Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


**Supplementary information**

# Antioxidant and Copper Chelating Power of New Molecules Proposed as Combined Multiple Targets Agent Against Alzheimer's Disease

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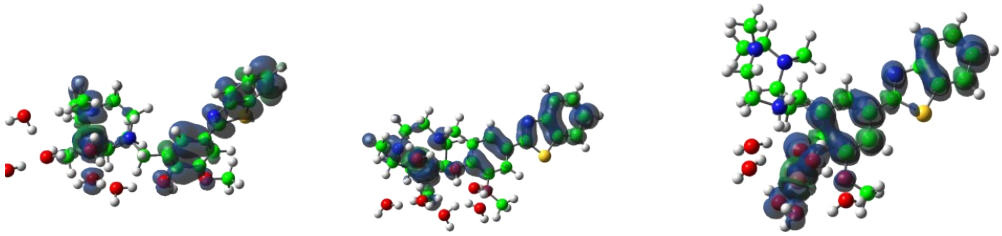
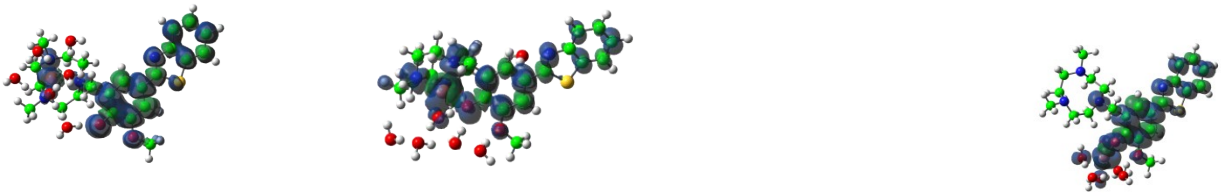
Table S1. Bond distances (Å) in the different complexes for $L_1(L_1^-)$ and $L_2(L_2^-)$.

| $L_1$ ($L_1^-$) | | | | | |
|---|---|---|---|---|---|
| Bond | Distance | Bond | Distance | Bond | Distance |
| N3 | | O,O | | N,O | |
| Cu-$N_1$ | 2.420 (2.208) | Co-$O_1$ | 1.931 (1.911) | Cu-$N_1$ | 2.273 (2.131) |
| Cu-$N_4$ | 2.068 (2.228) | Cu-$O_6$ | 2.862 (2.281) | Cu-$N_4$ | 2.048 ((2.254) |
| Cu-$N_7$ | 2.098 (2.015) | Cu-$O_{w1}$ | 2.264 (2.428) | Cu-$N_7$ | 2.193 (2.035) |
| Cu-$O_{w1}$ | 2.148 (2.015) | Cu-$O_{w2}$ | 2.433 (2.335) | Cu-$O_1$ | 2.812 (1.957) |
| Cu-$O_{w2}$ | 2.187 (3.055) | Cu-$O_{w3}$ | 2.086 (2.152) | Cu-$O_{w1}$ | 2.084 (3.171) |
| Cu-$O_{w3}$ | 3.086 (3.508) | Cu-$O_{w4}$ | 2.196 (2.375) | Cu-$O_{w2}$ | 2.355 (3.292) |
| $L_2$ ($L_2^-$) | | | | | |
| Bond | Distance | Bond | Distance | | |
| N4 | | O,O | | | |
| Cu-$N_1$ | 3.699 (3.712) | Co-$O_1$ | 2.536 (1.918) | | |
| Cu-$N_4$ | 2.085 (2.098) | Cu-$O_6$ | 2.844 (2.343) | | |
| Cu-$N_7$ | 3.641 (3.638 | Cu-$N_7$ | | | |
| Cu-$N_{10}$ | 2.073(2.066) | Cu-$O_{w1}$ | 2.033 (2.537) | | |
| Cu-$O_{w1}$ | 2.051 (2.093) | Cu-$O_{w2}$ | 2.244 | | |
| Cu-$O_{w2}$ | 2.103 (3.827) | Cu-$O_{w3}$ | 2.275 (2.031) | | |
| Cu-$O_{w3}$ | (2.098) | Cu-$O_{w4}$ | 1.993 (2.423) | | |



$L_1$(N3) $L_1$(N3,O) $L_1$(O,O)

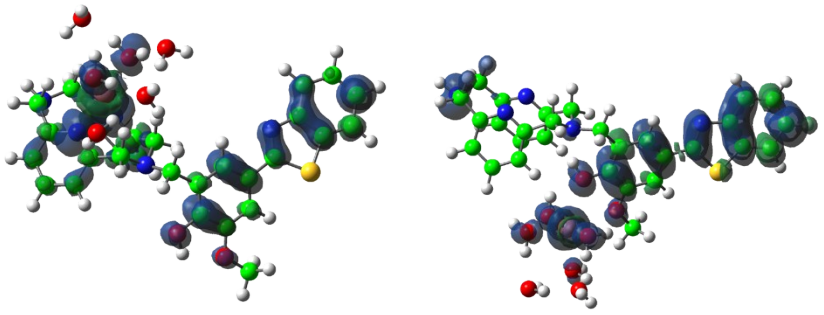
**a**



$L_1^-$(N3) $L_1^-$(N3,O) $L_1^-$(O,O)

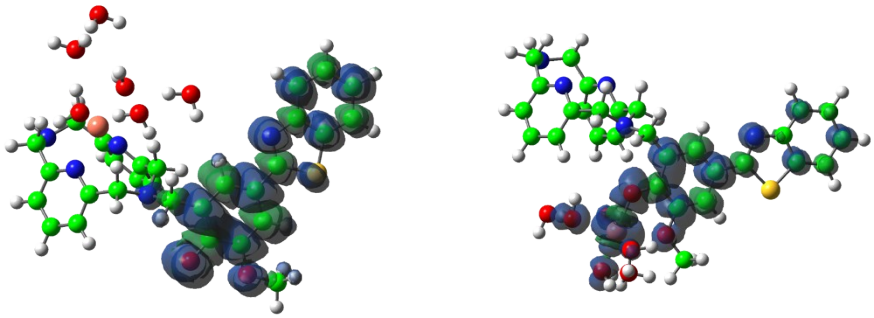
**b**

Figure S1. Spin density distribution for Cu-$L_1$ (a) and Cu-$L_1^-$ (b) complexes.



$L_2$(N4) $L_2$ (O)

**a**



$L_2^-$ (N4) $L_2^-$ (O)

**b**

Figure S2. Spin density distribution for Cu-$L_2$ (a) and Cu-$L_2^-$ (b) complexes.

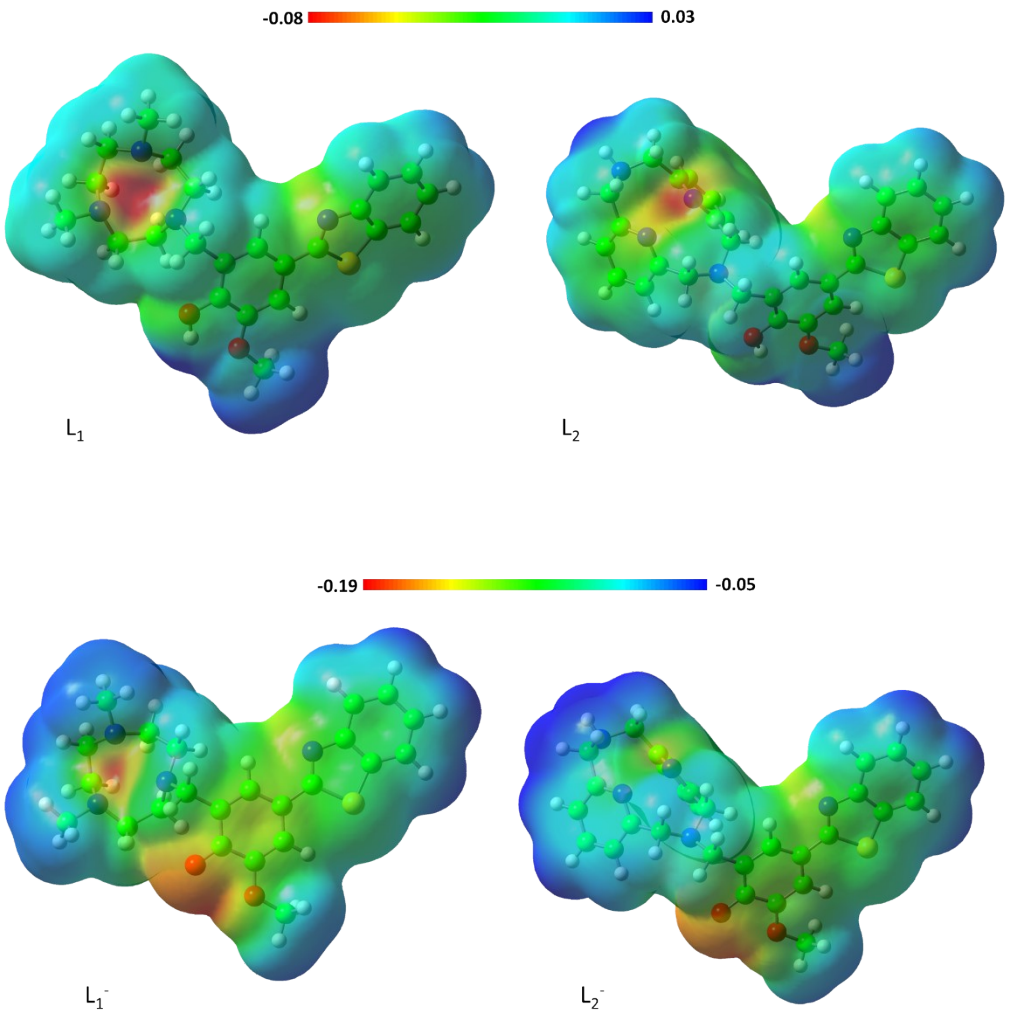



Figure S3. Molecular electrostatic potential maps for neutral and anionic considered species.