SUPPLEMENTARY MATERIAL

Type of the Paper (Article)

Unraveling the antibacterial activity of *Terminalia* sericea root bark through a metabolomic approach

Chinedu P Anokwuru ^{1,2}, Sidonie Tankeu ², Sandy van Vuuren ³, Alvaro Viljoen ^{2,4}. Isaiah D.I Ramaite¹, Orazio Taglialatela-Scafati ^{5,1}, Sandra Combrinck ^{2*}

- ¹ Department of Chemistry, University of Venda, Private Bag X5050, Thohoyandou 0950, South Africa Affiliation 1; <u>anokwuruchi@gmail.com; Isaiah.Ramaite@univen.ac.za</u>
- ² Department of Pharmaceutical Sciences, Tshwane University of Technology, Private Bag X680, Pretoria, 001, South Africa; <u>anokwurucp@tut.ac.za</u>; <u>tankeus@tut.ac.za</u>; <u>combrincks@tut.ac.za</u>
- ³ Department of Pharmacy and Pharmacology, Faculty of Health Sciences, University of the Witwatersrand, 7 York Road, Parktown, 2193, South Africa; <u>sandy.vanyuuren@wits.ac.za</u>
- ⁴ SAMRC Herbal Drugs Research Unit, Faculty of Science, Tshwane University of Technology, Private Bag X680, Pretoria 0001, South Africa; <u>viljoenam@tut.ac.za</u>
- ⁵ Department of Pharmacy, University of Naples, Federico II Via D. Montesano 49, 1-80131 Napoli, Italy; scatagli@unina.it
- * Correspondence: combrincks@tut.ac.za



Figure S1: Chemical profile of selected *T. sericea* root bark samples from population A) P6, B) P3, C) P4, D) P8. Peaks of each chromatogram highlighted are major constituents clustered in branch X (red), Y (green) and Z (blue)



Figure S2: ¹H NMR spectrum of sericic acid



Figure S3: ¹³C NMR spectrum of sericoside



Figure S4: A) ¹H NMR , B) ¹³C NMR spectra of 3',5',4–trihydroxy-resveratrol-3-O- β -rutinoside



Figure S5: A) ¹H NMR , B) ¹³C NMR spectra of ellagic acid



Figure S6: A) ¹H NMR spectrum of flavogallonic acid dilactone, B) ¹H NMR of spectrum of methylflavogallonate. The methoxy proton (OCH₃) at $\delta_{\rm H}$ 3.4 confirms the presence of a methyl group. C) ¹³C NMR spectrum of flavogallonic acid dilactone



Figure S7: A) ¹H and B) ¹³C NMR spectra of Resveratrol 3-(6"-galloyl)-O-β-D-glucopyranoside



Figure S8: A) ¹H NMR , B) ¹³C NMR spectra and C) UPLC-MS² fragment ions of quercetin-3-(2"-galloylrhamnoside)



Figure S9: A) ¹H NMR , B) ¹³C NMR spectra and C) UPLC-MS² fragment ions of ajunetin



Figure S10: Orthogonal projection to latent structure-discriminant analysis (OPLS-DA) model of the active (RED) and non-active (GREEN) samples of *T. sericea* root bark.



Figure S11: Variable importance for project (VIP) scores of compounds associated with the antibacterial activities of the active and non-active classes