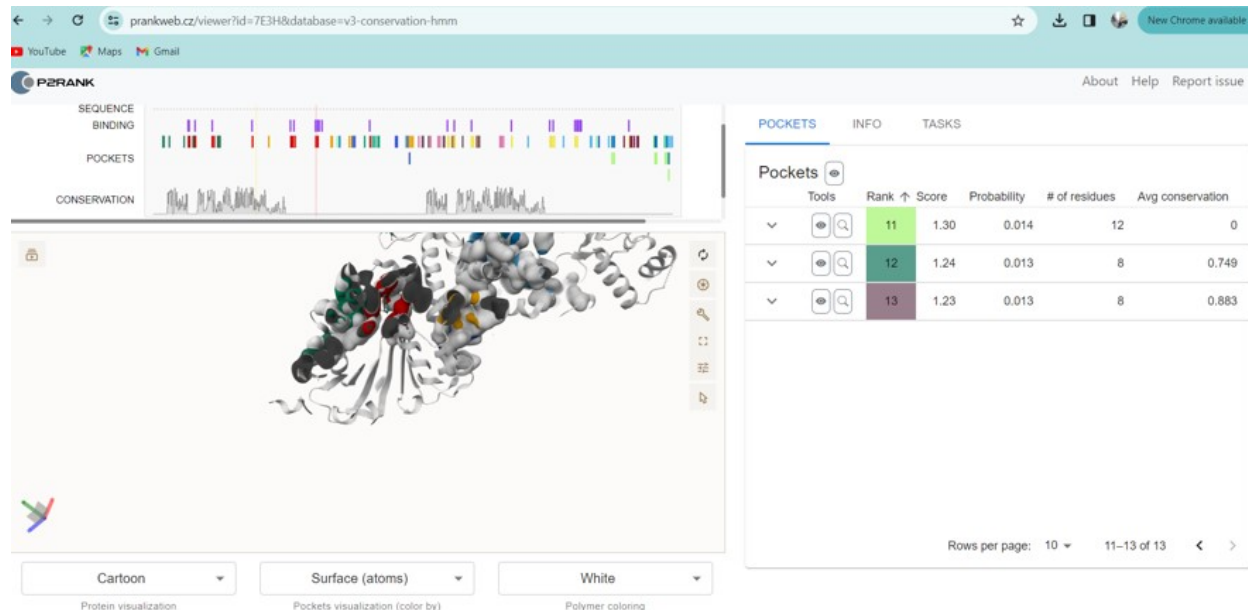
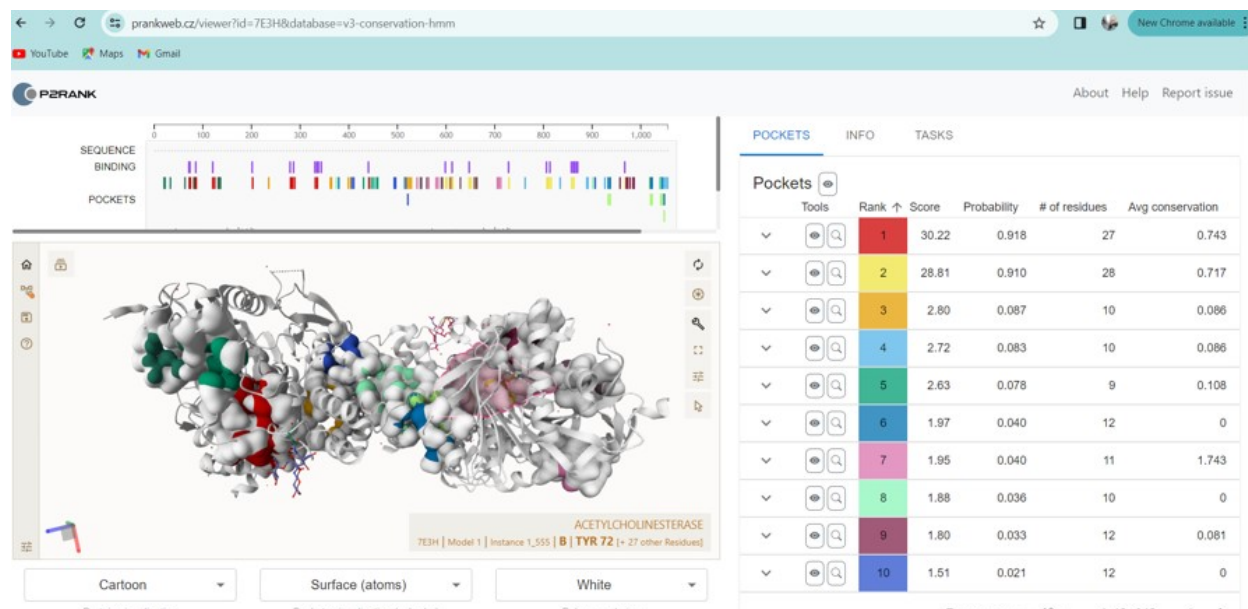


PrankWeb predictions:

A)



B)

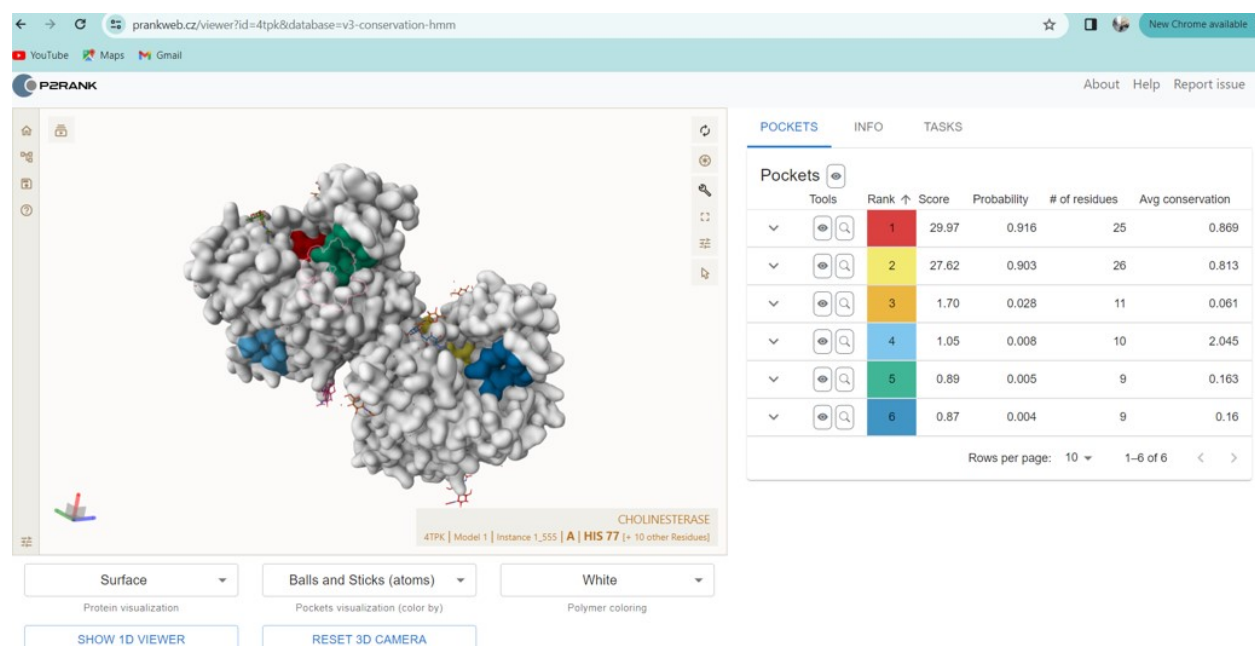


Fig. S1. PrankWeb server predictions: A) 7E3H, B) 4TPK.

DeepSite Predictions: Chain A

A)



B)



Fig.S2. DeepSite Predictions Chain A, Pocket 1: A) 7E3H, B) 5TPK.

DeepSite Predictions: Chain B

A)



playmolecule.org/deepsite/

Queue Status: running | Log out | Hello Asma

DEEPSITE sessions

Description	JobID	Url
pdbid: 7E3H chain: B	797C8728	G
pdbid: 4TPK chain: A	00ED9395	G
pdbid: UNK chain: A	55156505	G

Job Configuration

DeepSite prediction results

id	centers	score
1	$[-44.1, 11.3, -82.8]$	1.00
2	$[-32.1, 15.3, -66.8]$	0.98
3	$[-18.1, 13.3, -98.8]$	0.94
4	$[-50.1, 21.3, -94.8]$	0.89

DOWNLOAD RESULTS

DOWNLOAD CUBE FILE

Polymer 1
/static/apps/deepsite/output... | Model 1 | Instance 1_555 | B | PHE 286 (auth 295)

B)



playmolecule.org/deepsite/

Queue Status: running | Log out | Hello Asma

DEEPSITE sessions

Description	JobID	Url
pdbid: 4TPK chain: B	266CF208	G
pdbid: 7E3H chain: B	797C8728	G
pdbid: 4TPK chain: A	00ED9395	G
pdbid: UNK chain: A	55156505	G

Job Configuration

DeepSite prediction results

id	centers	score
1	$[-17.5, -24.7, 41.1]$	1.00
2	$[-47.5, -24.7, 31.1]$	0.92
3	$[-23.5, -54.7, 45.1]$	0.94
4	$[-27.5, -34.7, 25.1]$	0.64

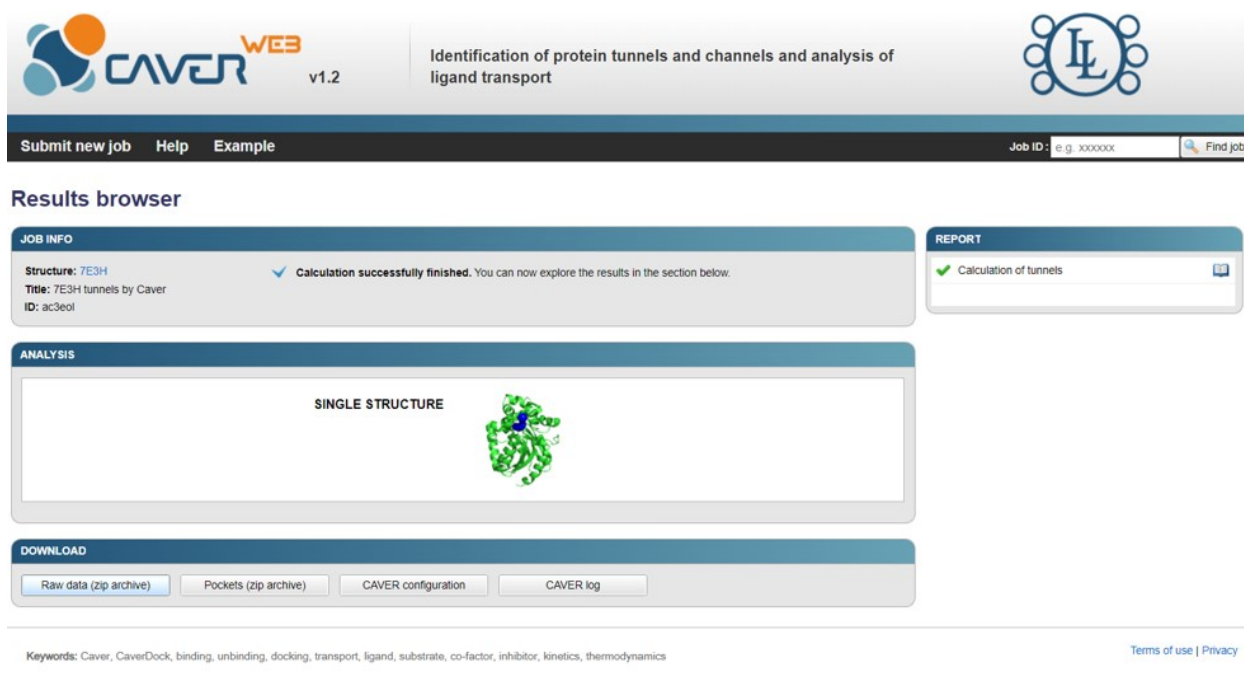
DOWNLOAD RESULTS

DOWNLOAD CUBE FILE

Polymer 1
/static/apps/deepsite/output... | Model 1 | Instance 1_555 | B | TRP 79 (auth 82)

Fig.S3. DeepSite Predictions Chain B, Pocket 1: A) 7E3H, B) 5TPK.

Tunnel Prediction by CAVER



The screenshot displays the CAVER web interface. At the top, the CAVER logo and version (v1.2) are shown, along with the description: "Identification of protein tunnels and channels and analysis of ligand transport". A navigation bar includes links for "Submit new job", "Help", and "Example". A search bar for "Job ID" is present with a "Find job" button. The main content area is titled "Results browser" and is divided into three sections: "JOB INFO", "ANALYSIS", and "DOWNLOAD".

JOB INFO

Structure: 7E3H
Title: 7E3H tunnels by Caver
ID: ac3e0f

✓ Calculation successfully finished. You can now explore the results in the section below.

ANALYSIS

SINGLE STRUCTURE

The analysis section displays a 3D visualization of a protein structure (green) with a tunnel highlighted in blue.

DOWNLOAD

Raw data (zip archive) Pockets (zip archive) CAVER configuration CAVER log

REPORT

✓ Calculation of tunnels

Keywords: Caver, CaverDock, binding, unbinding, docking, transport, ligand, substrate, co-factor, inhibitor, kinetics, thermodynamics

Terms of use | Privacy

Fig.S4. 7E3H CAVER Tunnel Predictions.

Way2Drug Predictions:

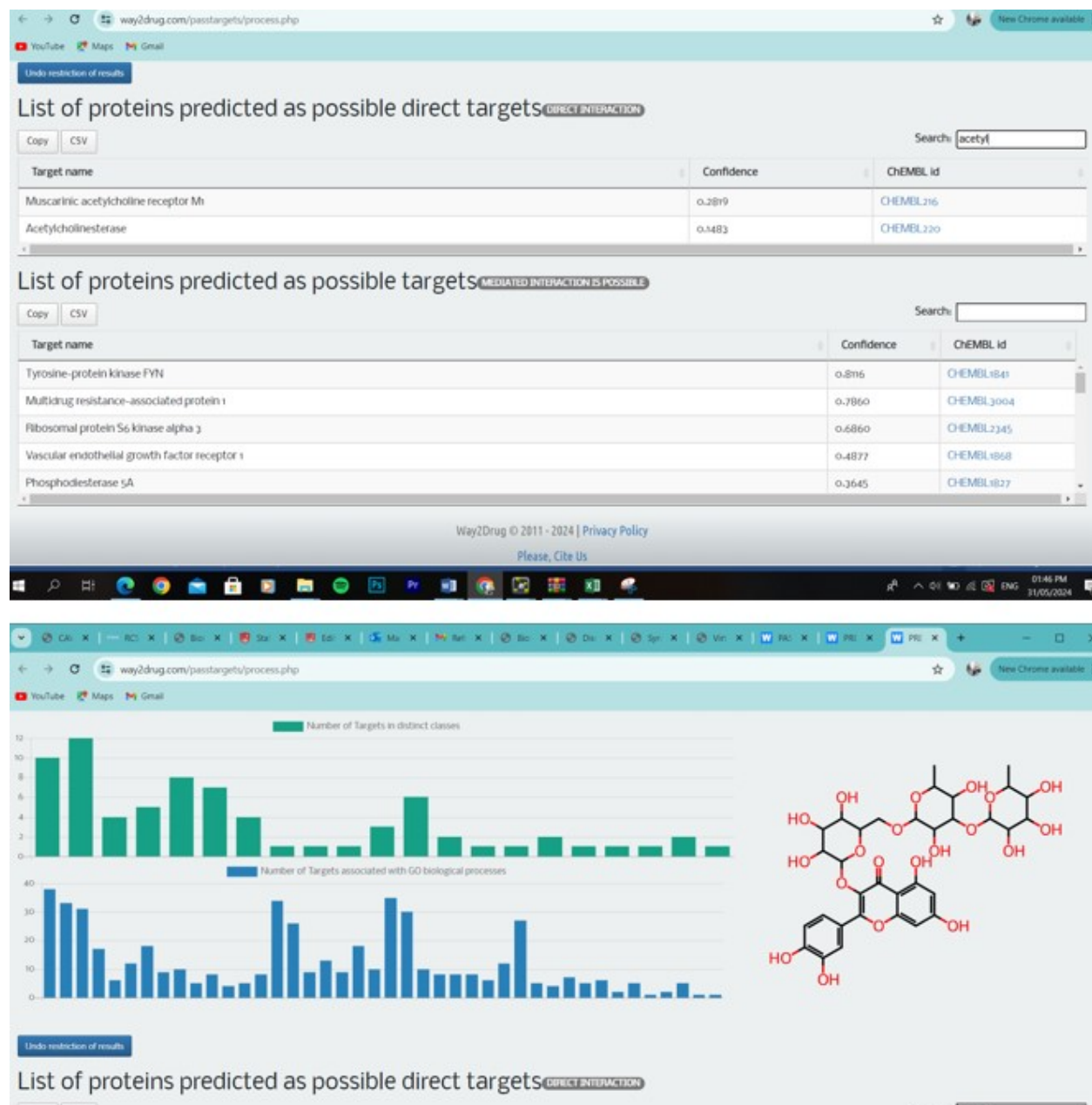
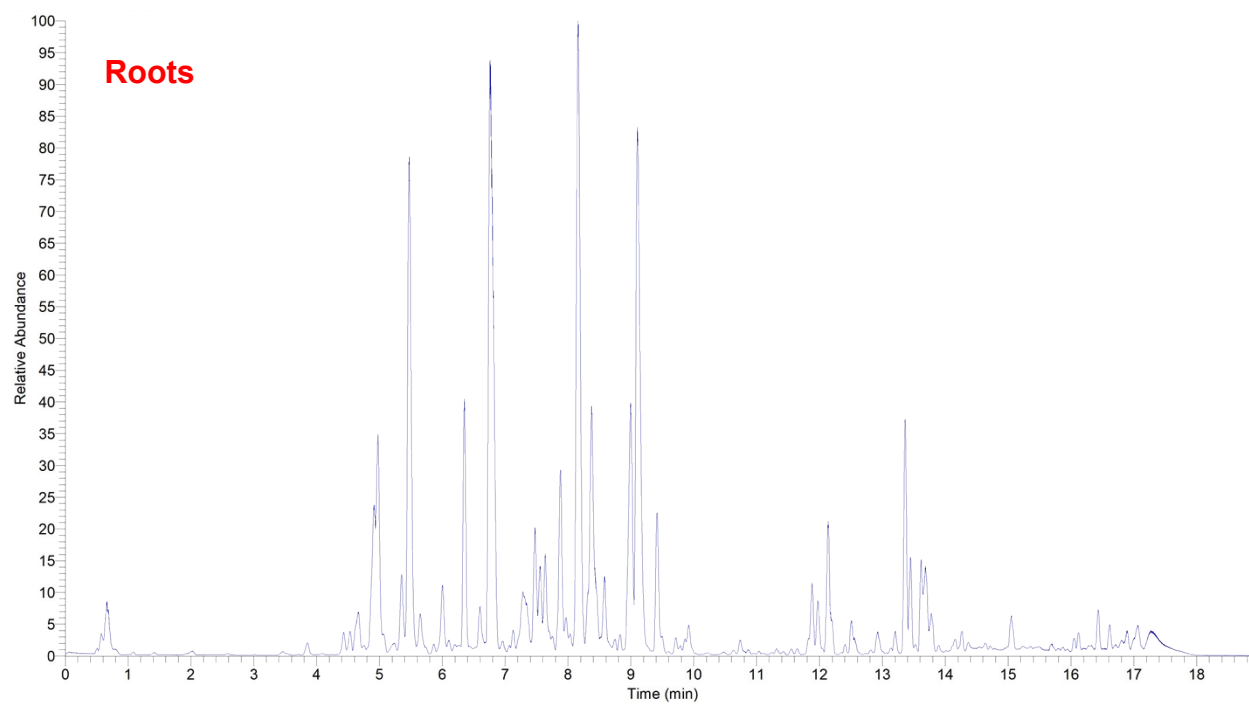
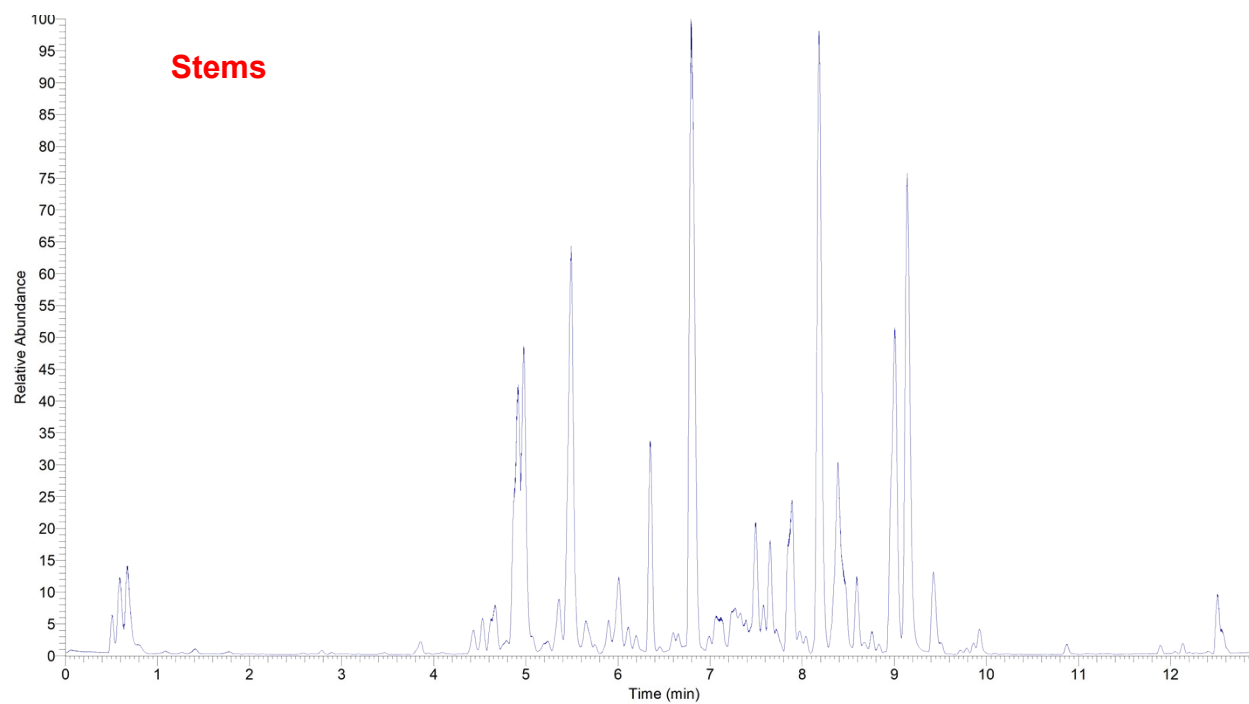


Fig. S5. Compound 12 Activity Prediction.



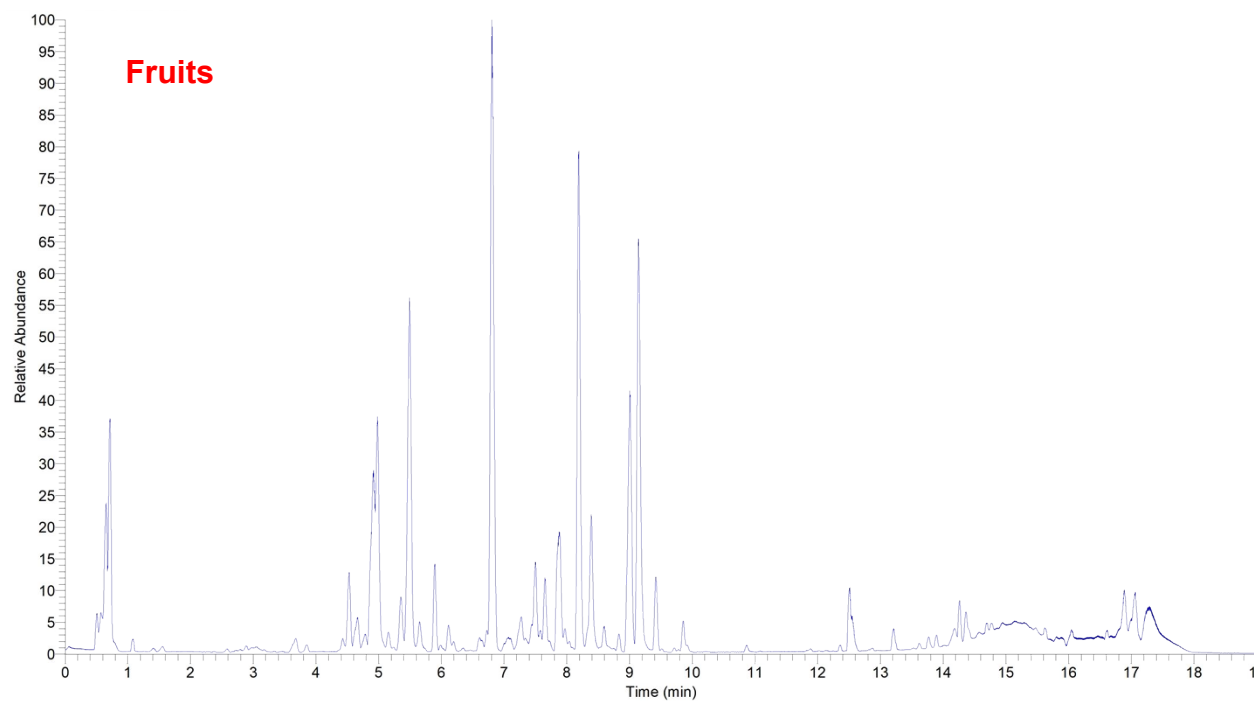
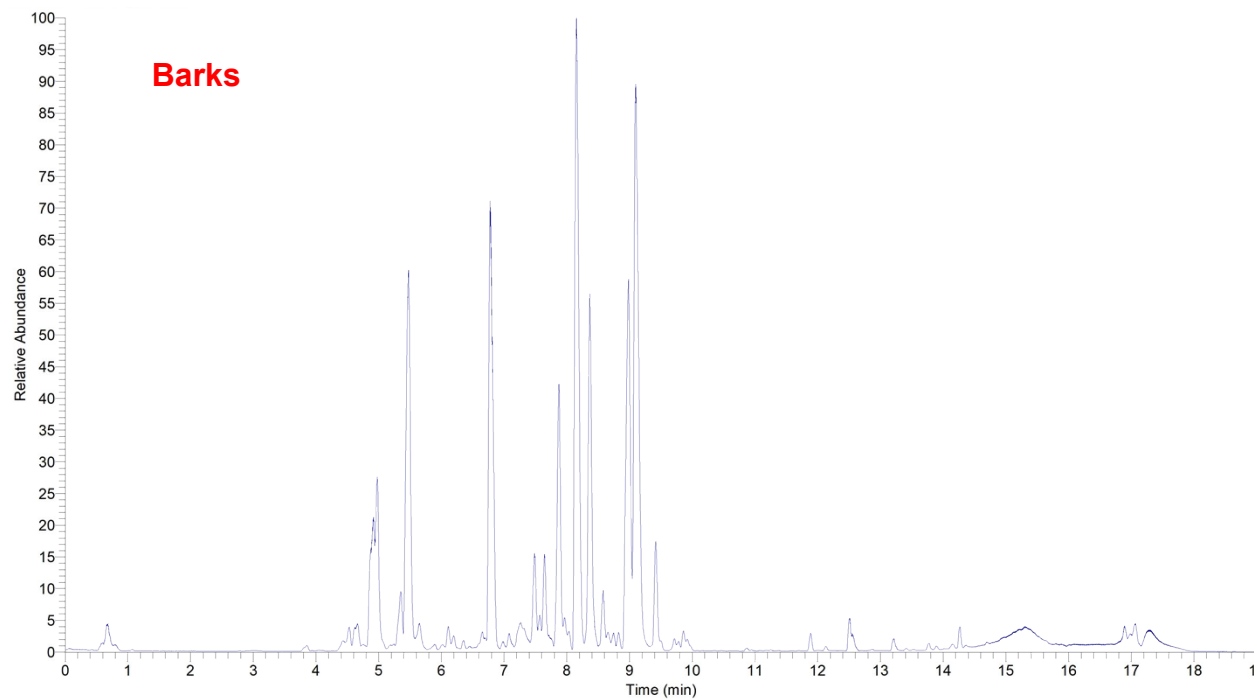


Fig. S6. Total ion chromatograms (TIC, +ESI) of the hydroalcoholic extracts prepared from the different organs of *Ochrosia elliptica* Labill.

