Electronic Supporting Information

Discovery of New Series of Jatrophane and Lathyrane Diterpenes as Potent and Specific P-Glycoprotein Modulators†

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†1H NMR spectra for compounds 1–8, purity criteria for isolated compounds, and minimum energy conformations obtained for each stereoisomers of 1.

Contents
S2-S9 1H NMR spectra for compounds 1-8
S10 Purity criteria for target compounds 1,2,4,5,6,8
S11 Fully optimized AM1 conformers of the possible four stereoisomers of 1 at C-8 and C-13 atoms.
S12 Superimposition of two low energy conformers of 8S,13R stereoisomer of 1
Spectrum S1.

$^1$H NMR spectrum of compound 1 (500 MHz, solvent CDCl$_3$)
Spectrum S2.

$^1$H NMR spectrum of compound 2 (500 MHz, solvent CDCl$_3$)
Spectrum S3.

$^1$H NMR spectrum of compound 3 (500 MHz, solvent CDCl$_3$)
Spectrum S4.

$^1$H NMR spectrum of compound 4 (500 MHz, solvent CDCl$_3$)
Spectrum S5.
$^1$H NMR spectrum of compound 5 (500 MHz, solvent CDCl$_3$)
Spectrum S6.
$^1$H NMR spectrum of compound 6 (500 MHz, solvent CDCl$_3$)
Spectrum S7.

$^1$H NMR spectrum of compound 7 (500 MHz, solvent CDCl$_3$)
Spectrum S8.
$^1$H NMR spectrum of compound 8 (500 MHz, solvent CDCl$_3$)
Purity criteria for target compounds. The degree of purity of tested compounds was over 95% as indicated by the appearance of a single peak using two different HPLC eluent systems. Retention times (Rt) are expressed in minutes.

Euphoscopin M (1): Hexane/EtOAc 75:25 with Rt 54.6. CH₂Cl₂/EtOAc 8:2 with Rt 36.4.

Euphoscopin N (2): Hexane/EtOAc 75:25 with Rt 27.9. CH₂Cl₂/EtOAc 8:2 with Rt 18.6.

Euphoscopin C (4): Hexane/EtOAc 85:15 with Rt 75.0. CH₂Cl₂/EtOAc 9:1 with Rt 50.0.

Euphornin (5): Hexane/EtOAc 75:25 with Rt 59.4. CH₂Cl₂/EtOAc 8:2 with Rt 39.6.

Epieuphoscopin B (6): Hexane/EtOAc 8:2 with Rt 24.0. CH₂Cl₂/EtOAc 85:15 with Rt 16.1.

Euphohelioscopin A (8): Hexane/EtOAc 75:25 with Rt 42.0. CH₂Cl₂/EtOAc 8:2 with Rt 28.2.
Figure S1.

A-D. Fully optimized AM1 conformers of the possible four stereoisomers of euphoscopin M (1) at C-8 and C-13 atoms: A) $8R,13R$; B) $8S,13R$; C: $8R,13S$; D $8S,13S$. Atoms are coloured by atom type; hydrogens atoms, with the exceptions of those useful for NMR discussion, are omitted for clarity of presentation.
Figure S2.

Superimposition of two low energy conformers of 8S,13R stereoisomer of euphoscopin M (1). The relation between H-7/H-8 dihedral angle value and the relative orientation of C-7 C-3 substituents is evidenced. Atoms are coloured by atom type; hydrogens atoms, with the exceptions of those discussed in NMR data are omitted for clarity of presentation.