



HAL
open science

Molecular Networking-Based Approach of *Aloe djiboutiensis*, Antioxidant Activity and In Vivo Toxicity of This Endemic Species in Djibouti

Rosella Spina, Abdirahman Elmi, Fatouma Mohamed Abdoul-Latif, François Dupire, Stéphanie Philippot, Marie-France Champy, Benoît Petit-Demoulière, Hugues Jacobs, Dominique Laurain-Mattar

► To cite this version:

Rosella Spina, Abdirahman Elmi, Fatouma Mohamed Abdoul-Latif, François Dupire, Stéphanie Philippot, et al.. Molecular Networking-Based Approach of *Aloe djiboutiensis*, Antioxidant Activity and In Vivo Toxicity of This Endemic Species in Djibouti. Analytics 2022, Sep 2022, Nantes, France. 2022. hal-03788657

HAL Id: hal-03788657

<https://hal.univ-lorraine.fr/hal-03788657>

Submitted on 26 Sep 2022

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Rosella Spina^{1,2}, Abdirahman Elmi^{1,3}, Fatouma M. Abdoul-Latif³, Francois Dupire¹, Stephanie Philippot¹, Marie-France Champy⁴,
Benoit Petit-Demoulière⁴, Hugues Jacobs⁴, Dominique Laurain-Mattar^{1,2}

¹Université de Lorraine, CNRS, L2CM, F-54000 Nancy, ²Université de Lorraine, INRAE, LAE, F-54000 Nancy

³Medicinal Research Institute, Centre d'Etudes et de Recherche de Djibouti, IRM-CERD, Route de l'Aéroport, Haramous B.P. 486, Djibouti;

⁴PHENOMIN-ICS, Institut Clinique de la souris, CNRS, UMR7104, Illkirch, France ; INSERM, U1258, Illkirch, France; Université de
Strasbourg, France

Correspondance: rosella.spina@univ-lorraine.fr

INTRODUCTION

Aloe djiboutiensis is a native plant in Djibouti, named botanically in 2007. The leaves and the latex are used traditionally used in Djibouti. The present research work was conducted to assess the possible toxic effect and antioxidant the latex and the leave extract, as well as to detect rapidly the previously characterized known molecules in the genus Aloe and to create a metabolic fingerprinting of *A. djiboutiensis* [1].

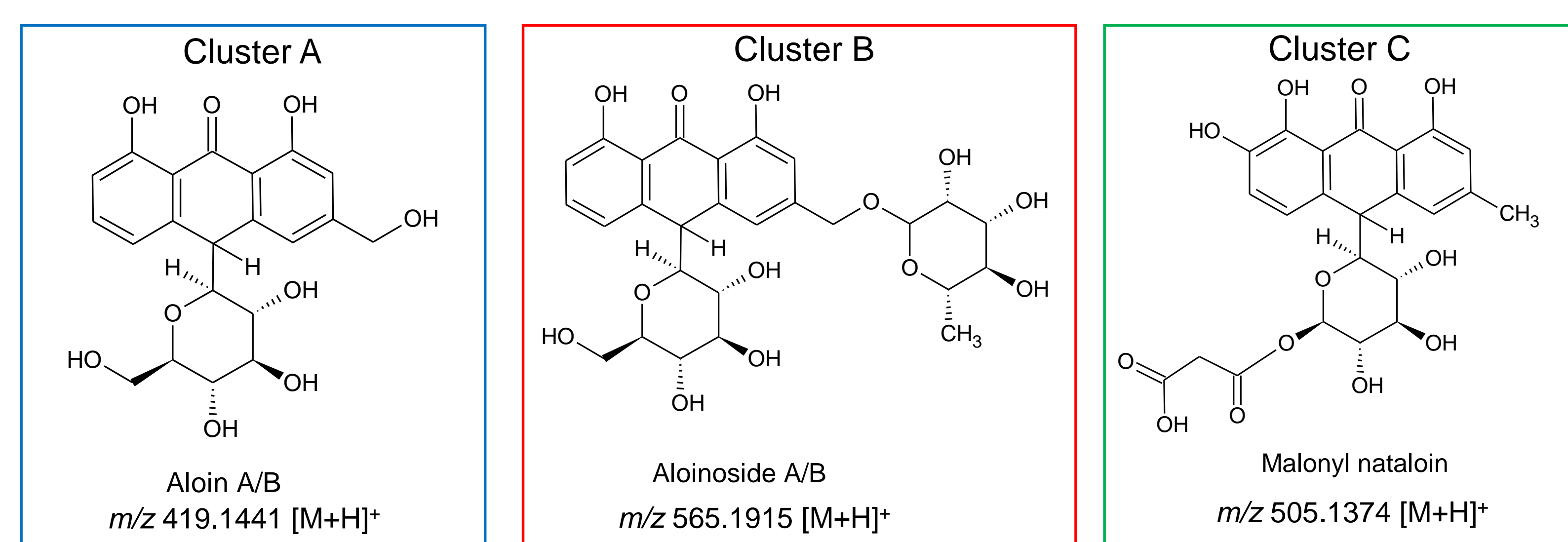
RESULTS AND DISCUSSION

The results for antioxidant activity, the *in vitro* and *in vivo* toxicity are reported in the figure. The latex (ADL) has the high level of phenol content (83.01 ± 0.8 mg GAE/g DW) and moderate level of flavonoid content (13.12 ± 0.11 mg QE/g DW).

The latex and five fractions of *Aloe djiboutiensis*, obtained after LH-20 fractionation of latex, were analyzed, and the phytochemical profile is evaluated using LC-MS/MS analysis. The identification/annotation of the chemical compounds is based on the comparison of commercial standards, the chemicals present in our in-house database (DataNat database, n° IDDN: FR.001.480019.000.S.P.2020.000.10300) and Global Natural Products Social Molecular Networking (GNPS) [2].

GNPS is used for the generation of molecular networking, and Cytoscape software 3.8.0 is used for the visualization of them.

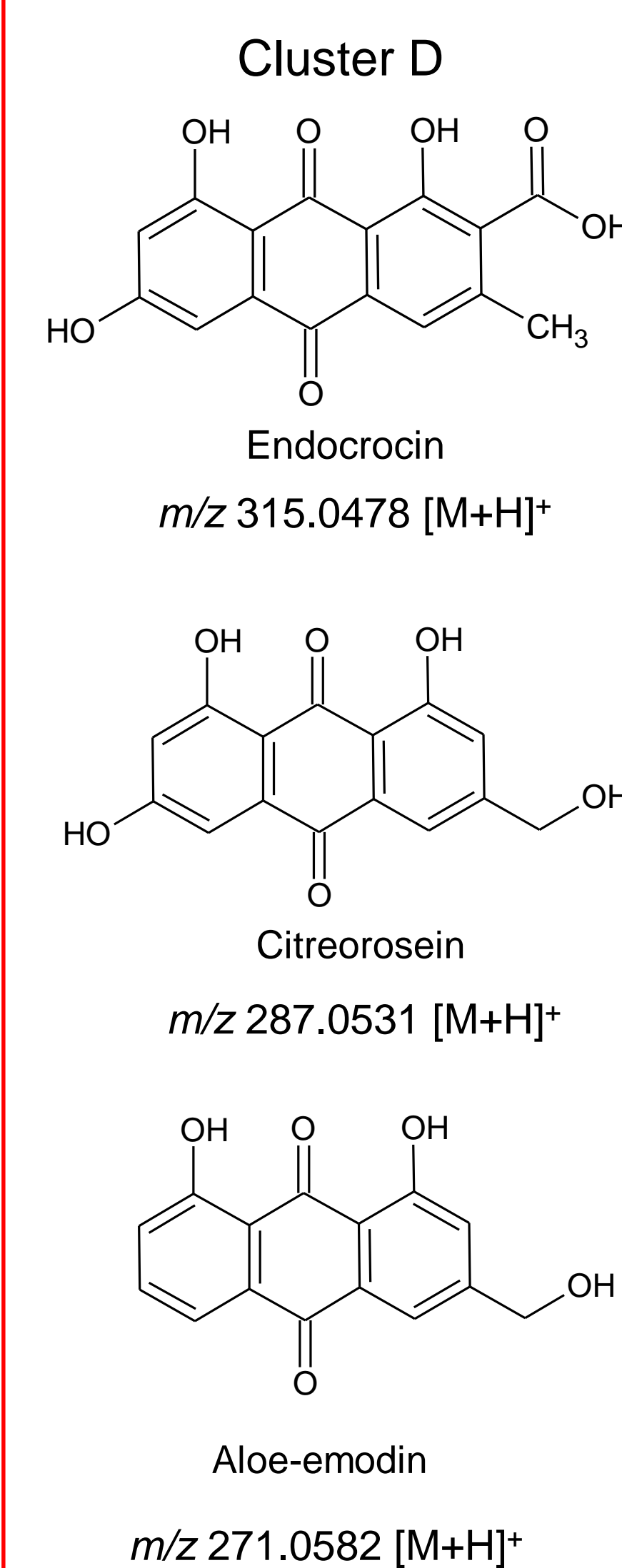
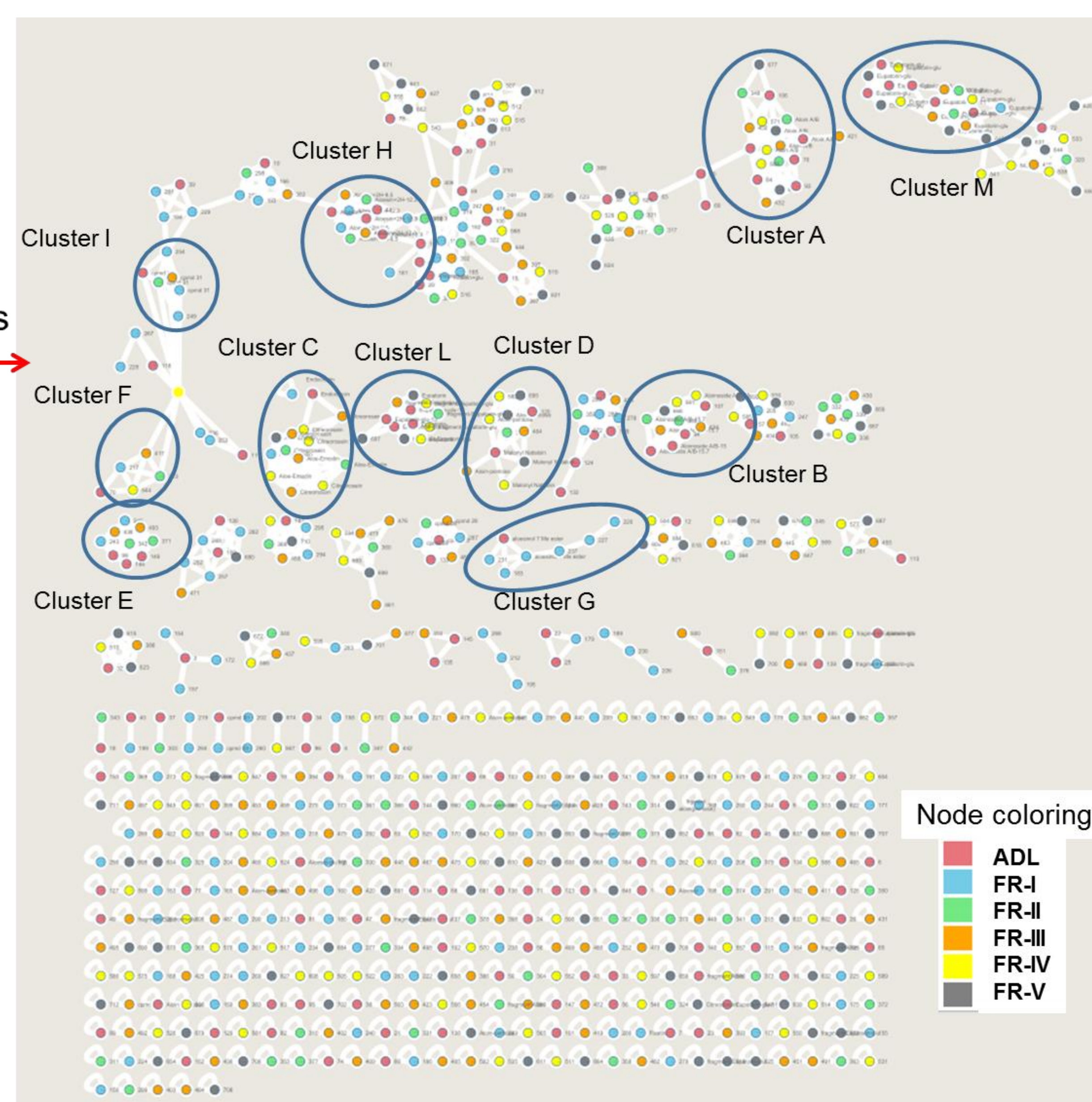
In total, 712 nodes are visible in molecular networking, which included 67 clusters (node>2). The observation of molecular network reveals the presence of eleven (11) annotated clusters named, respectively A, B, C, D, E, F, G, H, I, L, and M.



Fractionation
Sephadex®
LH-20
Five
fractions

Phytochemical analysis

LC-MS/MS
GNPS/ Cytoscape
Molecular networking



In vitro
toxicity

In vivo
toxicity

Antioxidant
activities

Any toxicity against
MRC-5 cells with
 $99 \pm 4.7\%$ of the
surviving cells

Any toxicity at 200 mg/kg
in mouse supplementation

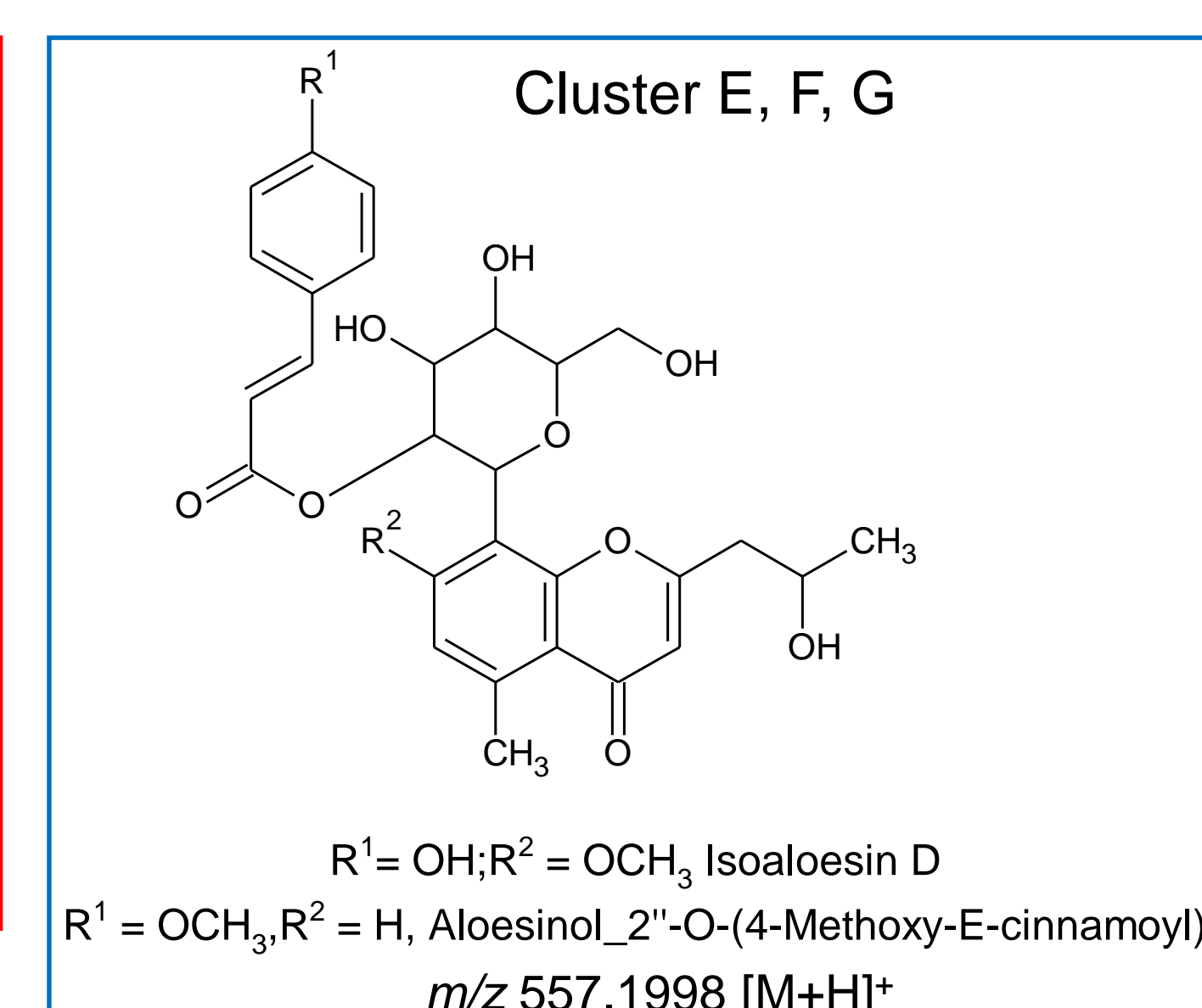
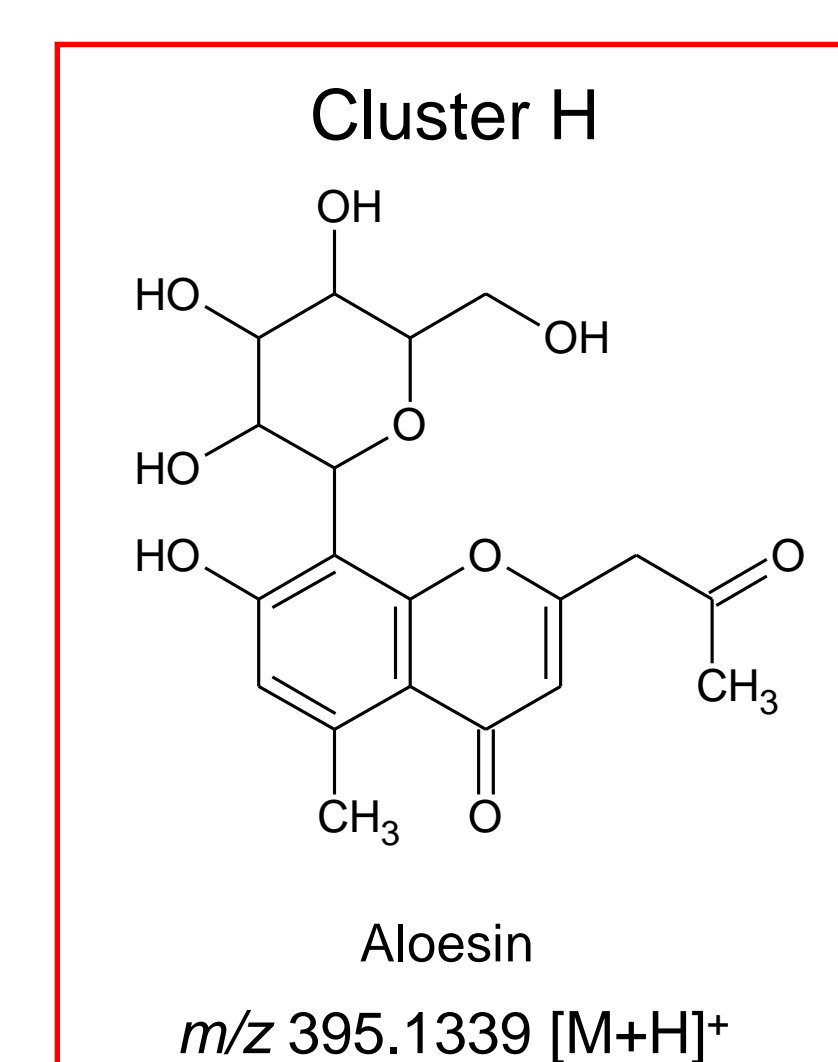
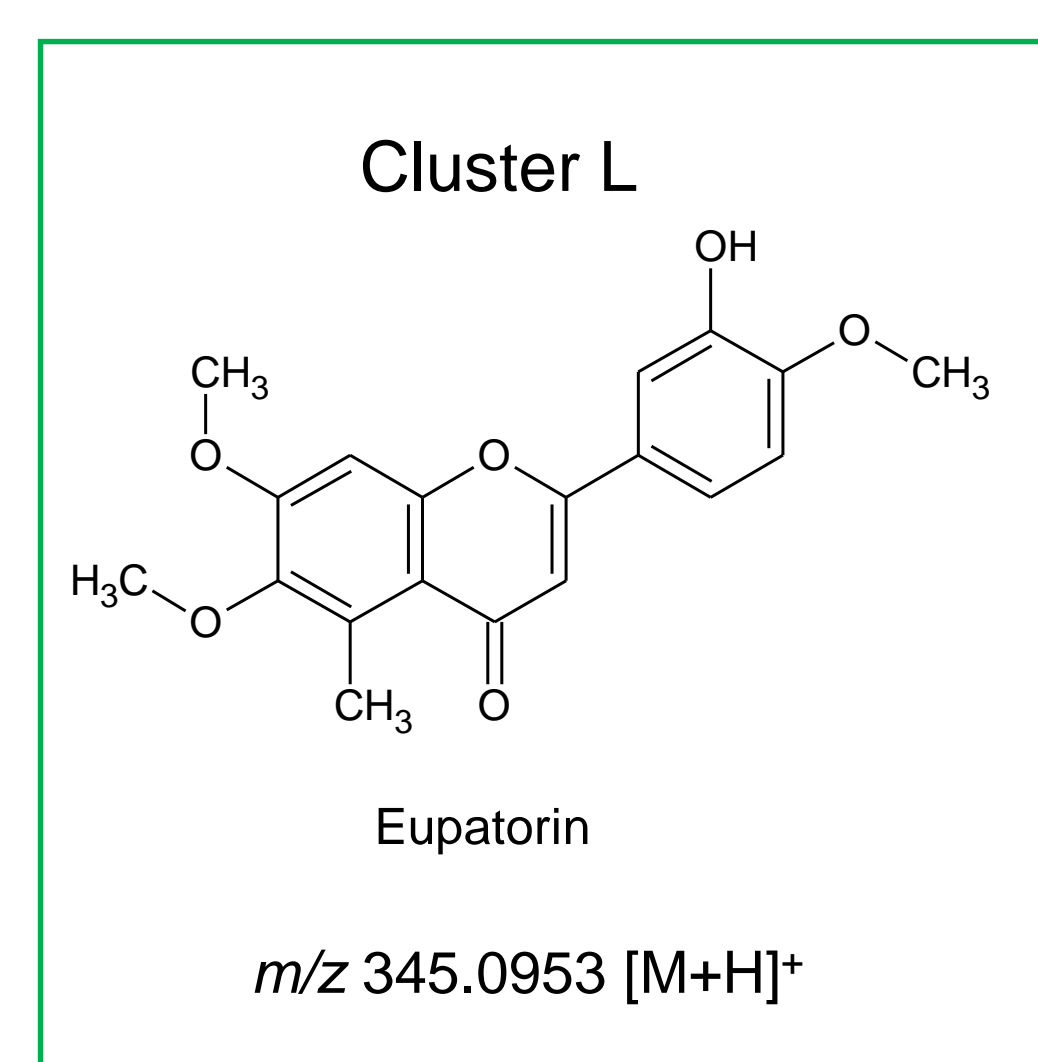
ABTS IC₅₀ = 600 ± 1.8 µg/mL
FRAP = 1.50 ± 0.12 mg EVC/g DW

CONCLUSION

According to the obtained results, the traditional use of the latex of *A. djiboutiensis* is safe until at less 18 mg/kg for human level and has beneficial effects for human health (following equations for dose conversion between animals and human).

In the figure are visible the relevant structures annotated in the molecular network.

In total twenty one (21) compounds are identified: nine (9) anthraquinones derivatives, ten (10) chromones derivatives, two (2) flavonols/ chromones isomers.



REFERENCES

1) A. Elmi, F. Mohamed Abdoul-Latif, R. Spina, F. Dupire, S. Philippot, C. Marie-France, H. Jacobs, D. Laurain-Mattar, *Molecules*, MDPI, **2021**, 26 (10), pp.3046. <https://doi.org/10.3390/molecules26103046>

2) Mingxun Wang, Jeremy J. Carver, Vanessa V. Phelan, Laura M. Sanchez, Neha Garg, Yao Peng, Don Duy Nguyen et al.; *Nature biotechnology* 34, no. 8 (2016): 828. PMID: 27504778