NMR Spectra

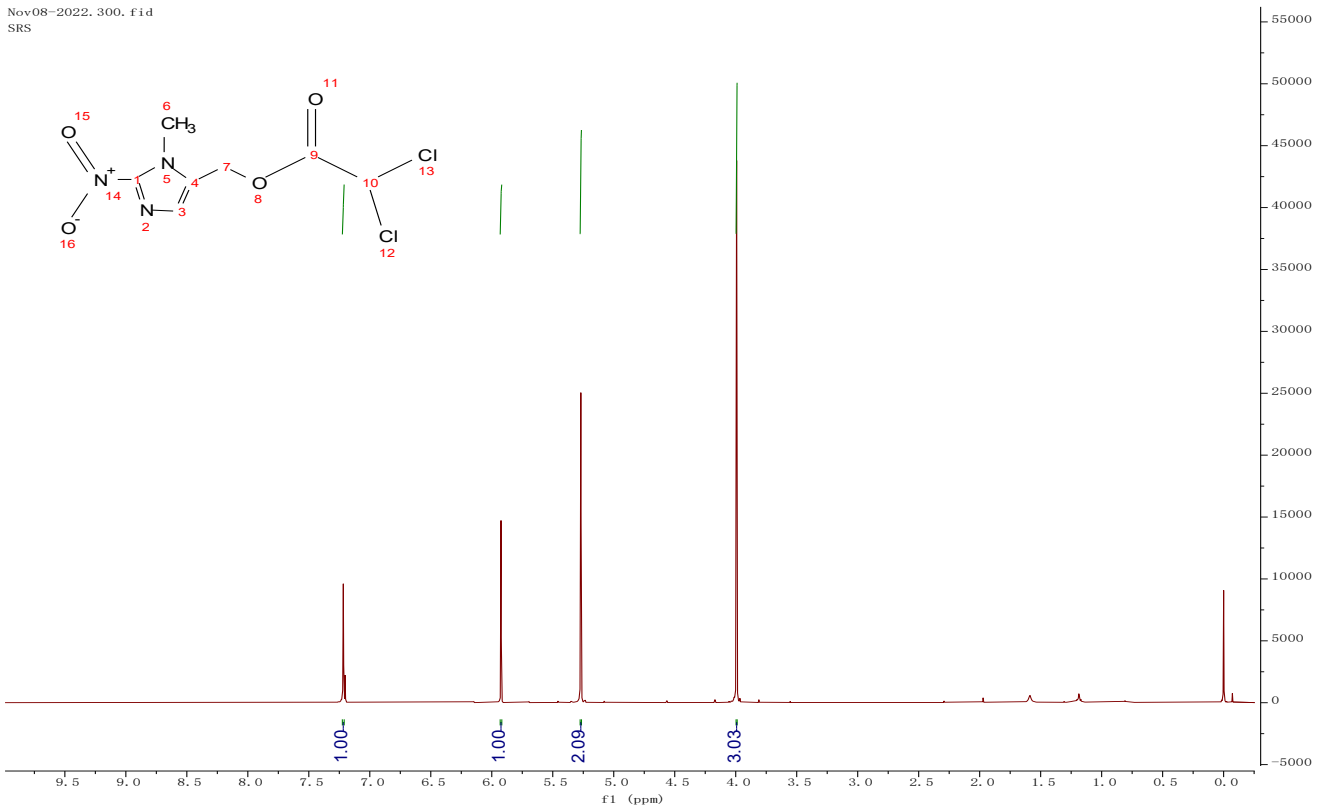


Fig. S1 ^{1}H NMR spectrum of **NIM-DCA**.

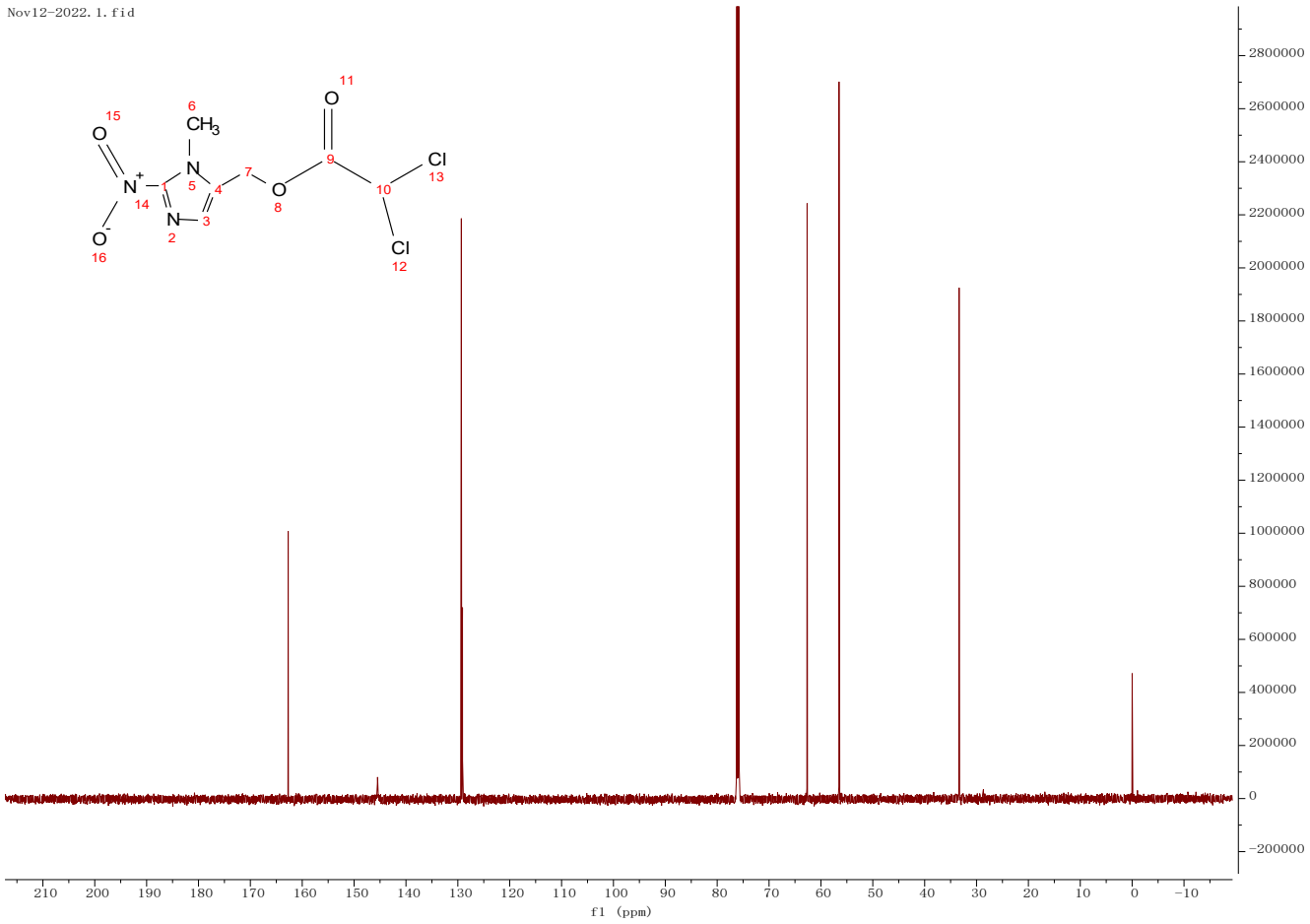
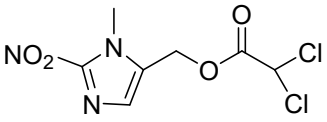


Fig. S2 ^{13}C NMR spectrum of **NIM-DCA**.

HRMS of Key Intermediates



Chemical Formula: $C_7H_7Cl_2N_3O_4$

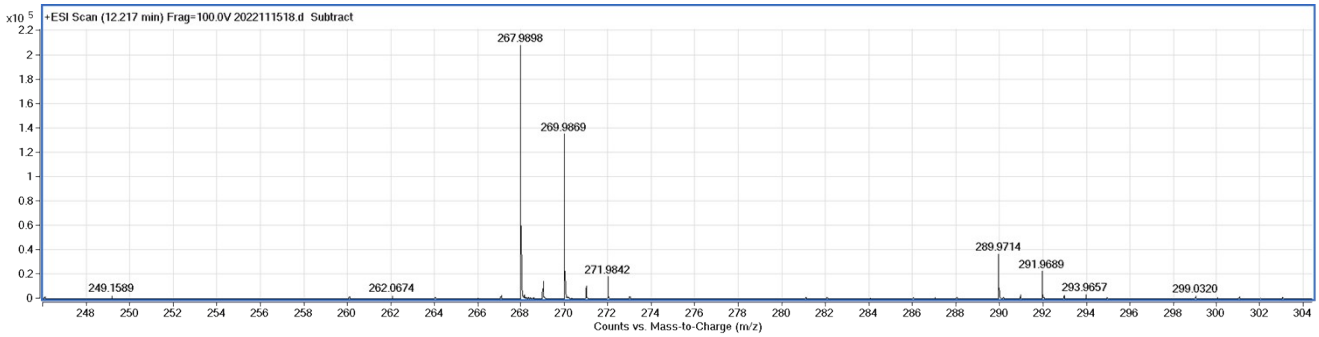


Fig. S3 HRMS of compound

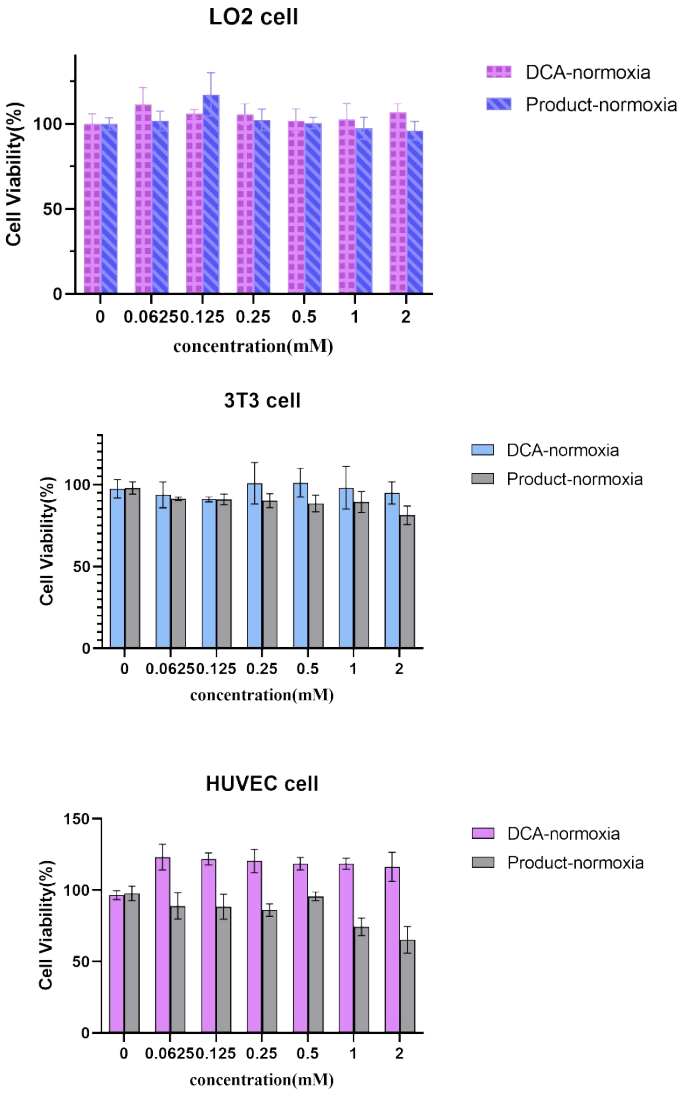


Fig. S4 Cell viability of LO2、NIH/3T3 and HUVEC fibroblast cells after incubation with various concentrations of DCA or **NIM-DCA** (product) under normoxia conditions for 24 hours.

Table S1. IC_{50} of NIM-DCA on tumor cells at 24h (mM)

Cell lines	Hela	MCF-7	HepG-2	4T1	A549	NCI-H1299	Sy5y
IC_{50}	0.9778	0.5441	0.2812	0.3992	0.214	0.6295	0.758

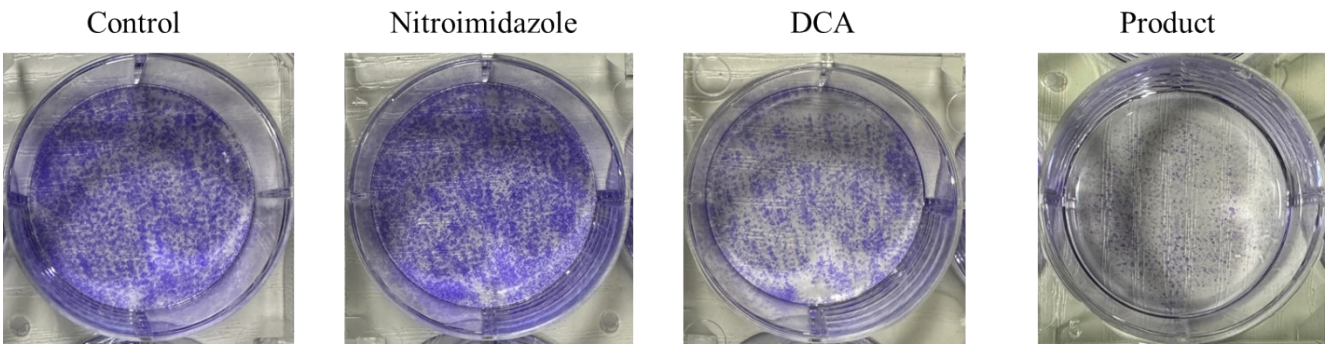


Figure S5. Colony formation assay images of A549 cells with the treatment of Control, Nitroimidazole (**HM-NIM**), DCA and Product (**NIM-DCA)** under hypoxia conditions.

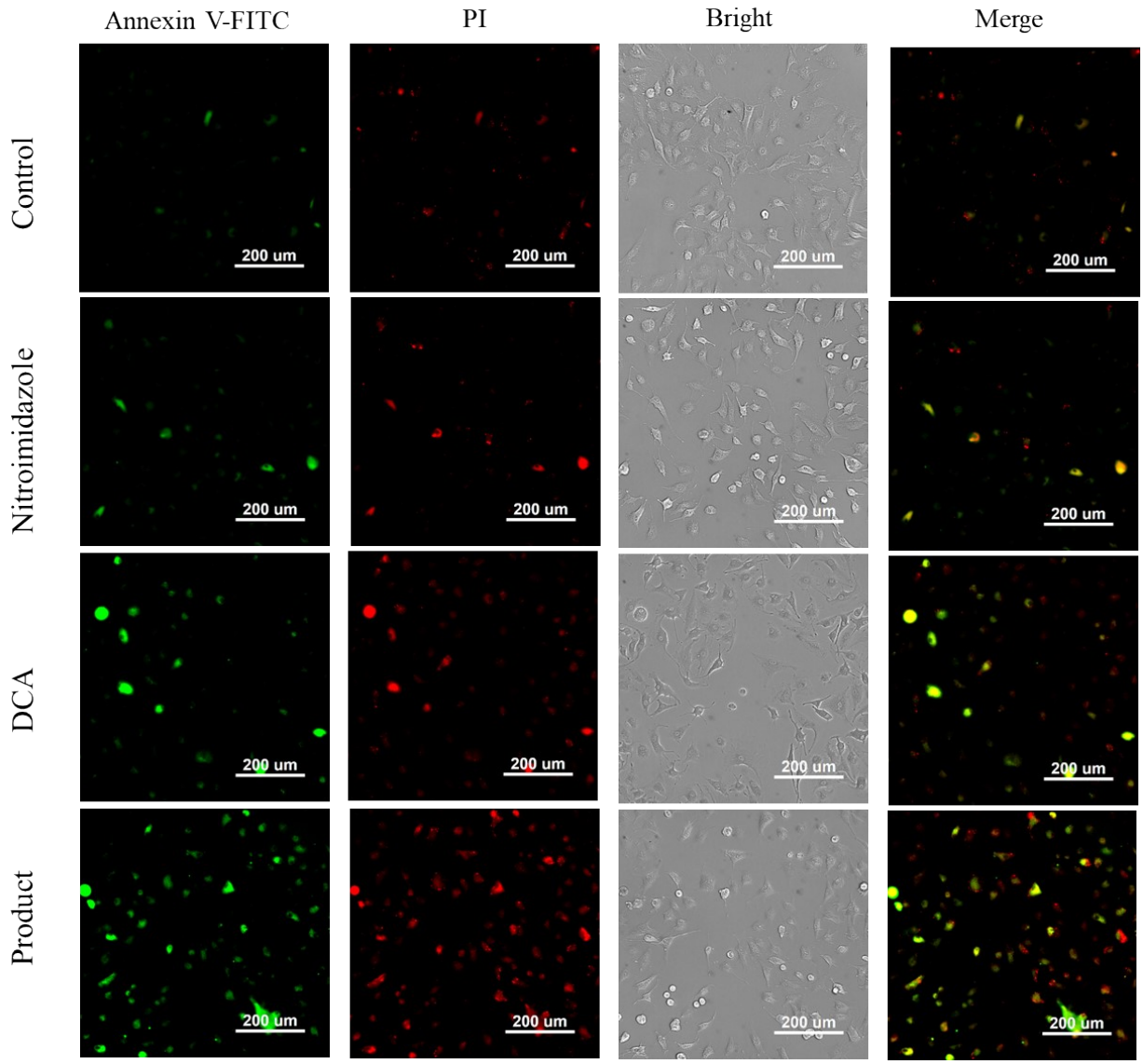


Figure S6. Confocal fluorescence images of A549 cells with the treatment of Control (blank), Nitroimidazole (**HM-NIM**), DCA and Product (**NIM-DCA**) under hypoxia conditions.

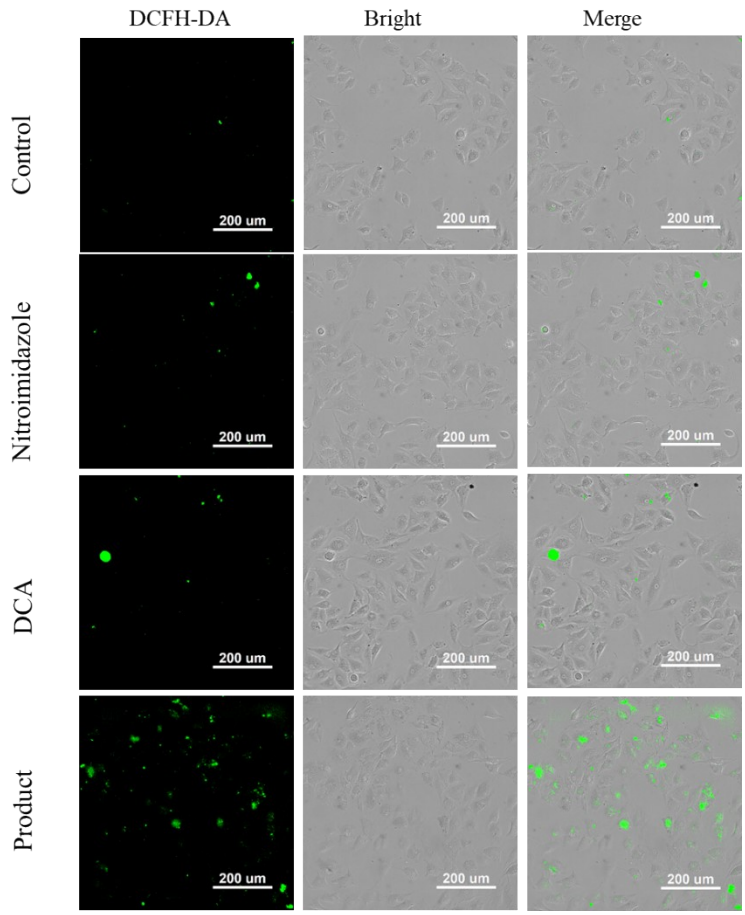


Figure S7. ROS production of A549 cells under hypoxic conditions when incubated with Control (blank), Nitroimidazole (**HM-NIM**), DCA and Product (**NIM-DCA**). Fluorescent probe used is DCFH-DA.

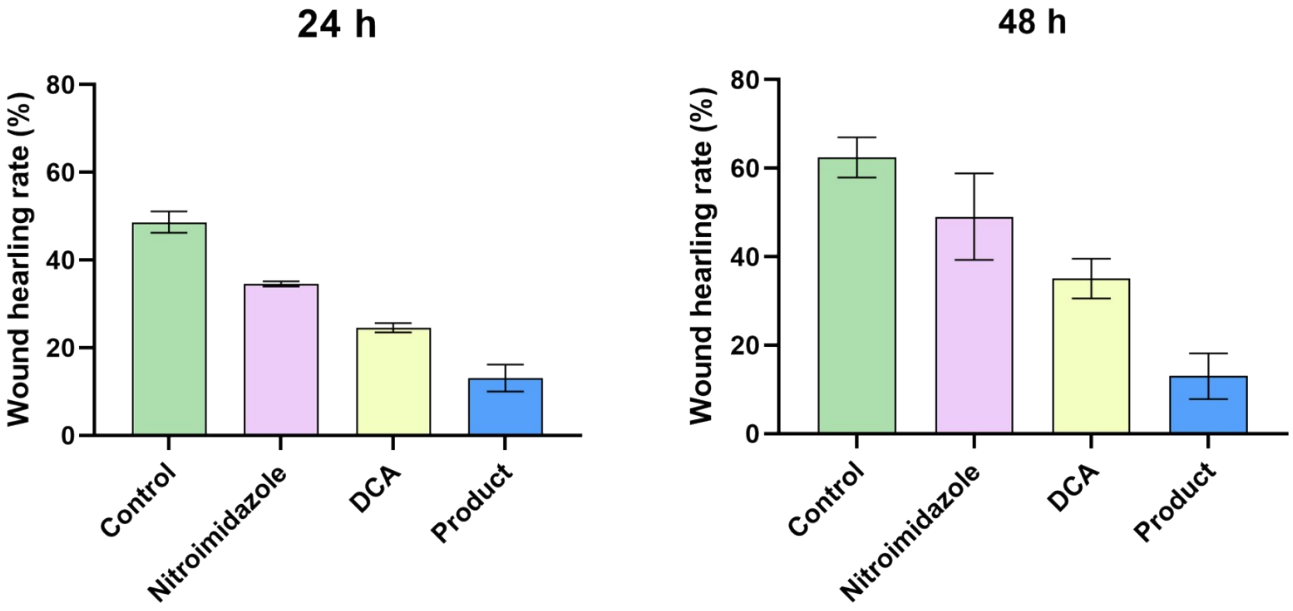


Figure S8. In vitro wound healing assay of with Control (blank), Nitroimidazole (**HM-NIM**), DCA and Product (**NIM-DCA**) using A549 cells. The wound healing rates of each group under hypoxia condition after 24 h and 48 h treatment.