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

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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].

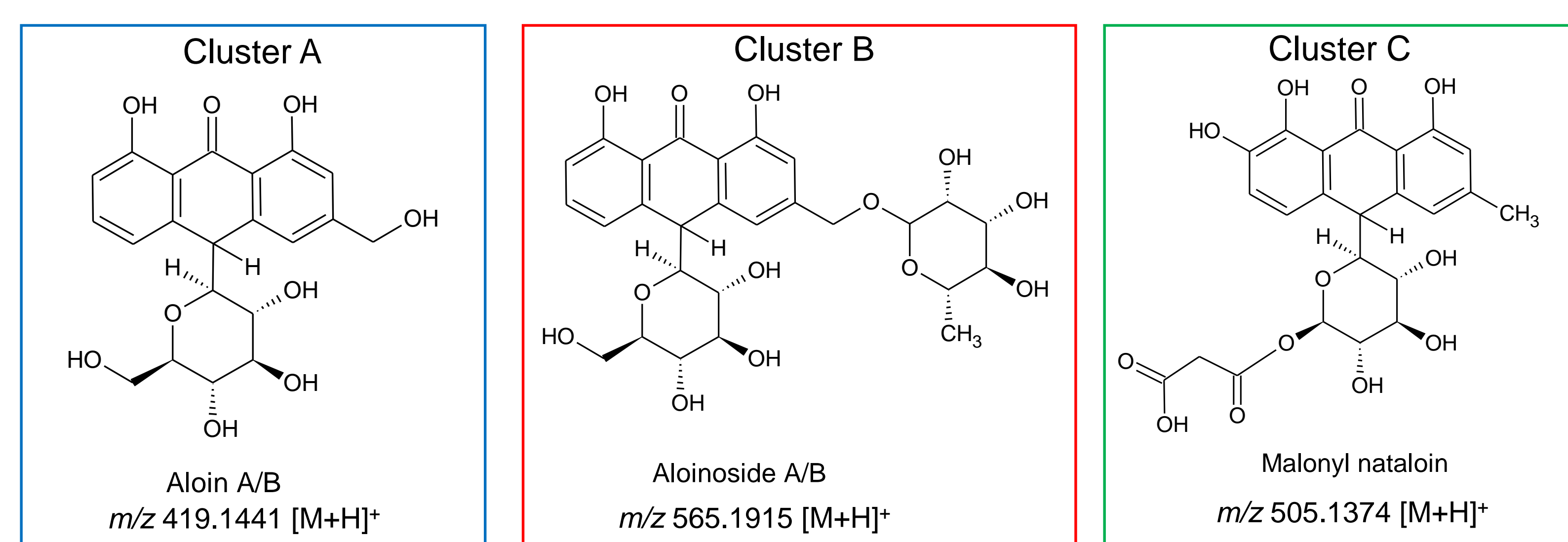
RESULTS AND DISCUSSION

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.



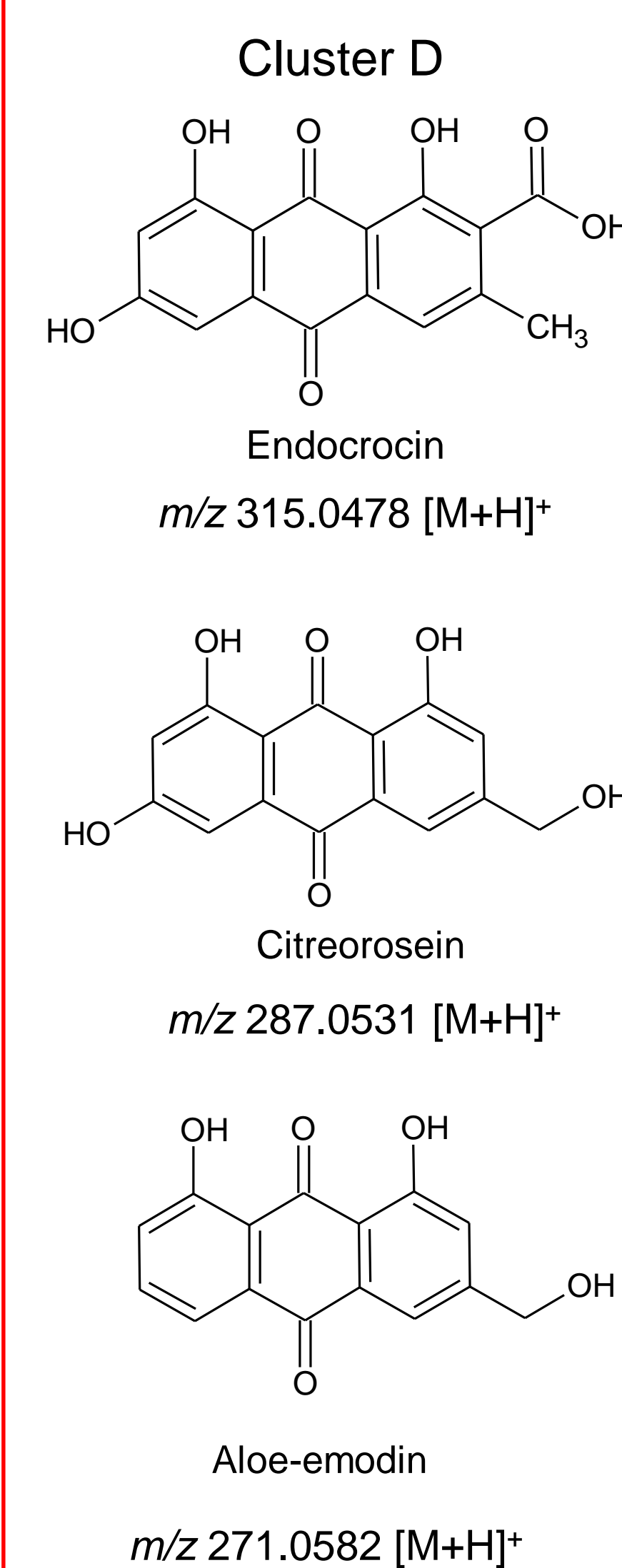
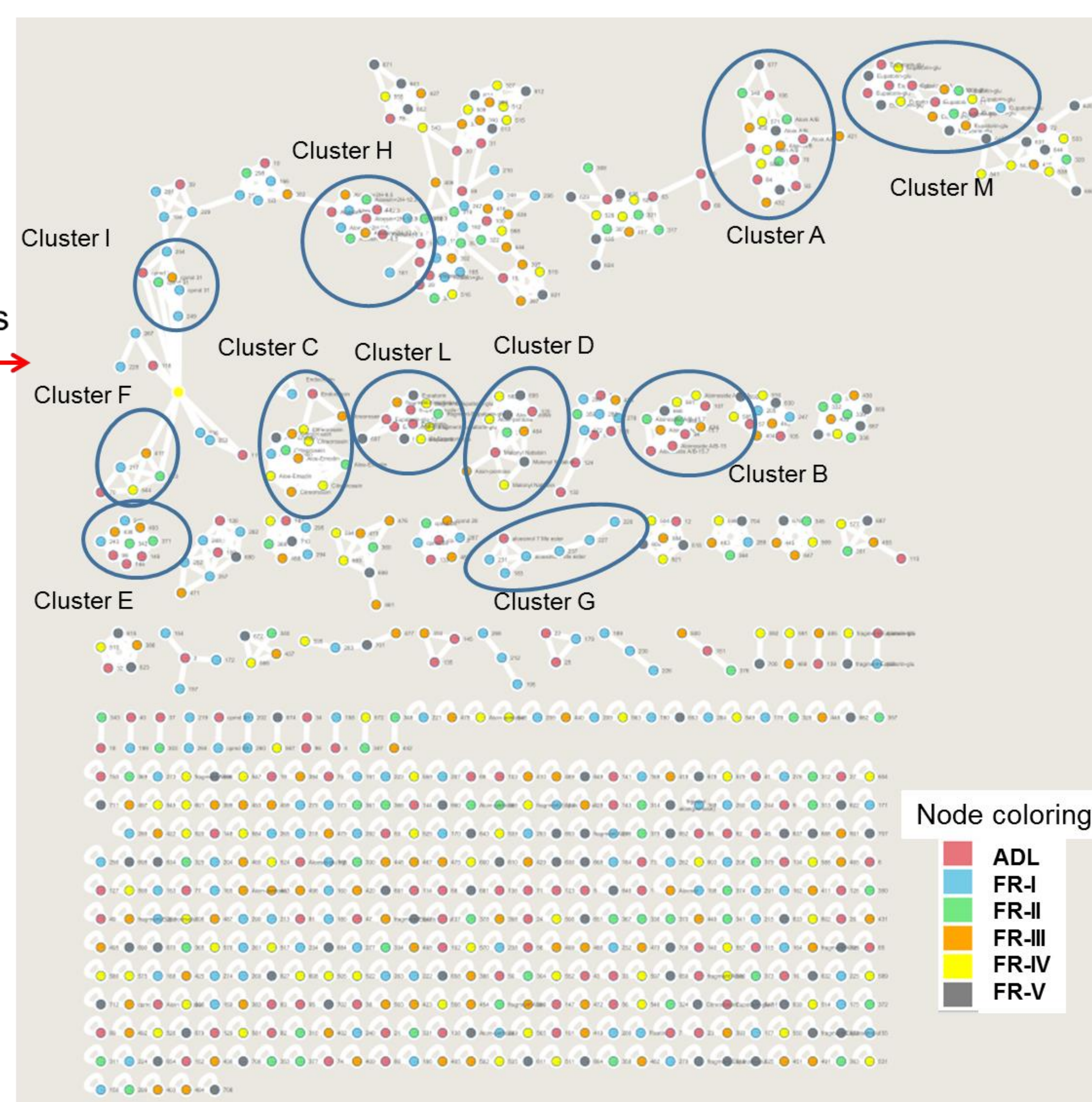
Fractionation

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

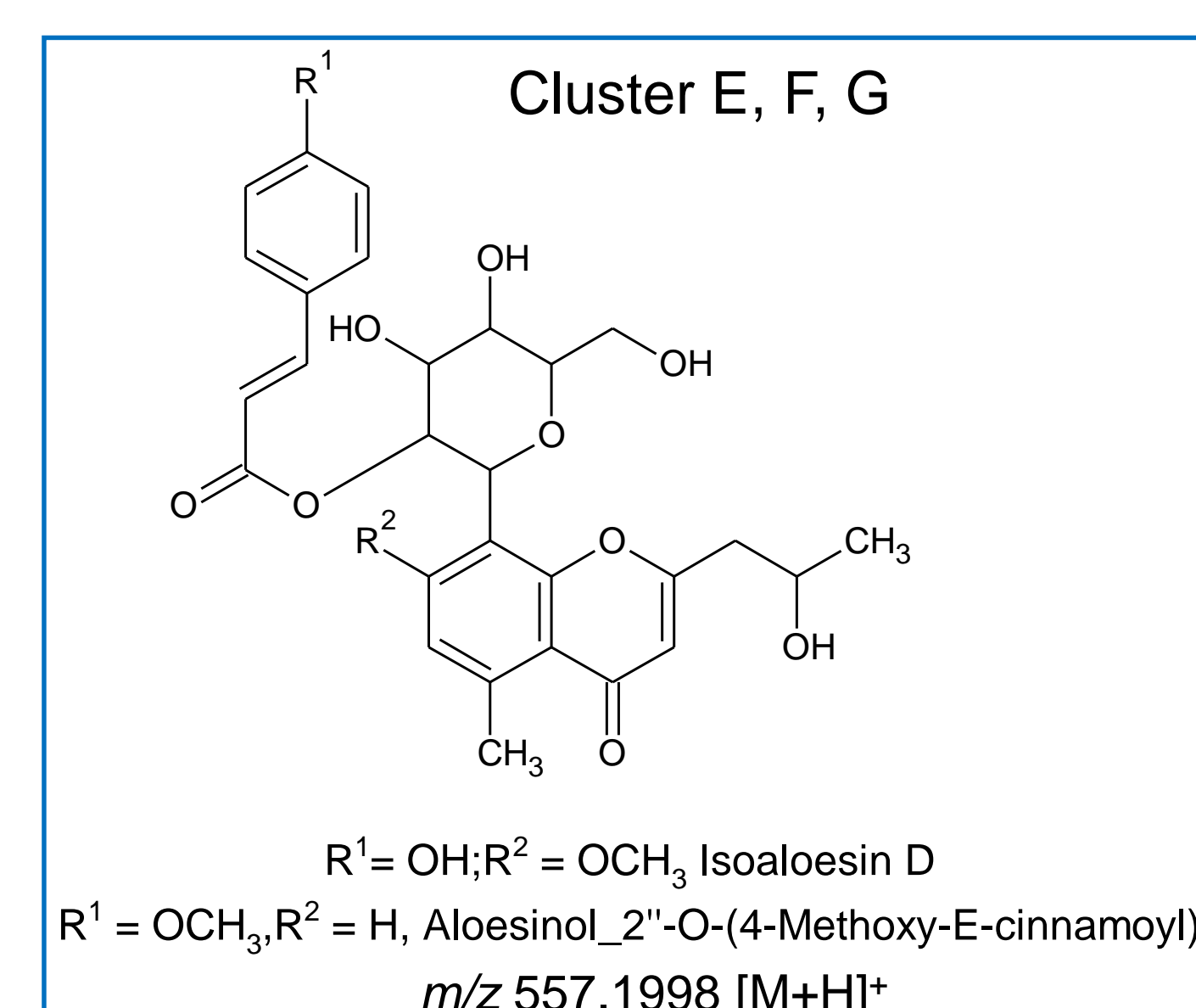
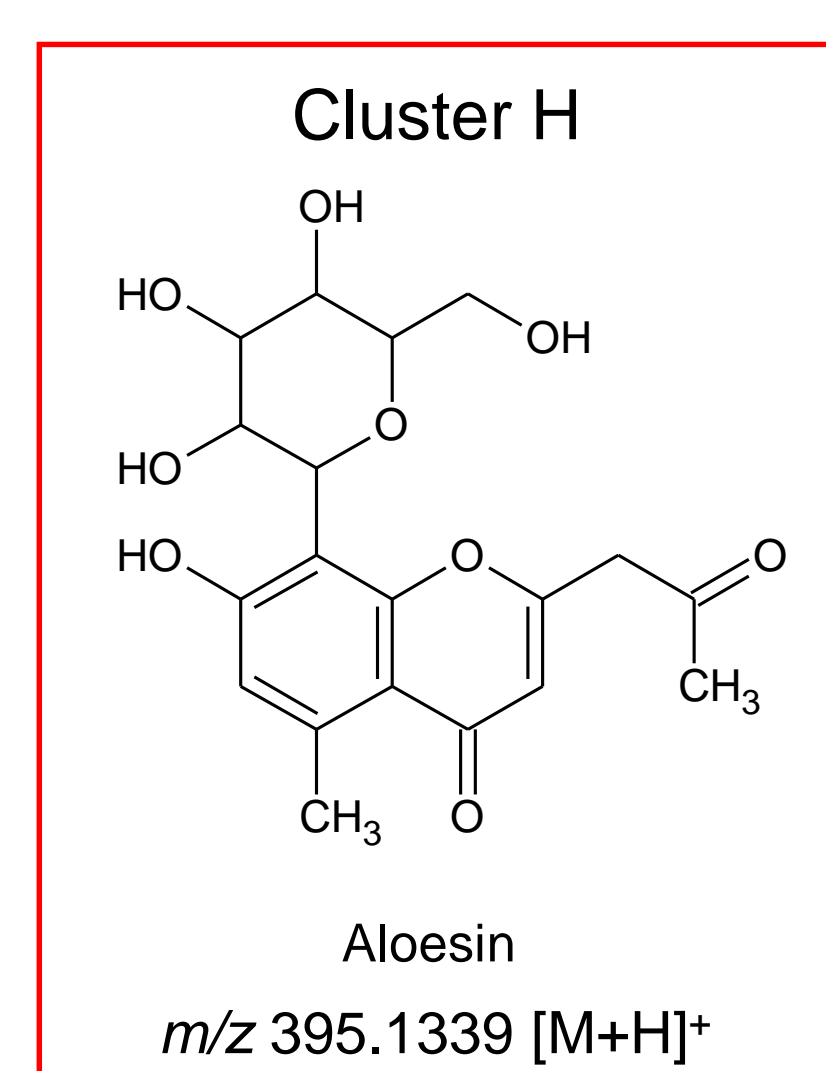
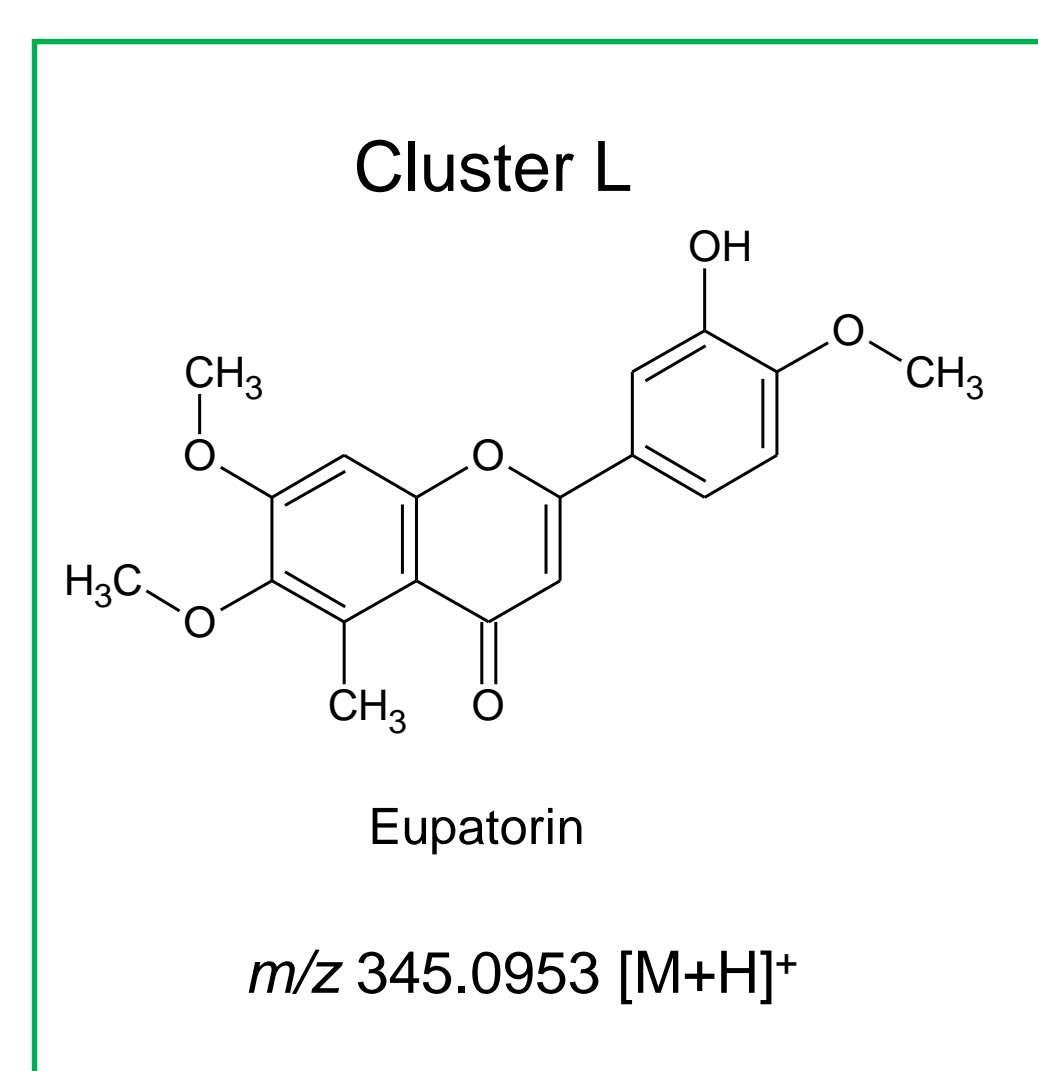
ABTS IC₅₀ = 600 ± 1.8 µg/mL
FRAP = 1.50 ± 0.12 mg EVC/g DW

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