

SCREENING OF MEDICINAL PLANT EXTRACTS FOR ANTIRETROVIRAL ACTIVITY: PRELIMINARY INSIGHTS TOWARDS HIV THERAPY

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INTRODUCTION

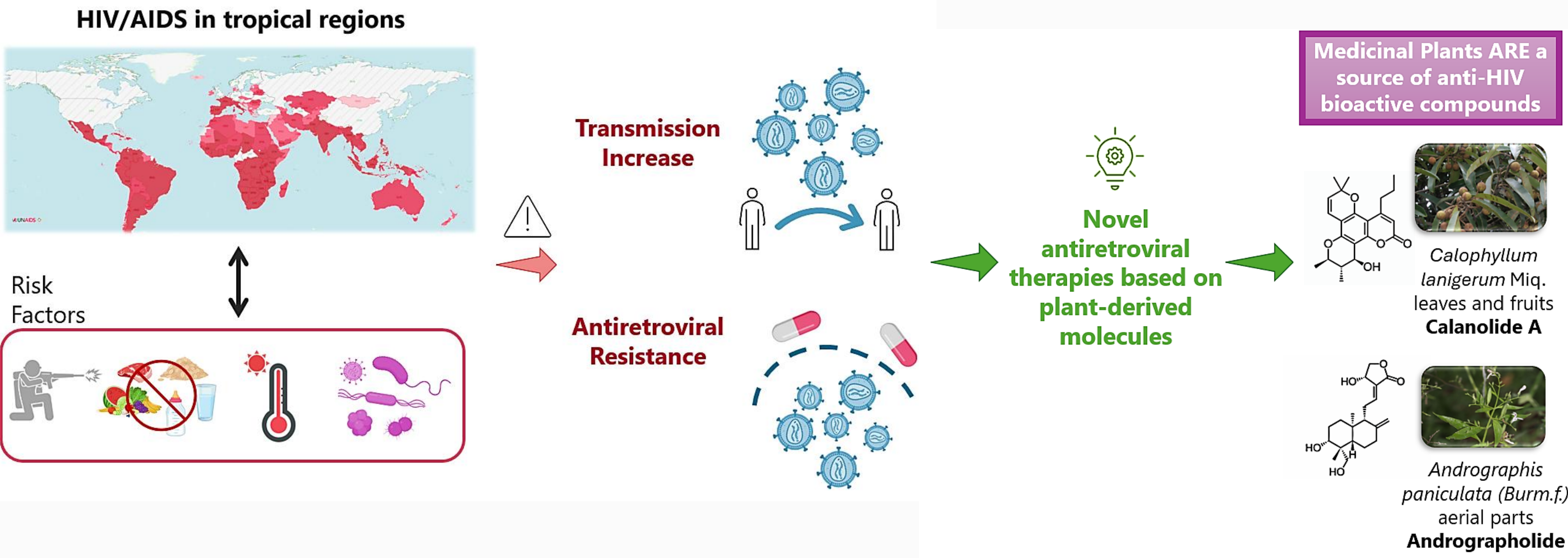
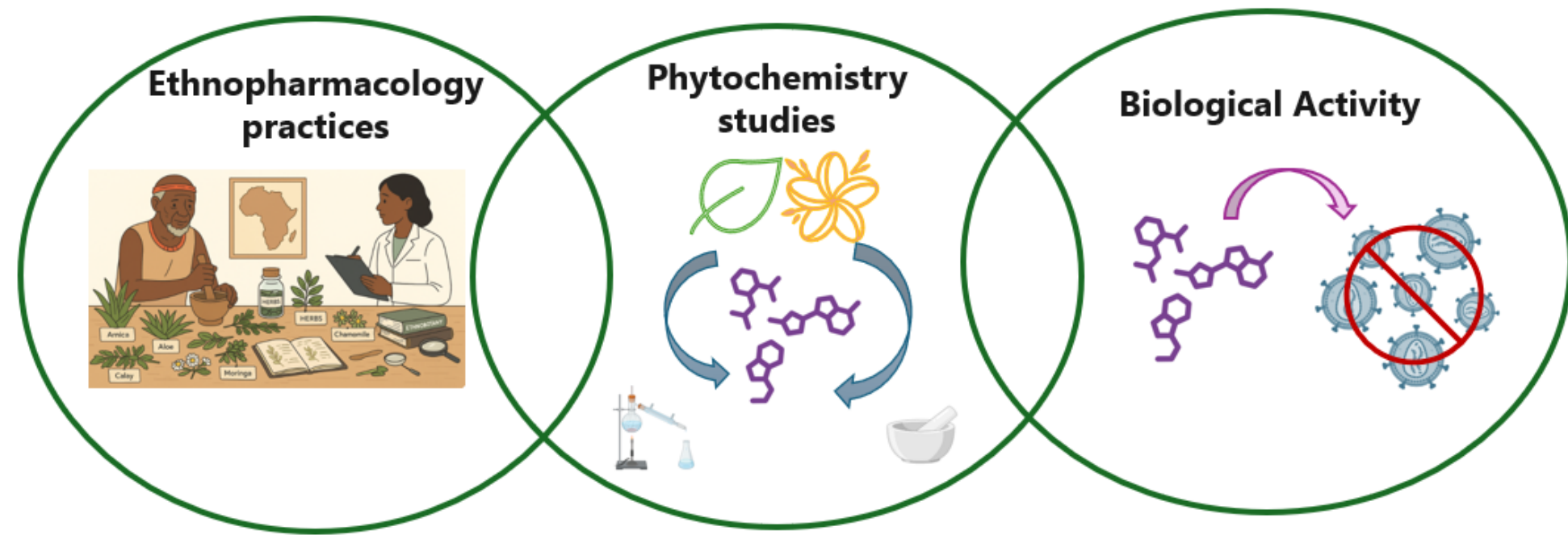


Figure 1: Plant-derived compounds can help combat HIV/AIDS challenges.

AIMS

To discover and develop natural, effective, and affordable novel plant-derived molecules with antiretroviral activity



MATERIALS AND METHODS

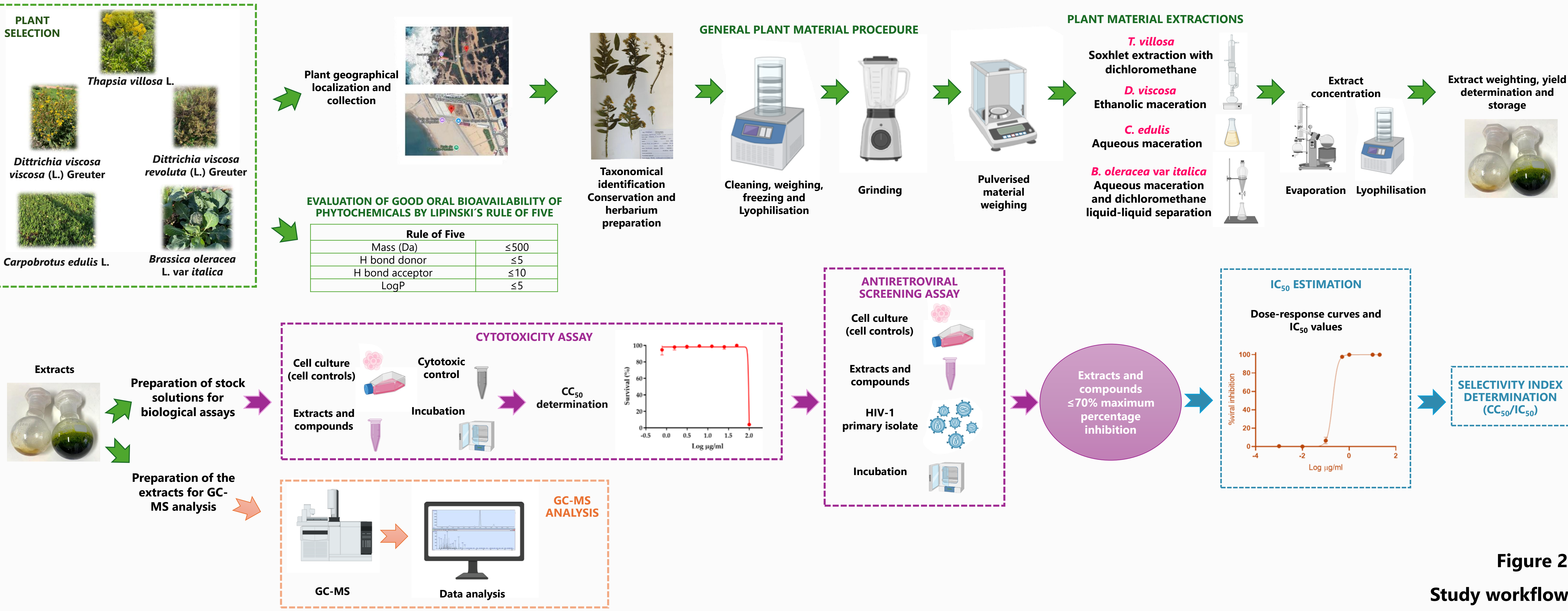


Figure 2: Study workflow.

RESULTS

Table 2: Medicinal plant extracts' anti-HIV activity and cytotoxicity.

Extracts, compounds and growth controls	Cytotoxic concentration 50% in TZM-bl cells (CC ₅₀)	Maximum percentage of inhibition	Inhibition concentration 50% against HIV-1 primary isolate (IC ₅₀)	Selectivity index (CC ₅₀ /IC ₅₀)
<i>T. villosa</i> L. extract 1	99.55 ± 0.55 µg/ml	92.5 ± 3.3	0.19 ± 0.03 µg/ml	517.51
<i>T. villosa</i> L. extract 2	> 100 µg/ml	80.1 ± 0.7	0.68 ± 0.02 µg/ml	> 148.15
<i>D. viscosa viscosa</i> extract 1	> 100 µg/ml	87.3 ± 4.2	4.34 ± 0.28 µg/ml	> 23.06
<i>D. viscosa viscosa</i> extract 2	> 100 µg/ml	89.3 ± 1.9	3.86 ± 0.89 µg/ml	> 25.88
<i>D. viscosa viscosa</i> extract 3	> 100 µg/ml	41.8 ± 2.4	-----	-----
<i>D. viscosa revoluta</i> extract 4	> 100 µg/ml	18.9 ± 3.2	-----	-----
<i>C. edulis</i> L. extract	> 100 µg/ml	25.5 ± 2.0	-----	-----
<i>B. oleracea</i> L. var <i>italica</i> extract 1	> 100 µg/ml	19.8 ± 2.3	-----	-----
<i>B. oleracea</i> L. var <i>italica</i> extract 2	> 100 µg/ml	18.6 ± 6.1	-----	-----
BITC (benzyl isothiocyanate)	50.51 ± 1.19 µg/ml	Not active	-----	-----
AITC (allyl isothiocyanate)	50.85 ± 1.85 µg/ml	Not active	-----	-----
DMSO	3.5 %	-----	-----	-----
BSS-730A (antiretroviral control)	76.84 µM (50.54 µg/ml) ^a	92.2 ± 2.3 (0.0053 µg/ml)	0.008 µM (0.0053 µg/ml) ^{a,b}	9605 ^a

^a Published in Bártolo *et al.* 2021 ^b The positive control was used at the MPI concentration in the IC₅₀ determination

Table 1: Examples of compounds from each plant evaluated by the Lipinsky Rule of Five.

Plant compounds	Class of compound	Rule of Five				Good oral bioavailability ?
		Mass (Da) ≤ 500	H bond donor ≤ 5	H bond acceptor ≤ 10	LogP ≤ 5	
<i>T. villosa</i> L.	Sesquiterpene Lactone	344.16	0	5	3.4	YES
<i>D. viscosa viscosa</i> L.	Sesquiterpene Lactone	248.14	0	3	1.9	YES
<i>D. viscosa revoluta</i> L.	Flavonoid	304.05	5	7	1.5	YES
<i>C. edulis</i> L.	Flavonoid	290.08	5	6	0.4	YES
<i>B. oleracea</i> var. <i>italica</i>	Indole derivative	147.03	1	2	0.8	YES

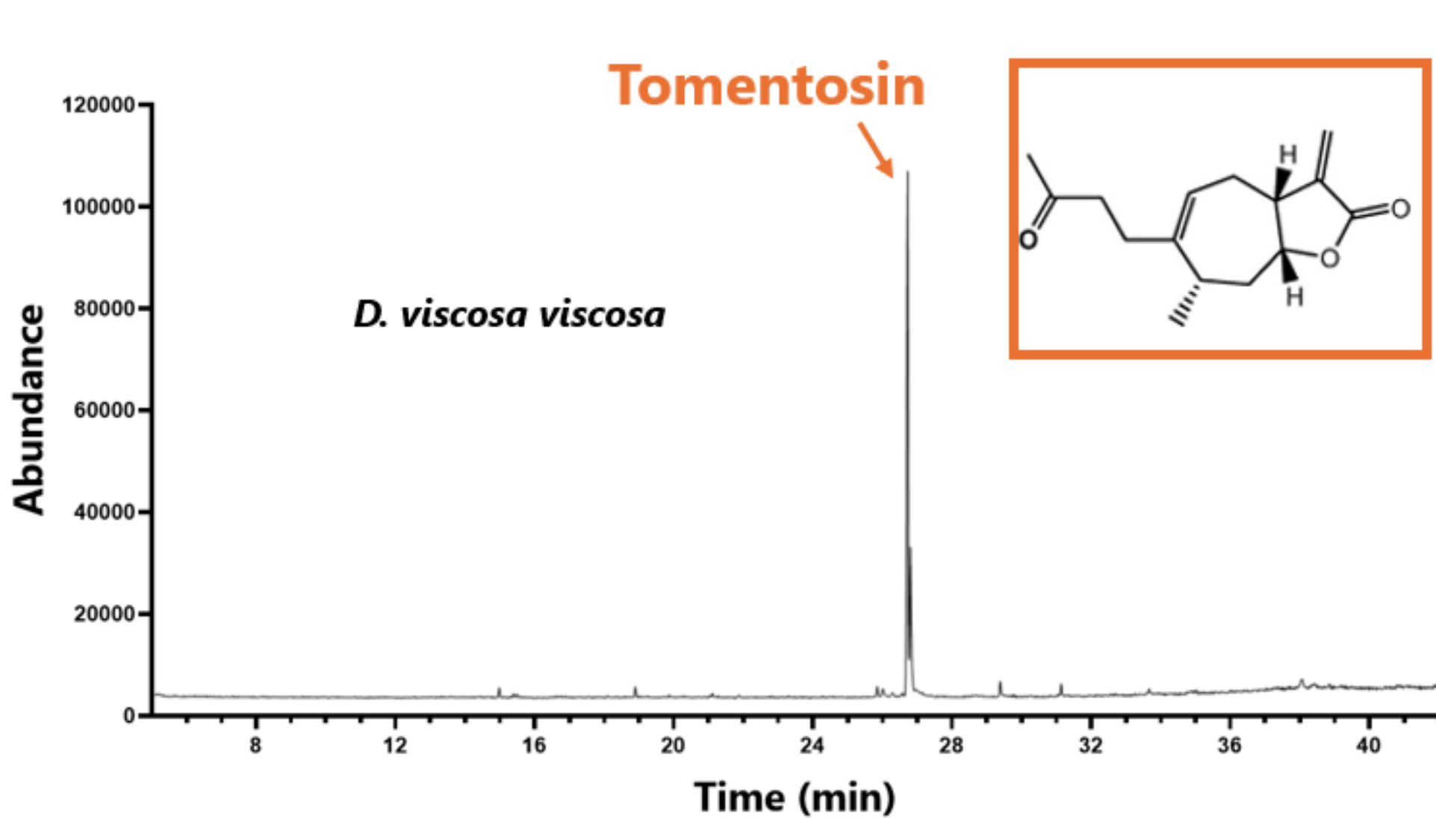


Figure 3: GC-MS chromatogram of tomentosin from *D. viscosa viscosa* L.

CONCLUSIONS

- T. villosa* L. and *D. viscosa viscosa* L. extracts 1 and 2 with maximum antiviral activity and minimal cell toxicity
- The remaining plant extracts also showed some activity without cell toxicity
- Possible active compounds are being identified by GC-MS

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