Electronic Supplementary Material (ESI) for New Journal of Chemistry.

An alternative Mechanism of Action for the Apoptotic Activity of Terpenoid-like Chalcone Derivatives

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Suplementar material

Table S1. Molecular mass calculated and exact molecular mass.

Compound	Calculated Molecular mass	Exact molecular mass
I	298,1733	298,1827
II	314,1437	314,1567
III	358,0932	358,1058
IV	325,1678	325,1791

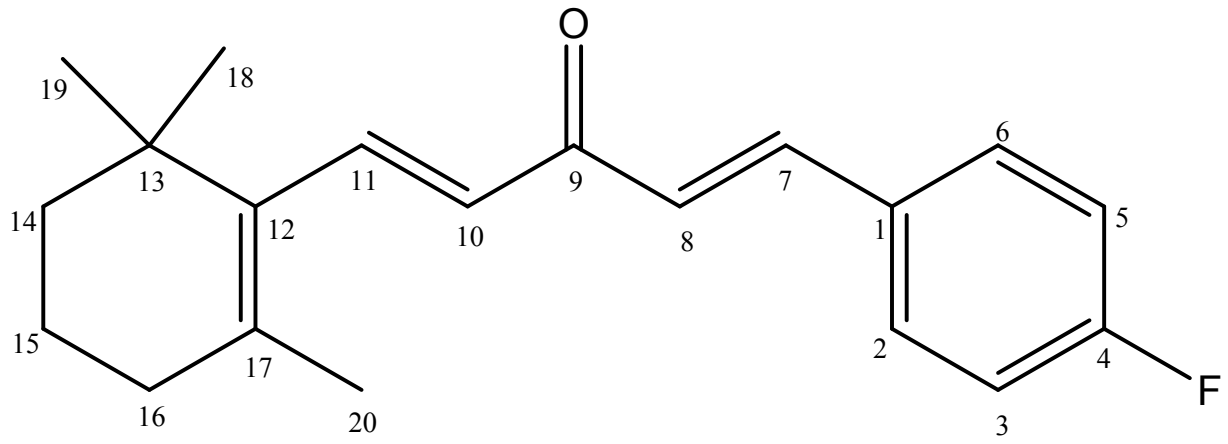


Figure S1. Numbering scheme used for the spectroscopic characterization

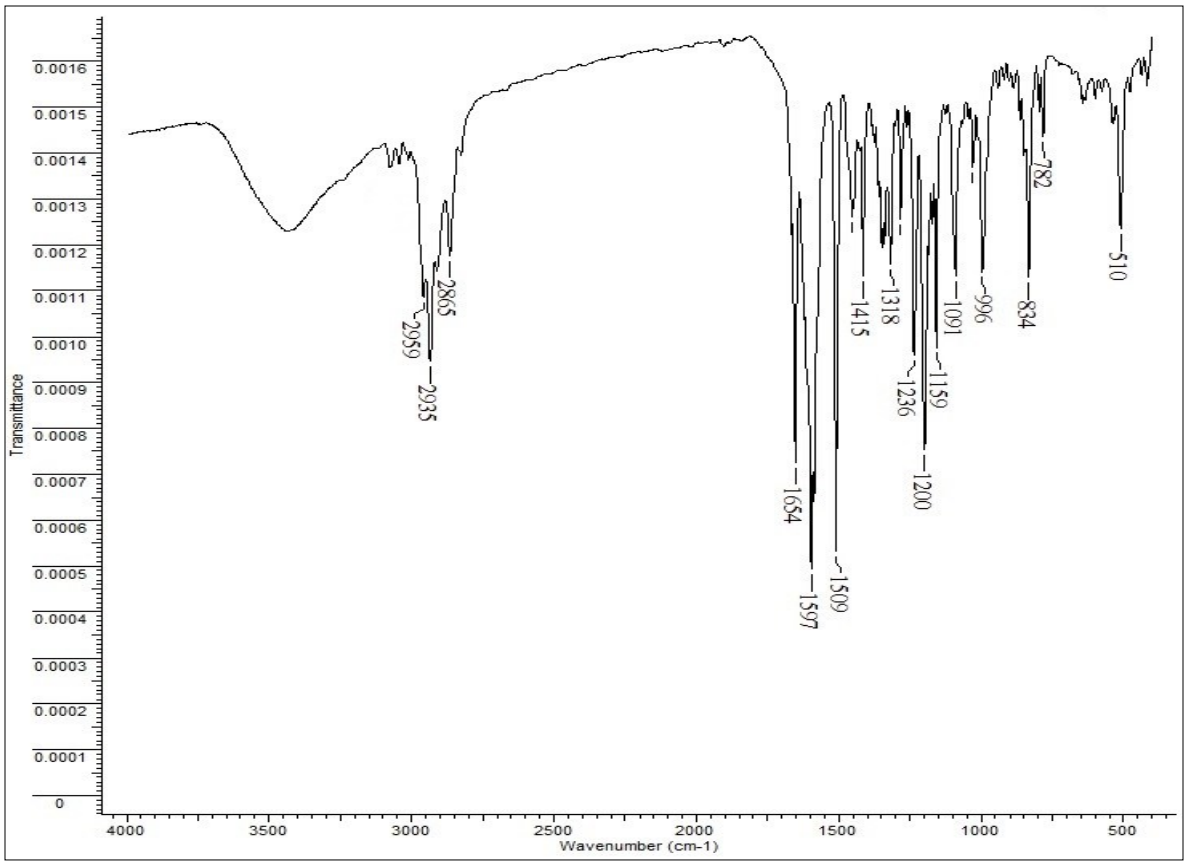


Figure S2. IR spectrum of compound **I** ((1*E*,4*E*)-1-(4-fluorophenyl)-5-(2,6,6-trimethylcyclohex-1-enyl)penta-1,4-dien-3-one).

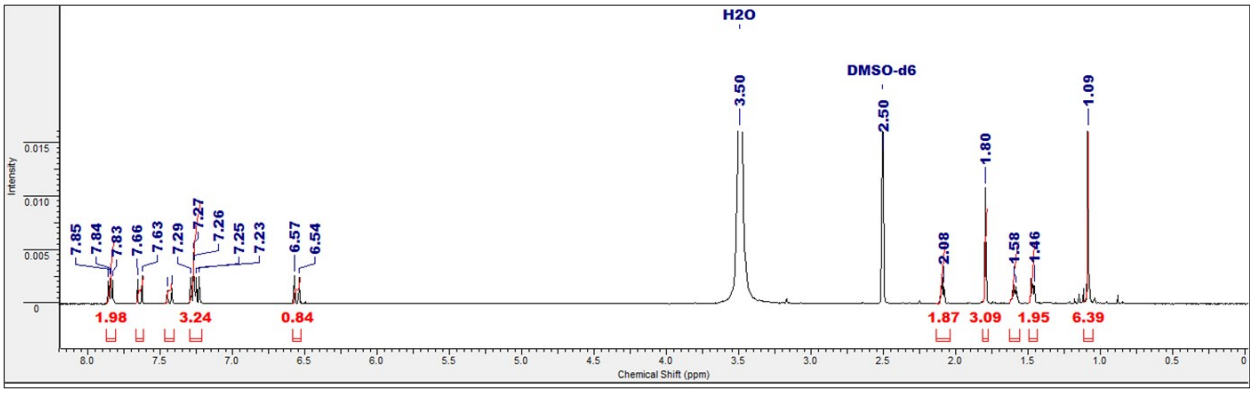


Figure S3. ^{1}H-NMR spectrum of compound **I** ((1*E*,4*E*)-1-(4-fluorophenyl)-5-(2,6,6-trimethylcyclohex-1-enyl)penta-1,4-dien-3-one).

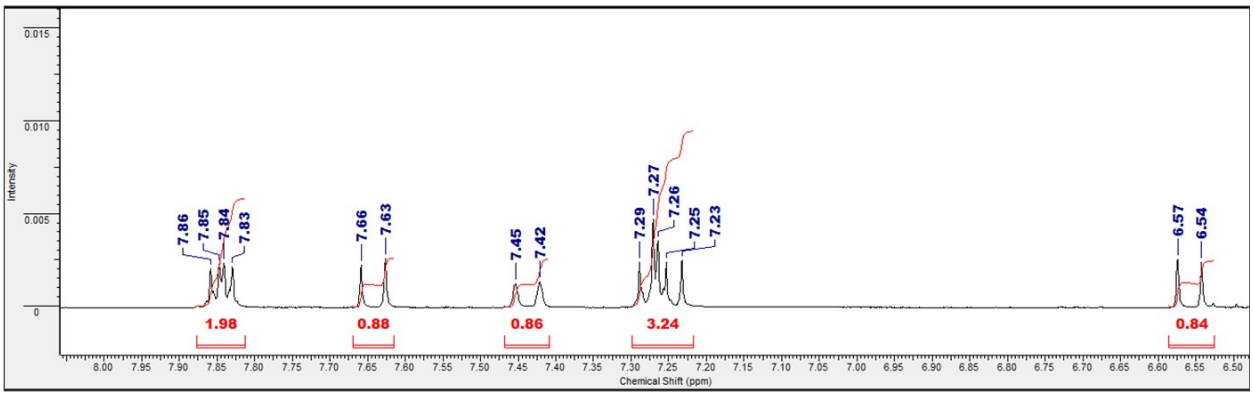


Figure S4. [1]H-NMR expanded spectrum of compound **I** ((1*E*,4*E*)-1-(4-fluorophenyl)-5-(2,6,6-trimethylcyclohex-1-enyl)penta-1,4-dien-3-one).

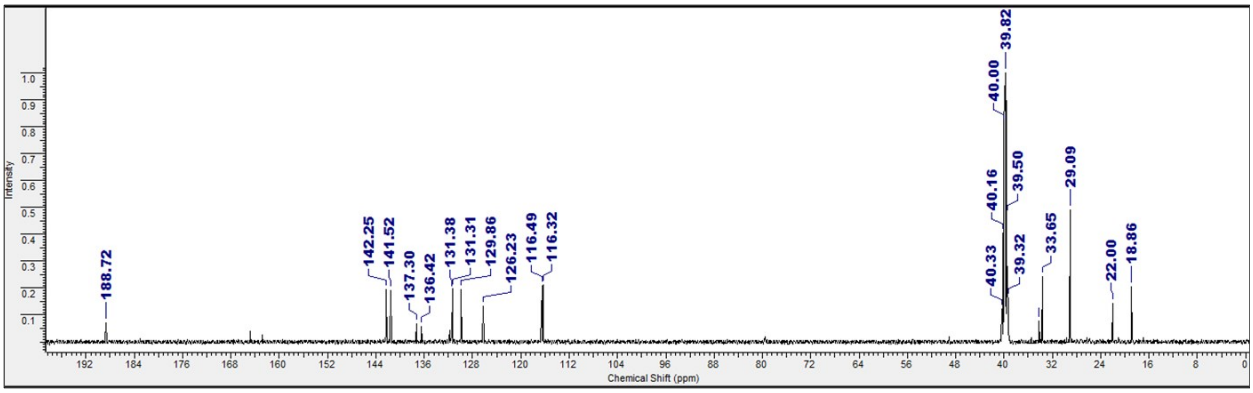


Figure S5. [13]C-NMR spectrum of compound **I** ((1*E*,4*E*)-1-(4-fluorophenyl)-5-(2,6,6-trimethylcyclohex-1-enyl)penta-1,4-dien-3-one).

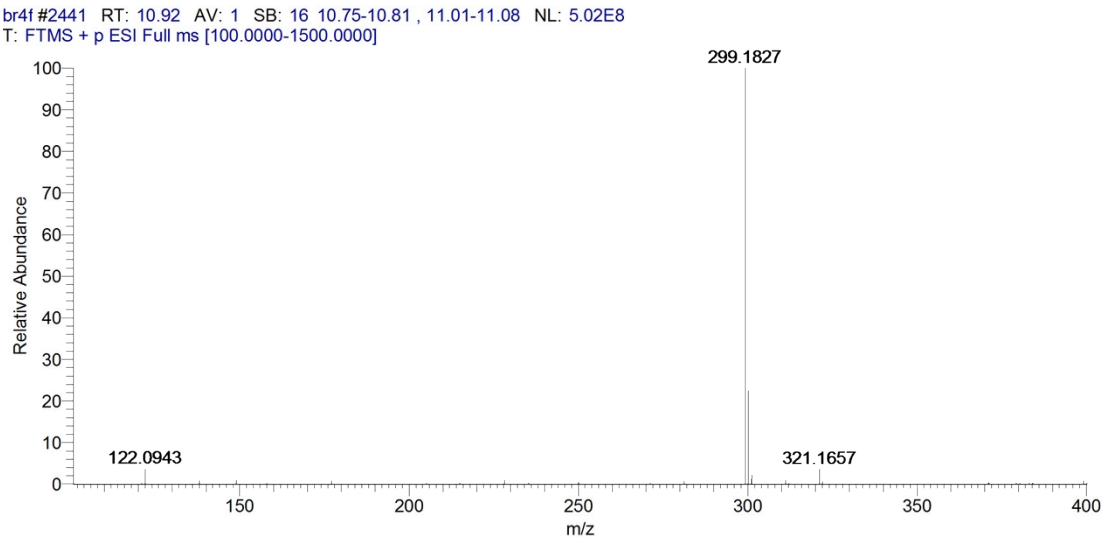
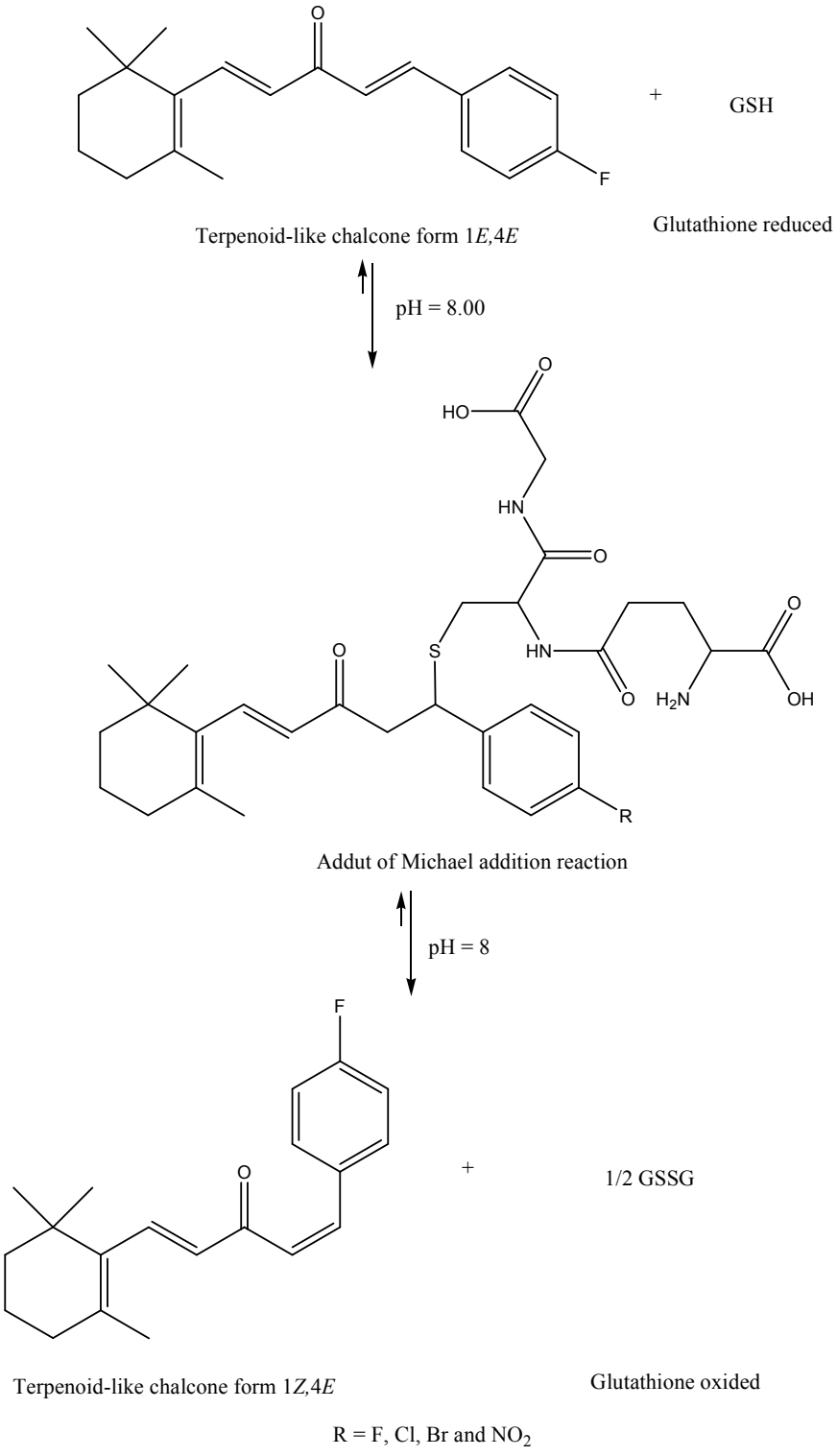


Figure S6. Mass spectrum of compound **I** ((1*E*,4*E*)-1-(4-fluorophenyl)-5-(2,6,6-trimethylcyclohex-1-enyl)penta-1,4-dien-3-one).

Target	Target Pref. Name	Organism	Confidence 70%	Confidence 80%	Confidence 90%	Activity Threshold
CHEMBL2390810	Microtubule-associated protein 2	Homo sapiens	empty	active	active	6
CHEMBL2283	Carbonic anhydrase II	Bos taurus	empty	active	both	6
CHEMBL1907591	Neuronal acetylcholine receptor; alpha4/beta4	Homo sapiens	active	active	active	5
CHEMBL4556	Glycine transporter 1	Rattus norvegicus	empty	active	active	6
CHEMBL3922	Methionine aminopeptidase 2	Homo sapiens	active	active	active	6
CHEMBL5163	Sodium channel protein type III alpha subunit	Homo sapiens	active	active	active	5
CHEMBL4244	Legumain	Homo sapiens	empty	active	both	6.5
CHEMBL3891	Calpain 1	Homo sapiens	empty	active	both	6
CHEMBL2094116	Serotonin 3 (5-HT3) receptor	Rattus norvegicus	empty	active	both	6.5
CHEMBL3486	Dihydroorotate dehydrogenase	Plasmodium falciparum	empty	active	active	6
CHEMBL2411	Serotonin 3a (5-HT3a) receptor	Rattus norvegicus	empty	active	active	6.5
CHEMBL2304404	Adenosine A1 receptor	Cavia porcellus	active	active	active	6
CHEMBL3242	Carbonic anhydrase XII	Homo sapiens	empty	active	both	6
CHEMBL276	Muscarinic acetylcholine receptor M1	Rattus norvegicus	empty	active	active	7
CHEMBL2304402	Phosphodiesterase 5A	Canis lupus familiaris	active	active	active	6.5
CHEMBL2617	Tryptase beta-1	Homo sapiens	empty	active	active	6
CHEMBL2096680	Glutamate NMDA receptor; Grin1/Grin2a	Rattus norvegicus	empty	active	both	5
CHEMBL5285	Mitogen-activated protein kinase kinase 5	Homo sapiens	active	active	active	6.5
CHEMBL3368	Glucocorticoid receptor	Rattus norvegicus	active	active	both	7
CHEMBL3712907	Transmembrane domain-containing protein TMIGD3	Homo sapiens	active	active	active	6

Figure S7. Target predicted by ChemBL for compound **I**.



Scheme S1. Michael's addition reaction of GSH to retinoid-like chalcones tested.