

NMR-Based Chemical Profiling, Isolation and Evaluation of the Cytotoxic Potential of the Diterpenoid Siderol from Cultivated *Sideritis euboea* Heldr.

Ekaterina-Michaela Tomou¹, Maria V. Chatziathanasiadou², Paschalina Chatzopoulou³, Andreas G. Tzakos^{2,*} and Helen Skaltsa^{1,*}

¹Department of Pharmacognosy & Chemistry of Natural Products, School of Pharmacy, National and Kapodistrian University of Athens, Panepistimiopolis, Zografou, 15771, Athens, Greece; ktomou@pharm.uoa.gr; skaltsa@pharm.uoa.gr

²Department of Chemistry, Section of Organic Chemistry and Biochemistry, University of Ioannina, 45110, Ioannina, Greece; m.chatziathanasiadou@gmail.com; atzakos@uoi.gr

³Hellenic Agricultural Organization DEMETER, Institute of Breeding and Plant Genetic Resources, IBPGR, Department of Medicinal and Aromatic Plants, Thermi, 57001 Thessaloniki, Greece; xatzlin@yahoo.gr

Correspondence: atzakos@uoi.gr (A.G.T.); skaltsa@pharm.uoa.gr (H.S.); Tel./Fax.: +30 2107274593(H.S.)

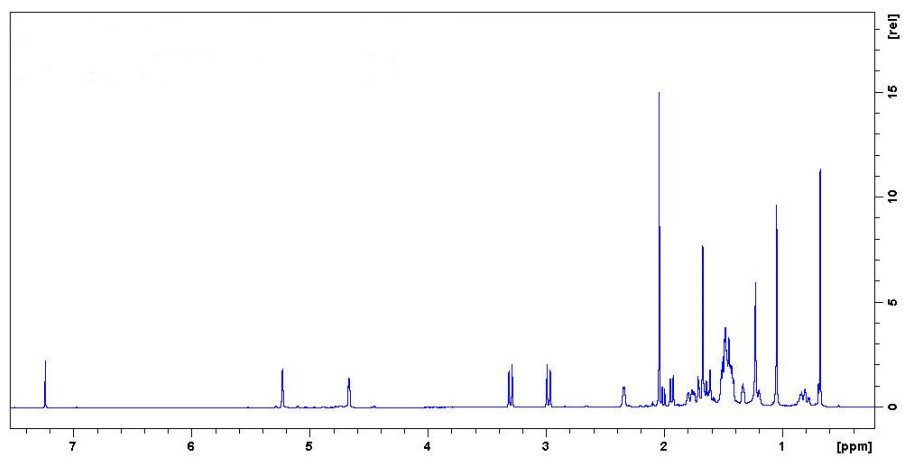


Figure S1. ^1H -NMR spectrum of compound **6** (CDCl_3 , 400 MHz) ($T=295\text{ K}$; number of scans, 16).

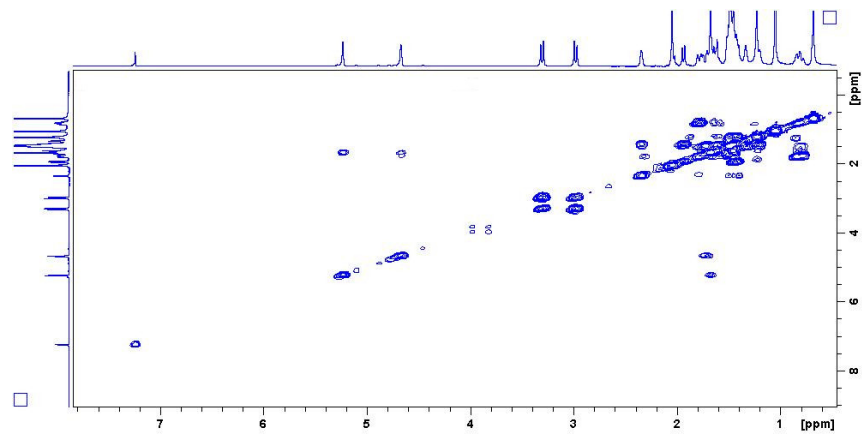


Figure S2. ^1H - ^1H COSY 2D spectrum of compound **6** (CDCl_3 , 400 MHz) ($T=295\text{ K}$, number of scans, 4).

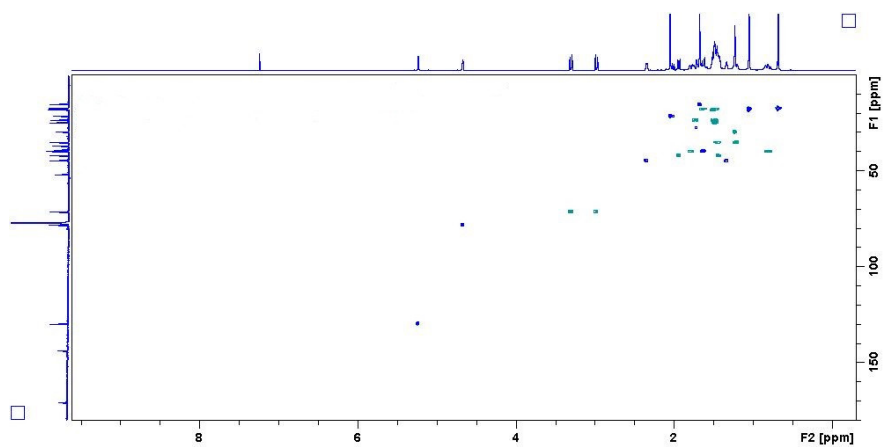


Figure S3. ^1H - ^{13}C HSQC 2D spectrum of compound **6** (CDCl_3 , 400 MHz) ($T=295$ K, number of scans, 20).

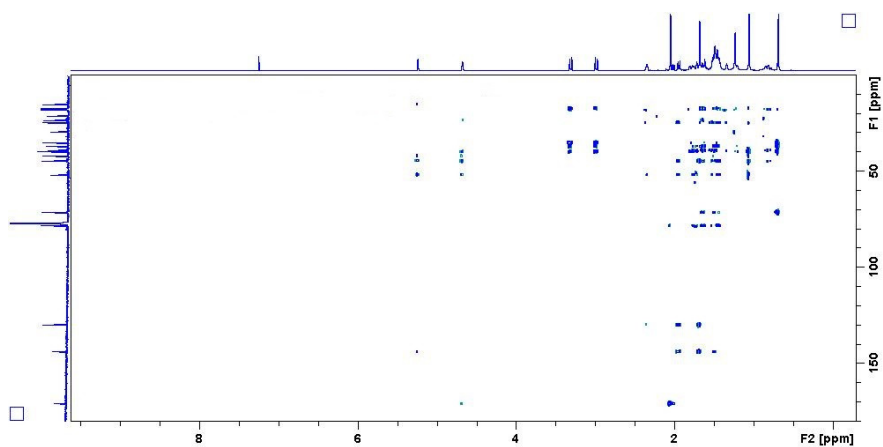


Figure S4. ^1H - ^{13}C HMBC 2D spectrum of compound **6** (CDCl_3 , 400 MHz) ($T=295$ K; number of scans, 48).

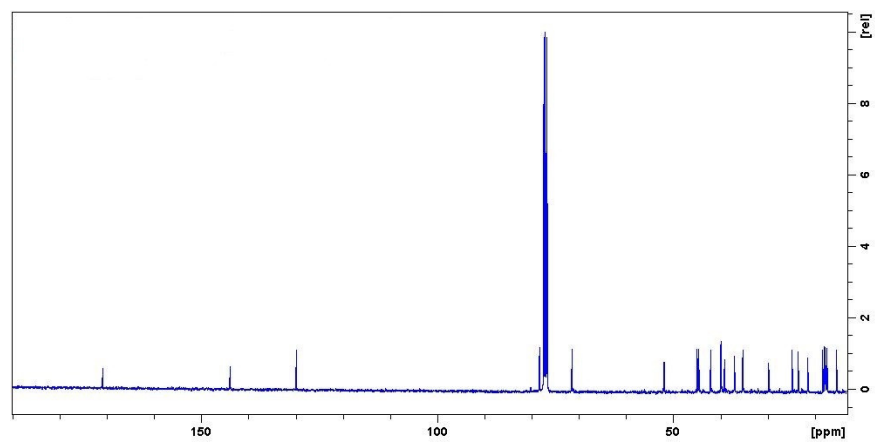


Figure S5. ¹³C-NMR spectrum of compound **6** (CDCl₃, 100.3 MHz) (T=295 K; number of scans, 9024).

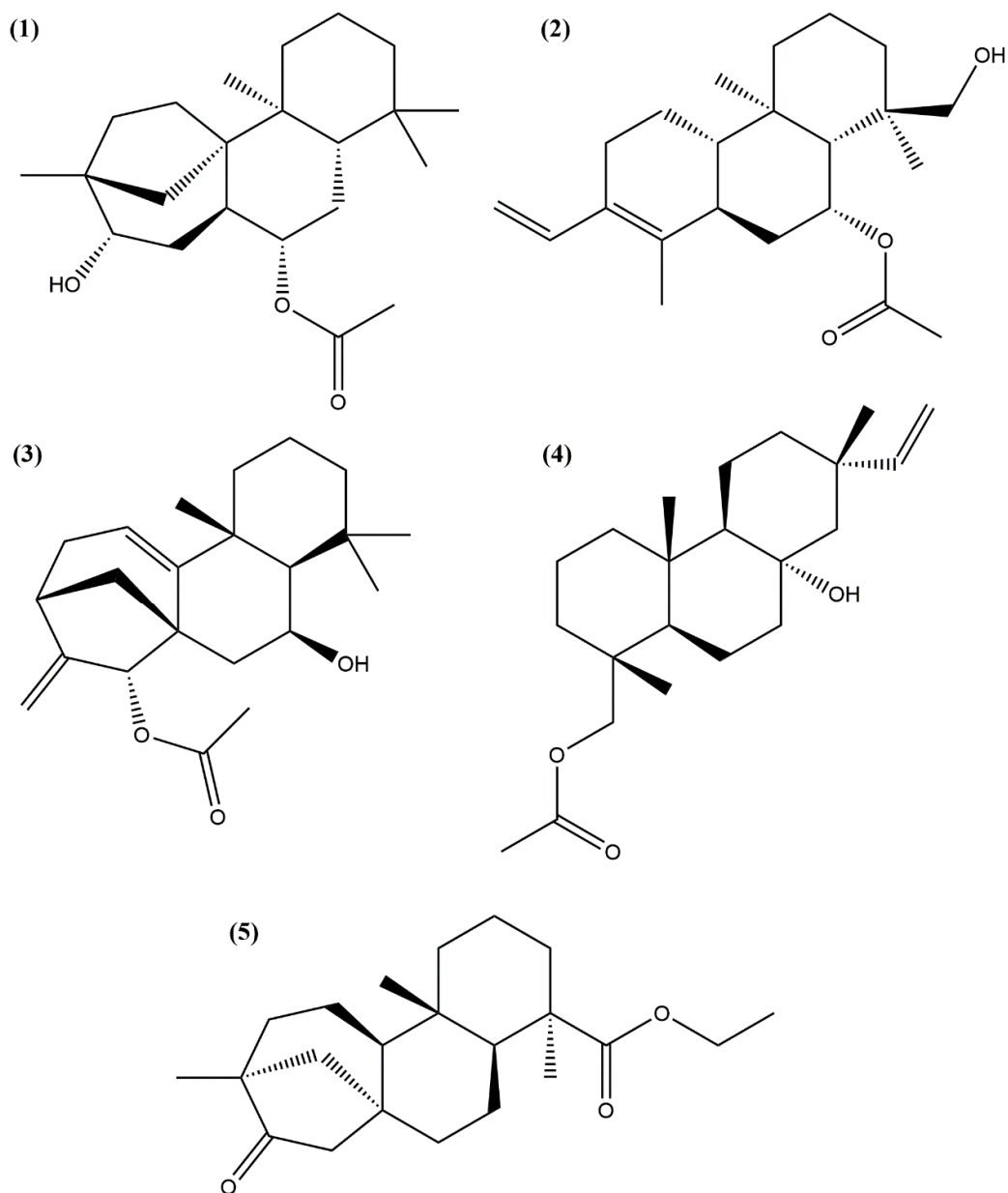


Figure S6. 2D Structures of (1) (4*aS*,6*S*,6*aS*,8*S*,9*R*,11*aS*,11*bS*)-8-hydroxy-4,4,9,11b-tetramethyltetradecahydro-9,11a-methanocyclohepta[*a*]naphthalen-6-yl acetate [CHEMBL494391], (2) (4*aS*,4*bR*,8*R*,8*aR*,9*R*,10*aR*)-8-(hydroxymethyl)-1,4*b*,8-trimethyl-2-vinyl-3,4,4*a*,4*b*,5,6,7,8,8*a*,9,10,10*a*-dodecahydrophenanthren-9-yl acetate [CHEMBL482794], (3) (4*aR*,5*S*,6*aS*,7*R*,9*R*,11*bR*)-5-hydroxy-4,4,11*b*-trimethyl-8-methylene-1,2,3,4,4*a*,5,6,7,8,9,10,11*b*-dodecahydro-6*a*,9-methanocyclohepta[*a*]naphthalen-7-yl acetate [CHEMBL448113], (4) ((1*R*,4*aS*,4*bR*,7*S*,8*aS*,10*aR*)-8*a*-hydroxy-1,4*a*,7-trimethyl-7-vinyltetradecahydrophenanthren-1-yl)methyl acetate [CHEMBL509521] and (5) ethyl (4*R*,4*aS*,6*aR*,9*S*,11*aR*,11*bS*)-4,9,11*b*-trimethyl-8-oxotetradecahydro-6*a*,9-methanocyclohepta[*a*]naphthalene-4-carboxylate [CHEMBL455441]