Supporting Information

Rec. Nat. Prod. 16:2 (2022) 128-143

¹H NMR-Based Metabolomics Profiling of *Syzygium grande* and *Oenanthe javanica* and Relationship Between Their Metabolite Compositions and Antimicrobial Activity Against *Bacillus* species

Khaled Bashir Abdusalam ^{1,2}, Lee Soo Yee ¹, Ahmed Mediani ³, Muhammad Tayyab Akhtar ⁴, Nawal Buzgaia ^{1,5}, Yaya Rukayadi ¹, Intan Safinar Ismail ^{1,6} and Khozirah Shaari ^{1,6*}

¹ Natural Medicine and Products Research Laboratory, Institute of Bioscience, Universiti Putra Malaysia, 43400 Serdang, Selangor, Malaysia

²Department of Botany, Faculty of Science, University of Gharyan, Libya

³Institute of Systems Biology (INBIOSIS), Universiti Kebangsaan Malaysia, 43600, UKM Bangi, Selangor, Malaysia

⁴Institute of Industrial Biotechnology, Government College University, Lahore, Pakistan

⁵Department of Chemistry, Faculty of Science, University of Benghazi, Libya

⁶Department of Chemistry, Faculty of Science, Universiti Putra Malaysia, 43400 UPM, Serdang, Selangor, Malaysia

Table of Contents	Page
Figure S1: ¹ H-NMR spectra of hexane (A), EtOAc (B), MeOH (C) and 70% MeOH (D)	3
extracts of S. grande leaves from δ 0.5 to 3.0 ppm	
Figure S2: ¹ H-NMR spectra of hexane (A), EtOAc (B), MeOH (C) and 70% MeOH (D)	4
extracts of S. grande leaves from δ 3.0 to 8.0 ppm	
Figure S3: ¹ H-NMR spectra of hexane (A), EtOAc (B), MeOH (C) and 70% MeOH (D)	5
extracts of O. javanica from δ 0.5 to 3.0 ppm.	
Figure S4: ¹ H-NMR spectra of hexane (A), EtOAc (B), MeOH (C) and 70% MeOH (D)	6
extracts of O. javanica from δ 3.0 to 5.0 ppm.	
Figure S5: ¹ H-NMR spectra of hexane (A), EtOAc (B), MeOH (C) and 70% MeOH (D)	7
extracts of O. javanica from δ 5.0 to 8.0 ppm.	
Figure S6: The permutation plots of the developed PLS model developed for the	8
antimicrobial activity of S. grande extract against B. cereus	
Figure S7: The permutation plots of the developed PLS model developed for the	9
antimicrobial activity of S. grande extract against B. subtilis	
Figure S8: The permutation plots of the developed PLS model developed for the	10

© 2021 ACG Publications. All rights reserved.

antimicrobial activity of S. grande extract against B. megaterium	
Figure S9: The permutation plots of the developed PLS model developed for the	11
antimicrobial activity of S. grande extract against B. pumilus	
Figure S10: The permutation plots of the developed PLS model developed for the	12
antimicrobial activity of O. javanica extract against B. cereus	
Figure S11: The permutation plots of the developed PLS model developed for the	13
antimicrobial activity of O. javanica extract against B. subtilis	
Figure S12: The permutation plots of the developed PLS model developed for the	14
antimicrobial activity of O. javanica extract against B. megaterium	
Figure S13: The permutation plots of the developed PLS model developed for the	15
antimicrobial activity of O. javanica extract against B. pumilus	



Figure S1: ¹H NMR spectra of hexane (A), EtOAc (B), MeOH (C) and 70% MeOH (D) extracts of *S. grande* leaves from δ 0.5 to 3.0 ppm.



Figure S2: ¹H NMR spectra of hexane (A), EtOAc (B), MeOH (C) and 70% MeOH (D) extracts of *S. grande* leaves from δ 3.0 to 8.0ppm.



Figure S3: ¹H NMR spectra of hexane (A), EtOAc (B), MeOH (C) and 70% MeOH (D) extracts of *O*. *javanica* from δ 0.5 to 3.0 ppm.



Figure S4: ¹H NMR spectra of hexane (A), EtOAc (B), MeOH (C) and 70% MeOH (D) extracts of *O*. *javanica* from δ 3.0 to 5.0 ppm.



Figure S5: ¹H NMR spectra of hexane (A), EtOAc (B), MeOH (C) and 70% MeOH (D) extracts of *O*. *javanica* from δ 5.0 to 8.0 ppm



Figure S6: The permutation plots of the developed PLS model developed for the antimicrobial activity of *S. grande* extract against *B. cereus*



Figure S7: The permutation plots of the developed PLS model developed for the antimicrobial activity of *S. grande* extract against *B. subtilis*



Figure S8: The permutation plots of the developed PLS model developed for the antimicrobial activity of *S. grande* extract against *B. megaterium*



Figure S9: The permutation plots of the developed PLS model developed for the antimicrobial activity of *S. grande* extract against *B. pumilus*



Figure S10: The permutation plots of the developed PLS model developed for the antimicrobial activity of *O. javanica* extract against *B. cereus*



Figure S11: The permutation plots of the developed PLS model developed for the antimicrobial activity of *O. javanica* extract against *B. subtilis*



Figure S12: The permutation plots of the developed PLS model developed for the antimicrobial activity of *O. javanica* extract against *B. megaterium*



Figure S13: The permutation plots of the developed PLS model developed for the antimicrobial activity of *O. javanica* extract against *B. pumilus*