000	0.492212000	5.925747000
C	2.266734000	-2.892937000	0.391181000	C	0.735568000	0.713065000	4.410153000
C	1.638265000	-4.545196000	-0.833099000	O	1.640090000	0.249829000	3.702834000
N	1.323031000	-3.298969000	-0.520159000	N	-0.269036000	1.466843000	3.918126000

H	2.520895000	-1.133870000	4.979894000
H	0.904139000	-1.070401000	7.415644000
H	-0.200613000	0.854457000	6.382302000
H	1.569707000	1.071838000	6.354322000
H	-1.072460000	1.670572000	4.503827000
H	-0.430710000	1.535575000	2.906212000
N	-0.186631000	-2.755454000	4.915916000
C	-1.384922000	-3.301966000	4.300337000
C	-2.133332000	-2.187686000	3.559531000
O	-1.618271000	-1.176329000	3.134316000
C	-1.112989000	-4.510800000	3.376260000
C	-0.368016000	-4.234836000	2.059857000
S	-1.318087000	-3.359085000	0.726019000
C	-2.223736000	-4.748185000	-0.014229000
H	0.740122000	-3.006128000	4.589117000
H	-2.060902000	-3.641154000	5.101624000
H	-0.533224000	-5.244554000	3.969166000
H	-2.085026000	-4.987461000	3.163809000
H	0.510755000	-3.590645000	2.230678000
H	0.010671000	-5.183366000	1.642415000
H	-2.857586000	-4.296298000	-0.792913000
H	-1.529313000	-5.462541000	-0.486878000
H	-2.857228000	-5.250665000	0.735798000
H	-3.833545000	-1.783771000	2.853620000
Cu	-0.218046000	-2.285844000	-0.879904000
H	0.843630000	-0.281430000	0.803499000
H	-0.376818000	-0.918914000	1.557040000
H	-0.015470000	-0.274266000	-1.842833000