SUPPORTING INFORMATION

Azide-mediated unusual *in situ* transformation of Mannich base to Schiff-Mannich base and isolation of their Cu(II) complexes: crystal structure, theoretical inspection and anticancer activities

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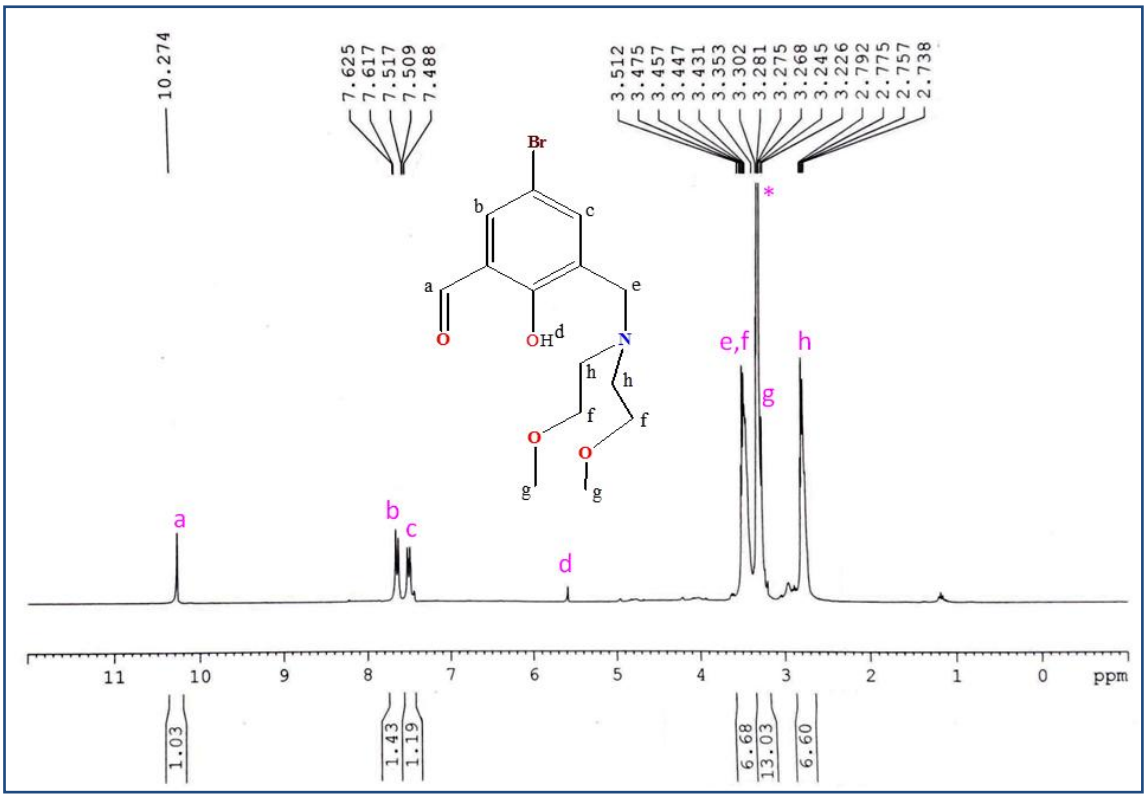

Fig. S1 ^{1}H-NMR spectrum of ligand HL[1] in $CDCl_3$.

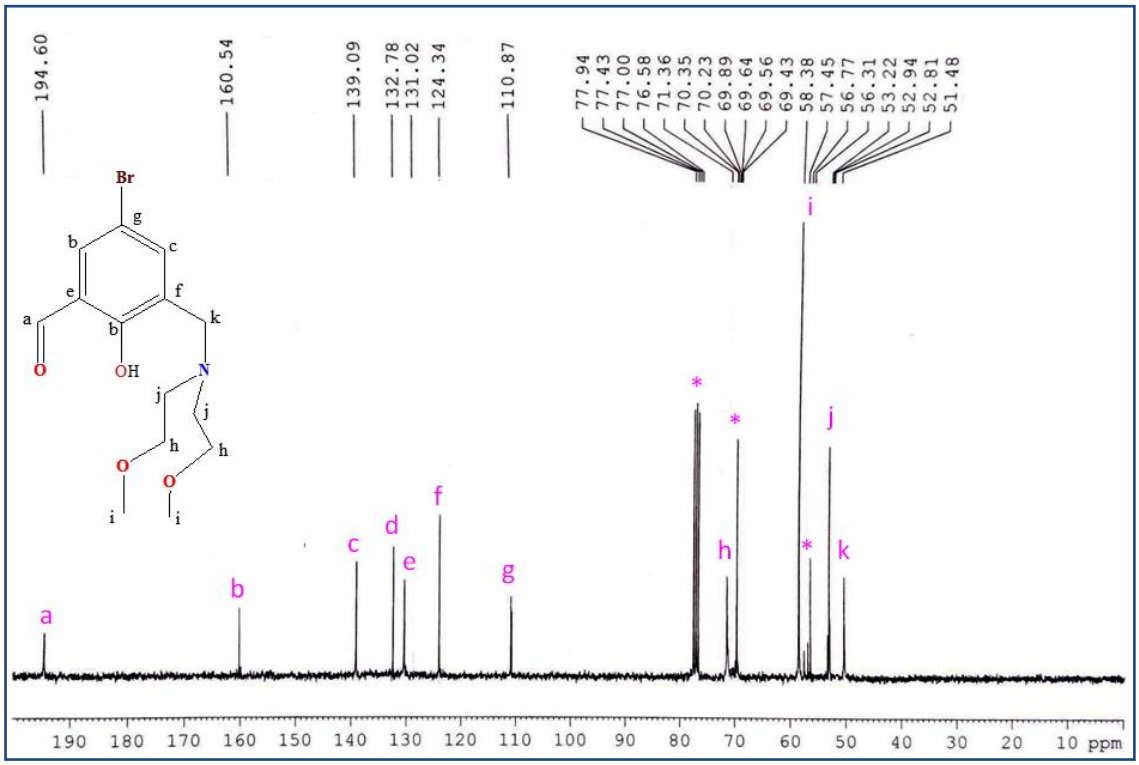

Fig. S2 ^{13}C-NMR spectrum of ligand HL[1] in DMSO-d_6.

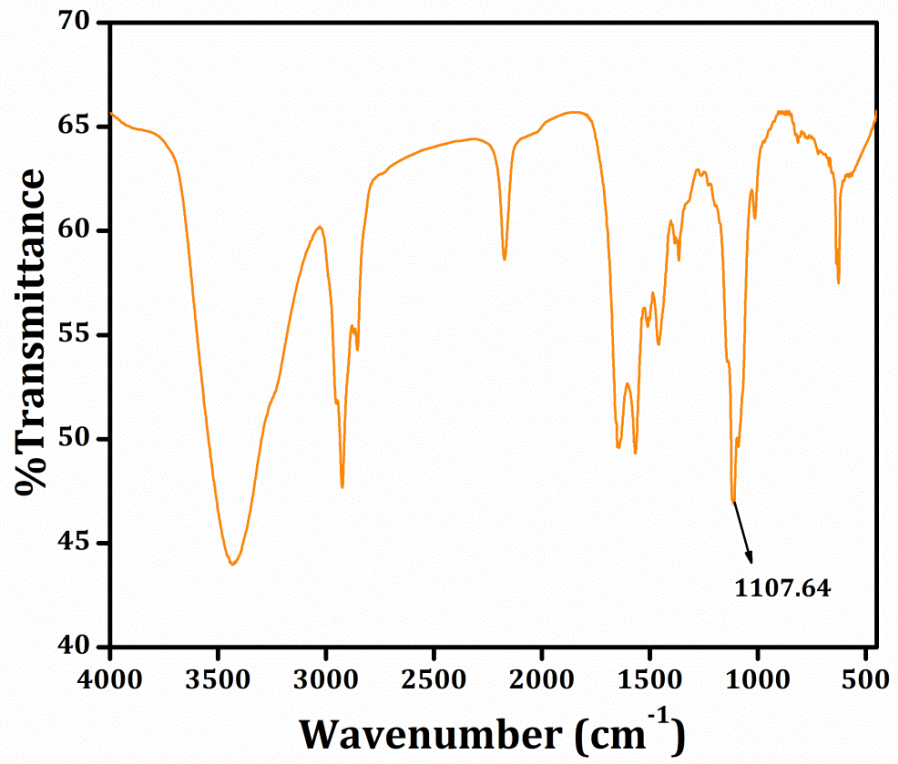

Fig. S3 FT-IR spectrum of ligand HL^1.

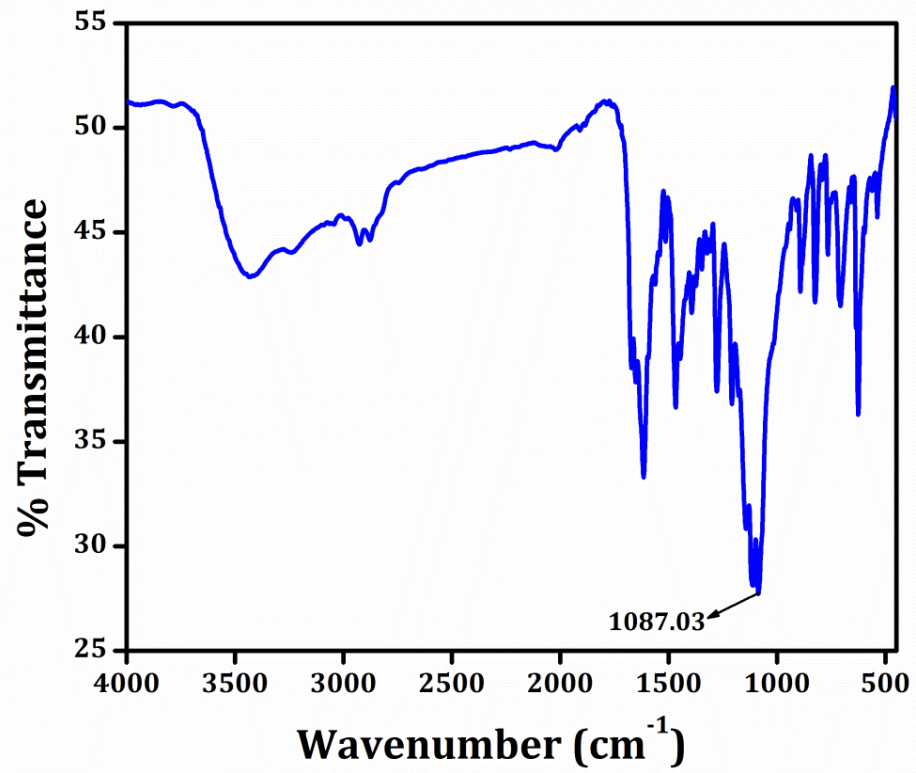

Fig. S4 FT-IR spectrum of complex **1**.

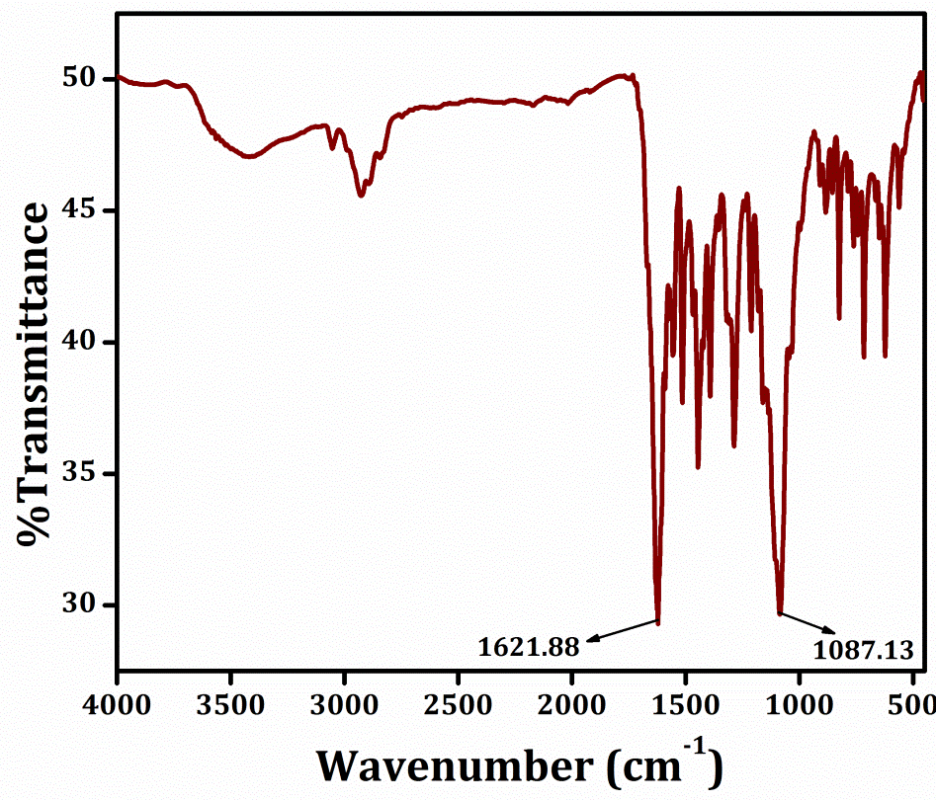

Fig. S5 FT-IR spectrum of complex **2**.

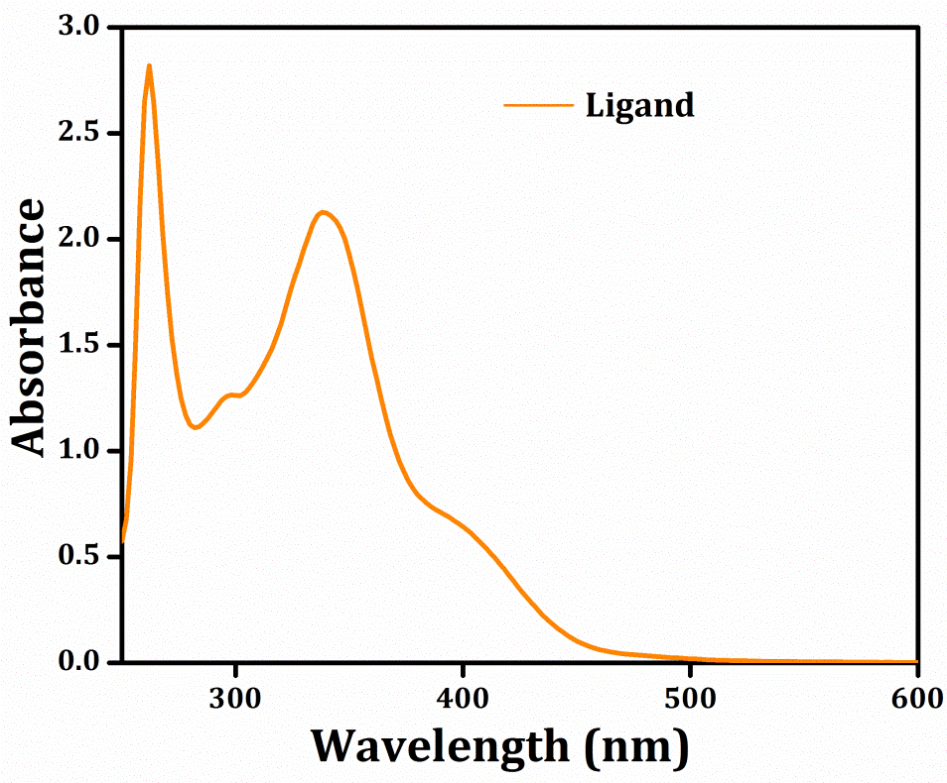

Fig. S6 UV-visible spectral plot of ligand HL^1.

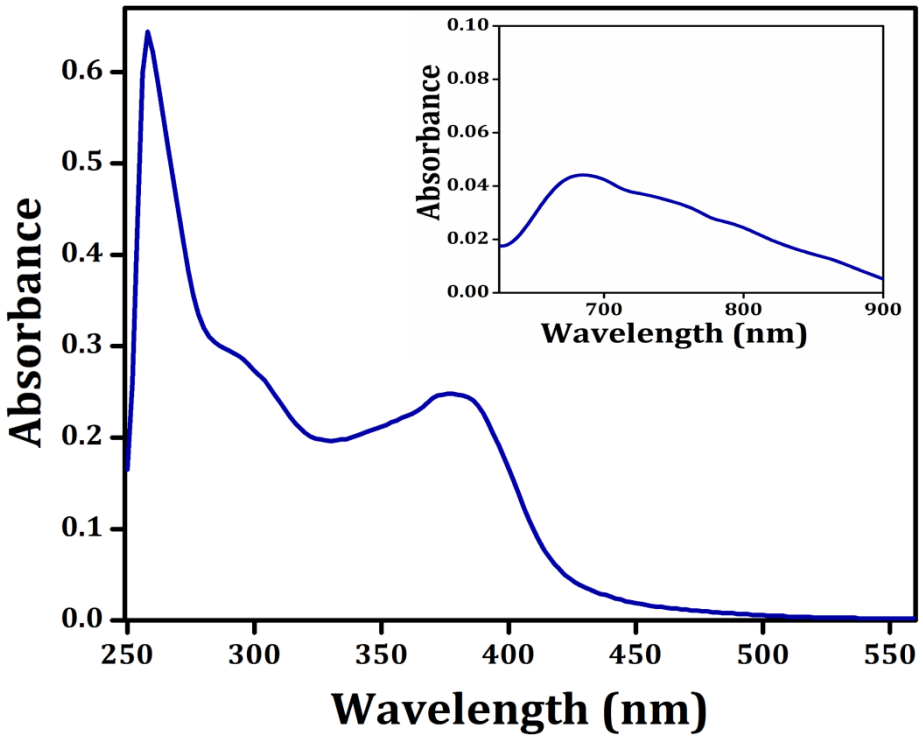

Fig. S7 UV-visible spectral plot of complex **1** solution [5×10^{-5} (M)]. Inset shows the d-d transition for [5×10^{-3} (M)] solution.

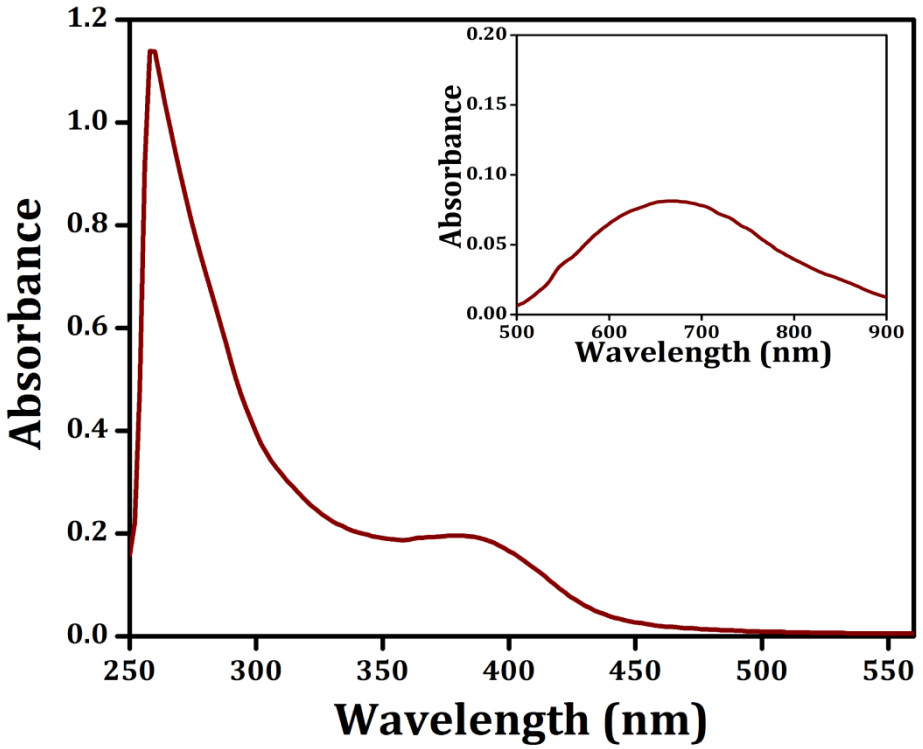

Fig. S8 UV-visible spectral plot of complex **2** solution [5×10^{-5} (M)]. Inset shows the d-d transition for [5×10^{-3} (M)] solution.

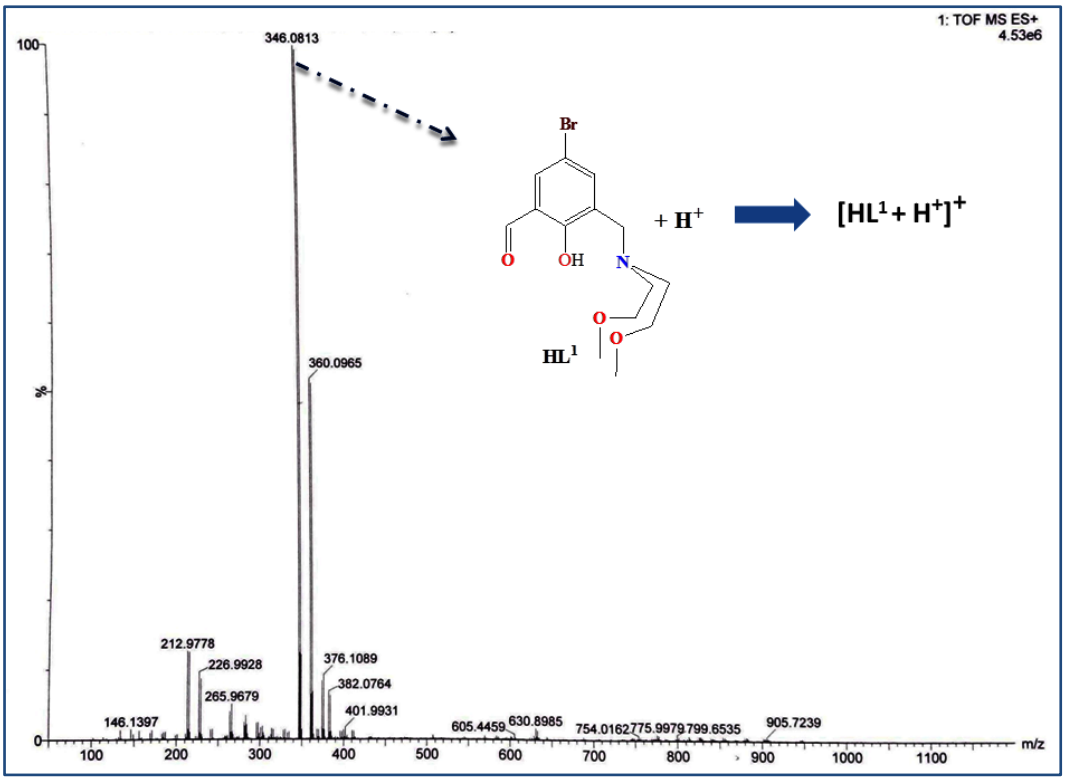

Fig. S9 ESI-MS spectrum of ligand HL^1.

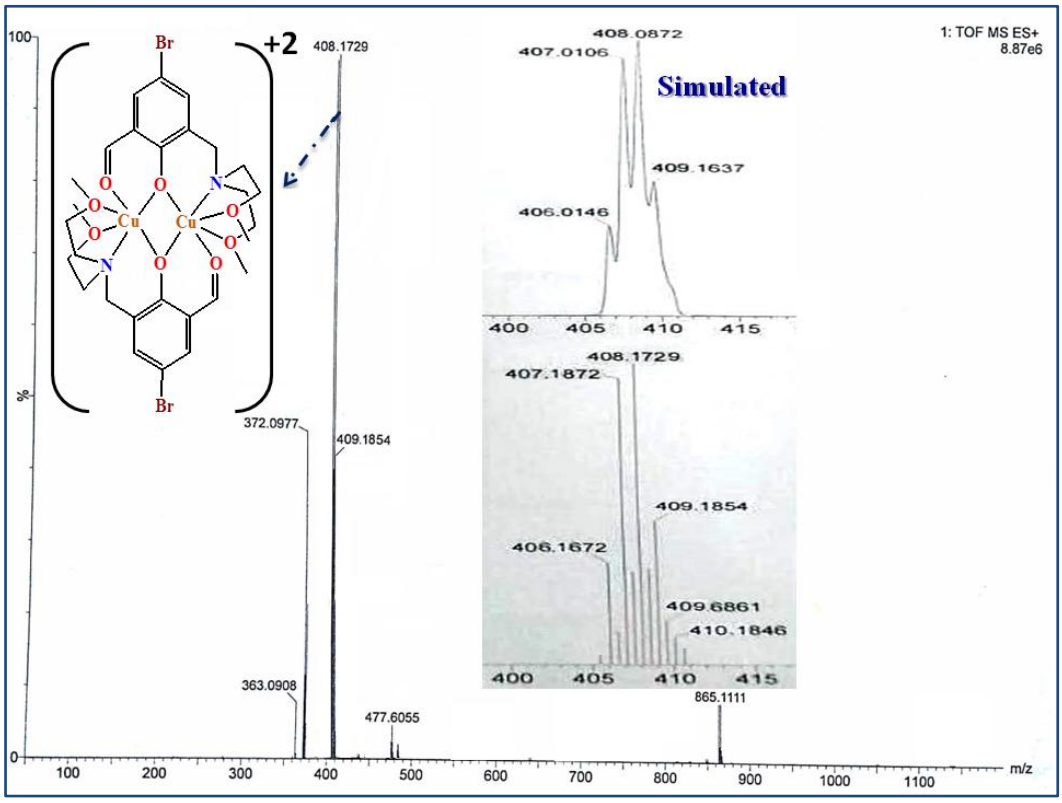

Fig. S10 ESI-MS spectrum of complex **1**.

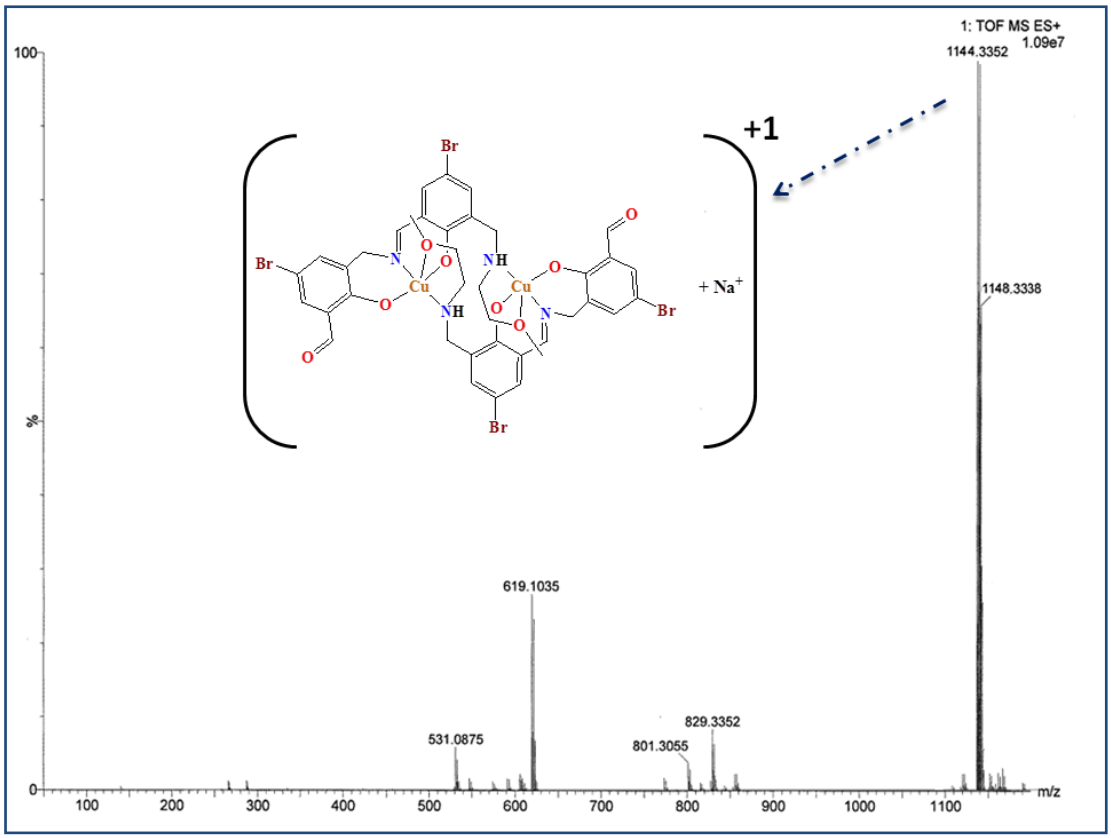

Fig. S11 ESI-MS spectrum of complex **2**.

Table S1: Coordination bond lengths (Å) and angles (°) for complex **1**.

Bond distances			
Cu1-O1	1.964(4)	Cu2-O1	1.923(4)
Cu1-O3	2.335(5)	Cu2-O2	1.979(5)
Cu1-O4	2.252(5)	Cu2-O5	1.956(4)
Cu1-O5	1.915(4)	Cu2-O7	2.425(5)
Cu1-O6	1.984(5)	Cu2-O8	2.223(6)
Cu1-N1	1.999(5)	Cu2-N2	1.986(6)
Bond Angles			
O1-Cu1-O3	93.97(19)	O1-Cu2-O2	91.80(19)
O1-Cu1-O4	105.71(19)	O1-Cu2-O5	78.29(17)
O1-Cu1-O5	78.29(17)	O1-Cu2-O7	108.98(19)
O1-Cu1-O6	167.20(19)	O1-Cu2-O8	96.7(2)
O1-Cu1-N1	94.7(2)	O1-Cu2-N2	170.2(2)
O3-Cu1-O4	150.9(2)	O2-Cu2-O5	166.9(2)
O3-Cu1-O5	106.04(19)	O2-Cu2-O7	78.61(19)

O3-Cu1-O6	81.5(2)	O2-Cu2-O8	81.4(2)
O3-Cu1-N1	79.8(2)	O2-Cu2-N2	95.9(2)
O4-Cu1-O5	98.9(2)	O5-Cu2-O7	96.37(19)
O4-Cu1-O6	83.1(2)	O5-Cu2-O8	108.1(2)
O4-Cu1-N1	77.4(2)	O5-Cu2-N2	95.0(2)
O5-Cu1-O6	91.37(18)	O7-Cu2-O8	147.6(2)
O5-Cu1-N1	171.0(2)	O7-Cu2-N2	78.6(2)
O6-Cu1-N1	96.3(2)	O8-Cu2-N2	78.5(3)

Table S2: Hydrogen bonding parameters of complex **1**.

D-H····A	**D-H(Å)**	**H····A(Å)**	**D····A(Å)**	**<D-H····A (°)**	**Symmetry code**
O9-H9c…O10	0.85	2.13	2.93(2)	157	-
O9-H9c...O13b	0.85	2.01	2.78(3)	150	-
O9-H9d...O16	0.85	2.28	3.033(14)	148	-
C6-H6...O12b	0.93	2.51	3.34(2)	149	x,3/2-y,-1/2+z
C8-H8a...O4	0.97	2.56	3.090(9)	114	-
C9-H9b...O18	0.97	2.54	3.49(3)	167	-
C9-H9b...O19	0.97	2.44	3.34(6)	153	-
C11-H11b…O6	0.97	2.43	2.953(9)	113	-
C13-H13b…O12b	0.96	2.50	3.32(3)	143	2-x,-1/2+y,3/2-z
C20-H20...O17	0.93	2.54	3.316(12)	141	1-x,1-y,2-z
C22-H22A...O8	0.97	2.55	3.079(10)	114	-
C24-H24b...O2	0.97	2.54	3.025(10)	111	-
C25-H25a...O9	0.97	2.31	3.261(14)	166	1-x,1-y,2-z
C25-H25b…O2	0.97	2.45	2.929(11)	110	-
C28-H28a...Br1	0.96	2.81	3.558(11)	135	1-x,1-y,1-z
C28-H28c...O13	0.96	2.59	3.49(2)	155	1-x,-1/2+y,3/2-z

Table S3: Coordination bond lengths (Å) and angles (°) for complex **2**.

Bond Distances		**Bond Angles**			
Cu1-O1	1.918(7)	O1-Cu1-O2	161.6(3)	O2-Cu1-O4'	100.0(3)
Cu1-O2	1.924(7)	O1-Cu1-N1	92.1(3)	O2-Cu1-N2'	90.5(3)
Cu1-O4'	2.413(8)	O1-Cu1-O4	97.2(3)	O4'-Cu1-N1	90.9(3)
Cu1-N1	1.952(8)	O1-Cu1-N2'	86.3(3)	O4'-Cu1-N2'	78.7(3)
Cu1-N2'	2.019(8)	O2-Cu1-N1	94.3(3)	N1-Cu1-N2'	169.1(3)

Primed atoms at -x+1/2,-y+3/2,-z+1.

Table S4: Hydrogen bonding parameters of complex **2**.

D-H····A	**D-H(Å)**	**H····A(Å)**	**D····A(Å)**	**<D-H····A (°)**	**Symmetry code**
N2-H2...O1	0.98	2.20	2.898(11)	127	-
C7-H7...O3	0.93	2.57	3.249(15)	130	1/2-x,-1/2+y,1/2-z
C15-H15...O2	0.93	2.47	2.811(17)	102	-
C16-H16b...Br1	0.97	2.89	3.614(10)	132	1-x,1-y,1-z

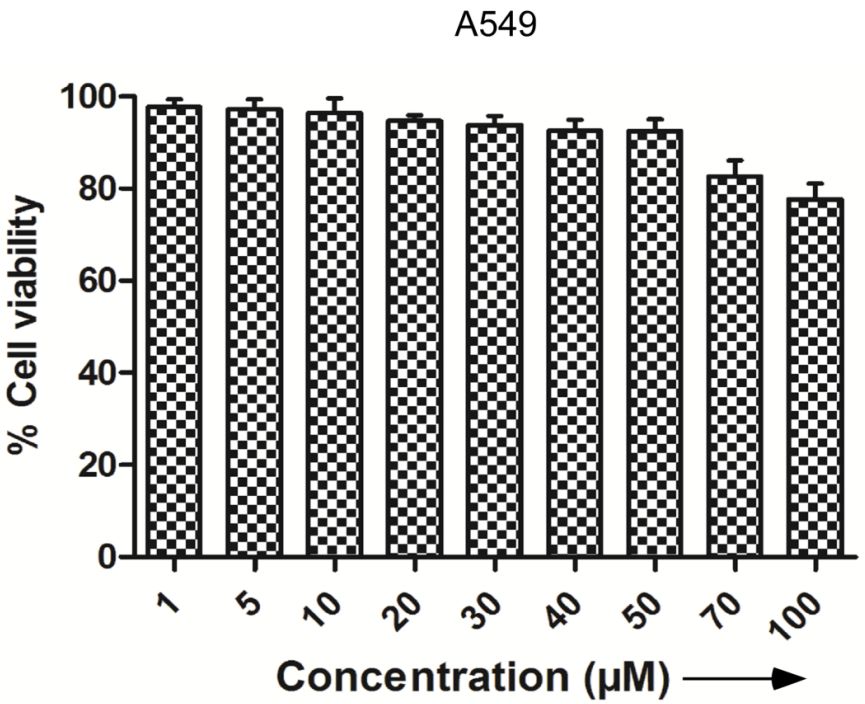

Fig. S12 Anti-proliferative activity of ligand HL^1 on A549 cell line. At 70 µM concentration HL^1 inhibits the cell viability by 17% and at the highest dose of 100 µM the cell viability was prevented by 22%.

Table S5: Theoretical calculations.

XYZ Coordinates of the Optimized Structures

L1

Charge = 0, Multiplicity = 1

C	2.970825000	-0.845522000	0.380639000	C	-1.234781000	1.232138000	-0.887934000
C	1.663404000	-1.185563000	-0.083343000	H	-0.652167000	1.583888000	-1.760439000
C	1.143113000	-0.589597000	-1.266549000	H	-2.252596000	1.642409000	-1.009573000
C	1.950783000	0.314619000	-1.970210000	C	-3.442162000	-0.597700000	0.337988000
C	3.250919000	0.657200000	-1.533515000	H	-2.902076000	-1.056854000	1.192743000
C	3.746244000	0.083516000	-0.366032000	H	-3.554169000	0.484660000	0.563275000
H	1.551148000	0.768695000	-2.881943000	C	-0.615501000	1.817800000	0.392787000
H	3.852895000	1.367781000	-2.104792000	H	-1.215319000	1.508149000	1.275445000
H	4.741988000	0.327571000	0.011765000	H	0.410542000	1.421403000	0.535403000
O	0.833262000	-2.081149000	0.542837000	C	-0.003935000	3.890189000	1.394211000
C	-0.279529000	-0.898916000	-1.711830000	H	-0.027571000	4.973896000	1.200768000
H	-0.400582000	-0.598233000	-2.776951000	H	-0.565466000	3.677620000	2.327927000
H	-0.450367000	-1.985692000	-1.656079000	H	1.049089000	3.572351000	1.543871000
C	3.542325000	-1.407895000	1.617736000	C	-5.571209000	-1.060305000	1.299657000
H	2.887525000	-2.113474000	2.194911000	H	-6.526824000	-1.552735000	1.062128000
O	4.669791000	-1.151527000	2.059422000	H	-5.128922000	-1.542021000	2.196413000
N	-1.277761000	-0.248607000	-0.829544000	H	-5.763477000	0.006466000	1.538617000
C	-2.632109000	-0.814900000	-0.952796000	O	-0.596193000	3.247868000	0.258521000
H	-3.201716000	-0.401250000	-1.815752000	O	-4.729352000	-1.204374000	0.148443000
H	-2.543989000	-1.901444000	-1.115550000	H	1.286014000	-2.499863000	1.305992000

TS1

Charge = -1, Multiplicity = 1

C	3.299122000	-0.732898000	0.303009000	H	5.062026000	0.369630000	-0.276033000
C	1.959982000	-1.203370000	-0.060660000	O	1.201045000	-1.875578000	0.739481000
C	1.494886000	-0.831246000	-1.401694000	C	0.124617000	-1.322965000	-1.830194000
C	2.288396000	-0.058807000	-2.245872000	H	-0.147259000	-0.928669000	-2.824371000
C	3.586591000	0.386922000	-1.865441000	H	0.120934000	-2.432574000	-1.902966000
C	4.070007000	0.043154000	-0.606932000	C	3.840859000	-1.059350000	1.614581000
H	1.900673000	0.211969000	-3.236112000	H	3.154967000	-1.671278000	2.251219000
H	4.184411000	0.988743000	-2.555763000	O	4.963472000	-0.721117000	2.055920000

N	-0.925487000	-0.906255000	-0.854474000
C	-2.258803000	-1.470074000	-1.140797000
H	-2.683994000	-0.951773000	-2.018962000
H	-2.188787000	-2.546716000	-1.400997000
C	-1.000300000	1.352376000	-0.727496000
H	-2.070275000	1.225236000	-0.839905000
C	-3.209947000	-1.325023000	0.057783000
H	-2.774135000	-1.818164000	0.953228000
H	-3.364249000	-0.261924000	0.324772000
C	-0.379972000	1.371655000	0.649176000
H	0.621700000	0.909878000	0.598672000
H	-0.237646000	2.405782000	1.028414000
C	-0.555766000	0.317998000	2.779063000
H	-1.293413000	-0.192158000	3.417397000
H	0.292400000	-0.363255000	2.575905000
H	-0.186504000	1.221554000	3.306525000
C	-5.430108000	-1.869520000	0.719759000
H	-6.336284000	-2.367759000	0.342290000
H	-5.093417000	-2.382476000	1.644591000
H	-5.674408000	-0.817669000	0.975817000
O	-1.239374000	0.654620000	1.557859000
O	-4.446610000	-1.948864000	-0.320458000
H	-0.366746000	1.326435000	-1.605835000
N	-1.329453000	3.366453000	-1.205613000
N	-1.274090000	4.062601000	-0.210170000
N	-1.205940000	4.738770000	0.762378000
H	-0.580843000	-1.221401000	0.069133000

L2

Charge = -1, Multiplicity = 1

C	3.092058000	0.282147000	-0.148854000
C	1.777014000	0.527365000	0.475119000
C	0.903527000	-0.656900000	0.585301000
C	1.327359000	-1.901456000	0.128830000
C	2.605631000	-2.105259000	-0.471529000
C	3.460623000	-1.016379000	-0.601905000
H	0.650026000	-2.759888000	0.235607000
H	2.898926000	-3.101058000	-0.817515000
H	4.451568000	-1.128641000	-1.057404000
O	1.409877000	1.673266000	0.906469000
C	-0.484924000	-0.481471000	1.166955000
H	-0.779503000	-1.391864000	1.740031000
H	-0.480078000	0.370282000	1.867942000
C	4.021554000	1.386601000	-0.302734000
H	3.632740000	2.361701000	0.085071000
O	5.168627000	1.333804000	-0.812114000
N	-1.478722000	-0.164239000	0.097613000
C	-2.860564000	-0.135283000	0.613925000
H	-3.178843000	-1.089897000	1.095118000
H	-2.924217000	0.646740000	1.392063000
C	-3.847834000	0.205510000	-0.511608000
H	-3.592231000	1.190097000	-0.956975000
H	-3.783127000	-0.550978000	-1.325575000
C	-6.170301000	0.533949000	-0.927516000
H	-7.141125000	0.525517000	-0.408070000
H	-6.010251000	1.535652000	-1.378360000
H	-6.192760000	-0.214432000	-1.747306000
O	-5.170152000	0.223204000	0.050289000
H	-1.411751000	-0.918702000	-0.600968000

P1

Charge = 0, Multiplicity = 1

C	0.274629000	0.970572000	-0.239551000
H	-0.038727000	1.989244000	0.026662000

H	0.351813000	0.904091000	-1.338487000
C	-0.756554000	-0.047995000	0.283061000
H	-0.436381000	-1.081126000	0.027970000
H	-0.828088000	0.017750000	1.388793000
C	-3.060563000	-0.607636000	0.065867000
H	-3.968636000	-0.278776000	-0.461533000
H	-2.842813000	-1.660597000	-0.206252000
H	-3.236523000	-0.557306000	1.159728000
O	-2.002980000	0.274695000	-0.342007000
N	1.612827000	0.783306000	0.402618000
N	2.274142000	-0.204458000	0.028622000
N	3.009907000	-1.067489000	-0.219395000

L2H

Charge = 0, Multiplicity = 1

C	2.991566000	0.357749000	-0.112886000
C	1.685038000	0.346387000	0.466151000
C	0.923744000	-0.854840000	0.497077000
C	1.486468000	-2.018014000	-0.048484000
C	2.778839000	-2.029433000	-0.621178000
C	3.516515000	-0.849157000	-0.650696000
H	0.899691000	-2.941647000	-0.021425000
H	3.188754000	-2.953943000	-1.034722000
H	4.517656000	-0.812909000	-1.086864000
O	1.082737000	1.444997000	1.027920000
C	-0.486346000	-0.864641000	1.064137000
H	-0.745026000	-1.899228000	1.382446000
H	-0.539896000	-0.227855000	1.963096000
C	3.813991000	1.579006000	-0.188674000
H	3.356622000	2.517104000	0.224548000
O	4.950635000	1.640264000	-0.675048000
N	-1.444055000	-0.313751000	0.070452000
C	-2.837185000	-0.347079000	0.559601000
H	-3.194857000	-1.369815000	0.818266000
H	-2.894012000	0.254655000	1.484124000
C	-3.781094000	0.263315000	-0.486775000
H	-3.475002000	1.307070000	-0.709898000
H	-3.724671000	-0.308167000	-1.440116000
C	-6.077973000	0.772676000	-0.856943000
H	-7.059184000	0.697873000	-0.363340000
H	-5.866995000	1.838561000	-1.083300000
H	-6.111955000	0.214801000	-1.815977000
O	-5.112942000	0.219096000	0.046995000
H	1.694480000	2.211902000	1.035212000
H	-1.382035000	-0.902813000	-0.772133000

TS2

Charge = -1, Multiplicity = 1

C	-3.691586000	-0.435094000	-0.139768000
C	-2.247110000	-0.660751000	-0.008323000
C	-1.517361000	0.338613000	0.784021000
C	-2.170702000	1.434302000	1.339494000
C	-3.574316000	1.632423000	1.187105000
C	-4.307597000	0.700043000	0.459598000
H	-1.588503000	2.163025000	1.918297000
H	-4.058431000	2.502376000	1.640456000
H	-5.388490000	0.817143000	0.322338000
O	-1.628306000	-1.653440000	-0.546101000
C	-0.028135000	0.108412000	0.968084000
H	0.428003000	0.903479000	1.580344000
H	0.153080000	-0.856021000	1.476229000
C	-4.495699000	-1.377616000	-0.901556000
H	-3.911148000	-2.227760000	-1.334014000
O	-5.731873000	-1.308311000	-1.099817000
N	0.710498000	0.026798000	-0.328441000
C	2.872673000	-0.325173000	-0.234321000
H	2.762158000	-0.663076000	-1.258814000
C	3.157700000	1.140023000	0.040053000

H	2.627262000	1.465492000	0.958324000
H	4.239910000	1.287562000	0.214198000
C	2.971879000	3.315960000	-0.913210000
H	2.617281000	3.820284000	-1.824483000
H	2.419707000	3.715744000	-0.038170000
H	4.050920000	3.531160000	-0.774149000
O	2.729709000	1.912785000	-1.097805000
H	2.633188000	-1.004822000	0.578648000
N	4.815697000	-0.997366000	-0.287293000
N	4.872068000	-2.041992000	0.340281000
N	4.938763000	-3.054795000	0.950832000
H	0.631177000	0.905835000	-0.854983000
H	0.249973000	-0.724064000	-0.869148000

L3

Charge = -1, Multiplicity = 1

C	1.245126000	-0.085573000	-0.021293000
C	-0.124276000	-0.594116000	-0.195070000
C	-1.185664000	0.425944000	-0.230217000
C	-0.879977000	1.774947000	-0.086576000
C	0.458615000	2.240517000	0.090962000
C	1.492142000	1.311624000	0.118153000
H	-1.696893000	2.508753000	-0.115976000
H	0.657983000	3.311181000	0.199296000
H	2.532897000	1.629066000	0.249846000
O	-0.408082000	-1.841908000	-0.310470000
C	-2.613586000	-0.066010000	-0.410595000
H	-3.303805000	0.789999000	-0.521036000
H	-2.684503000	-0.666762000	-1.336238000
C	2.353957000	-1.021805000	0.015239000
H	2.046415000	-2.091962000	-0.098706000
O	3.568755000	-0.736981000	0.158314000
N	-3.127736000	-0.944661000	0.692343000
H	-2.977130000	-0.432488000	1.575457000
H	-2.444212000	-1.717222000	0.734595000

Complex 1

Charge = 1 Multiplicity = 2

C	2.981604000	-0.389694000	-0.365484000
C	1.663373000	0.093045000	-0.691275000
C	1.359610000	1.484486000	-0.459612000
C	2.348818000	2.321734000	0.072038000
C	3.650571000	1.847176000	0.359370000
C	3.956477000	0.501202000	0.136450000
H	2.106277000	3.371567000	0.261176000
H	4.403836000	2.530779000	0.756872000
H	4.950289000	0.102618000	0.355259000
O	0.758266000	-0.743277000	-1.184629000
C	-0.016103000	2.022193000	-0.805525000
H	-0.062741000	3.105526000	-0.596347000
H	-0.219994000	1.866365000	-1.876520000
C	3.304653000	-1.821029000	-0.547327000
H	2.461854000	-2.450840000	-0.916566000
O	4.409735000	-2.322778000	-0.299150000
N	-1.149417000	1.326264000	-0.071024000
C	-2.485226000	1.727230000	-0.631211000
H	-2.800496000	2.711877000	-0.241672000
H	-2.358749000	1.808713000	-1.720291000
C	-1.022557000	1.419767000	1.422061000
H	0.037275000	1.598691000	1.643304000
H	-1.597529000	2.281228000	1.804367000
C	-3.576356000	0.689710000	-0.337452000
H	-3.867183000	0.671938000	0.724311000
H	-4.472034000	0.902110000	-0.943136000

C	-1.475891000	0.133771000	2.163077000	C	-3.914563000	-1.742234000	-0.330778000
H	-1.216477000	0.230915000	3.230661000	H	-3.427786000	-2.647182000	-0.714684000
H	-2.557571000	-0.027104000	2.086399000	H	-4.004041000	-1.789085000	0.766869000
C	0.453841000	-1.365779000	2.118444000	H	-4.905159000	-1.613379000	-0.793837000
H	0.802982000	-2.237343000	1.550421000	O	-0.877919000	-1.066363000	1.607512000
H	1.148942000	-0.525674000	1.956917000	O	-3.052762000	-0.627276000	-0.717633000
H	0.393206000	-1.604062000	3.193029000	Cu	-1.035760000	-0.724945000	-0.617063000

TS3

Charge = 0 Multiplicity = 2

C	3.228220000	-0.306004000	0.299406000	C	-3.150070000	-1.183033000	-0.992139000
C	2.006912000	-0.737099000	-0.331586000	H	-3.411840000	-0.251486000	-0.464284000
C	1.618424000	-0.102260000	-1.568620000	H	-4.059391000	-1.634137000	-1.421220000
C	2.427423000	0.907526000	-2.105514000	C	-0.570400000	1.458871000	0.678875000
C	3.633314000	1.317791000	-1.486833000	H	0.508673000	1.237726000	0.622143000
C	4.023299000	0.706846000	-0.296747000	H	-0.699460000	2.361755000	1.305256000
H	2.115679000	1.389066000	-3.038374000	C	-0.927043000	0.308042000	2.762374000
H	4.241146000	2.104816000	-1.939934000	H	-1.486187000	-0.543799000	3.173005000
H	4.942530000	0.998819000	0.218742000	H	0.157105000	0.138687000	2.897284000
O	1.273898000	-1.698577000	0.232112000	H	-1.226840000	1.238728000	3.276227000
C	0.349078000	-0.541855000	-2.284286000	C	-3.397498000	-2.257231000	1.185570000
H	0.202003000	0.079920000	-3.189841000	H	-2.872338000	-2.972764000	1.831334000
H	0.445716000	-1.590953000	-2.636718000	H	-3.494633000	-1.282325000	1.691804000
C	3.640170000	-0.897061000	1.582281000	H	-4.389995000	-2.648822000	0.909657000
H	2.936067000	-1.658758000	1.994806000	O	-1.265433000	0.367263000	1.352747000
O	4.675618000	-0.599058000	2.202537000	O	-2.576808000	-2.116784000	-0.011841000
N	-0.847645000	-0.440054000	-1.421268000	Cu	-0.615653000	-1.564046000	0.213228000
C	-2.077917000	-0.941764000	-2.061746000	H	-0.475156000	1.909121000	-1.528901000
H	-2.462936000	-0.213518000	-2.803654000	N	-1.613121000	3.730421000	-0.744768000
H	-1.878297000	-1.887586000	-2.603812000	N	-1.818423000	4.110687000	0.392628000
C	-1.134678000	1.664820000	-0.706041000	N	-1.995541000	4.466305000	1.510898000
H	-2.188405000	1.503069000	-0.893977000				

P2

Charge = 0 Multiplicity = 2

C	3.177400000	-0.335530000	-0.162831000	C	1.960660000	1.820108000	-0.085947000
C	1.986463000	0.425974000	-0.462893000	C	3.064236000	2.379043000	0.565811000

C	4.231190000	1.626167000	0.858075000
C	4.277696000	0.284482000	0.489365000
H	3.027113000	3.436948000	0.849211000
H	5.076509000	2.099771000	1.364359000
H	5.157938000	-0.331916000	0.694478000
O	0.954905000	-0.150797000	-1.068930000
C	0.742981000	2.656832000	-0.440622000
H	0.900175000	3.697597000	-0.087908000
H	0.640779000	2.723778000	-1.551069000
C	3.260288000	-1.753171000	-0.530374000
H	2.361841000	-2.151852000	-1.059878000
O	4.229223000	-2.501320000	-0.300191000
N	-0.496617000	2.126684000	0.155892000
C	-1.665287000	2.935195000	-0.211075000
H	-1.607279000	3.946287000	0.245315000
H	-1.742532000	3.089212000	-1.312896000
C	-0.124144000	-2.647397000	0.843778000
H	0.518993000	-1.754077000	0.893861000
C	-2.931685000	2.238885000	0.289809000
H	-2.911338000	2.133120000	1.389598000
H	-3.848489000	2.772022000	-0.015919000
C	-0.687892000	-2.808941000	-0.569137000
H	0.153470000	-2.853811000	-1.282204000
H	-1.295555000	-3.726325000	-0.654359000
C	-1.976010000	-1.692661000	-2.280449000
H	-2.644004000	-0.830476000	-2.405742000
H	-1.105468000	-1.598069000	-2.951498000
H	-2.521002000	-2.628447000	-2.487200000
C	-4.024397000	0.066175000	0.157422000
H	-3.810909000	-0.946602000	-0.203311000
H	-4.067164000	0.063123000	1.258983000
H	-4.977072000	0.435784000	-0.258831000
O	-1.538514000	-1.670602000	-0.888176000
O	-2.930435000	0.902831000	-0.305322000
Cu	-0.865814000	0.306381000	-0.449671000
H	0.486555000	-3.532108000	1.077548000
N	-1.208599000	-2.590749000	1.875601000
N	-1.534729000	-1.457764000	2.268748000
N	-1.924966000	-0.469724000	2.738798000