

Supplementary Materials

Phytochemical Analysis and *In Vitro* Antileukemic Activity of Alkaloid-Enriched Extracts from *Vinca sardoa* (Stearn) Pignatti

Daniela De Vita ^{1,*}, Claudio Frezza ¹, Fabio Sciubba ^{1,2}, Chiara Toniolo ¹, Camilla Badiali ¹, Rita Petrucci ³, Martina Bortolami ³, Paola Di Matteo ³, Daniele Rocco ³, Annarita Stringaro ⁴, Marisa Colone ⁴, Andrea Maxia ⁵, Maria Teresa Petrucci ⁶, Mauro Serafini ¹ and Sebastiano Foddai ¹

¹ Department of Environmental Biology, “Sapienza” University of Rome, Piazzale Aldo Moro 5, 00185 Rome, Italy; claudio.frezza@uniroma1.it (C.F.); fabio.sciubba@uniroma1.it (F.S.); chiara.toniolo@uniroma1.it (C.T.); camilla.badiali@uniroma1.it (C.B.); mauro.serafini@uniroma1.it (M.S.); sebastiano.foddai@uniroma1.it (S.F.)

² NMR-Based Metabolomics Laboratory, “Sapienza” University of Rome, Piazzale Aldo Moro 5, 00185 Rome, Italy

³ Department of Basic and Applied Sciences for Engineering, “Sapienza” University of Rome, Via Castro Laurenziano 7, 00161 Rome, Italy; rita.petrucci@uniroma1.it (R.P.); martina.bortolami@uniroma1.it (M.B.); p.dimatteo@uniroma1.it (P.D.M.); daniele.rocco@uniroma1.it (D.R.)

⁴ National Center for Drug Research and Evaluation, Italian National Institute of Health, Viale Regina Elena 299, 00161 Rome, Italy; annarita.stringaro@iss.it (A.S.); marisa.colone@iss.it (M.C.)

⁵ Laboratory of Economic and Pharmaceutical Botany, Department of Life and Environmental Sciences, Università degli Studi di Cagliari, Viale S. Ignazio da Laconi 13, 09123 Cagliari, Italy; a.maxia@unica.it

⁶ Department of Cellular Biotechnologies and Hematology, “Sapienza” University of Rome, Via Benevento 6, 00161 Rome, Italy; petrucci@bce.uniroma1.it

* Correspondence: daniela.devita@uniroma1.it; Tel.: +39-06-4991-2788

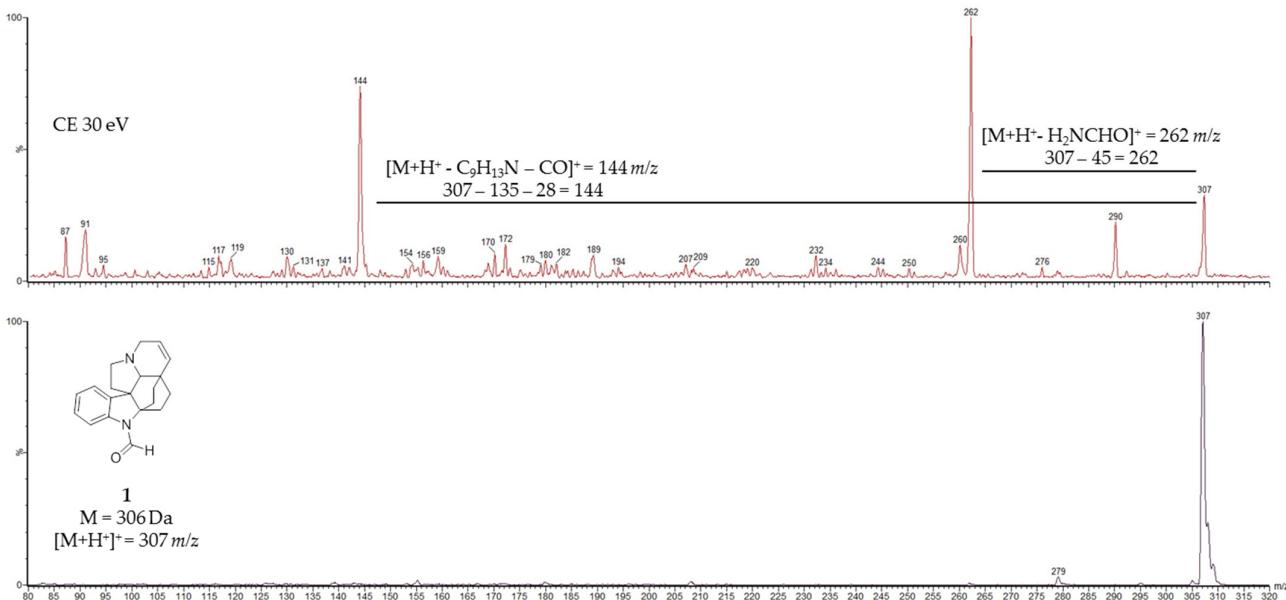


Figure S1. Alkaloid 1: structure, molecular mass, m/z monoisotopic value of the protonated ion $[M + H^+]$, mass spectrum (bottom), fragmentation spectrum at 30 eV (CE) (top), tentatively assigned principal fragments.

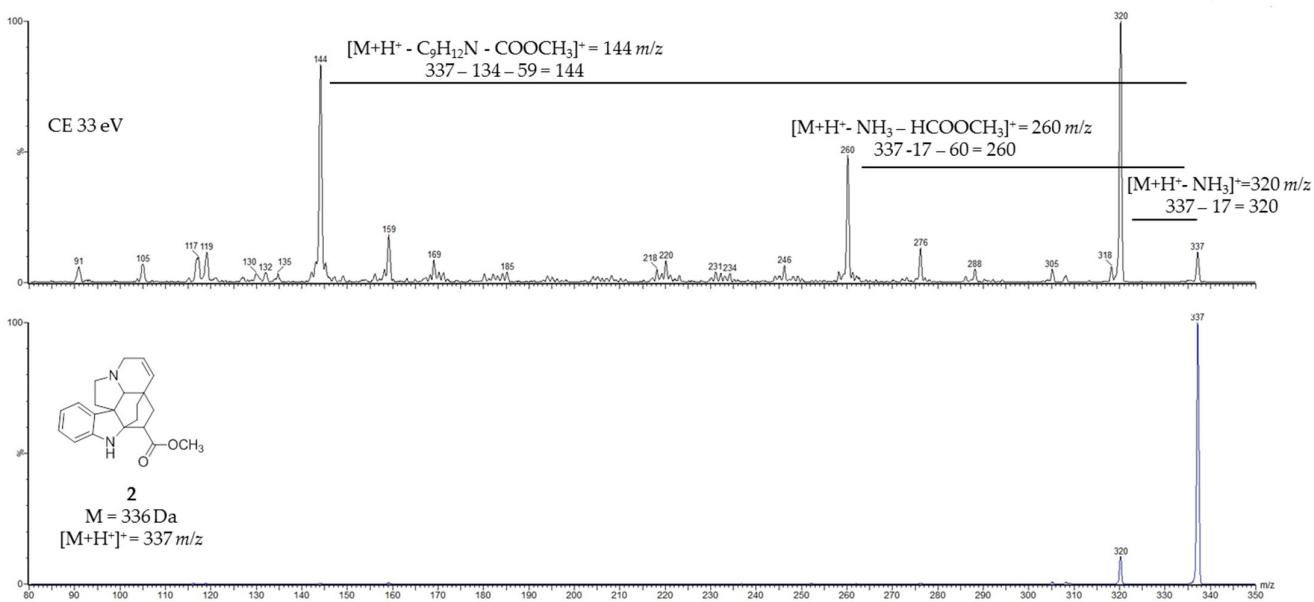


Figure S2. Alkaloid 2: structure, molecular mass, m/z monoisotopic value of the protonated ion $[M + H^+]$, mass spectrum (bottom), fragmentation spectrum at 33 eV (CE) (top), tentatively assigned principal fragments.

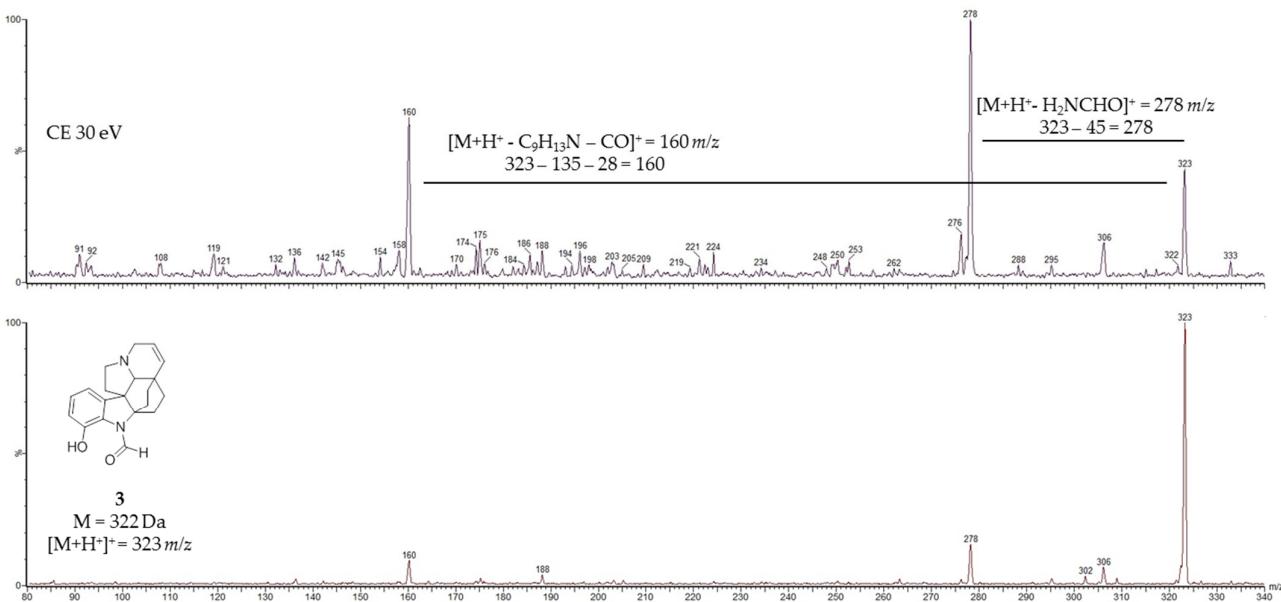


Figure S3. Alkaloid 3: structure, molecular mass, m/z monoisotopic value of the protonated ion $[M + H^+]^+$, mass spectrum (bottom), fragmentation spectrum at 30 eV (CE) (top), tentatively assigned principal fragments.

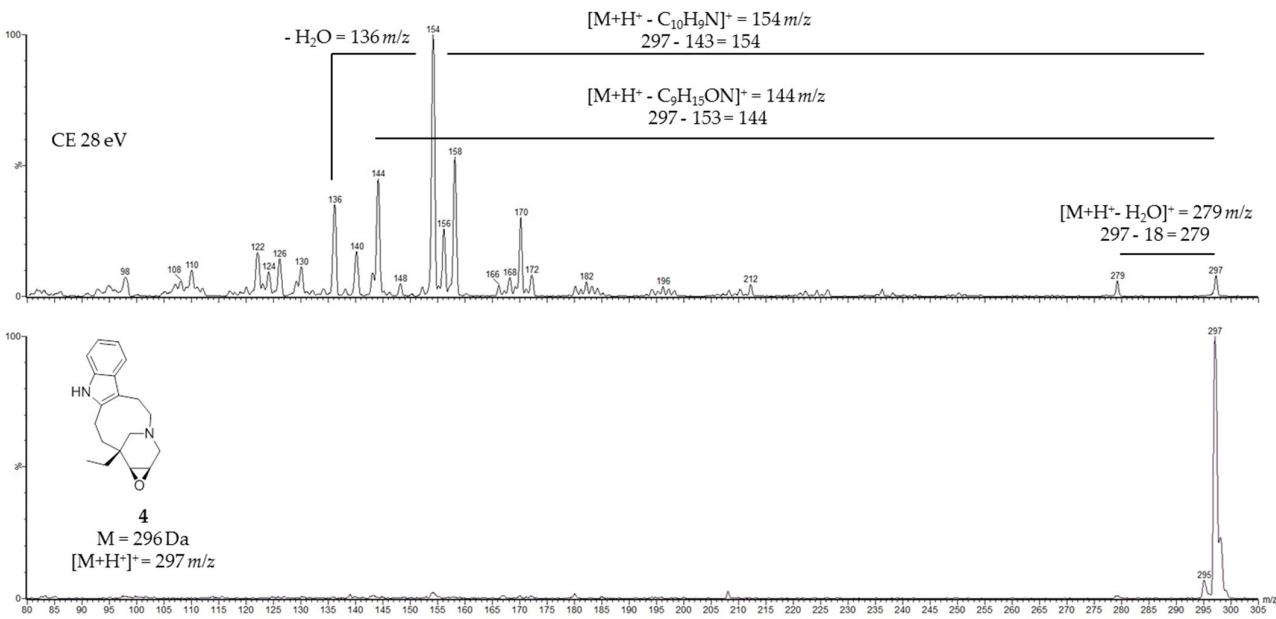


Figure S4. Alkaloid 4: structure, molecular mass, m/z monoisotopic value of the protonated ion $[M + H^+]^+$, mass spectrum (bottom), fragmentation spectrum at 28 eV (CE) (top), tentatively assigned principal fragments.

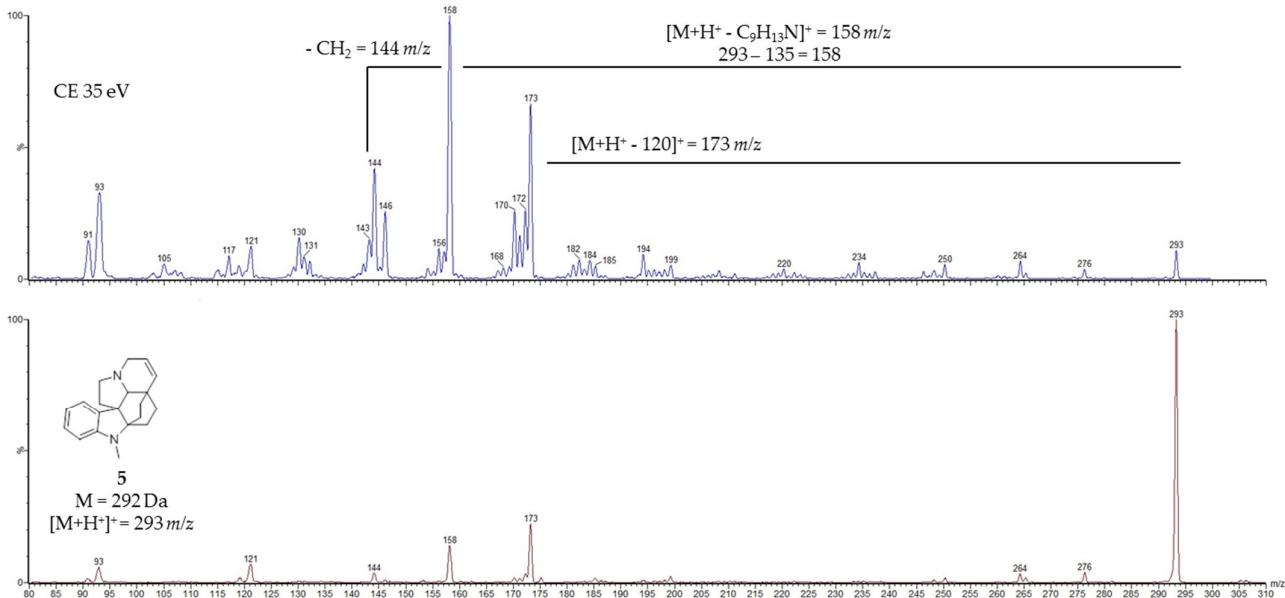


Figure S5. Alkaloid 5: structure, molecular mass, m/z monoisotopic value of the protonated ion $[M + H^+]^+$, mass spectrum (bottom), fragmentation spectrum at 35 eV (CE) (top), tentatively assigned principal fragments.

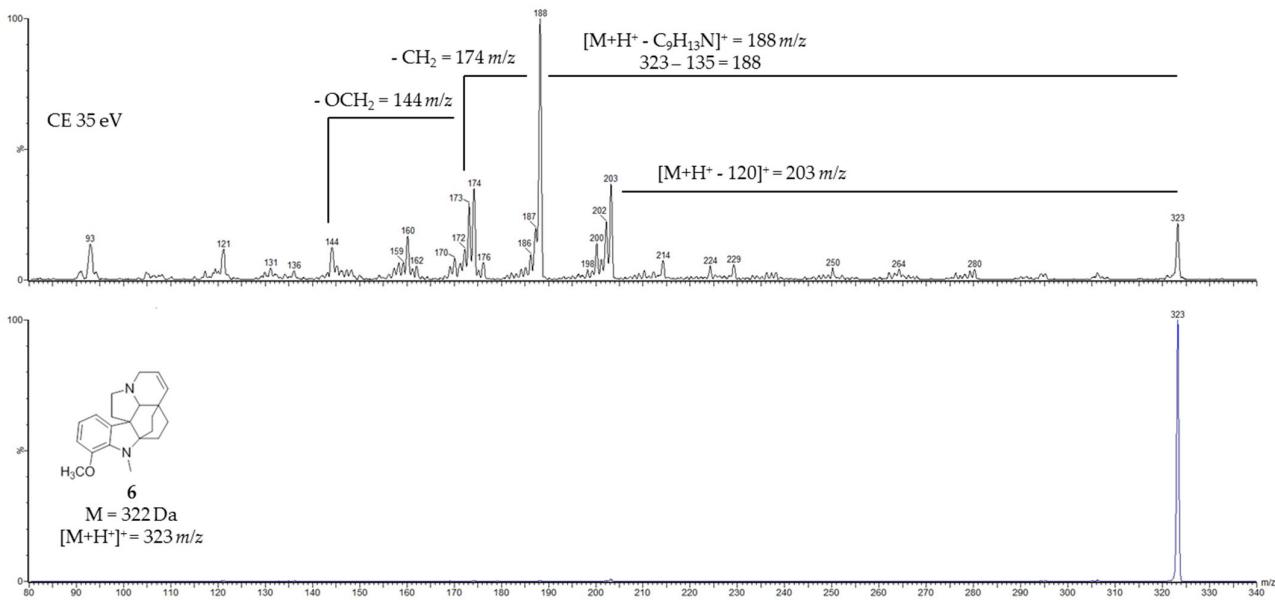


Figure S6. Alkaloid 6: structure, molecular mass, m/z monoisotopic value of the protonated ion $[M + H^+]^+$, mass spectrum (bottom), fragmentation spectrum at 35 eV (CE) (top), tentatively assigned principal fragments.

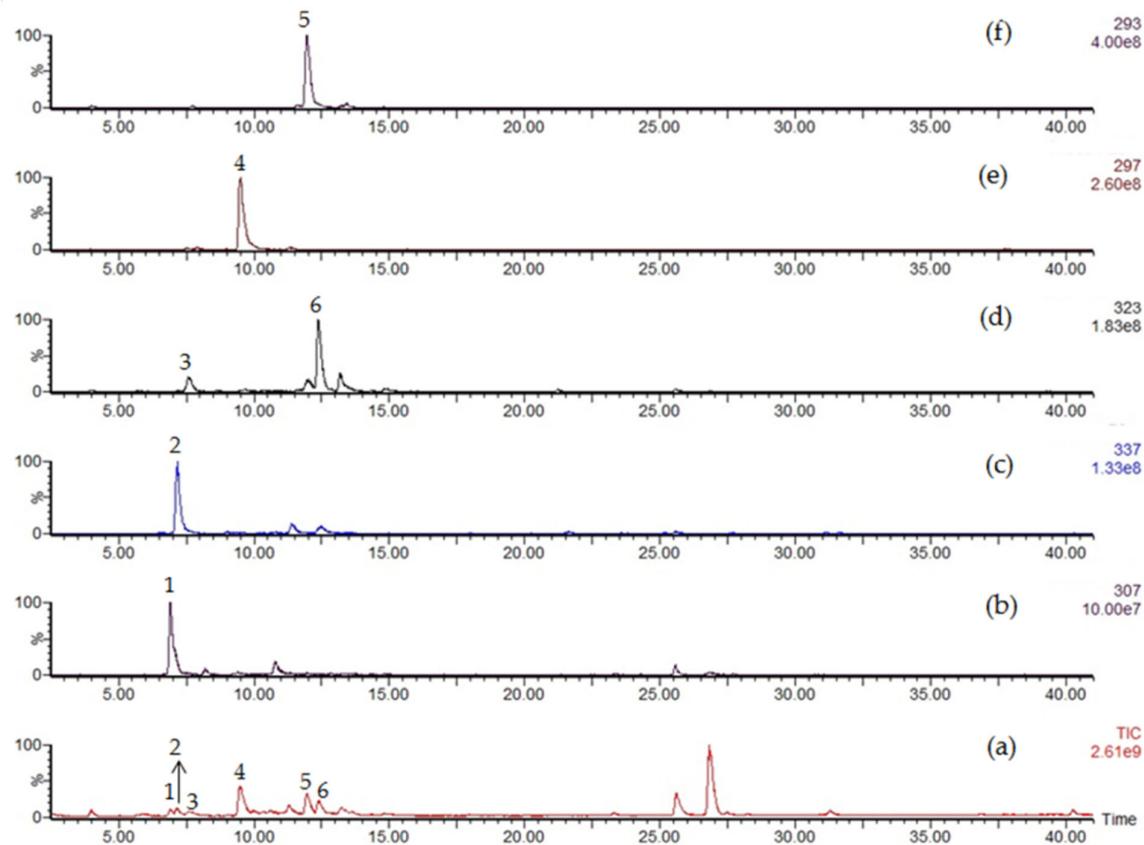


Figure S7. Total Ion Chromatogram (TIC) and Selected Ion Recording (SIR) chromatograms of the extracts of *V. sardoa*, RM2019 sample. (a) TIC; (b) SIR chromatogram obtained for the selected m/z value 307, corresponding to the protonated ion $[M + H]^+$ of alkaloid 1, $t_R = 6.77$ min; (c) SIR chromatogram obtained for the selected m/z value 337, corresponding to the protonated ion $[M + H]^+$ of alkaloid 2, $t_R = 7.04$ min; (d) SIR chromatogram obtained for the selected m/z value 323, corresponding to the isobaric protonated ions $[M + H]^+$ of alkaloid 3, $t_R = 7.41$ min, and alkaloid 6, $t_R = 12.22$ min; (e) SIR chromatogram obtained for the selected m/z value 297, corresponding to the protonated ion $[M + H]^+$ of alkaloid 4, $t_R = 9.29$ min; (f) SIR chromatogram obtained for the selected m/z value 293, corresponding to the protonated ion $[M + H]^+$ of alkaloid 5, $t_R = 11.74$ min.

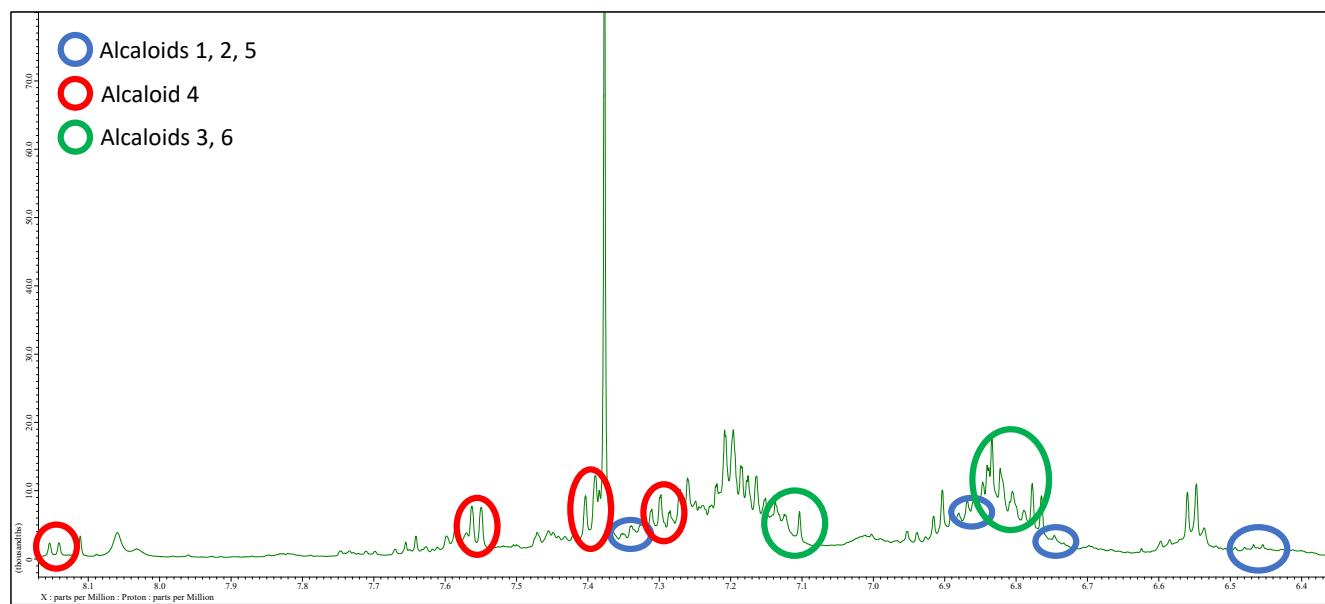


Figure S8. ^1H -NMR (600 MHz, CDCl_3) spectrum of *V. sardoa* extract.

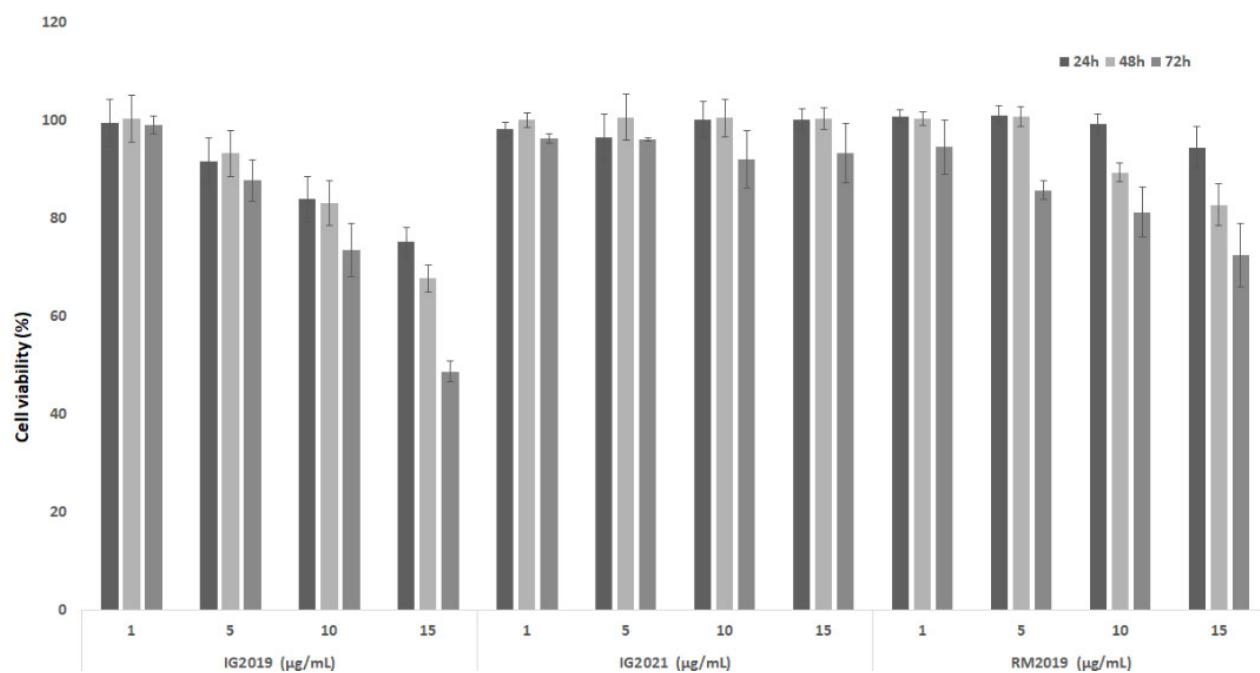


Figure S9. Cell viability analysis in fibroblast cell treated with IG2019, IG2021, RM2019 for 24, 48 and 72 h. All experiments were performed in triplicate and all data were expressed at mean \pm SD values.

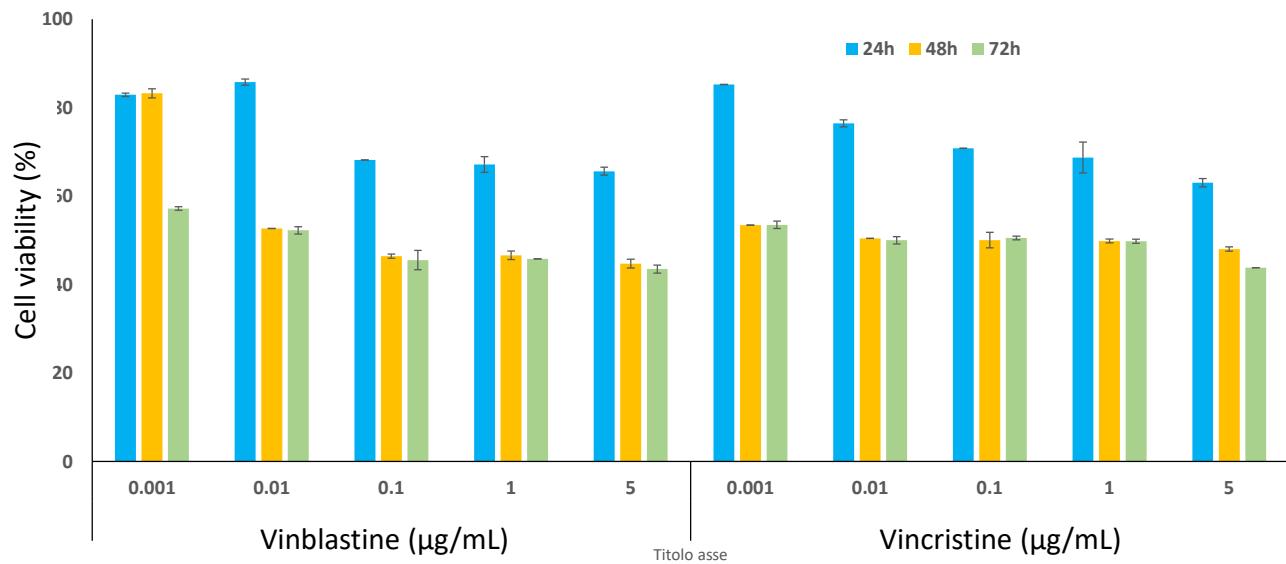


Figure S10. Cell viability analysis in SUP-B15 cells treated with Vincristine and Vinblastine for 24, 48 and 72 h. All experiments were performed in triplicate and all data were expressed at mean \pm SD values.