Supplementary Material

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Candesartan and Valsartan Zn(II) complexes as inducing agents of reductive stress: mitochondrial dysfunction and apoptosis.

Valeria R. Martínez,[a] María V. Aguirre,[b] Juan S. Todaro,[b] Evelina G. Ferrer,[a] Patricia A.M. Williams*[,a]

[a] Centro de Química Inorgánica (CEQUINOR-CONICET-CICPBA-UNLP) 120 Nº 1465. La Plata, Argentina

[b] Laboratorio de Investigaciones Bioquímicas. Facultad de Medicina. UNNE. Moreno 1240. Corrientes. Argentina

Table S1. Assignment of the main vibrational frequencies of candesartan (Cand) and ZnCand, wavenumbers are in cm^{-1}

Assignments	Cand	ZnCand
ν NH	3445 (w)	
ν OH	3410 (w)	3383 (s)
ν $CH_{arom\ iph}$	3059 (m)	3061 (sh)
ν $CH_{arom\ oph}$	3025 (sh)	3026 (sh)
ν_{as} CH CH_3	2989 (m) 2963 (sh)	2987 (m) 2943 (sh)
ν_s CH CH_2, CH_3	2937 (m)	2934 (sh)
ν_{as} CH CH_2, CH_3	2905 (sh) 2901 (m)	2899 (sh)
ν_s CH CH_3	2871 (m)	2856 (sh)
ν NH OCOH	2300	
ν C=O+ δ COH	1705 (vs)	1706 (vs)
ν C=C + ν C=NBz + ν_{as} COO-		1652 (sh)
ν C=C + ν C=NBz	1610 (m)	1621 (m)
δ_{ip} NNH_{tz} + δ_{ip} CCH_{arom} + ν C=C	1549 (vs)	1548 (vs)
δ_{ip} CCH_{arom} + $_{scissor}$ CH_2 + def CH_3+ ν C-$C_{tz\text{-}biph}$	1517 (sh)	1511 (sh)
δ NNH + ν C-$C_{tz\text{-}biph}$ + δ_{ip} CCH_{arom}	1479 (s)	1489 (sh)
δ NNH + δ CCH_{ip} + $_{scissor}$ CH_2 + δ COH + ν CN_{Bz}	1461 (sh)	1463 (m)
ν $C=N_{Bz,tz}$ + δ_{ip} CCH_{Bz}+ ω CH_2 + τ CH_2 + δ COH	1426 (s)	1429 (m) 1409 (m)
δs CH_3 + ω CH_2 + ν CN_{Bz} + ν C-COO-	1387 (m)	1387 (m)
δ NNH + ω CH_2 + ν C=C + ν CN_{Bz}+ ν_s COO-	1353 (m)	1356 (m)
ν NN + ν NH + δ NNH	1238 (vs)	1251 (w)
ν CO (COH)	1212 (sh)	
+ ν NN + δ CCH_{arom}	1190 (sh)	
δ_{ip} CCH_{arom} + ρ CH_2	1134 (m)	1154 (m)
+ ω CH_2 + δ_{ip} NNH + ν CN_{Bz} + ν (Bz)C-C(COO-)	1112 (sh)	1111 (w)
δ NNN +	1039 (s)	1038 (s)
δ NCN + δ_{op} CCH + ν (Bz)C-C(COO-)	1002 (sh)	1008 (sh)
δ_{op} COH + $\delta_{op}$$CCH_{Bz}$ + δ CCC (Et) + π CCOO (COO-)	823 (m)	818 (d)
ν_{op} NH + δ_{op} CCH + δ_{op} CCC_{arom}+π NNCC	754 (s)	763 (m) 745 (sh)
δ OCO (COOH) +δ (Bz)COC (Et)	698 (m)	697 (vw)
π NNNH + ring biphenyl breathing	674 (sh)	
ring biphenyl breathing		670 (vw)

Abbreviations: s, strong; m, medium; w, weak; vw, very weak; sh, shoulder. ν, stretching; δ, bending; ω, wagging; τ, twisting; ρ , rocking; π , out of plane deformation (4 atoms); s, symmetric; as, antisymmetric; arom, aromatic; oph, out of phase; iph, in phase; op, out of plane; ip, in plane. Bz, benzimidazole; biph, biphenyl; tz, tetrazole;

Table S2. Assignment of the main vibrational frequencies of valsartan (Vals), and ZnCand, wavenumbers are in cm^{-1}

Assignments	Vals	ZnVals
ν NH, ν OH_{COOH}	3436 (m)	
ν OH_{water}		3416 (m)
ν $CH_{arom\ iph}$	3129 (sh), 3054 (sh)	3061 (w)
ν $CH_{arom\ oph}$	3063 (m)	3028(m)
ν_{as} CH, CH_3	2965 (vs)	2965 (s)
ν_s CH, CH_3		2932 (sh)
ν_{as} CH CH_2, CH_3	2908 (sh)	2905 (sh)
ν_s CH, CH_2	2882 (sh), 2737 (m)	2872 (m)
ν C=O	1730 (s)	
ν_{as} COO^-		1625 (vs)
ν C=N, ν C=O amide	1605(vs)	1605 (vs)
δ_{ip} NNH_{tz} + δ_{ip} CCH_{arom} + ν C=C	1556 (sh)	1568 (sh)
δ_{ip} CCH_{arom} + $_{scissor}$ CH_2	1513 (w)	1510 (w)
δ NNH + δ CCH_{ip} + ν C_{23}–C_{18} + ν CN	1467 (s) 1453 (sh)	1463 (s)
δ NNH + δ CCH_{ip} + ν C_{23}–C_{18}	1410 (m)	1428 (sh)
ν_s COO^-	1390 (w)	1408 (s) 1390 (s)
δ NNH + ν NN + δ CC $_{bridge\ bound\ biphenyl}$	1274 (m), 1210 (m)	1265 (w), 1244 (w), 1206 (m)
δ_{ip} CCH + ω CH_2 + ρ CH_2	1172 (sh)	1175 (w)
δ NNH + ν NN	1108 (w)	1106 (w)
ω CH_2 + ρ CH_2	1062 (w) 1051 (w)	
δ NNN+ ν NN + ring biphenyl breathing	1006 (w), 993 (w)	1016 (w), 1007 (w)

Abbreviations: s, strong; m, medium; w, weak; vw, very weak; sh, shoulder. ν, stretching; δ, bending; ω, wagging; τ, twisting; ρ , rocking; π , out of plane deformation (4 atoms); s, symmetric; as, antisymmetric; arom, aromatic; oph, out of phase; iph, in phase; op, out of plane; ip, in plane. Bz, benzimidazole; biph, biphenyl; tz, tetrazole;

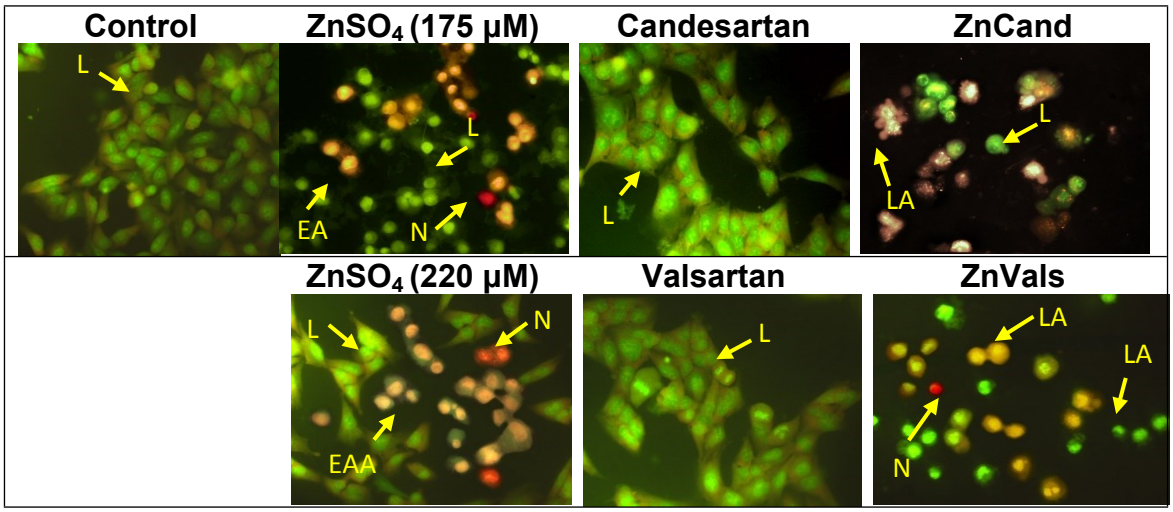

Fig. S1. Representative fluorescence microscopy images of cells at different stages. Magnification 40x. Live cells (L), early apoptosis (EA), late apoptosis (LA) and necrosis (N)