

Supporting Material to

X-Ray diffraction, IR spectrum, optical properties, AIM, NBO, RDG, HS, Fukui function, biological and molecular docking analysis of a novel hybrid compound (C₉H₁₅N₃)[CuCl₄(H₂O)]

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Figure S - 1: The cristal photo of (C₉H₁₅N₃)[CuCl₄(H₂O)]

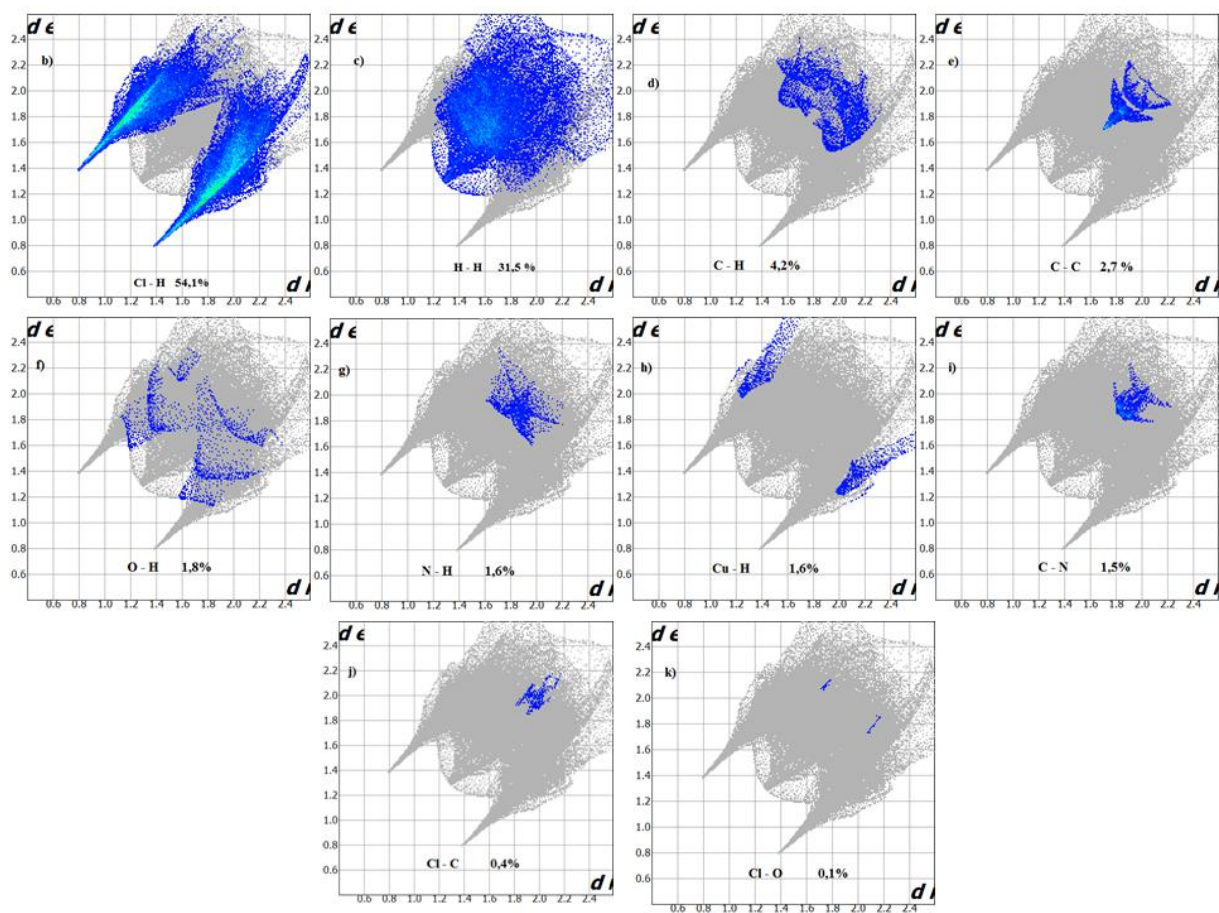


Figure S - 2 : The two-dimensional fingerprint plots for the title compound delineated into: (b) Cl...H, (b) H...H, (c) C...H, (d) C...C, (e) O...H, (f) N...H, (g) Cu...H, (h) C...N, (i) Cl...H, (j) Cl...C and (k) Cl...O

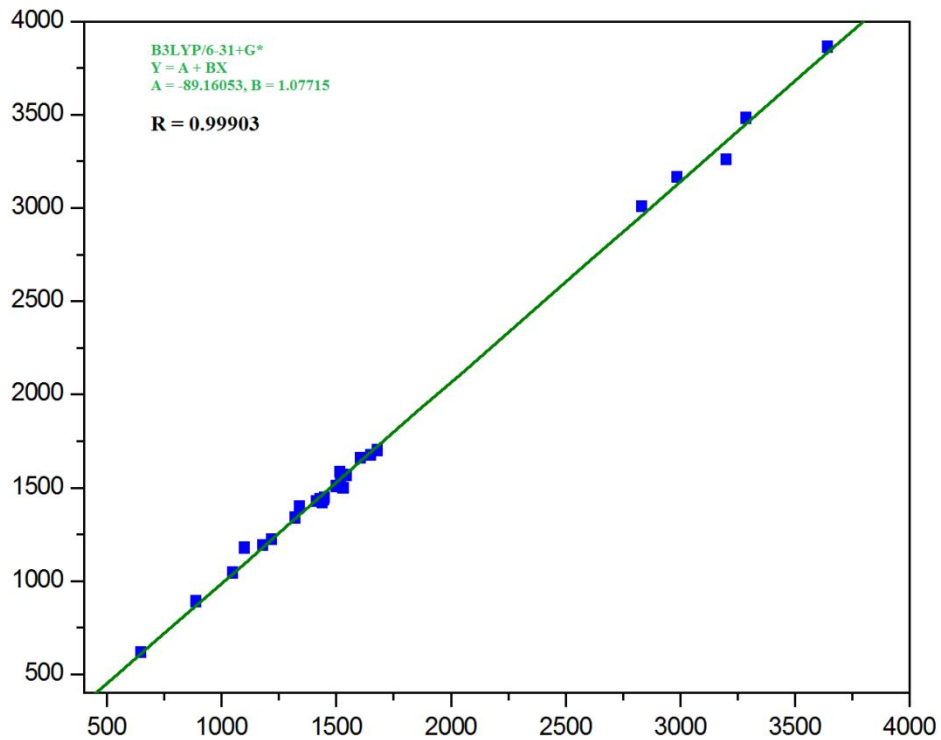


Figure S - 3 : Correlation graph between the experimental and calculated wave numbers (cm^{-1}) of $(\text{C}_9\text{H}_{15}\text{N}_3)[\text{CuCl}_4(\text{H}_2\text{O})]$

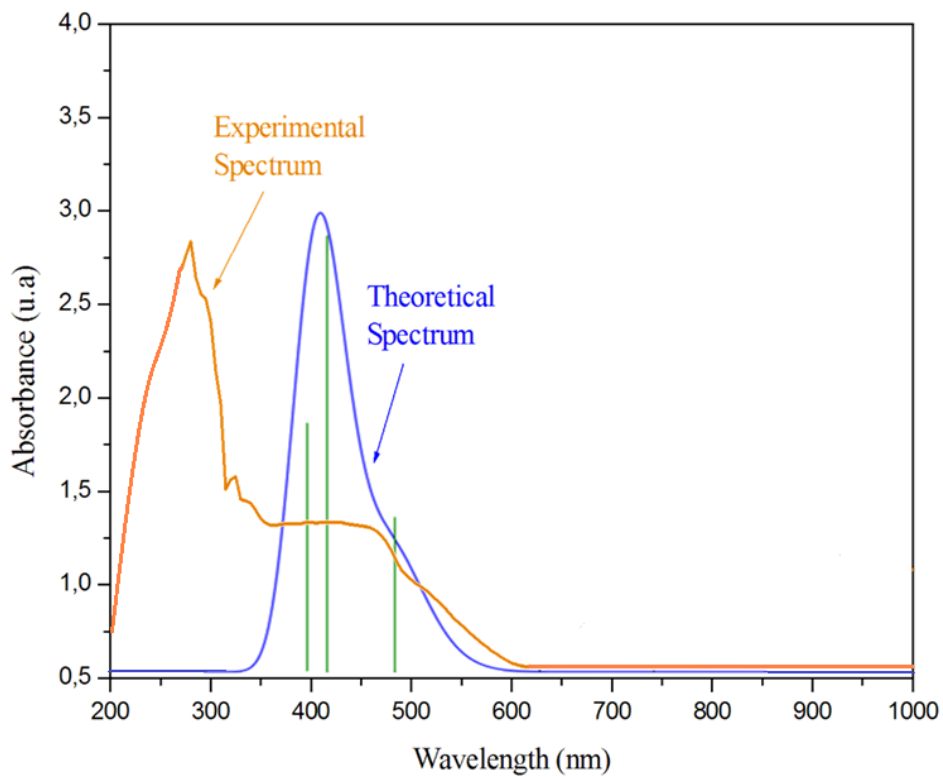


Figure S - 4 : Correlation graph between the experimental and calculated wavelength (nm) of $(\text{C}_9\text{H}_{15}\text{N}_3)[\text{CuCl}_4(\text{H}_2\text{O})]$

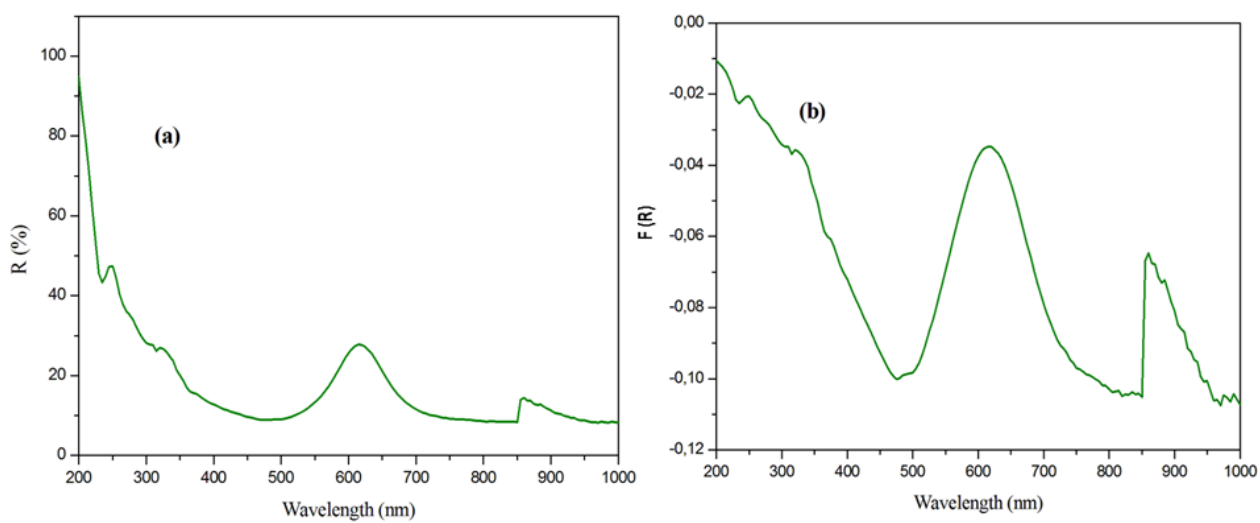


Figure S - 5 : (a): The diffuse reflectance spectra and (b): the Kubelka-Munk absorption spectra of $(C_9H_{15}N_3)[CuCl_4(H_2O)]$

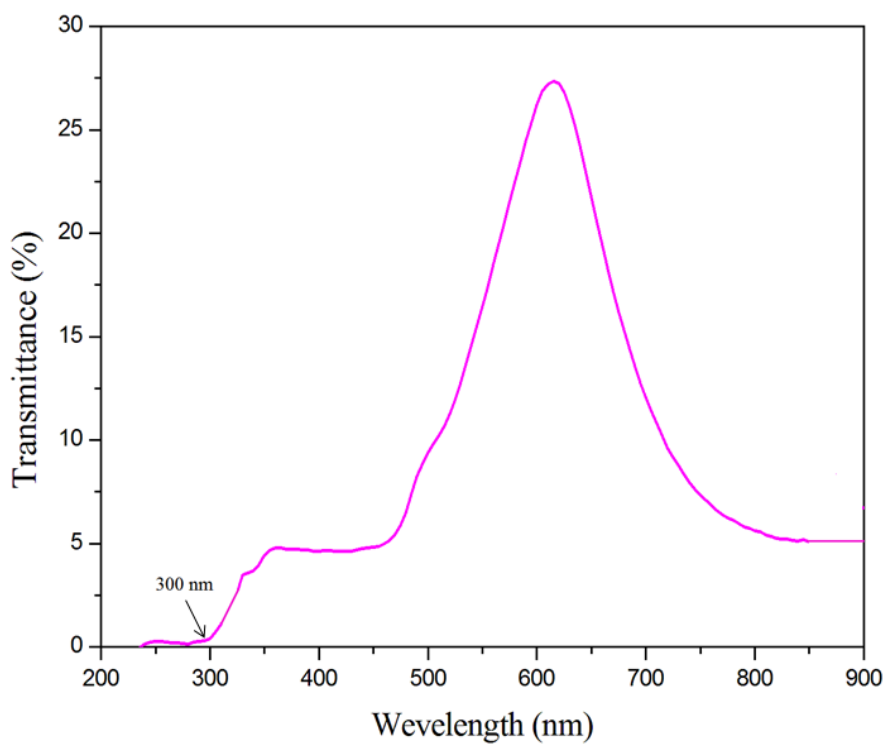


Figure S - 6 : Optical transmittance spectrum of $(C_9H_{15}N_3)[CuCl_4(H_2O)]$

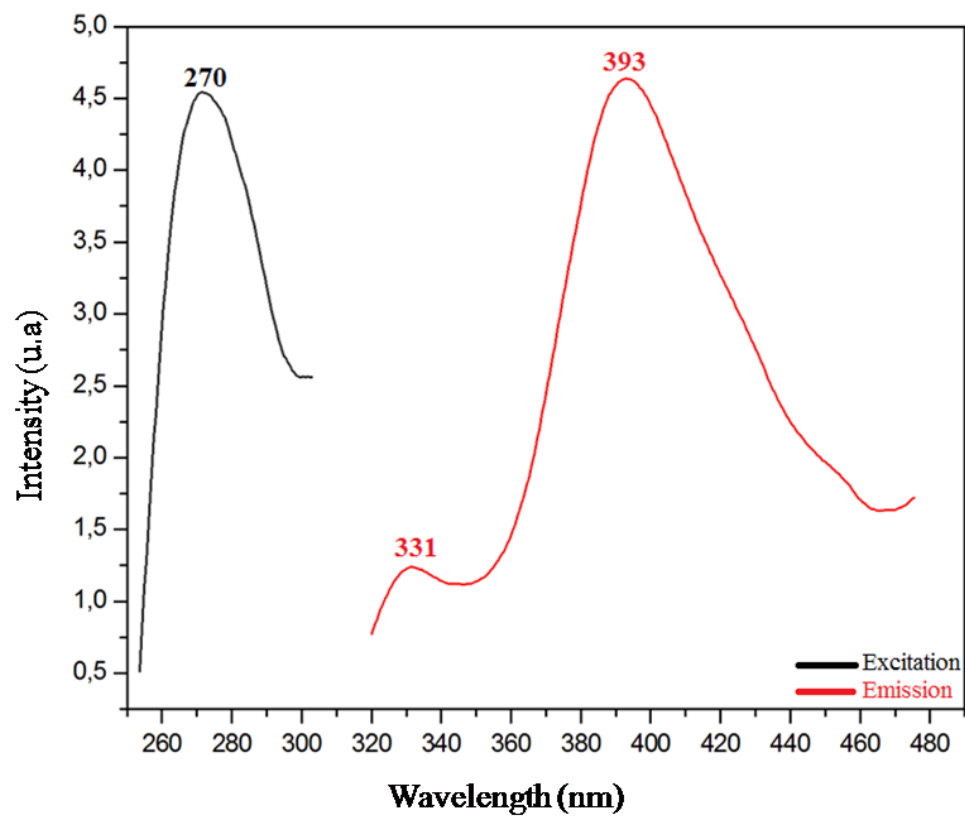


Figure S - 7 : The emission spectra of $(C_9H_{15}N_3)[CuCl_4(H_2O)]$

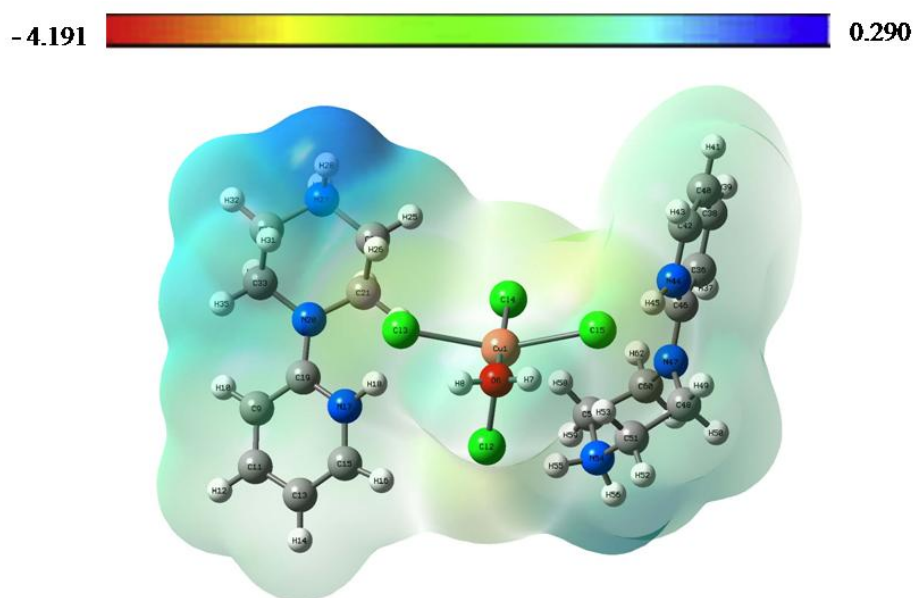


Figure S - 8 : Molecular electrostatic potential surface (between -4.191 and 0.290) of $(C_9H_{15}N_3)[CuCl_4(H_2O)]$

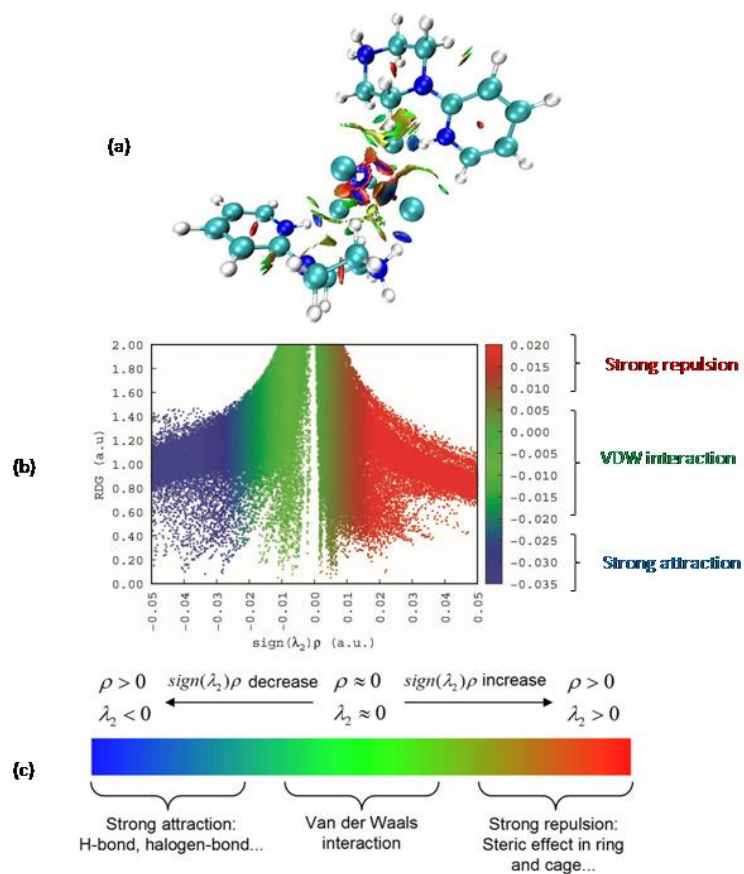


Figure S - 9 : Representation of different types of interactions in the monomer (a). Graph of the reduced density gradient vs. $\text{sign}(\lambda_2)\rho$ of $(\text{C}_9\text{H}_{15}\text{N}_3)[\text{CuCl}_4(\text{H}_2\text{O})]$ (b). Color code for different regions of interactions (c).

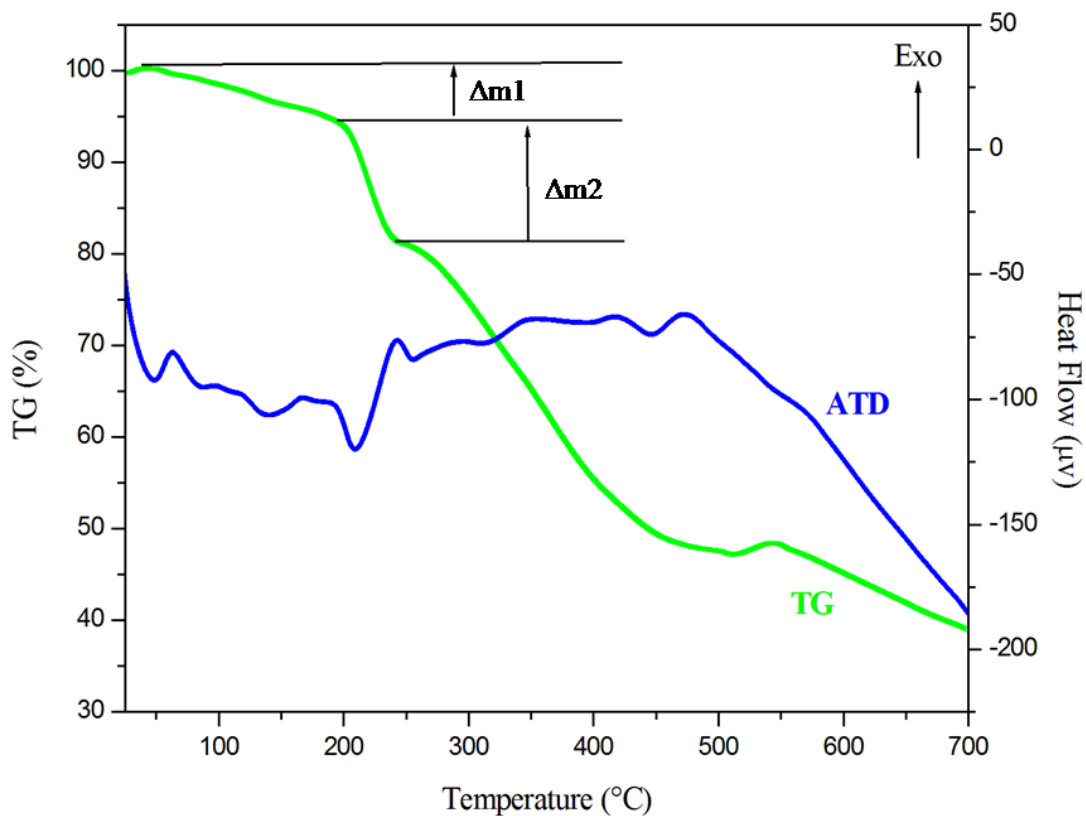


Figure S - 10 : Simultaneous curves of thermogravimetric analysis and differential thermal analysis of $(C_9H_{15}N_3)[CuCl_4(H_2O)]$.

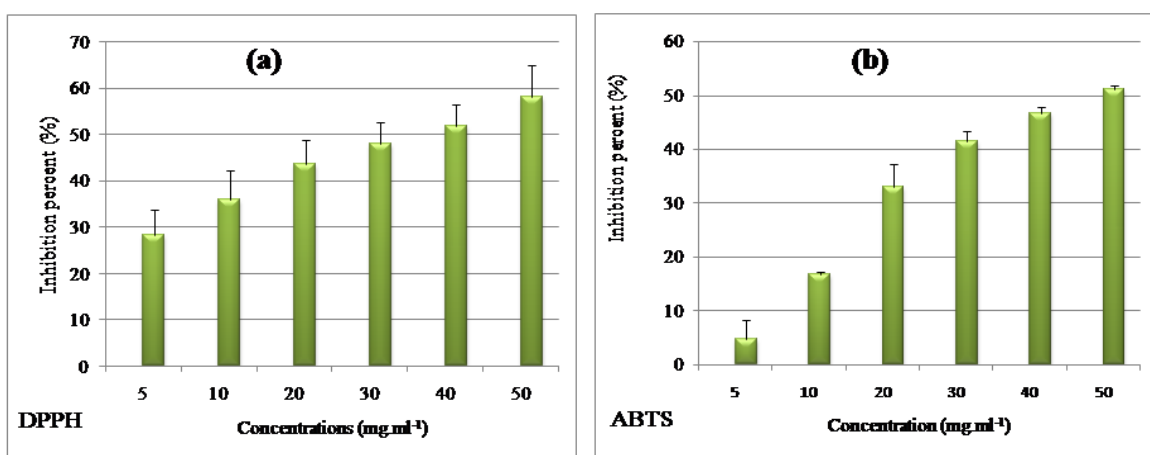


Figure S - 11 : Scavenging activity of $(C_9H_{15}N_3)[CuCl_4(H_2O)]$ in both (a) $DPPH^{++}$ and (b) $ABTS^{++}$ test. The data are reported as mean \pm standard deviation

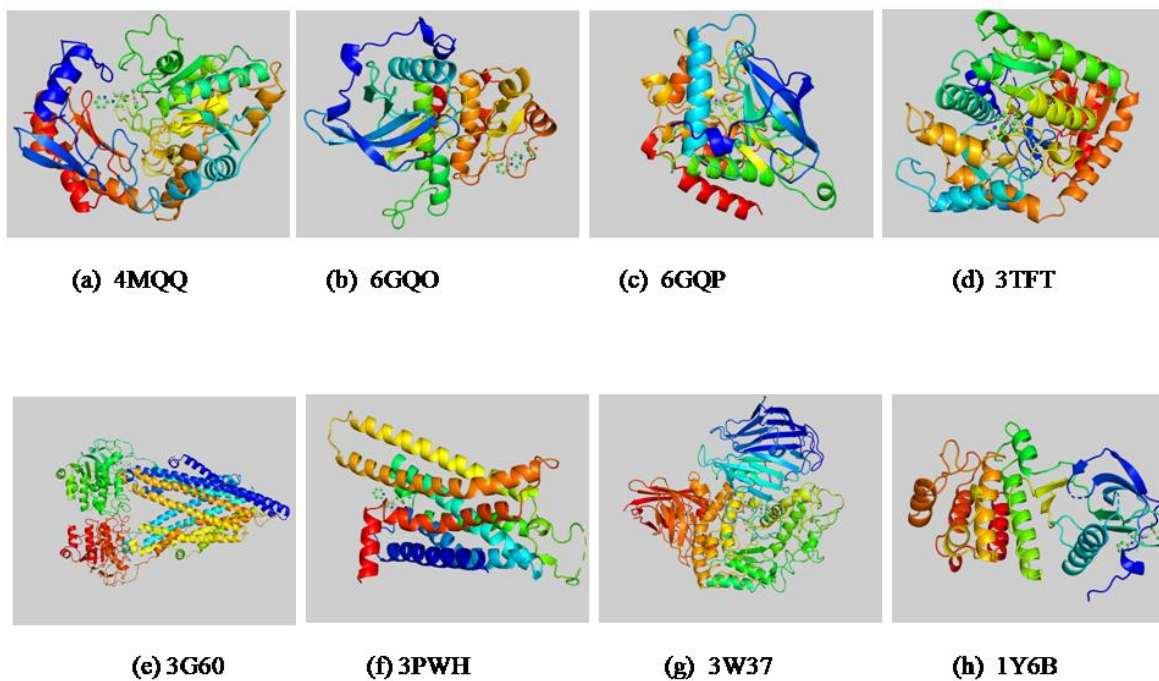


Figure S - 12: The best docked poses of 2PPCU compound with eight protein: (a) 4MQQ, (b) 6GQO, (c) 6GQP, (d) 3TFT, (e) 3G60, (f) 3PWH, (g) 3W37, (h) 1Y6B

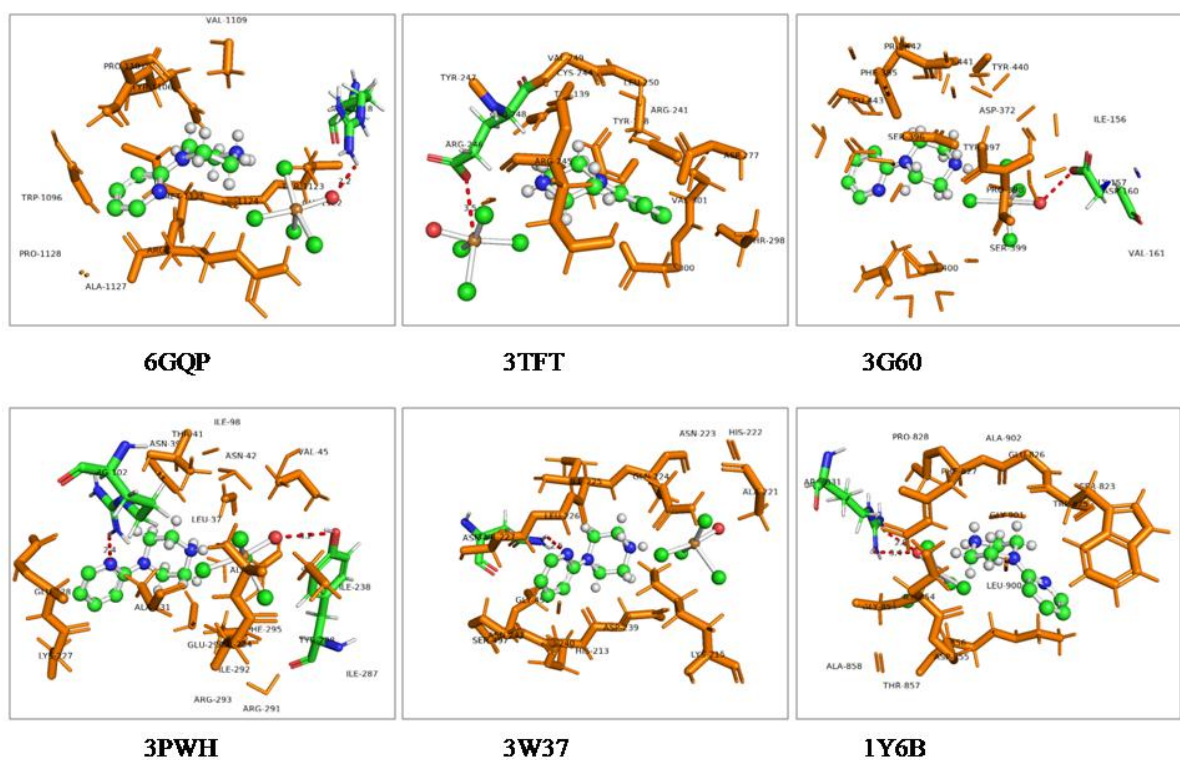


Figure S - 13 : Different types of interactions between $(C_9H_{15}N_3)[CuCl_4(H_2O)]$ and 6GQP, 3TFT, 3G60, 3PWH, 3W37, 1Y6B

Table S – 1: Assignments of IR vibrational modes in (C₉H₁₅N₃)[CuCl₄(H₂O)]

<u>IR Experimental</u>	<u>Frequency (cm⁻¹)</u>	<u>IR Theoretical</u>	<u>Attribution</u>
3642-3000		3695, 3863	ν_s (OH)
3288-3268		3481, 3406	ν_s (-NH ₂)
3200-3150		3260, 3235, 3247 3235, 3274	ν_s (CH)
2987		3164	ν_s (-NH)
2832-2800		3172, 3164, 3193, 3190 3193, 3190, 3158, 3112 3013, 3007	ν_s (CH ₂)
1627		1701, 1454, 1338, 1270	δ_s (-NH ₂)
1607		1674, 1659, 1128	ν_s (C=C)
1531		1674, 1659, 1499	δ_s (-NH)
1450		1674, 787, 386, 320	δ_s (CNC)
1414-900		1583, 1128, 1082, 899 1068, 1019, 1062, 941	ν_s (C-C)
1515-1220		1583, 1428, 1421, 1223 1499, 1128, 1331, 1297 1499, 1439, 1331 1318 1338, 1207, 1207	δ_s (C-C)
1547		1566	δ_s (H ₂ O)
1520-1510		1533, 1516, 1522	δ_s (CH)
1500		1508	δ_{as} (CH)
1450		1467, 1270, 738, 899 1190, 1062, 1082, 738	ν_s (C-N)
1445-1200		1467, 1297, 1207	δ_s (CN)
1438		1454, 1421, 1418 949, 898	τ_s (HNCC)
1430-750		1439, 1032, 1032, 386	τ_s (HCNC)
1340		1399	τ_{as} (HCCN)
1320		1338	τ_s (HCCN)
1220		1223	δ_{as} (CC)
1180		1190, 751	τ_s (CCNC)
1100-500		1177, 899, 505, 469 787, 613, 642, 642 286, 218, 162	δ_s (NCC)
1090-805		1056, 1053, 751, 811 1044, 1019, 949, 898	τ_s (HCCC)
1048-723		1044, 1019, 642 1019, 738	δ_s (CCC)
890		891	τ_s (CNCC)
650		891, 218	γ_s (CCCN)
--		616, 611	δ_s (CuO)
--		542, 414	τ_s (CCCC)
--		451	δ_{as} (NCC)
--		426	ν_s (Cu-O)

--	386	$\tau_s(\text{NCCN})$
--	368, 341	$t_s(\text{HOCuCl})$
--	320, 218	$\tau_s(\text{CCCN})$
--	263, 257, 250, 174	$v_s(\text{Cu-Cl})$
--	194, 162, 128	
--	174, 153, 103	$\gamma_s(\text{OCIClCu})$
--	153, 146, 140, 95	
--	143, 129, 113, 90	$\delta_s(\text{OCuCl})$
--	143, 129, 113, 103	$\delta_s(\text{ClCuCl})$
--	83, 32	$\tau_s(\text{CNCN})$
--	77, 72, 40	$\tau_s(\text{CuCIHN})$
--	77, 69, 43	$\tau_s(\text{CNHCl})$
--	43, 17, 5	$t_s(\text{HClCuCl})$
--	32	$\delta_{as}(\text{Cu-Cl})$

Table S – 2: NBO results showing the formation of Lewis and non-Lewis orbitals in $(\text{C}_9\text{H}_{15}\text{N}_3)[\text{CuCl}_4(\text{H}_2\text{O})]$

Bonde A-B	Occupancy	EDA(%)	EDB(%)	NBO	Orbital atomique (%)
σ O6-H7	0.99759	77.80	22.20	0.8820(sp2.43) O6 0.4712 s H7	s(29.17%)p(70.83) s(100%)
σ O6-H8	0.99755	77.77	22.23	0.819(sp2.44) O6 0.4715 s H8	s(29.08%)p(70.92) s(100%)
σ C9-H10	0.98708	62.17	37.83	0.7885(sp2.30) C9 0.6151 s H10	s(30.34%)p(69.66%) s(100%)
π C9-C11	0.82653	56.24	43.76	0.7499(sp99.99) C9 0.6615(sp1) C11	s(0.02%)p(99.98%) s(0.01%)p(99.99%)
σ C9-C19	0.98594	48.89	51.11	0.6992(sp1.97)C9 0.7149(sp1.59)C19	s(33.63%)p(66.37%) s(38.65%)p(61.35%)
σ C11-H12	0.98800	62.82	37.18	0.7926(sp2.35) C11 0.6097 s H12	s(29.84%)p(70.16%) s(100%)
σ C11-C13	0.99059	50.25	49.75	0.7089(sp1.86) C11 0.7053(sp1.89) C13	s(34.91%)p(65.09%) s(34.59%)p(65.41%)
σ C13-H14	0.98770	62.98	37.02	0.7936(sp2.2) C13 0.6085 s H14	s(31.29%)p(68.71%) s(100%)
π C13-C15	0.82257	54.80	45.20	0.7403(sp1)C13 0.6723(sp99.99) C15	s(0 %)p(100%) s(0.02%)p(99.98%)
σ C15-H16	0.98726	63.72	36.28	0.7983(sp2.02) C15 0.6023s H16	s(33.15%)p(66.85%) s(100%)
σ C15-N17	0.99247	35.99	64.01	0.5999(sp2.53) C15 0.8001(sp1.82) N17	s(28.33%)p(71.67%) s(35.46%)p(64.54%)
σ N17-H18	0.99003	76.09	23.91	0.8723(sp2.43) N17 0.4890s H18	s(29.11%)p(70.89%) s(100%)
π N17-C19	0.90737	72.54	27.46	0.8517(sp99.99) N17 0.5240(sp1)C19	s(0.10%)p(99.90%) s(0.01%)p(99.99%)
σ C19-N20	0.99069	38.07	61.93	0.6170(sp2.16) C19 0.7869(sp1.76) N20	s(31.63%)p(68.37%) s(36.28%)p(63.72%)
σ N20-C21	0.98888	63.55	36.45	0.7972(sp2.19) N20	s(31.34%)p(68.66%)

σ N20-C33	0.99051	62.50	37.50	0.6037(sp3.38) C21	s(22.85%)p(77.15%)
				0.7906(sp2.22) N20	s(31.10%)p(68.90%)
				0.6124(sp3.22) C33	s(23.69%)p(97.31%)
σ C21-H22	0.98389	64.22	35.78	0.8014(sp2.87) C21	s(25.84%)p(74.16%)
				0.5981s H22	s(100%)
σ C21-H23	0.98935	61.48	38.52	0.7841(sp3.16) C21	s(24.05%)p(75.95%)
				0.6207 s H23	s(100%)
σ C21-C24	0.99076	49.58	50.42	0.7041(sp2.67) C21	s(27.27%)p(72.73%)
				0.7101 (sp2.46 C24	s(28.92%)p(71.08%)
σ C24-H25	0.98731	63.15	36.85	0.7947(sp2.88) C24	s(25.75%)p(74.25%)
				0.6071 s H25	s(100%)
σ C24-H26	0.98836	63.98	36.02	0.7999(sp2.74) C24	s(26.74%)p(73.26%)
				0.6002s H260	s(100%)
σ C24-N27	0.99501	32.04	67.96	0.5660(sp4.38) C24	s(18.58%)p(81.42%)
				0.8244(sp2.57) N27	s(28.03%)p(71.97%)
σ N27-H28	0.99328	74.21	25.79	0.8614(sp3.47) N27	s(22.36%)p(77.64%)
				0.5152s H28	s(100%)
σ N27-H29	0.99475	73.46	26.54	0.8571(sp3.52) N27	s(22.13%)p(77.87%)
				0.5152s H29	s(100%)
σ N27-C30	0.99505	66.48	33.52	0.8153(sp2.65) N27	s(27.40%)p(72.60%)
				0.5790(sp4.13) C30	s(19.50%)p(80.50%)
σ C30-H31	0.98959	62.86	37.14	0.7928(sp2.9) C30	s(25.67%)p(74.33%)
				0.6094s H31	s(100%)
σ C30-H32	0.98874	62.63	37.37	0.7914(sp2.93) C30	s(25.46%)p(74.54%)
				0.6113s H32	s(100%)
σ C30-C33	0.99013	50.66	49.34	0.7118(sp2.41) C30	s(29.34%)p(70.66%)
				0.7024(sp2.74) C33	s(26.77%)p(73.23%)
σ C33-H34	0.99021	61.66	38.34	0.7852(sp3.04) C33	s(24.74%)p(75.26%)
				0.6192s H34	s(100%)
σ C33-H35	0.98519	62.90	37.10	0.79321(sp3.03) C33	s(24.80%)p(75.20%)
				0.6091s H35	s(100%)
LP(1)-Cu1	0.99987	-	-	spd1.00	s(0%)p(0%)d(100%)
LP(2)-Cu1	0.99980	-	-	sp(0.66)d(99.99)	s(0.13)p(0.08)d(99.7
LP(3)-Cu1	0.99974	-	-	sp1d(99.99)	s(0)p(0.05)d(99.95)
LP(4)-Cu1	0.99931	-	-	sp1d(99.99)	s(0)p(0.01)d(99.99)
LP(5)-Cu1	0.99854	-	-	sp(0.03)d(99.99)	s(0.20)p(0.01)d(99.7
LP*(6)Cu1	0.18108	-	-	sp0.07d0	s(93.02)p(6.66)d0.32
LP*(7)Cu1	0.11518	-	-	sp(99.99)d(0.72)	s(0.08)p(99.86)d(0)
LP*(8)Cu1	0.09805	-	-	sp(21.28)d(0.03)	s(4.48)p(95.38)d(0.1
LP*(9)Cu1	0.09176	-	-	sp(47.83)d(0.08)	s(2.04)p(97.8)d(0.15
LP(1)-Cl2	0.99260	-	-	sp(0.97)	s(50.86%)p(49.14%)
LP(2)-Cl2	0.98804	-	-	sp(12.51)	s(7.4%)p(92.60%)
LP(3)-Cl2	0.93387	-	-	sp(3.75)	s(21.07%)p(78.93%)
LP(4)-Cl2	0.91972	-	-	sp(3.84)	s(20.67%)p(79.33%)
LP(1)-Cl3	0.99546	-	-	sp(0.83)	s(54.69%)p(45.31%)
LP(2)-Cl3	0.97946	-	-	sp(52.32)	s(1.88%)p(98.12%)
LP(3)-Cl3	0.95554	-	-	sp(45.21)	s(2.16%)p(97.84%)
LP(4)-Cl3	0.91127	-	-	sp(1.42)	s(41.27%)p(58.73%)
LP(1)-Cl4	0.99482	-	-	sp(0.75)	s(57.12%)p(42.88%)
LP(2)-Cl4	0.98230	-	-	sp(68.68)	s(1.44%)p(98.56%)

LP(3)-Cl4	0.97852	-	-	sp(1.00)	s(0.01%)p(99.99%)
LP(4)-Cl4	0.89802	-	-	sp(1.41)	s(41.43%)p(58.57%)
LP(1)-Cl5	0.99390	-	-	sp(1.07)	s(48.29%)p(51.71%)
LP(2)-Cl5	0.98171	-	-	sp(99.99)	s(0.62%)p(99.38%)
LP(3)-Cl5	0.94940	-	-	sp(4.73)	s(17.46%)p(82.54%)
LP(4)-Cl5	0.91088	-	-	sp(1.97)	s(33.63%)p(66.37%)
LP(1)-O6	0.99357	-	-	sp(69.45)	s(1.42)p(98.58%)
LP(2)-O6	0.95274	-	-	sp(1.48)	s(40.29%)p(59.71%)
LP(1)N20	0.87108	-	-	sp(76.08)	s(1.3%)p(98.70%)
RY*(1)Cu1	0.00168	-	-	sp(83.43)d(6.15)	s(1.10)p(92.10)d(6.7)
RY*(1)-O6	0.00091	-	-	sp(5.65)	s(15.04%)p(84.96%)
RY*(1)-H7	0.00063	-	-	s	s(100%)
RY*(2)-C9	0.00282	-	-	sp(99.99)	s(0.06%)p(99.94%)
RY*(1)C11	0.00338	-	-	sp(72.81)	s(1.35%)p(98.65%)
RY*(1)N17	0.00204	-	-	sp(99.99)	s(0.13%)p(99.87%)
RY*(1)N20	0.00593	-	-	sp(42.90)	s(2.28%)p(97.72%)
RY*(1)N27	0.00106	-	-	sp(28.87)	s(3.35%)p(96.65%)

Table S – 3: Second order perturbation theory analysis of Fock matrix basis in NBO basis corresponding to the intra molecular bonds in (C₉H₁₅N₃)[CuCl₄(H₂O)]

Donor	Acceptor	E⁽²⁾ Kcal/mol	E(j)-E(i) (a.u)	F(i,j) (a.u)
LP(3)-Cl2	LP*(9)-Cu(1)	4.07	0.47	0.056
LP(4)-Cl2	LP*(6)-Cu(1)	15.54	0.36	0.100
LP(4)-Cl2	LP*(9)-Cu(1)	13.99	0.45	0.101
LP(3)-Cl3	N17-H18	8.53	0.64	0.093
O6-H8	LP*(8)-Cu(1)	5.88	1.02	0.103
LP(2)-O6	LP*(6)-Cu(1)	6.23	0.63	0.085
LP(2)-O6	LP*(8)-Cu(1)	26.15	0.82	0.190
C9-C11	C13-C15	6.97	0.29	0.059
C9-C11	N17-C19	21.48	0.20	0.089
C13-C15	N17-C19	6.71	0.20	0.049
C15-H16	N17-C19	3.93	0.93	0.077
N17-C19	C9-C11	3.25	0.38	0.046
N17-C19	C13-C15	10.84	0.39	0.083
LP(1)-N20	N17-C19	22.94	0.21	0.096
N17-C19	C9-C11	23.72	0.09	0.087
N17-C19	C13-C15	11.66	0.09	0.064
LP(4)-Cl4	LP*(6)-Cu(1)	37.61	0.48	0.176
LP(4)-Cl4	LP*(8)-Cu(1)	23.92	0.67	0.160
LP(1)-Cl4	LP*(8)-Cu(1)	4.21	6.75	0.074
LP(4)-Cl3	LP*(6)-Cu(1)	13.50	0.48	0.106
LP(4)-Cl3	LP*(7)-Cu(1)	26.26	0.68	0.171
LP(4)-Cl5	LP*(6)-Cu(1)	10.79	0.44	0.092
LP(4)-Cl5	LP*(7)-Cu(1)	28.63	0.65	0.175

Table S – 4: Condensed Fukui function fr for (C₉H₁₅N₃)⁺

Atoms	<i>Mulliken atomic charges</i>			<i>Fukui functions</i>			
	N	(N+1)	(N-1)	f ⁺	f ⁻	f ⁰	Δf
1 C	0.407793	-1.661840	0.538042	-2.069633	-0.130249	-1.0998	-1.939
2 C	-0.482102	1.155124	-0.489425	1.637226	0.007323	0.815	1.629
3 C	-0.112434	0.988692	0.025185	1.101126	-0.137919	0.4815	1.239
4 C	-0.000424	-0.285987	0.002690	-0.285563	-0.002693	-0.1445	-0.283
5 C	-0.171389	1.130583	-0.259396	1.301972	0.088007	0.695	1.214
6 H	0.118978	-0.232473	0.152132	-0.3514253	-0.033154	-0.192	-0.318
7 H	0.142146	-1.032656	0.178080	-1.174802	-0.035934	-0.6055	-1.138
8 H	0.124726	-0.365836	0.176657	-0.507982	-0.051931	-0.279	-0.456
9 H	0.158463	-0.145898	0.197601	-0.304361	-0.039438	-0.1715	-0.265
10 N	-0.322383	-0.437578	-0.260069	-0.115195	-0.062314	-0.0875	-0.053
11 N	0.058895	0.106185	0.189098	0.04729	-0.130203	-0.0415	0.177
12 C	-0.313728	0.066287	-0.289230	0.380015	-0.024498	0.178	0.405
13 H	0.134630	0.127443	0.177358	-0.007187	-0.042728	0.025	0.036
14 H	0.101434	-0.042534	0.166661	-0.143968	-0.065227	-0.1045	-0.079
15 C	-0.103640	0.582586	-0.077874	0.686226	-0.025766	0.33	-0.660
16 H	0.108685	-0.017936	0.165159	-0.126621	-0.065474	-0.096	-0.061
17 H	0.100275	-0.132121	0.128167	-0.232396	-0.027892	-0.130	-0.205
18 C	-0.213840	1.533695	-0.148191	1.747535	-0.362031	0.693	2.109
19 H	0.097077	-0.093046	0.120993	-0.190123	-0.023916	-0.107	0.166
20 H	0.117045	-0.637908	0.168833	-0.754953	-0.051788	-0.403	-0.703
21 C	-0.084033	-0.288872	-0.136093	-0.204839	0.05206	-0.076	-0.257
2 H	0.133818	-0.036706	0.187320	-0.170524	-0.053502	-0.879	-0.117
23 H	0.091079	-0.519828	0.122008	-0.610907	-0.030929	-0.821	-0.579
24 N	-0.264193	-0.499932	-0.238865	-0.235739	-0.025328	-0.131	-0.210
25 H	0.173122	-0.259446	0.203161	-0.432568	-0.030039	-0.231	-0.403