Supplementary material

Simple avarone mimetics as selective agents against multidrug resistant cancer cells

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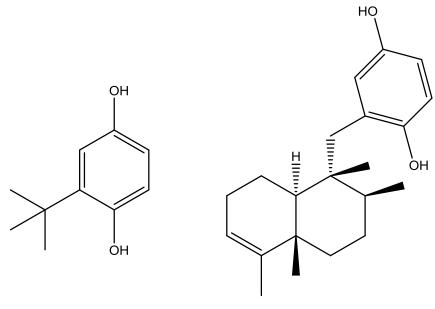
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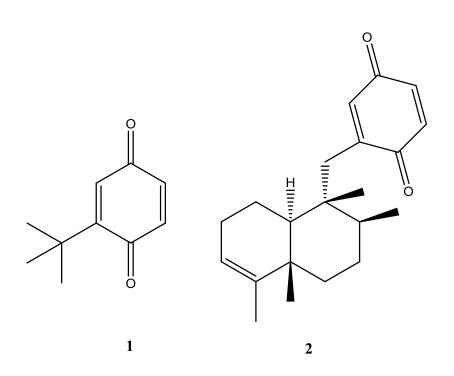
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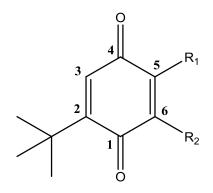
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tert-Butylhydroquinone (TBHQ)

Avarol



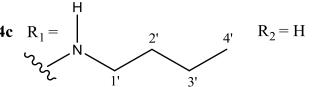


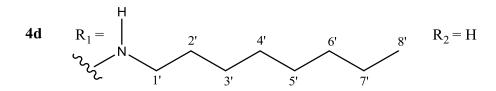
$$3a \qquad R_1 = H \qquad R_2 = NHMe$$

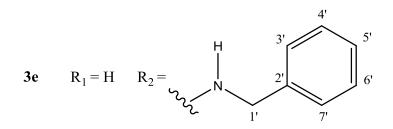
$$4a R_1 = NHMe R_2 = H$$

3b
$$R_1 = H$$
 $R_2 = \bigcup_{N=1}^{H} 2^{N}$ 4b $R_1 = \bigcup_{N=1}^{N} 2^{N}$

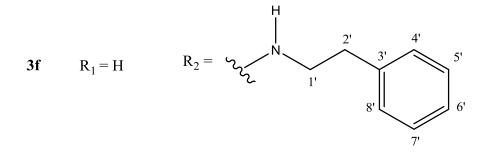
4b
$$R_1 = \bigcup_{N=1}^{n} P_1 = P_1$$

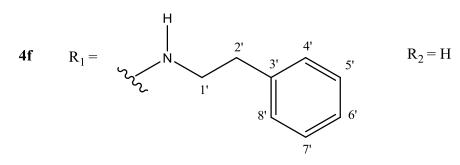


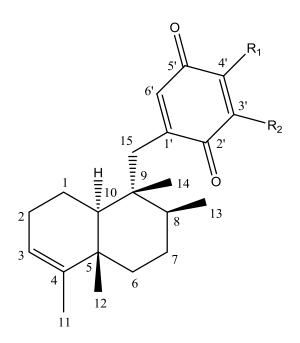


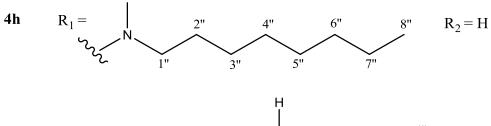


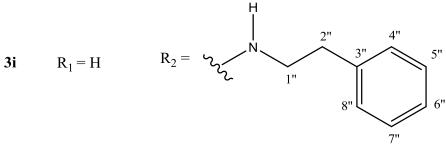
4e
$$R_1 = \begin{pmatrix} H & 3' \\ & & \\ &$$





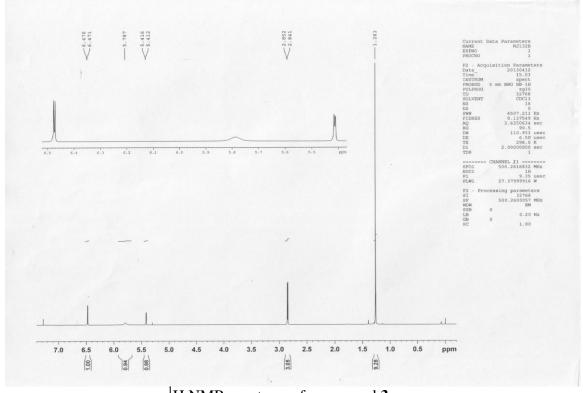




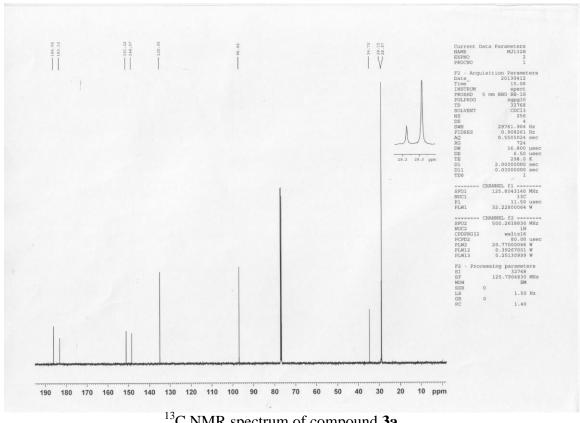


4i
$$R_1 = \frac{1}{N} \frac{2}{1} \frac{4}{3} \frac{4}{6}$$
 $R_2 = H$

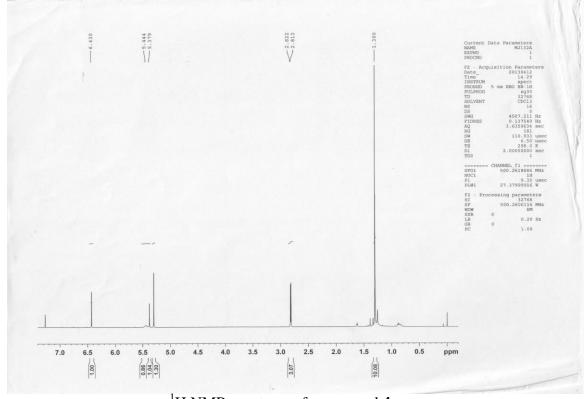
Scheme S1



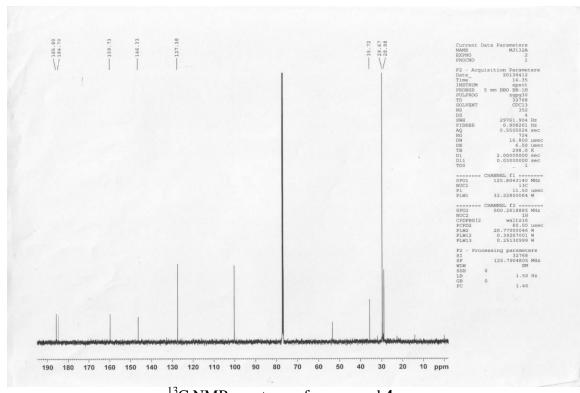
¹H NMR spectrum of compound **3a**



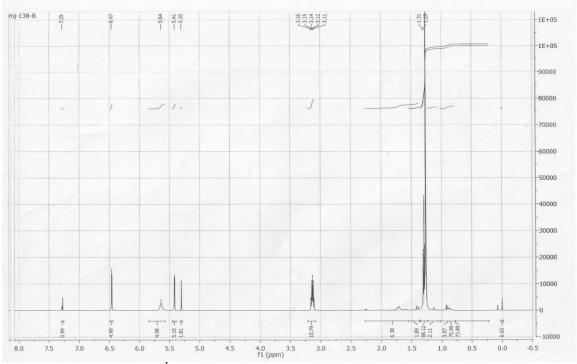
¹³C NMR spectrum of compound **3a**



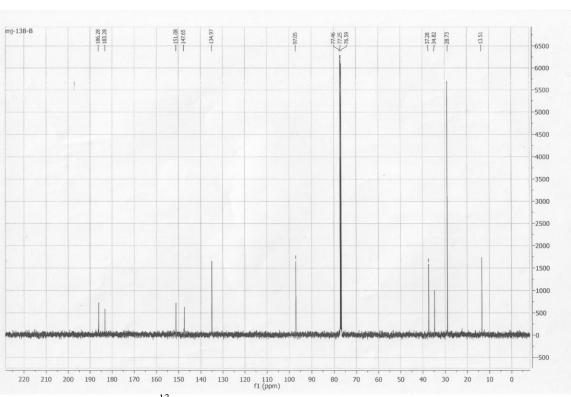
¹H NMR spectrum of compound **4a**



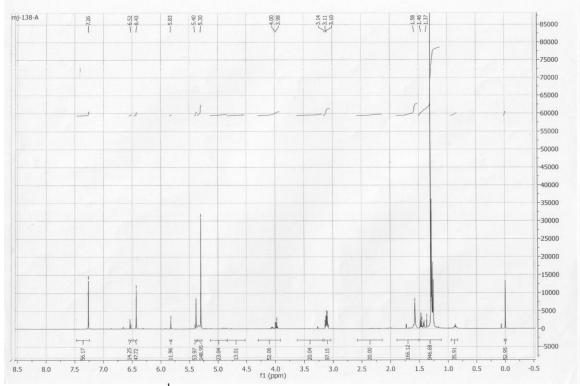
¹³C NMR spectrum of compound **4a**



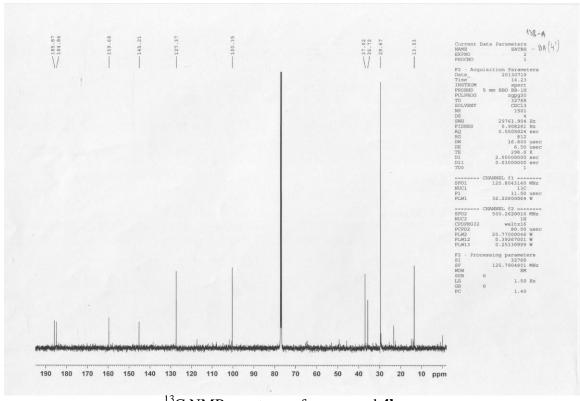
¹H NMR spectrum of compound **3b**



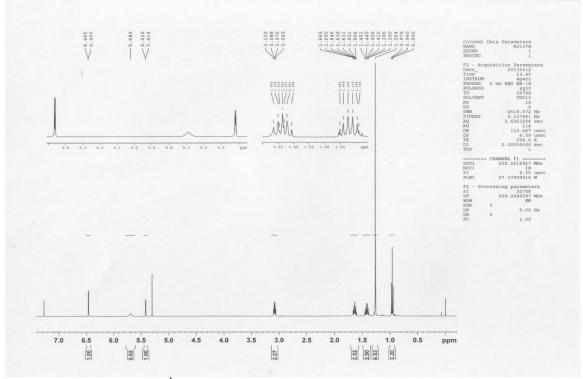
¹³C NMR spectrum of compound **3b**



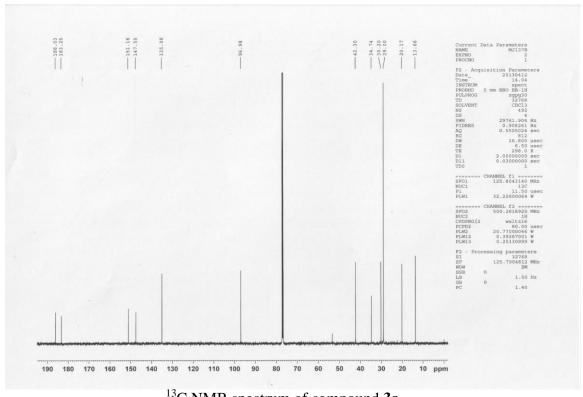
¹H NMR spectrum of compound **4b**



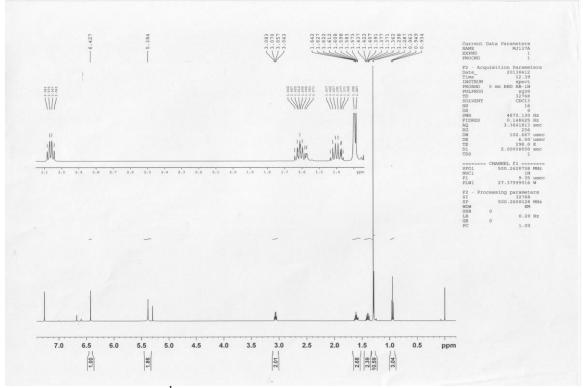
¹³C NMR spectrum of compound **4b**



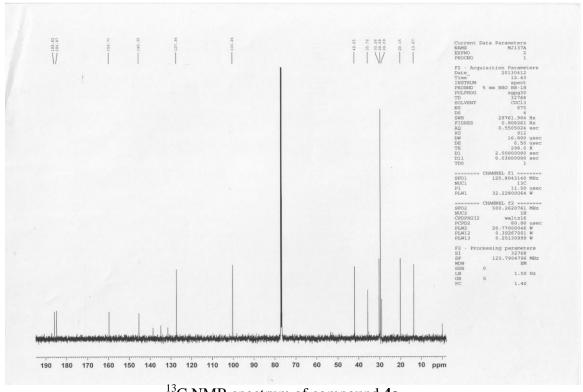
¹H NMR spectrum of compound **3c**



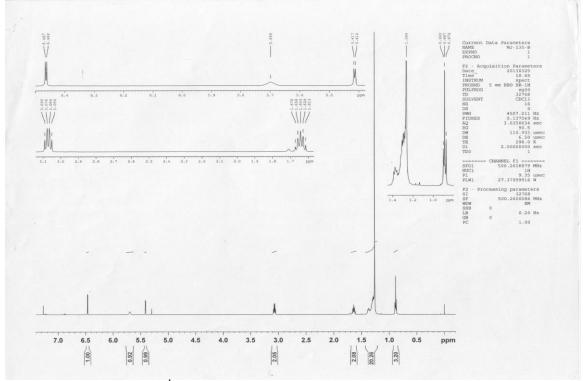
 13 C NMR spectrum of compound 3c



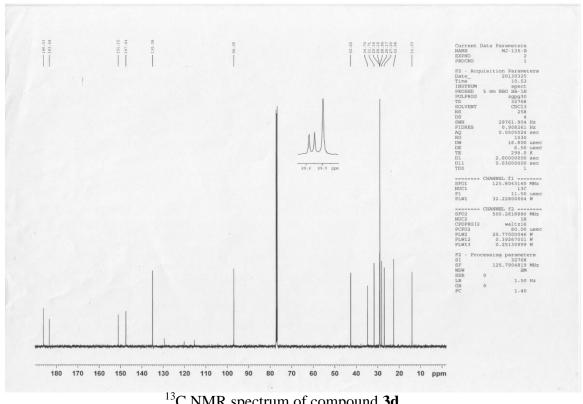
¹H NMR spectrum of compound **4c**



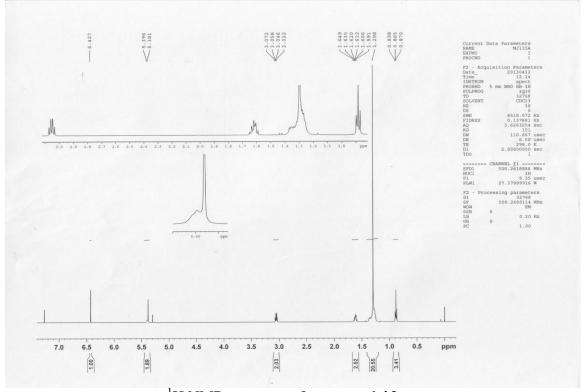
 13 C NMR spectrum of compound 4c



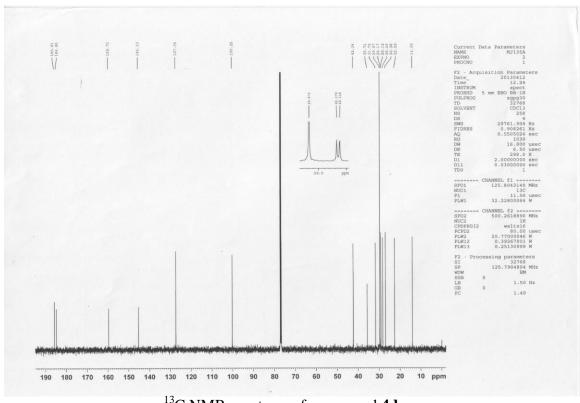
¹H NMR spectrum of compound **3d**



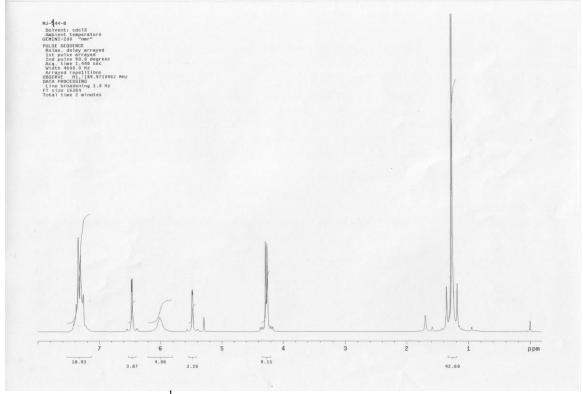
¹³C NMR spectrum of compound **3d**



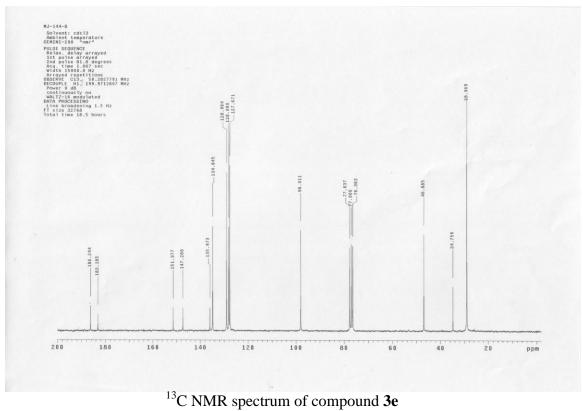
¹H NMR spectrum of compound **4d**

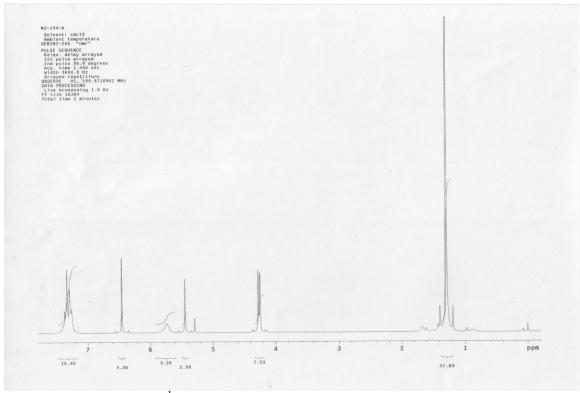


¹³C NMR spectrum of compound **4d**

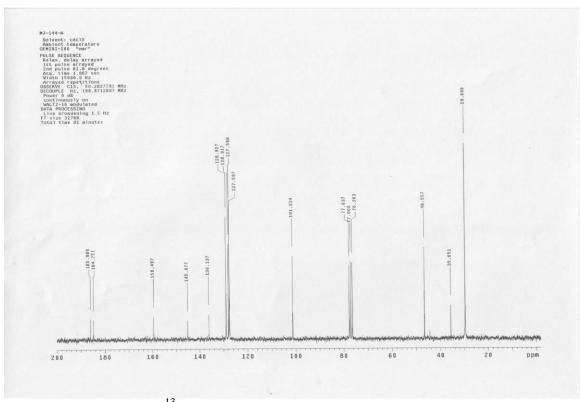


¹H NMR spectrum of compound **3e**

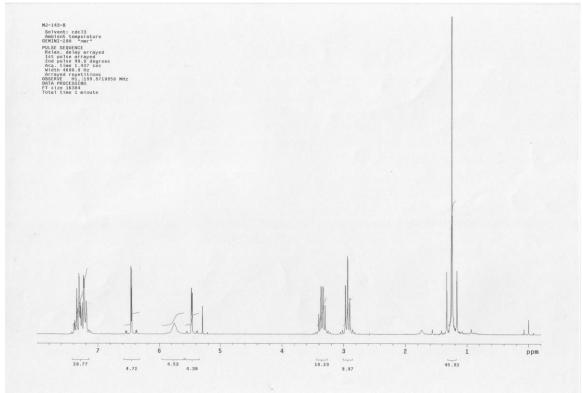




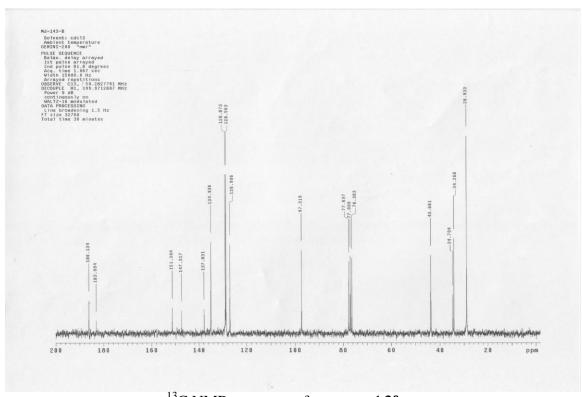
¹H NMR spectrum of compound **4e**



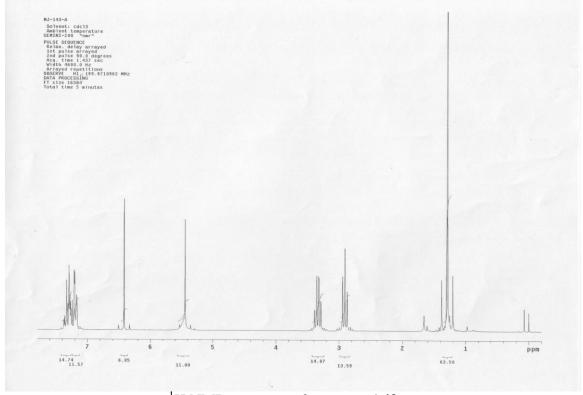
¹³C NMR spectrum of compound **4e**



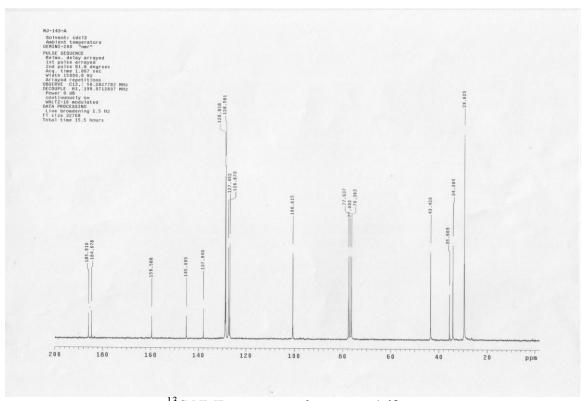
¹H NMR spectrum of compound **3f**



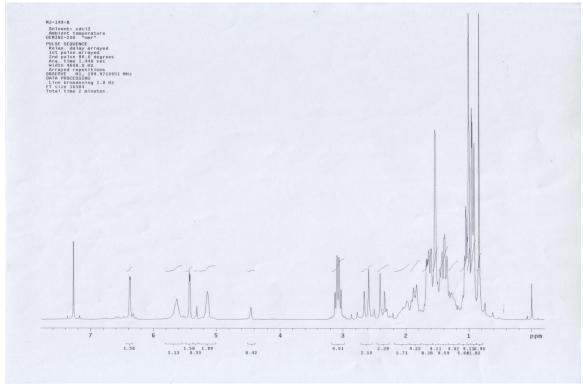
¹³C NMR spectrum of compound **3f**



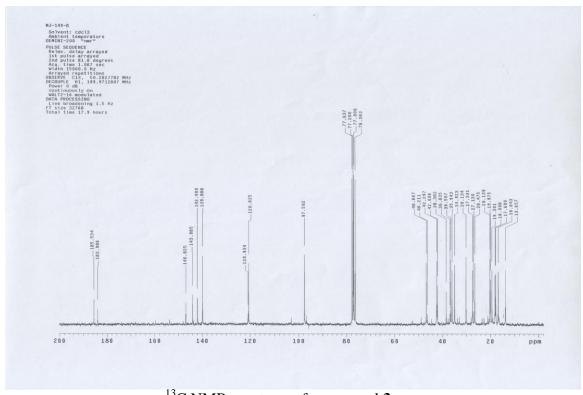
¹H NMR spectrum of compound **4f**



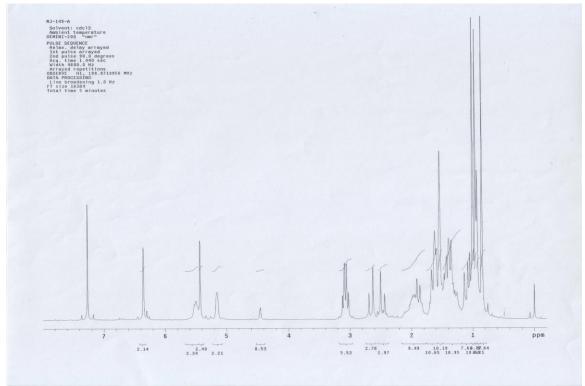
¹³C NMR spectrum of compound **4f**



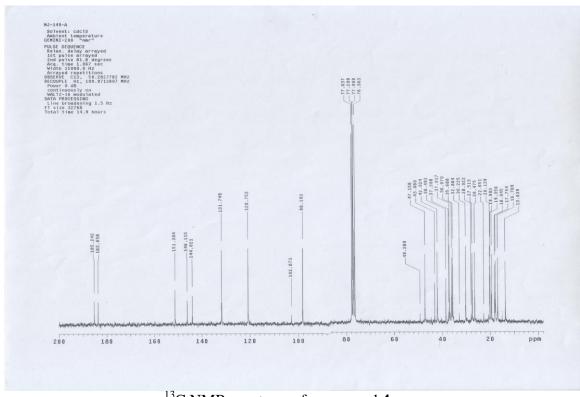
¹H NMR spectrum of compound **3g**



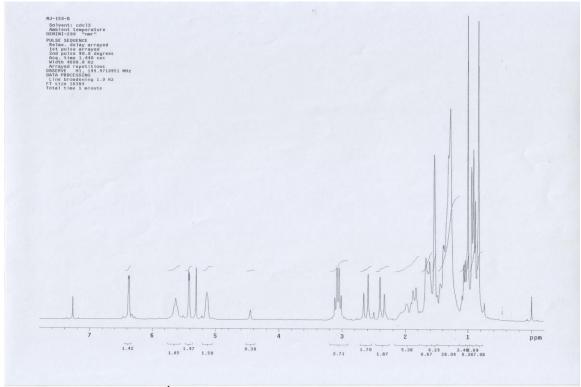
¹³C NMR spectrum of compound **3g**



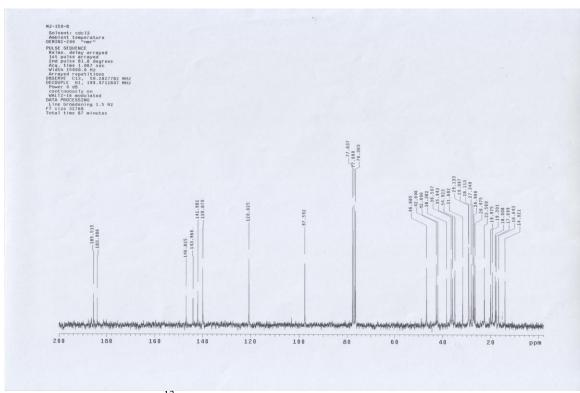
¹H NMR spectrum of compound **4g**



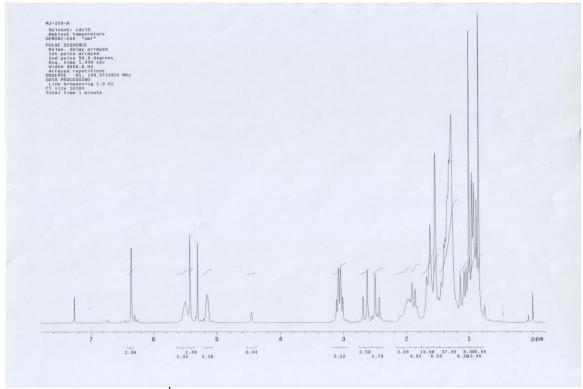
¹³C NMR spectrum of compound **4g**



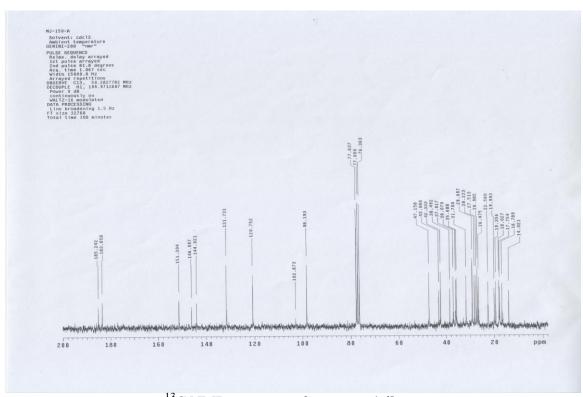
¹H NMR spectrum of compound **3h**



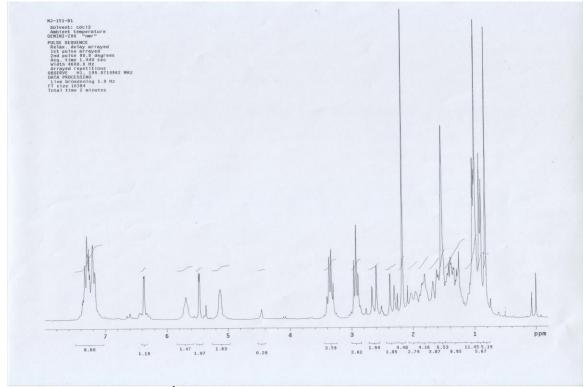
¹³C NMR spectrum of compound **3h**



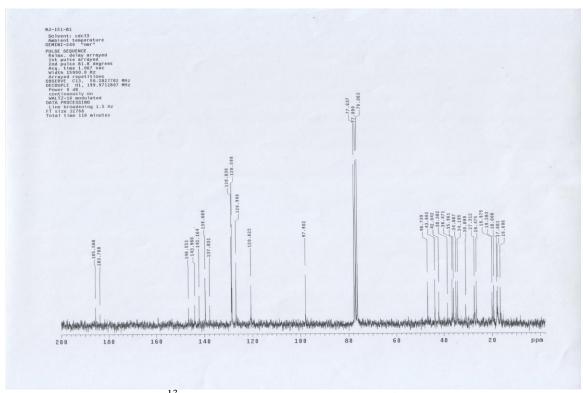
¹H NMR spectrum of compound **4h**



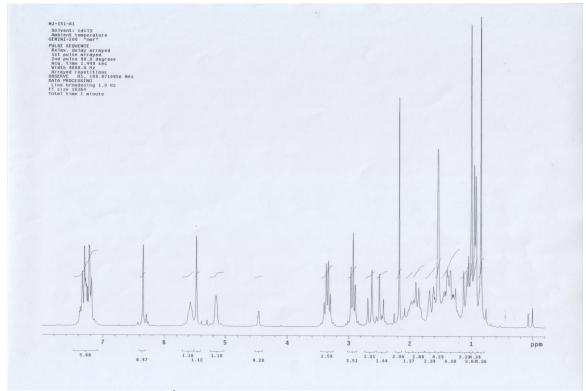
¹³C NMR spectrum of compound **4h**



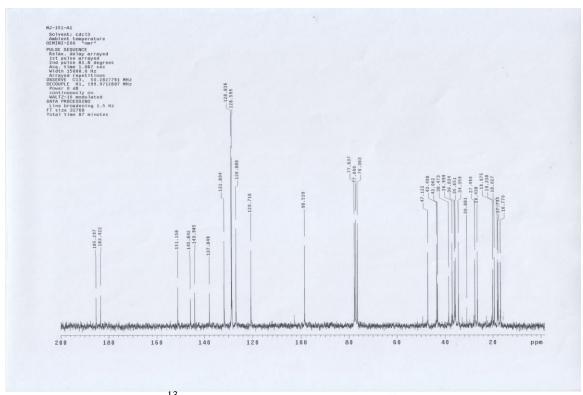
¹H NMR spectrum of compound **3i**



¹³C NMR spectrum of compound **3i**



¹H NMR spectrum of compound **4i**



¹³C NMR spectrum of compound **4i**

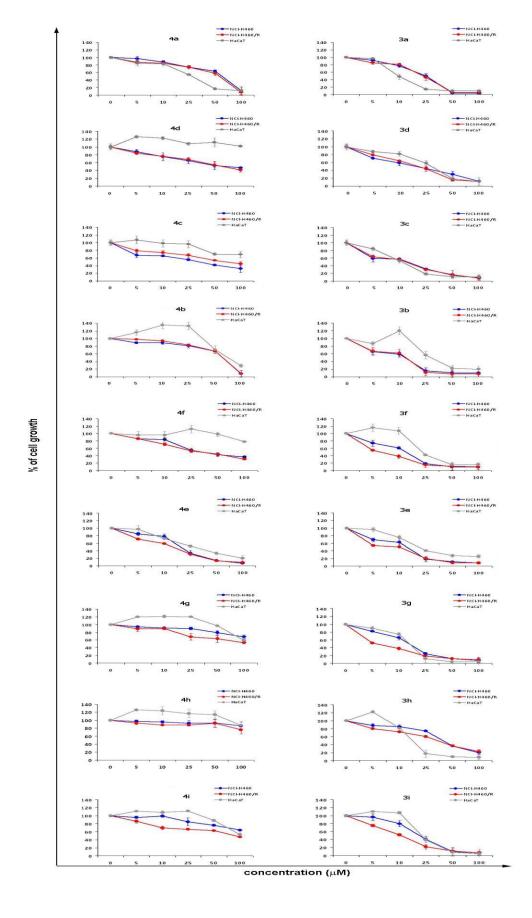
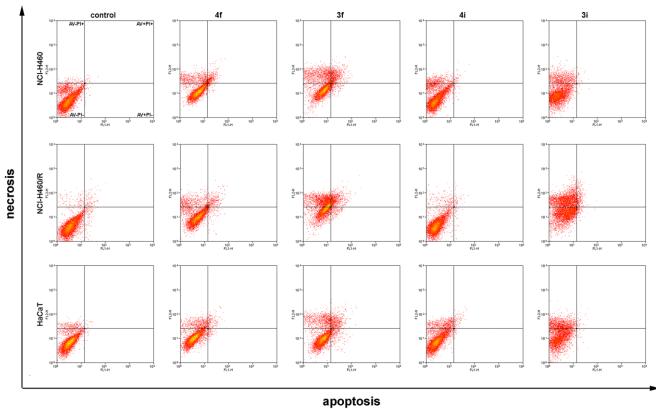
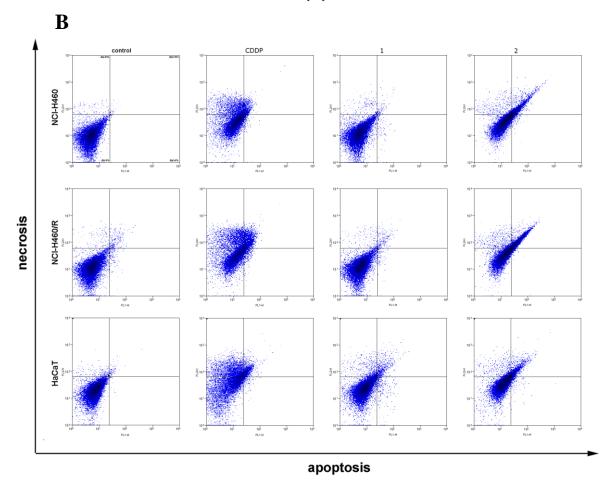


Figure S1. Cell growth inhibition by avarone, TBQ and their derivatives. Inhibitory potential of 18 compounds was studied in NCI-H460, NCI-H460/R and HaCaT cells after 72 h using MTT assay.









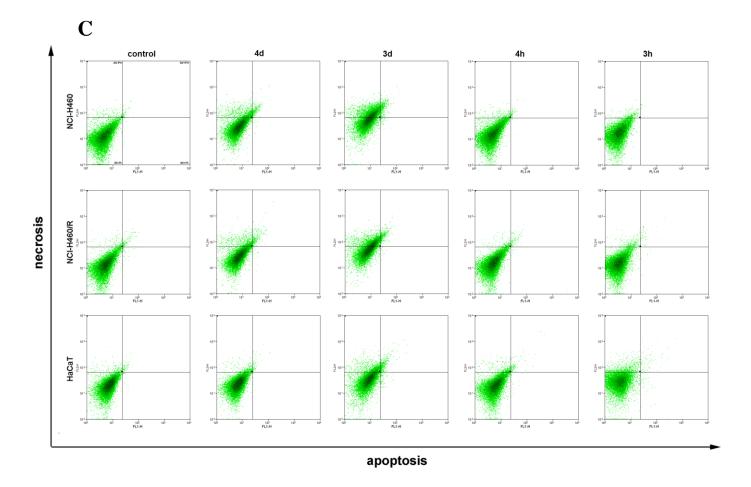


Figure S2 (A, B, C). Cell death induction by avarone, TBQ, their quinone mimetics and CDDP. The type of cell death investigated in NCI-H460, NCI-H460/R and HaCaT cells after 72 h by flow cytometry (AV/PI staining). The assay distinguishes viable cells (AV-PI-), apoptotic cells (AV+PI-), late apoptotic and necrotic cells (AV+PI+) and secondary necrotic or dead cells (AV-PI+).