

LC-MS based phytochemical profiling towards the identification of antioxidant markers in some endemic *Aloe* species from Mascarene Islands

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Table S1. MZmine parameters

Figure S1. DPPH inhibitory activity of inactive extracts.

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<i>Module</i>	<i>Parameters</i>
Raw data methods > Raw data import	Importation of all .mzXML files
Raw data methods > Mass detection	Scans MS level : 1 Mass detector : centroid Noise level : 2.0E2 ; 1.5E2
Raw data methods > Mass detection	Scans MS level : 2 Mass detector : centroid Noise level : 1.3E1
Feature detection > LC-MS > ADAP chromatogram builder	Scans MS level : 1 Min group group size in # of scans : 4 Group intensity threshold : 1.0E3 Min highest intensity : 1.0E3 Scan to scan accuracy (m/z) : 10 ppm
Feature detection > Chromatogram resolving > Local minimum resolver	Chromatographic threshold : 20% Minimum search range RT/Mobility (absolute) : 0.10 Minimum relative height : 15% Minimum absolute height : 2.0E3 ; 1.0E3 Min ratio of peak top/edge : 3 Peak duration range (min/mobility) : 0.01 -1.00 Min # of data points : 3
Feature list methods > Isotopes > ¹³ C isotope filter	m/z tolerance : 10 ppm Retention time tolerance : 0.1 absolute (min) Mobility tolerance : unchecked Monotonic shape : unchecked Maximum charge : 2 Representative isotope : most intense Never remove feature with MS2 : checked
Feature list methods > Alignment > Join aligner (within replicates)	m/z tolerance : 10 ppm Weight for m/z : 75 Retention time tolerance : 0.2 absolute (min) Weight for RT : 25 Mobility tolerance : unchecked Mobility weight : 1.00 Require same charge state : checked Require same ID : unchecked Compare isotope pattern : unchecked Compare spectra similarity : unchecked
Feature list methods > Processing > Assign MS ² to features	Retention time tolerance : 0.1 absolute (min) MS1 to MS2 precursor tolerance (m/z) : 10 ppm Limit by RT edges : unchecked Combine MS/MS spectra (TIMS) : unchecked Lock to feature mobility range : unchecked Minimum merged intensity : unchecked
Feature list methods > Feature list filtering > Feature list rows filter (within replicates)	Minimum features in a row (abs or %) : 3 Retention time : 0.6 - 30.0 min (auto range) Features with MS2 scans : checked

Feature list methods > Alignment > Join aligner (across all samples)	m/z tolerance : 10 ppm Weight for m/z : 75 Retention time tolerance : 0.2 absolute (min) Weight for RT : 25 Mobility tolerance : unchecked Mobility weight : 1.0 Require same charge state : checked Require same ID : unchecked Compare isotope pattern : unchecked Compare spectra similarity : unchecked
Feature list method > Feature list filtering > Feature list rows filter (across all samples)	Minimum features in a row (abs or %) : 3 Retention time : 0.6 - 30.0 min (auto range) Features with MS2 scans : checked Reset the feature number ID : checked
Feature list method > Export feature list > GNPS - feature based molecular networking	Merge MS/MS (experimental) : checked Select spectra to merge : across samples m/z merge mode : most intense intensity merge mode : maximum intensity Expected mass deviation : 5 ppm Cosine threshold : 70 % Signal count threshold : 20 % Isolation window offset : 0.0 Isolation window width (m/z) : 3.0 Filter rows : ALL Feature intensity : Peak area CSV export : ALL Submit to GNPS : unchecked Open folder : unchecked

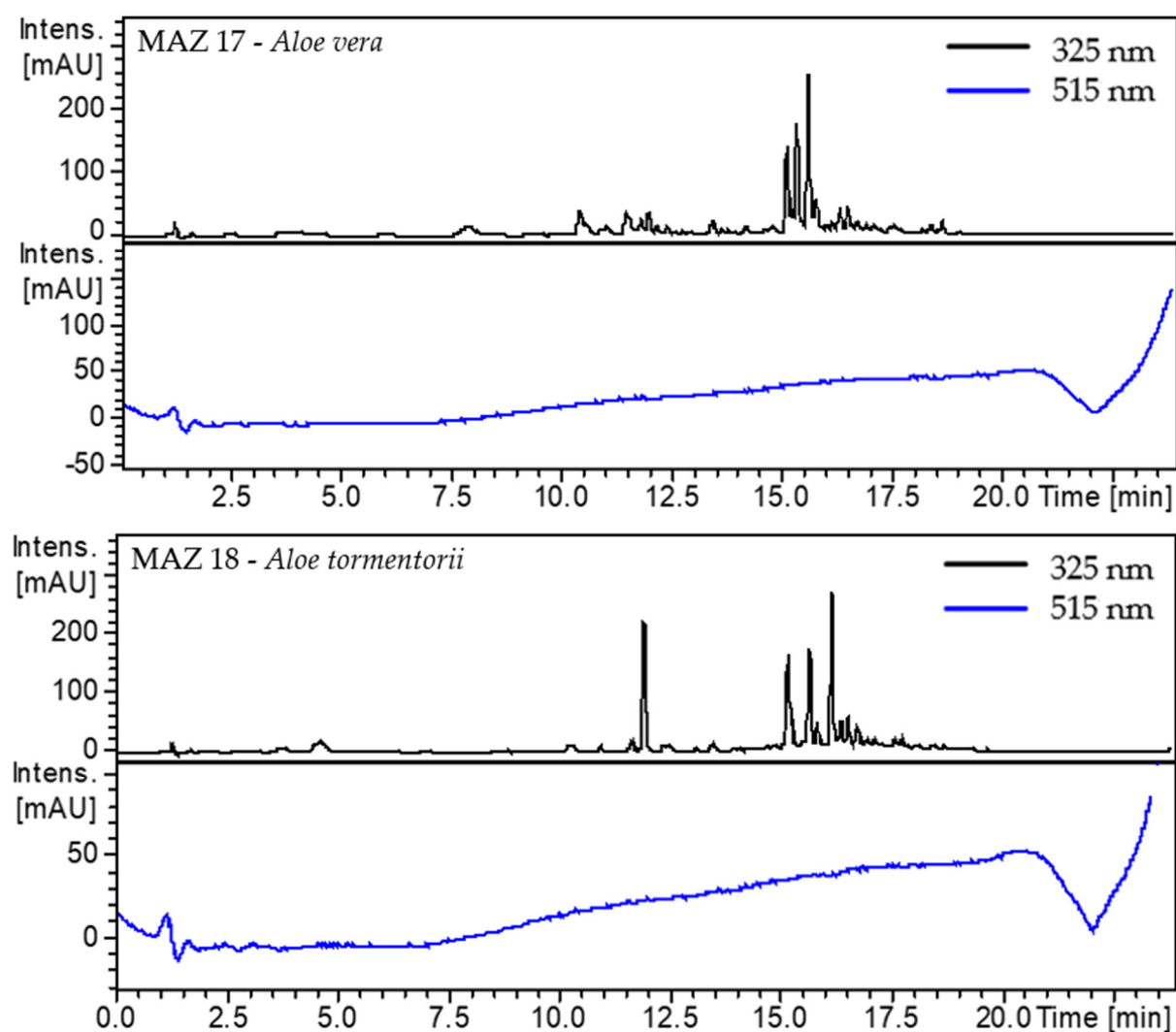


Figure S1. DPPH inhibitory activity of inactive extracts.