

SUPPLEMENTARY INFORMATION

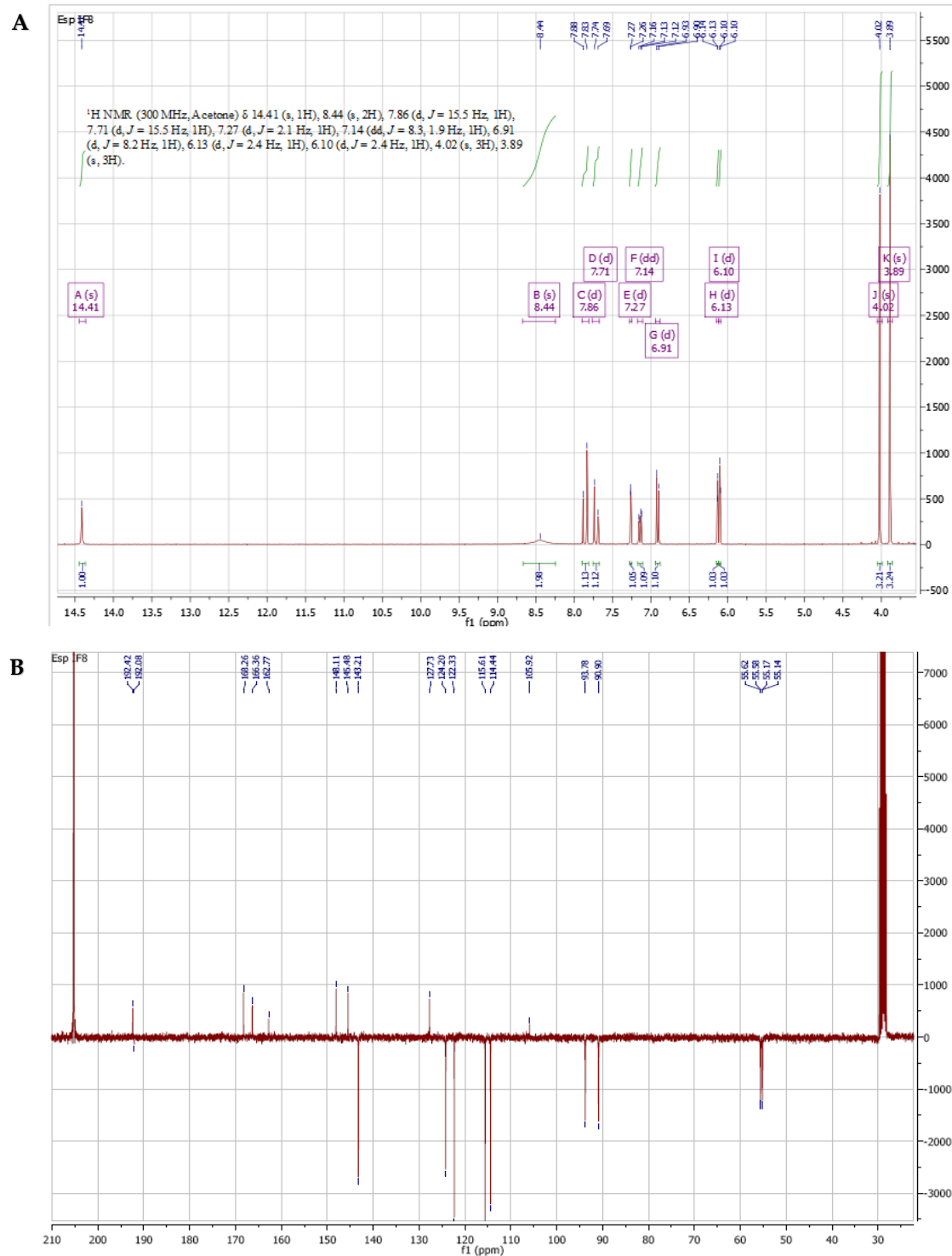


Figure S1: Nuclear Magnetic Resonance Spectroscopy of Chalcotanina (2',3,4-trihydroxy- 4',6'-dimetoxichalcone). A. ¹H NMR spectrum. B. ¹³C NMR spectrum (75 MHz, CDCl₃)

<Spectrum>

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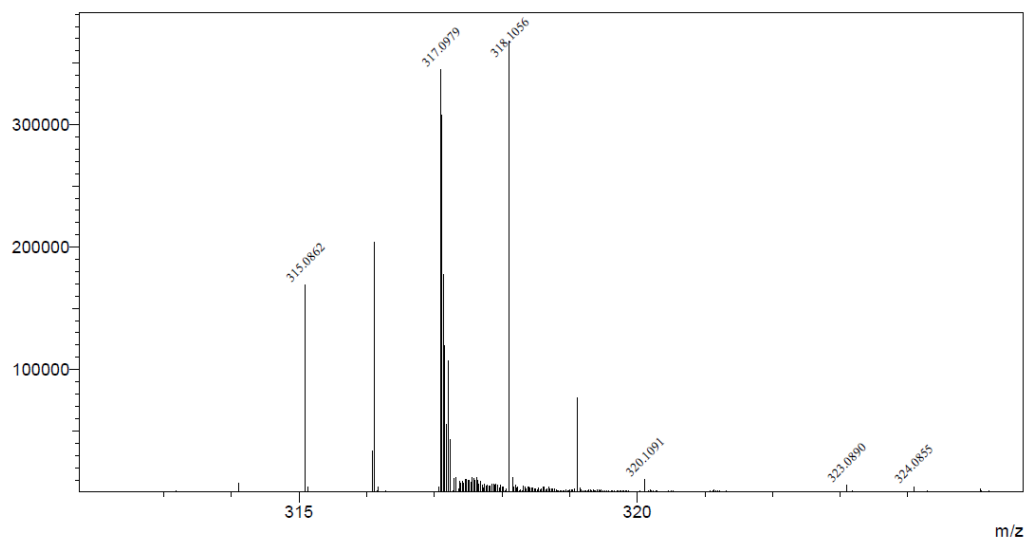


Figure S2. HPLC/QTOF analysis ESI positive ion mode of Chalcotanina $[M+H]^+$: 317,00979

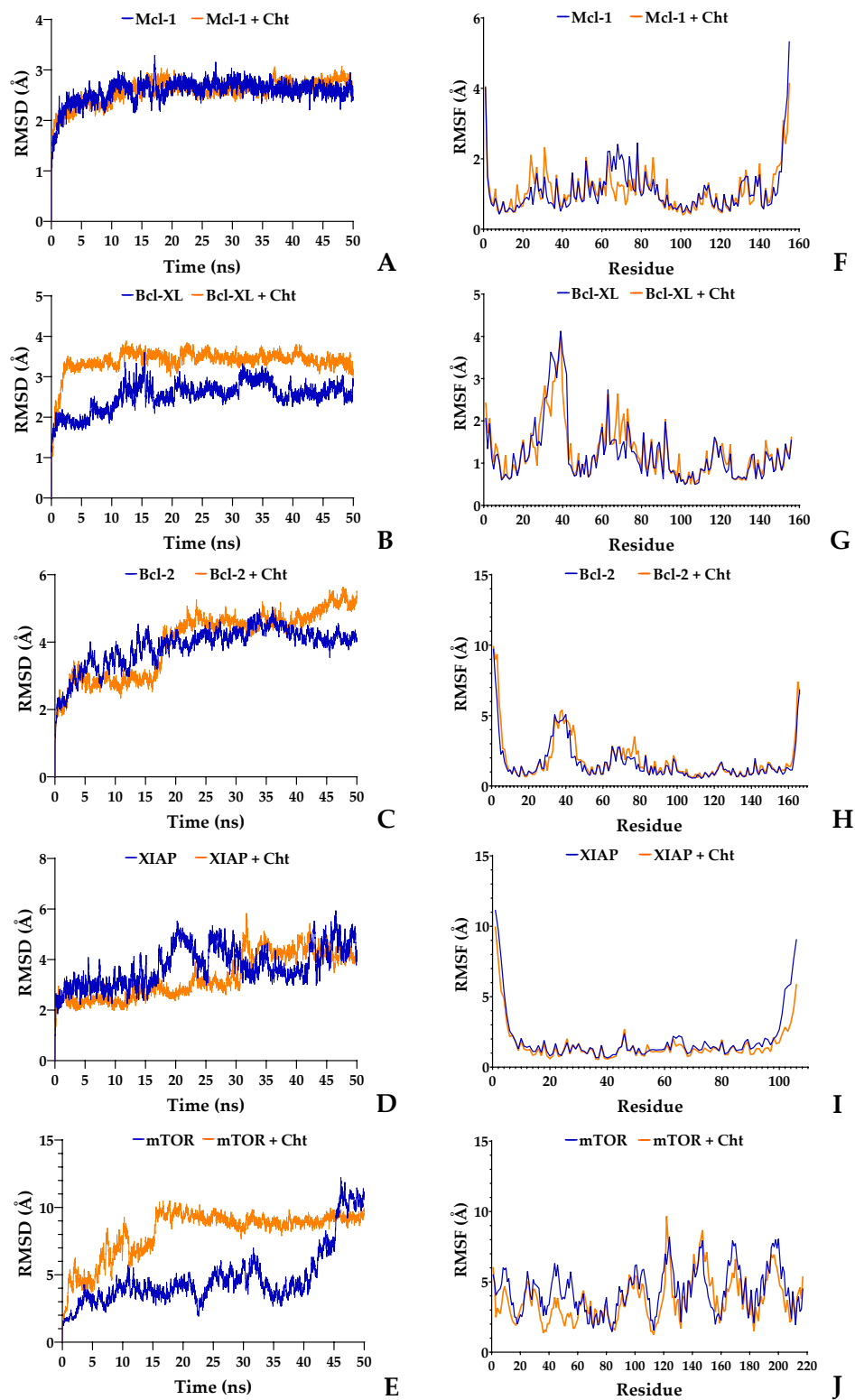


Figure S3. The root-mean-square deviation and fluctuation of pro-survival proteins in response to Chalcotanina. (A-D) RMSD trajectories for each protein: (A) Bcl-2, (B) Bcl-XL, (C) Mcl-1, (D) mTOR,

(E) XIAP. Blue traces represent the standalone protein, while the orange traces depict the protein-ligand complex with Chalcotanina. (F-J) RMSF profiles for each protein: (F) Mcl-1, (G) Bcl-XL, (H) Bcl-2, (I) XIAP and (J) mTOR. The blue shades indicate the protein in its unliganded state, while the orange traces represent the bound state with Chalcotanina.