QUALOME

Chemical profiling of a *Rhodiola rosea* extract by NMR and liquid chromatography coupled to mass spectrometry (LC/MS)

Internal R&D

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NatExplore SAS - 25, la chute des eaux - 51140 Prouilly
SIRET : 84288816600019 - TVA IC : FR28842888166
jane.hubert@nat-explore.com / alexis.kotland@nat-explore.com

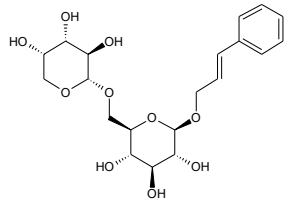
Chemical profiling and specific search of rosarin, rosavin, rosin and salidroside in *Rhodiola rosea* extract

Objective

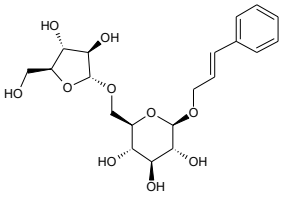
The objective of this work was to:

- Investigate the chemical profile of a *Rhodiola rosea* extract using liquid chromatography coupled to high resolution mass spectrometry and NMR.
- Search for the chemical markers rosavin, rosarin, rosin and salidroside.

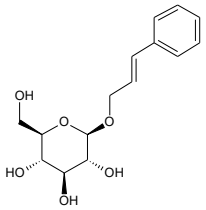
Rosavin



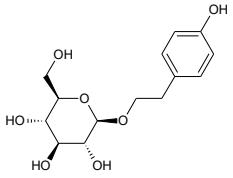
Rosarin



Rosin



Salidroside



Starting material

- Project QUALOME
- Sample description: 15 % vol, racines et rhizomes de *Rhodiola rosea*, eau de source, vodka, Les jardins de la Santé, Evoleina Rhodiola SARL (labeled RHOT-EXT) provided by Julien Héritier, MEDIPLANT.
- Quantity shipped ≈ 20 mL (two flasks of 10 mL)
- Analysis period: April 2026

Liquid-liquid extraction

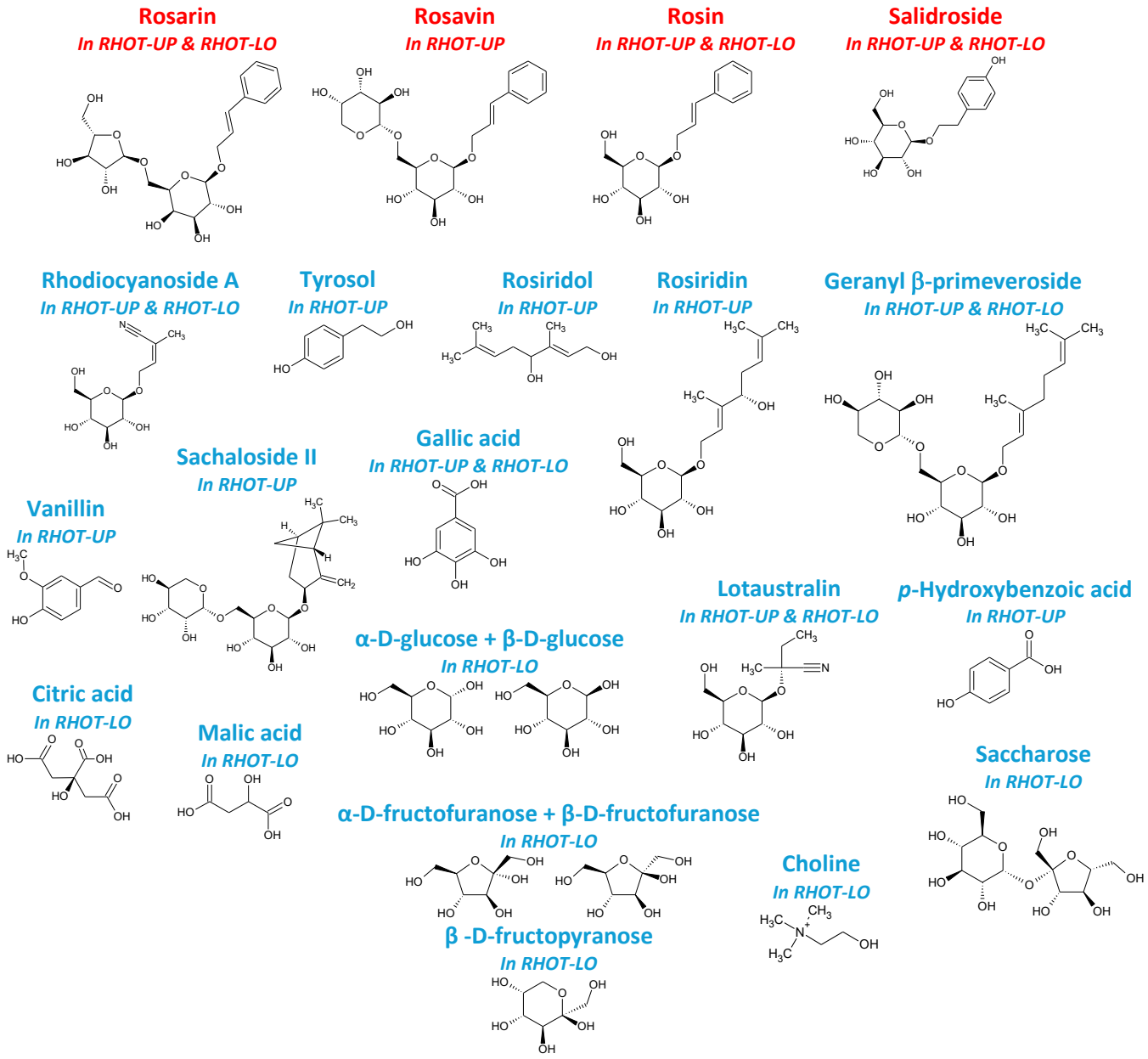
The liquid extract (21 mL) was mixed with 60 mL of water, 60 mL of acetonitrile and 60 mL of ethyl acetate. After a vigorous shaking, the biphasic solution was separated in two phases. The lower phase was re-extracted twice with 100 mL of the upper phase of the biphasic solvent system ethyl acetate/acetonitrile/water (3/3/4, v/v). The upper phases were combined and evaporated to dryness, resulting in 21 mg (RHOT-UP). The lower phase was also evaporated to dryness (RHOT-LO, 277 mg).

NMR analyses and metabolite identification

RHOT-UP (≈21 mg) and RHOT-LO (≈23 mg) were dissolved in 700 µL of DMSO-*d6* and analyzed by ^{1}H, ^{13}C, HSQC, HMBC, and COSY NMR at 298 K on a Bruker Avance AVIII-600 spectrometer (Karlsruhe, Germany) equipped with a cryoprobe. Data were processed with TopSpin 4.2.0. Data were processed with TopSpin 4.2.0. Structural elucidation was performed by rigorously scrutinizing all 1D and 2D NMR spectra. The metabolites identified by NMR are given in Figure 1.

The four chemical markers were searched by scrutinizing specific atom positions in HSQC spectra.

Figure 1. Chemical structures identified by NMR in RHOT-UP and RHOT-LO. The targeted compounds were highlighted in red.



Liquid Chromatography / Mass Spectrometry

RHOT-EXT was also analyzed at 2 g/L in MeOH/H_2O (80/20, v/v) by LC/HRMS.

Mass spectrometer: SYNAPT G2 si (Waters) – High Resolution

- HPLC column: Uptisphere C-18 ODB 150*2.1 mm, 2.2 µm (Interchim)
- Mass spectrometry parameters: ESI-, *m/z* 50-2000, scan 1s
- Data processing software: MassLynx

The resulting BPI chromatogram is given in Figure 2, and LC/MS data are summarized in Table 1.

Figure 2. LC/MS BPI chromatogram of RHOT-EXT (ESI-)

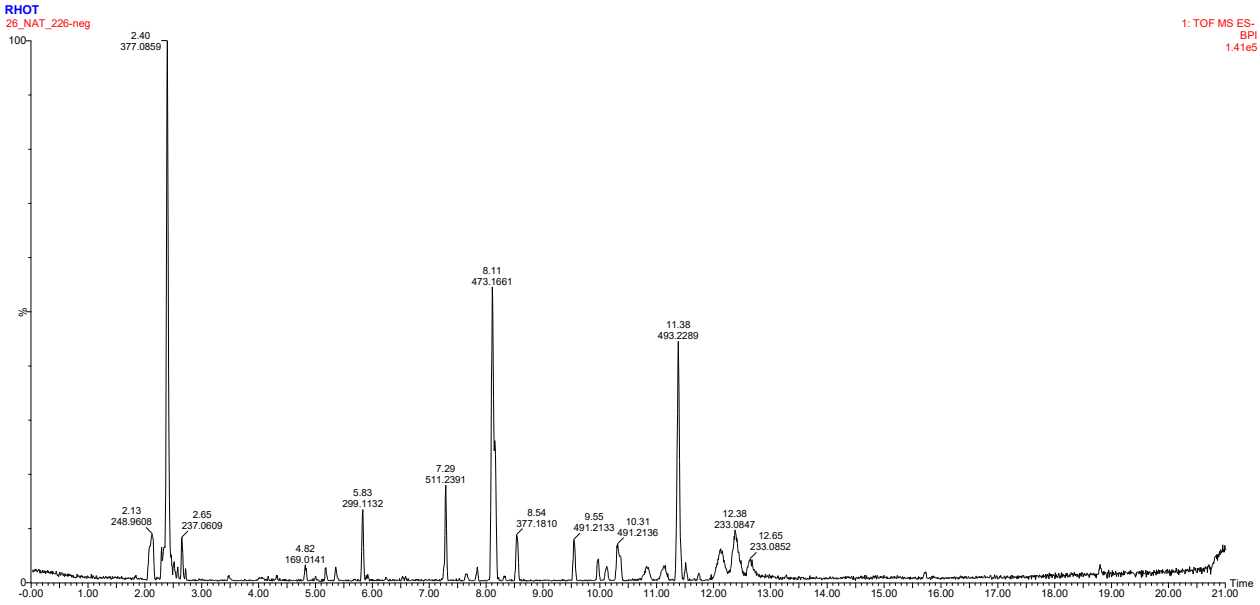


Table 1. Summary of LC/MS data

LC Rt (min)	Observed *m/z*	Elemental composition	Δppm	Annotation **
2.29	211.0816 $[M-H]^-$	$C_7H_{15}O_7$	-0.9	Volemitol*
2.40	341.1079 $[M-H]^-$	$C_{12}H_{21}O_{11}$	-1.5	Saccharose*
2.59	369.1041 $[M-H]^-$	$C_{13}H_{21}O_{12}$	2.2	Disaccharide*
2.64	237.0612 $[M-H]^-$	$C_8H_{13}O_8$	0.8	2-Keto-3-deoxyoctonate or isomer
3.48	191.0189 $[M-H]^-$	$C_6H_7O_7$	-1.6	Citric acid*
4.82	169.0145 $[M-H]^-$	$C_7H_5O_5$	4.7	Gallic acid*
5.17	306.1189 $[M-H]^-$	-	-	*Not assigned*
5.83	299.1132 $[M-H]^-$	$C_{14}H_{19}O_7$	0.3	**Salidroside***
7.29	511.2400 $[M+HCOO]^-$ 465.2321 $[M-H]^-$	$C_{22}H_{39}O_{13}$ $C_{21}H_{37}O_{11}$	1.8 -3.2	Rhodioloside E or isomer

7.84	509.2236 $[M+HCOO]^-$ 463.2164 $[M-H]^-$	$C_{22}H_{37}O_{13}$ $C_{21}H_{35}O_{11}$	0.4 -3.2	Rhodioloside F
8.11	473.1660 $[M+HCOO]^-$ 427.1601 $[M-H]^-$	$C_{21}H_{29}O_{12}$ $C_{20}H_{27}O_{10}$	0.2 -0.7	**Rosarin* or rosavin***
8.15	473.1659 $[M+HCOO]^-$ 427.1596 $[M-H]^-$	$C_{21}H_{29}O_{12}$ $C_{20}H_{27}O_{10}$	0.0 -1.9	**Rosarin* or rosavin***
8.54	377.1810 $[M-H]^-$	$C_{17}H_{29}O_9$	-0.5	*Not assigned*
9.54	491.2133 $[M+HCOO]^-$ 445.2085 $[M-H]^-$	$C_{22}H_{35}O_{12}$ $C_{21}H_{33}O_{10}$	0.8 2.5	Sachaloside II or isomer
9.96	489.1968 $[M+HCOO]^-$ 443.1895 $[M-H]^-$	$C_{22}H_{33}O_{12}$ $C_{21}H_{31}O_{10}$	-0.8 -5.0	Dihydrophaseic acid glucoside or isomer
10.12	187.0971 $[M-H]^-$	$C_9H_{15}O_4$	0.5	Column impurity
10.31	491.2135 $[M+HCOO]^-$ 445.2066 $[M-H]^-$	$C_{22}H_{35}O_{12}$ $C_{21}H_{33}O_{10}$	1.2 -1.8	Sachaloside II or isomer
11.41	493.2290 $[M+HCOO]^-$ 447.2232 $[M-H]^-$	$C_{22}H_{37}O_{12}$ $C_{21}H_{35}O_{10}$	-0.6 0.4	Geranyl β-primeveroside
11.50	469.2276 $[M+HCOO]^-$ 423.2213 $[M-H]^-$	$C_{20}H_{37}O_{12}$ $C_{19}H_{35}O_{10}$	-1.9 -4.0	Rhodiooctanoside or isomer

In blue: also identified by NMR

** in accordance with our internal LC/MS database*

*** in DOI: 10.1002/bmc.1198 ; DOI: 10.1055/s-2008-1034288 ; https://doi.org/10.3389/fphar.2025.1608767*

Conclusion

The four chemical markers rosarin, rosavin, rosin, and salidroside were identified by NMR In the *Rhodiola rosea* extract examined in this study.

A diversity of other metabolites were also identified by NMR and/or annotated by LC/MS, as listed below:

- Rosavin **CAS 84954-92-7**
- Rosarin **CAS 84954-93-8**
- Rosin **CAS 85026-55-7**
- Salidroside **CAS 10338-51-9**
- Rhodiocyanoside A **CAS 168433-86-1**
- Tyrosol **CAS 10597-60-1**
- Rosiridin **CAS 100462-37-1**
- Geranyl β-primeveroside **CAS 150995-11-2**
- Rosiridol **CAS 101391-01-9**
- Gallic acid **CAS 149-91-7**
- Lotaustralin **CAS 534-67-8**
- *p*-Hydroxybenzoic acid **CAS 99-96-7**
- Vanillin **CAS 121-33-5**
- Sachaloside II **CAS 1001645-53-9**
- α-D-glucose **CAS 492-62-6**
- β-D-glucose **CAS 492-61-5**
- α-D-fructofuranose **CAS 10489-79-9**

- β-D-fructofuranose **CAS 470-23-5**
- β-D-fructopyranose **CAS 7660-25-5**
- Saccharose **CAS 57-50-1**
- Choline **CAS 62-49-7**
- Citric acid **CAS 77-92-9**
- Malic acid **CAS 6915-15-7**