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Aliskiren Copper(II) Complex. Synthesis and Antioxidant Activity

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Supplementary Information

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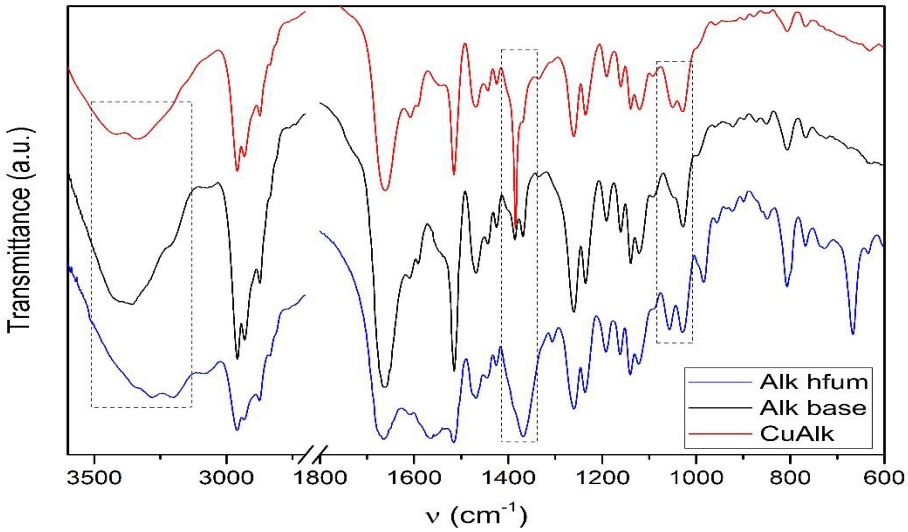

Fig. S1. FTIR spectra of Aliskiren base (Alk base, in black), Aliskiren hemifumarate (Alk hfum, in blue) and Aliskiren copper(II) complex (CuAlk, in red). The dotted squares show main differences among compounds.

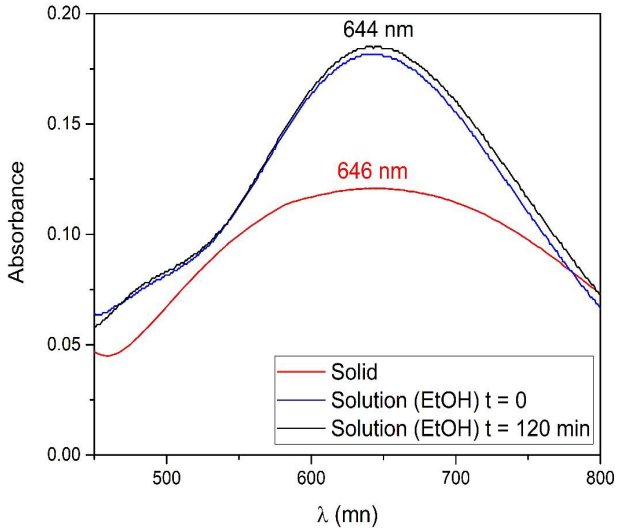

Fig. S2. UV-vis spectra of an ethanolic solution 0.0125 M of CuAlk at 0 (blue) and 120 min (black) and reflectance diffuse spectra of solid CuAlk (red).

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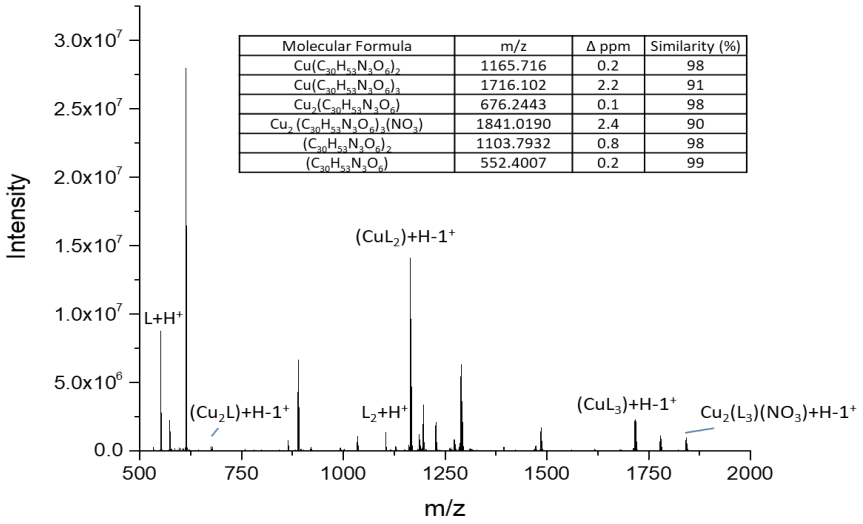
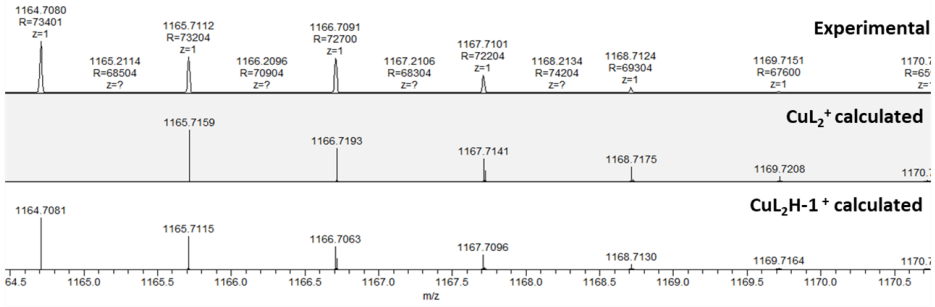


Fig. S3. FTMS spectrum of CuAlk (2 mM) in ethanolic solution. Ionization voltage +1.4 kV, gas pressure 0.30 psi, temperature 120°C. Inset: main peek assignation. L= Alk ($C_{30}H_{53}N_3O_6$).



Type	MF	Adduct	m/z	Δ ppm	z	Intensity	Similarity
(Cu) ($C_{30}H_{53}N_3O_6$)$_2$	$C_{60}H_{106}CuN_6O_{12}$	H-1+	1164.708	3.954946	1	37.56288	0.9892
(Cu) ($C_{30}H_{53}N_3O_6$)$_3$	$C_{90}H_{159}CuN_9O_{18}$	H-1+	1716.102	4.993142	1	5.083054	0.988085
(Cu)$_2$ ($C_{30}H_{53}N_3O_6$)	$C_{30}H_{53}Cu_2N_3O_6$	H-1+	676.2443	-6.43E-07	1	1.284747	0.984729
(Cu) ($C_{30}H_{53}N_3O_6$)$_3$	$C_{90}H_{159}CuN_9O_{18}$	+	1717.109	2.283159	1	5.377864	0.911861
(Cu)$_2$ ($C_{30}H_{53}N_3O_6$)$_3$ (NO_3)	$C_{90}H_{159}Cu_2N_{10}O_{21}$	H-1+	1841.019	2.477824	1	1.728231	0.898405
(Cu) ($C_{30}H_{53}N_3O_6$)$_2$	$C_{60}H_{106}CuN_6O_{12}$	+	1165.716	-0.17527	1	26.10583	0.893515
(Cu)$_4$ ($C_{30}H_{53}N_3O_6$)$_4$ (NO_3) (H_2O) $_3$	$C_{120}H_{218}Cu_4N_{13}O_{30}$	++	1286.655	-0.6615	2	1.033369	0.823566
(Cu) ($C_{30}H_{53}N_3O_6$)$_3$	$C_{90}H_{159}CuN_9O_{18}$	H+	1718.117	-2.48979	1	4.913273	0.822056
(Cu)$_2$ ($C_{30}H_{53}N_3O_6$)$_3$ (NO_3)	$C_{90}H_{159}Cu_2N_{10}O_{21}$	+	1842.027	-2.7052	1	2.330669	0.811346
(Cu) ($C_{30}H_{53}N_3O_6$)$_2$	$C_{60}H_{106}CuN_6O_{12}$	Na+	1188.706	-9.32974	1	2.187438	0.804462
(Cu) ($C_{30}H_{53}N_3O_6$)$_2$	$C_{60}H_{106}CuN_6O_{12}$	H+	1166.724	-8.72621	1	25.02378	0.80152

Fig. S4. Experimental FTMS spectrum of CuAlk (2 mM) in ethanolic solution, calculated spectrum for CuL_2^+ adduct and $CuL_2H\text{-}1^+$ adduct in 1164-1170 m/z range. Ionization voltage +1.4 kV, gas pressure 0.30 psi, temperature 120°C. Table: main fragment assignment. L= Alk ($C_{30}H_{53}N_3O_6$).

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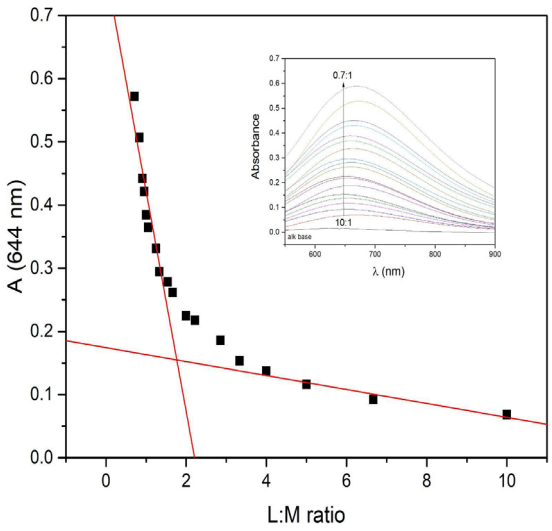

Fig. S5. Spectrophotometric determinations of CuAlk complex stoichiometry at 644 nm by the molar ratio method. Inset: UV–vis spectra of Alk base (0.002 M) with the addition of $Cu(NO_3)_2 \cdot 3H_2O$ in ligand-to-metal ratios (L/M) from 10.0 to 0.70 (pH 7.5) in ethanol. The arrow indicates increased metal additions.

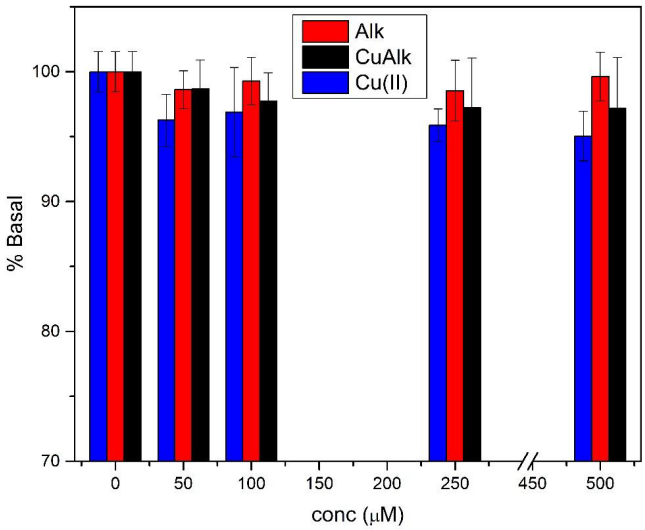

Fig. S6. Scavenging of 1,1-diphenyl-2-picrylhydrazyl radical (DPPH•) by Alk (red), CuAlk (black), and copper(II) (blue). The values are expressed as the mean ± standard error of at least three independent experiments.

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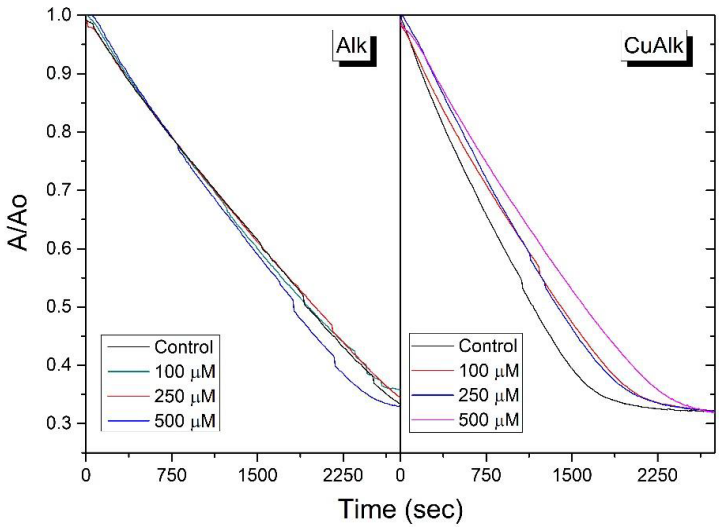

Fig. S7. Scavenge of peroxyl radicals measured as the decay of the intensity of pyranine by addition of different concentrations of Alk (left) and CuAlk (right) at different concentrations.

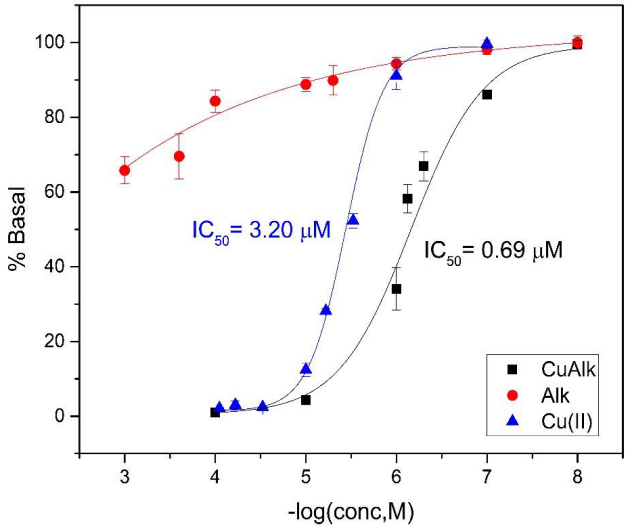

Fig. S8. Effect of CuAlk (in black), Alk (in red) and Cu(II) (in blue) [26] on the reduction of nitroblue tetrazolium by non-enzymatically generated superoxide (phenazine methosulfate and reduced nicotinamide adenine dinucleotide system).

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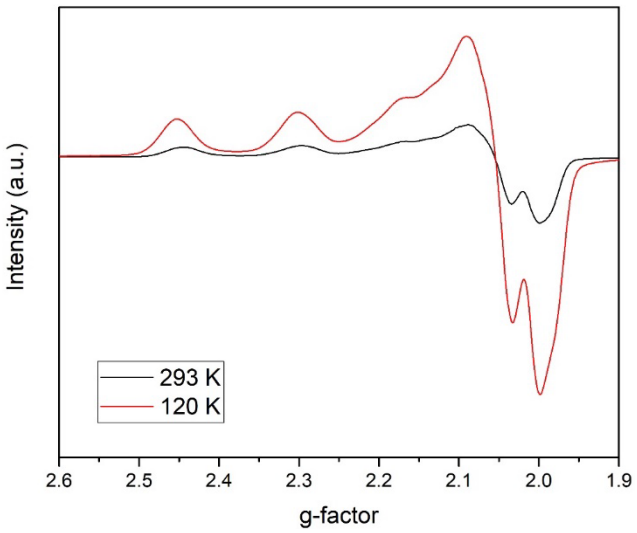

Fig. S9. Experimental Band-X EPR of solid CuAlk at 293 K (black) and at 120 K (red).

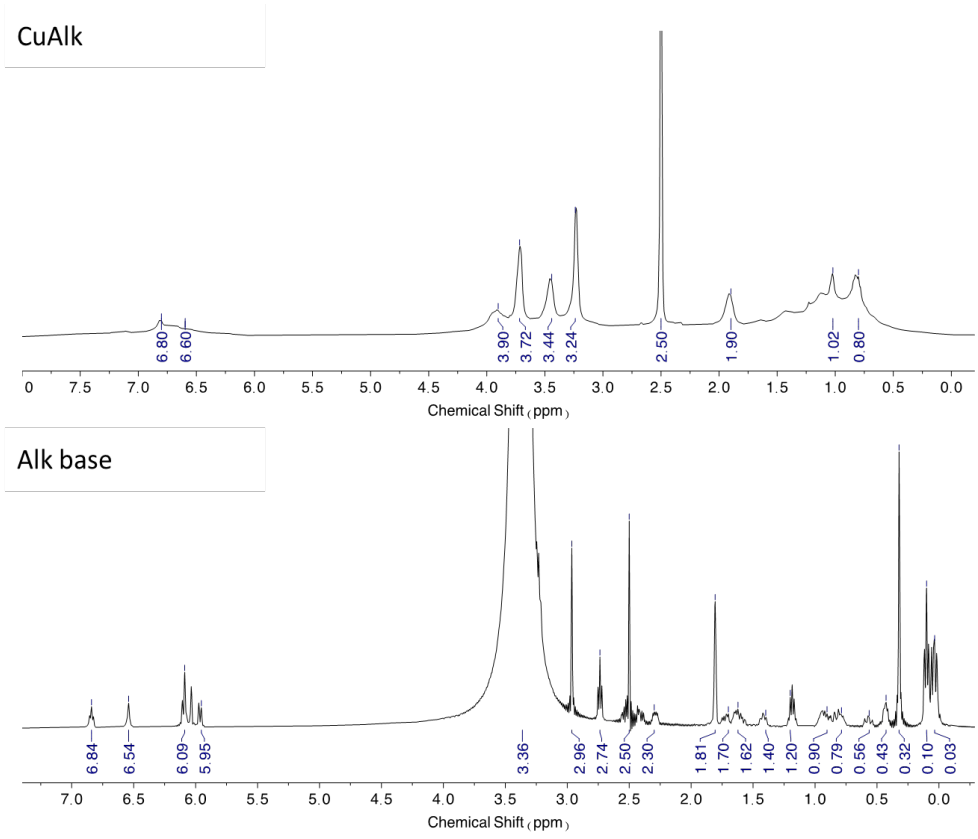

Fig. S10. ^{1}H NMR in d_6-DMSO of CuAlk and Alk base.

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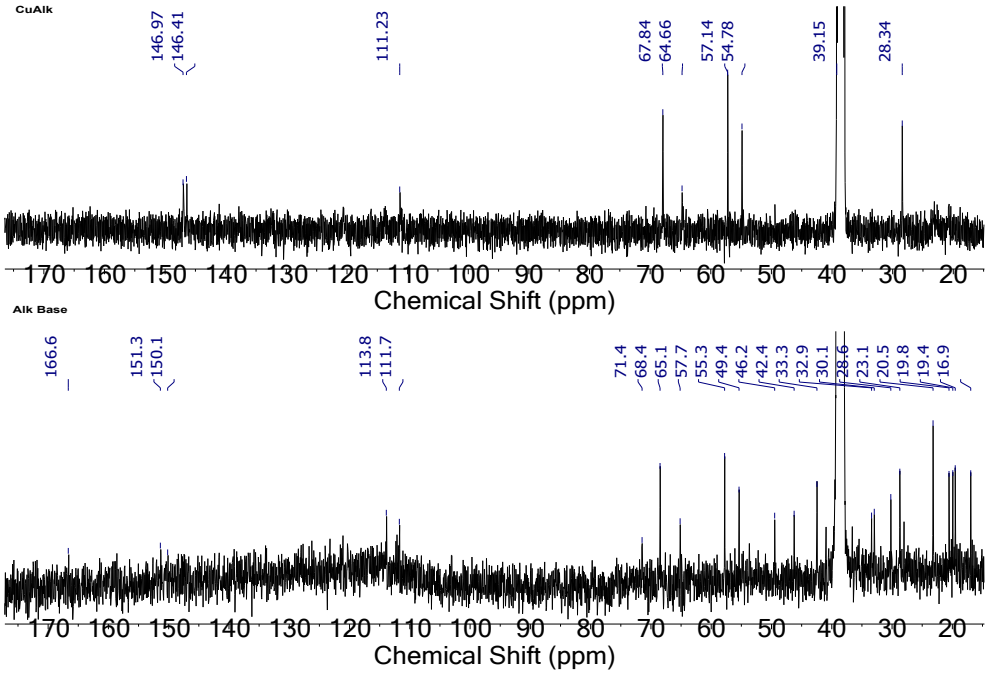

Fig. S11. ^{13}C NMR in d_6-DMSO of CuAlk and Alk base.