Supplementary Information

Chemicals

Salicylaldehyde and carbohydrazide and were purchased from Aldrich. Methanol, absolute ethanol (GR), N,N-dimethylformamide (DMF, GR, DMSO, Cu(OAc)2(H2O), 1,10-phenanthroline monohydrate (GR) were obtained from Merck. Calf thymus DNA was sourced from Sigma.

Physical measurements

C, H and N analysis were performed on a Perkin-Elmer model 2400 series II CHNS/O analyzer. Mass spectra were recorded on a Xevo-G2 XS QT of mass spectrometer, Waters UHPLC system. Infrared (IR) spectrum was recorded with a Shimadzu IR Affinity - 1 FT-IR spectrometer using KBr pellet. Conductivity measurement was done using a Mettler Toledo dual conductivity/pH meter model SevenMulti equipped with Inlab 730 and Inlab 413 electrodes. Electronic spectra were recorded on a Jasco V-570 UV/VIS/NIR spectrophotometer using a pair of matched quartz cell of path length of 1 cm. Electron paramagnetic resonance spectra were recorded on a JEOL, Japan Model: JES - FA200 ESR spectrometer with X and Q band. Room temperature solution EPR spectra were recorded using an aqueous cell and frozen glass spectra were recorded in liquid nitrogen using a quartz dewer. Fluorescence measurements were done using a Jasco fluorescence spectrophotometer FP-8500. X-ray crystal structure was determined using a Bruker Axs Kappa Apex2 diffractometer. Crystallographic data for the structural analysis has been deposited with the Cambridge Crystallographic Data Center, CCDC number is 2365897 for compound **1**.

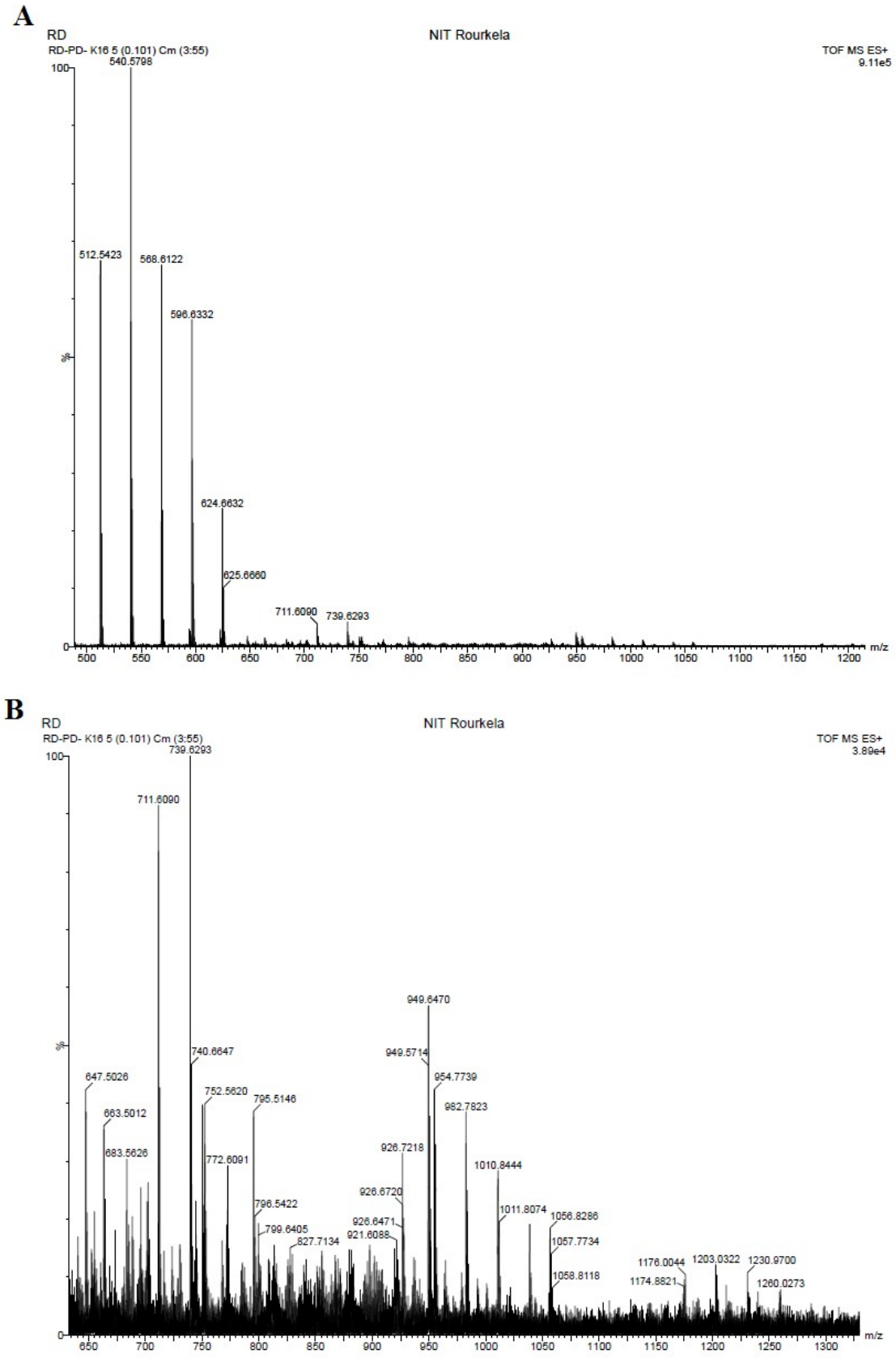

Fig. S1 HR-MS spectra of **1** in CH_3OH.

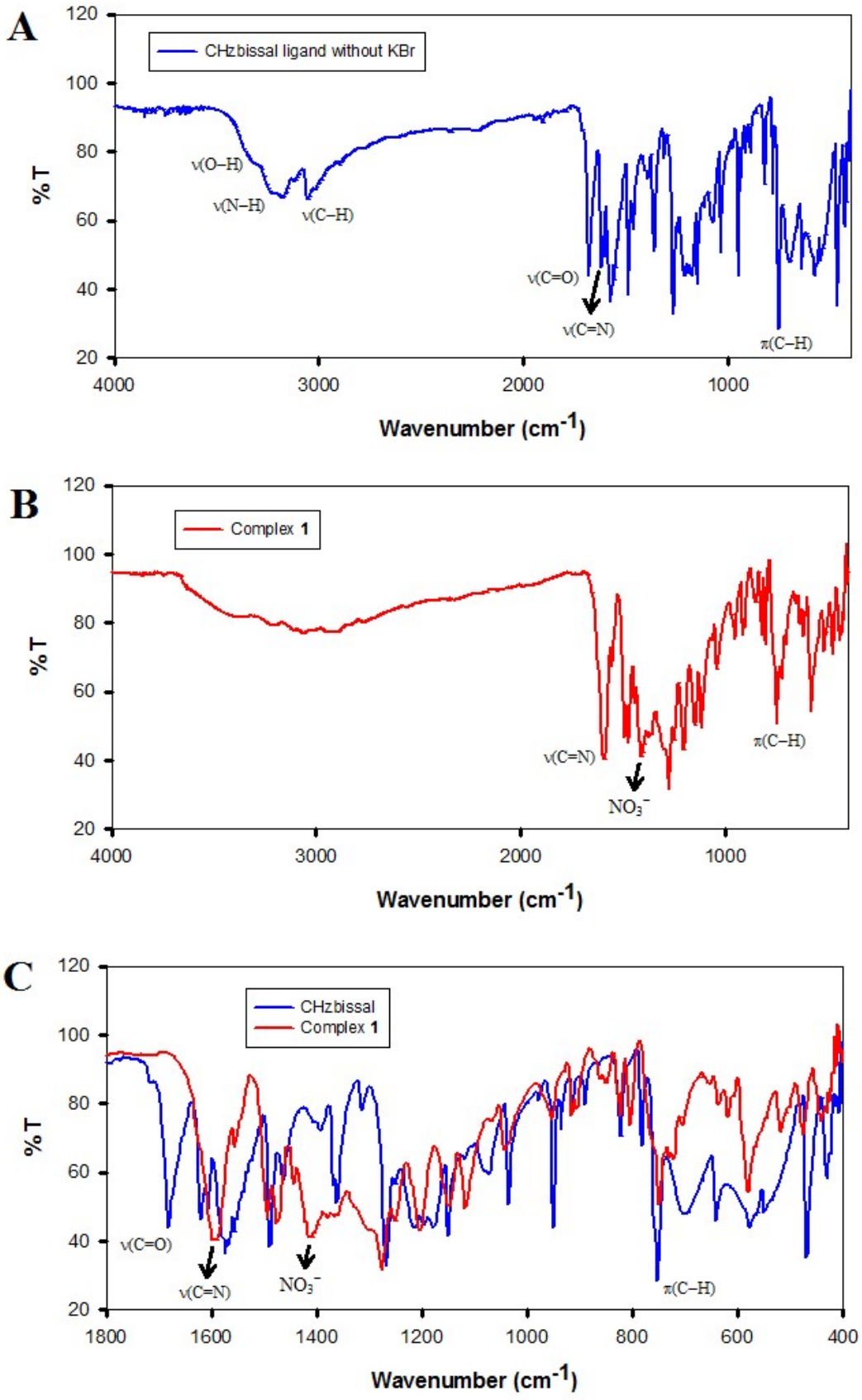

Fig. S2 IR spectra of (A) Schiff base ligand 1,5-bis(salicylidene)carbohydrazide, (B) **1**, and (C) overlay of Schiff base ligand and **1** in the 1800-400 cm^{-1} region.

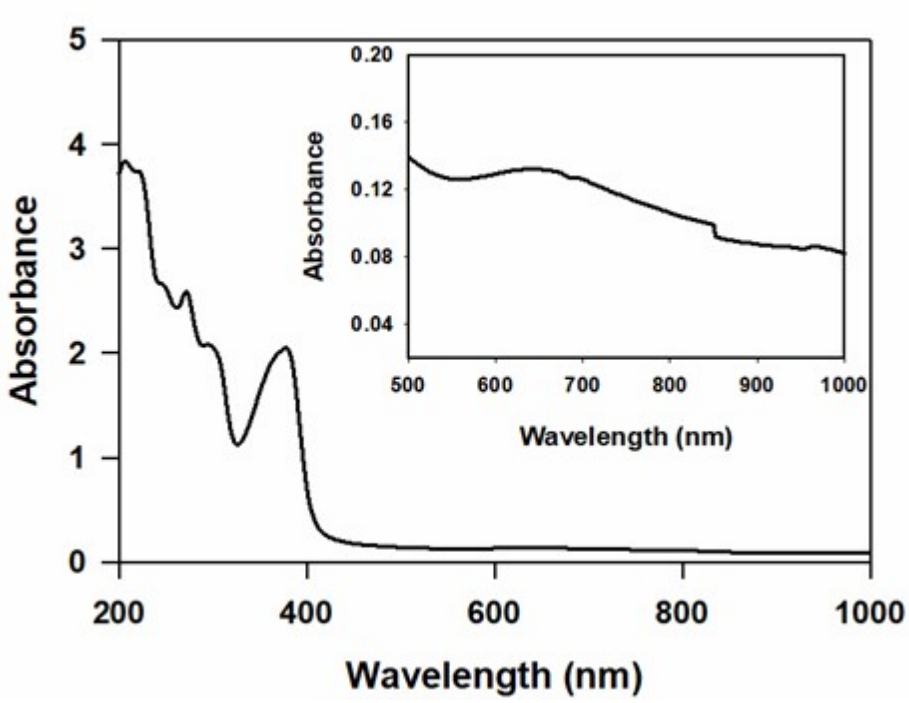

Fig. S3 Electronic spectra of **1** in water. [**1**] = 1.81×10^{-4} M.

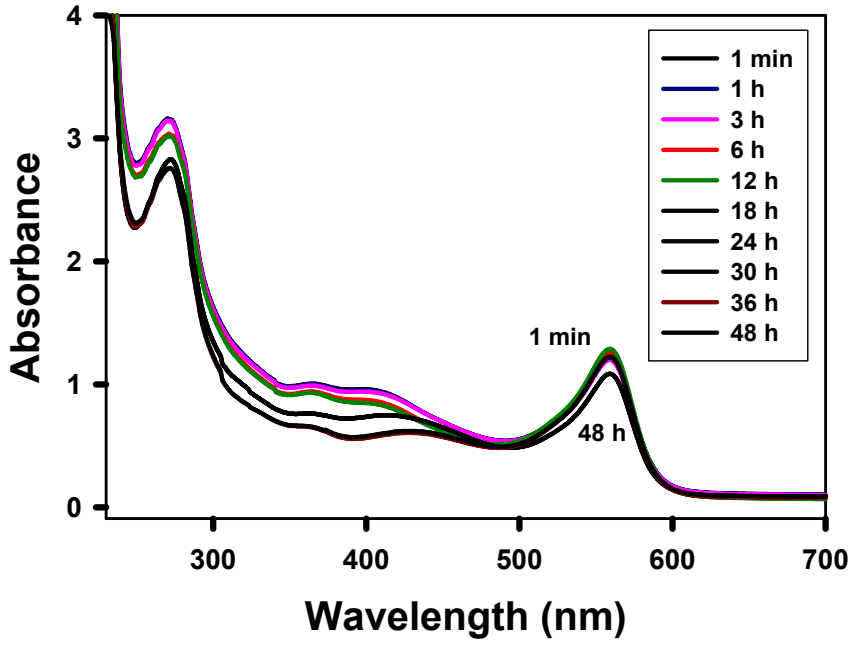

Fig. S4 Electronic spectral change with time to check stability of **1** in DMEM for 48 h.

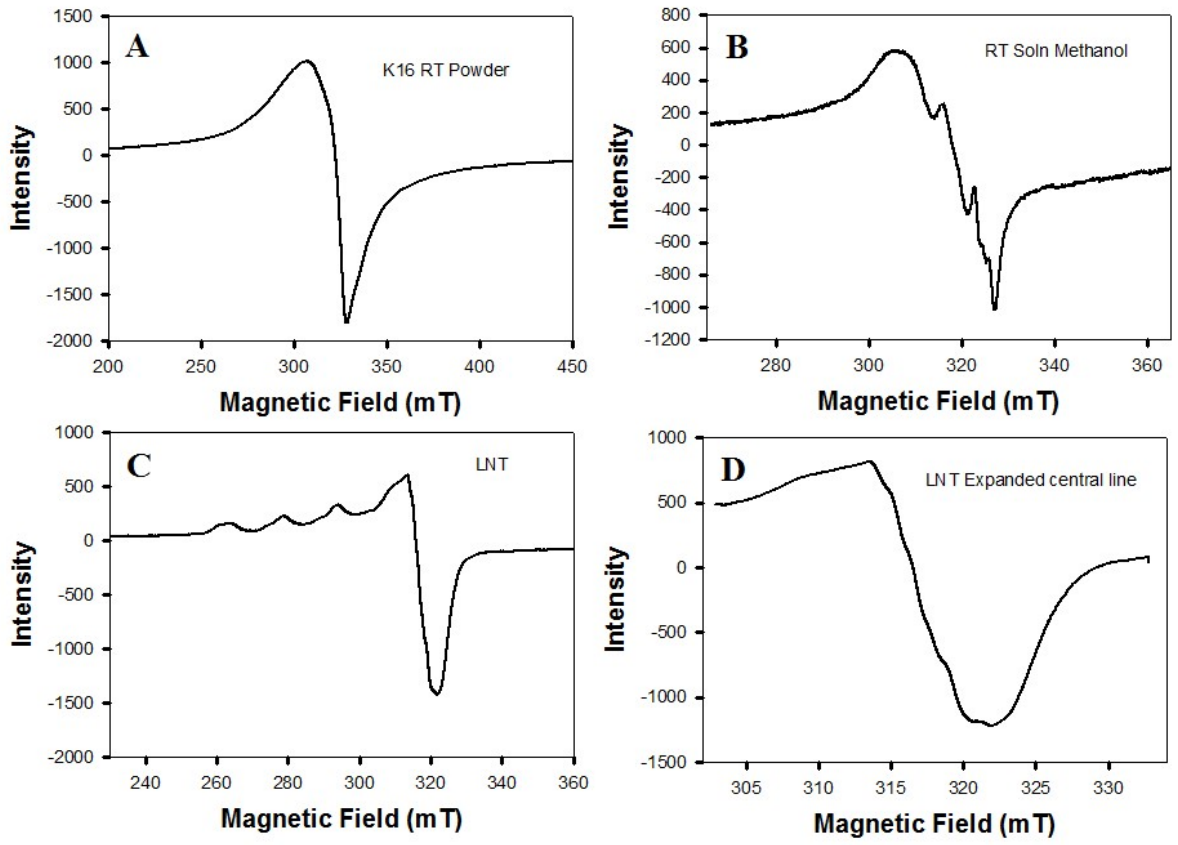

Fig. S5 X-band EPR spectra of **1**. (A) Powder sample at RT. (B) CH_3OH solution spectrum at RT. (C) Frozen glass spectrum in CH_3OH at LNT. (D) Expanded view of the central line of the frozen glass spectrum shown in C.

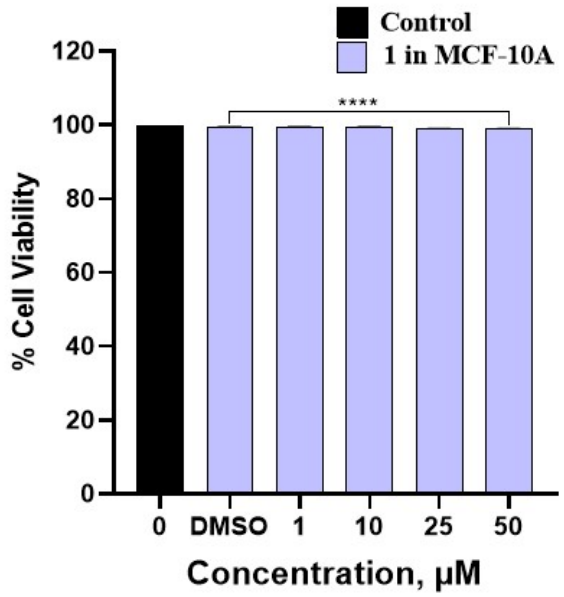

Fig. S6 Cell viability of MCF-10A cells against **1**.

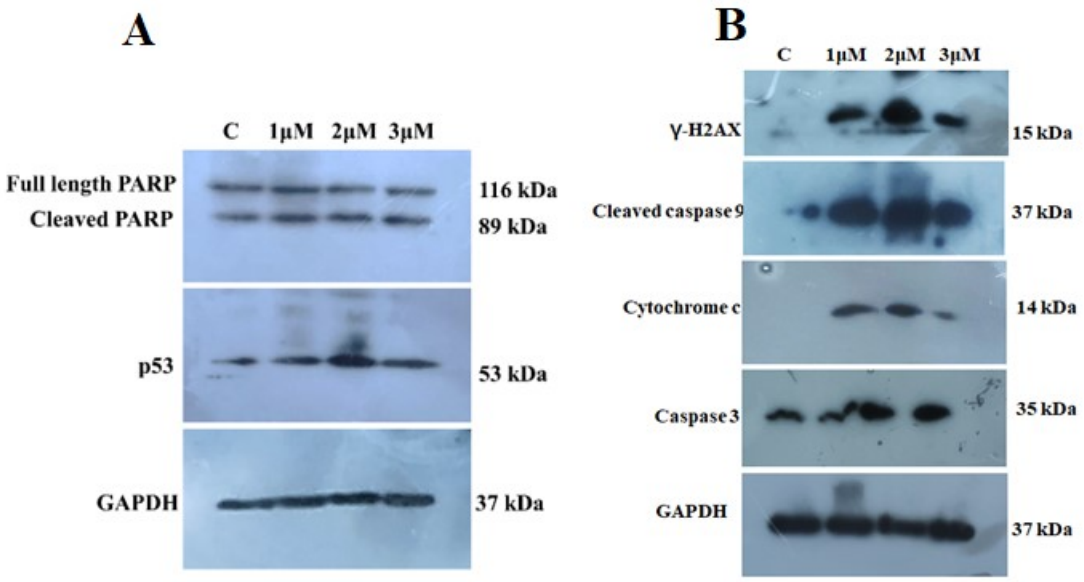

Fig. S7 Western blot detection of apoptotic protein expression after treatment with complex **1** (1, 2 and 3 μM) for 24 h. (A) PARP, p53. (B) Gamma H2AX, cleaved caspase 9, cytochrome c, caspase 3. GAPDH was used as loading control for all.