

SUPPLEMENTARY MATERIALS

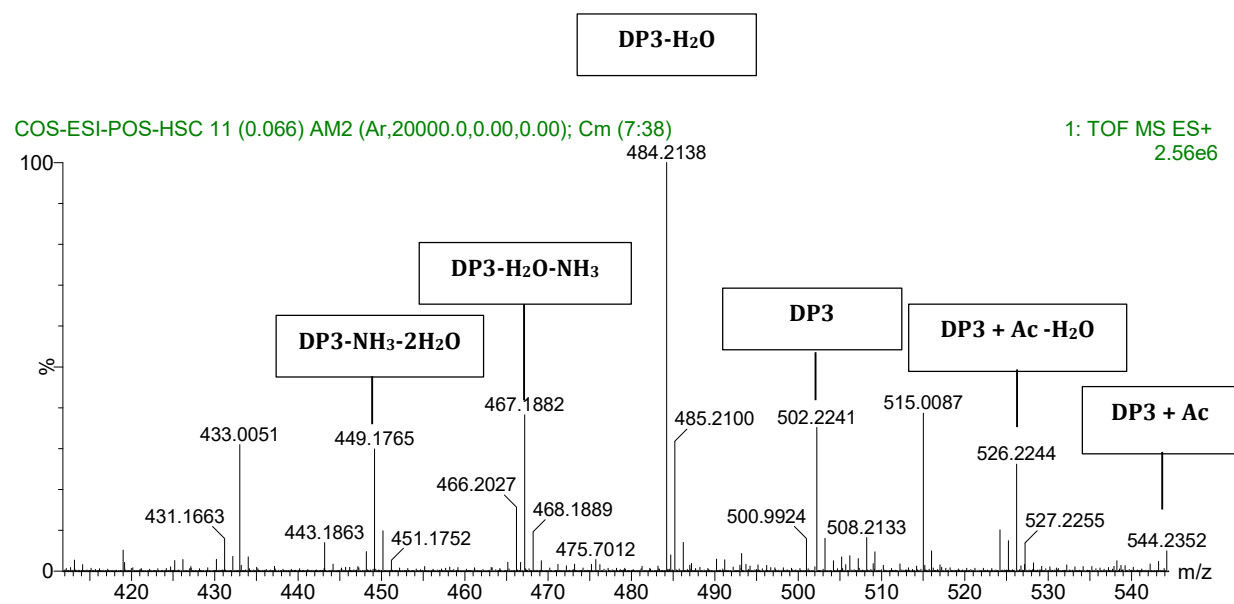


Figure S1. Electrospray-ionization high resolution mass spectrometry (ESI-HRMS) analysis of selected DP3 of chitosan oligosaccharides obtained from fungal chitosan by acetic acid hydrolyzed method using autoclaving-cooling process (10 cycles, 30 min at 121 °C and 15 min cooling).

Table S1: Mass spectrometric data for COS oligomers produced during the acid hydrolysis process.

| | Elemental composition | Experimental m/z | Theoretical m/z | Error (ppm) | Error (mDa) |
|-----------------------|--|------------------|-----------------|-------------|-------------|
| DP1-H ₂ O | C ₆ H ₁₁ O ₄ N | 162.0766 | 162.0767 | 0.4 | 0.1 |
| DP2-H ₂ O | C ₁₂ H ₂₂ O ₈ N ₂ | 323.1454 | 323.1453 | -0.4 | -0.1 |
| DP3-H ₂ O | C ₁₈ H ₃₃ O ₁₂ N ₃ | 484.2143 | 484.2138 | -0.9 | -0.5 |
| DP4-H ₂ O | C ₂₄ H ₄₄ O ₁₆ N ₄ | 645.2831 | 645.2837 | 1.0 | 0.6 |
| DP5-H ₂ O | C ₃₀ H ₅₅ O ₂₀ N ₅ | 806.3519 | 806.3519 | 0.0 | 0.0 |
| DP6-H ₂ O | C ₃₆ H ₆₆ O ₂₄ N ₆ | 967.4207 | 967.4202 | -0.5 | -0.5 |
| DP7- H ₂ O | C ₄₂ H ₇₇ O ₂₈ N ₇ | 1128.4895 | 1128.4868 | -2.4 | -2.7 |
| DP8-H ₂ O | C ₄₈ H ₈₈ O ₃₂ N ₈ | 1289.5583 | 1289.5535 | -3.7 | -4.8 |
| DP9-H ₂ O | C ₅₄ H ₉₉ O ₃₆ N ₉ | 1450.6271 | 1450.621 | -4.2 | -6.1 |
| DP10-H ₂ O | C ₆₀ H ₁₁₀ O ₄₀ N ₁₀ | 1611.6959 | 1611.6892 | -4.2 | -6.7 |

Table S2: ¹H-NMR and ¹³C-NMR spectral data for a solution of chitosan oligosaccharides solubilized in deuterium oxide (10 mg/mL).

| Chemical shifts (δ) relative to TMSP * | | | |
|--|------|-----------------|-------|
| H ₁ | 4.69 | C ₁ | 102.6 |
| H ₂ | 2.98 | C ₂ | 59.0 |
| H ₃ | 3.73 | C ₃ | 74.6 |
| H ₄ | 3.82 | C ₄ | 79.8 |
| H ₅ | 3.68 | C ₅ | 77.9 |
| H ₆ | 3.79 | C ₆ | 62.9 |
| H _{6'} | 3.95 | - | - |
| C=O | - | C=O | 177.4 |
| CH ₃ | 2.07 | CH ₃ | 24.9 |

* 3-(trimethylsilyl)-propionic acid D₄, sodium salt

Table S3: Identification of phenolics compounds in roots and shoots of flax seedlings by UPLC-MS/MS.

| N | Family | Compounds | Part used | RT (min) | CCS (Å ²) | [M-H] ⁻ precursor ion (m/z) | MS ² fragment ions (m/z) | m/z (Expected) | Error (mDa) | Error (ppm) | Elemental Composition | Collision energy (eV) | References |
|---|---|-------------------------------------|---------------|----------|--------------------------|--|---|-------------------|-------------|----------------|---|-----------------------------|------------|
| 1 | Cyanogenic glycoside | Linamarin | shoots, roots | 0,54 | 165 | 292,1045 | | 292,1038 | 0,7 | 2,2 | C ₁₁ H ₁₈ O ₈ N* | 16 | [I, II] |
| | | | | | | | 161,0454 | 161,0455 | -0,2 | -1,2 | C ₆ H ₉ O ₅ | | |
| | | | | | | | 159,0304 | 159,0299 | 0,5 | 3,4 | C ₆ H ₇ O ₅ | | |
| | | | | | | | 113,0240 | 113,0244 | -0,4 | -3,6 | C ₅ H ₅ O ₃ | | |
| | | | | | | | 101,0240 | 101,0244 | -0,4 | -4,4 | C ₄ H ₅ O ₃ | | |
| | | | | | | | 95,0133 | 95,0139 | -0,5 | -5,4 | C ₅ H ₃ O ₂ | | |
| | | | | | | | 89,0239 | 89,0244 | -0,5 | -6,0 | C ₃ H ₅ O ₃ | | |
| | | | | | | | 85,0289 | 85,0295 | -0,6 | -6,7 | C ₄ H ₅ O ₂ | | |
| | | | | | | | 83,0137 | 83,0139 | -0,2 | -2,0 | C ₄ H ₅ O ₂ | | |
| | | | | | | | 73,0289 | 73,0295 | -0,6 | -8,5 | C ₃ H ₅ O ₂ | | |
| | | | | | | | 71,0133 | 71,0139 | -0,5 | -7,4 | C ₃ H ₃ O ₂ | | |
| 2 | Cyanogenic glycoside | Lotaustralin | shoots, roots | 0,81 | 169 | 306,1204 | | 306,1194 | 0,9 | 3,1 | C ₁₂ H ₂₀ O ₈ N* | 17 | [I, II] |
| | | | | | | | 161,0456 | 161,0455 | 0,0 | 0,0 | C ₆ H ₉ O ₅ | | |
| | | | | | | | 159,0302 | 159,0299 | 0,3 | 1,8 | C ₆ H ₇ O ₅ | | |
| | | | | | | | 113,0242 | 113,0244 | -0,2 | -1,7 | C ₅ H ₅ O ₃ | | |
| | | | | | | | 101,0243 | 101,0244 | -0,2 | -1,6 | C ₄ H ₅ O ₃ | | |
| | | | | | | | 99,0088 | 99,0088 | 0,0 | 0,2 | C ₄ H ₃ O ₃ | | |
| | | | | | | | 95,0139 | 95,0139 | 0,0 | 0,0 | C ₅ H ₃ O ₂ | | |
| | | | | | | | 89,0241 | 89,0244 | -0,3 | -3,1 | C ₃ H ₅ O ₃ | | |
| | | | | | | | 85,0293 | 85,0295 | -0,2 | -2,2 | C ₄ H ₅ O ₂ | | |
| | | | | | | | 73,0292 | 73,0295 | -0,3 | -3,9 | C ₃ H ₅ O ₂ | | |
| 6 | Flavonoids (luteolin derivatives) | <i>Carlinoside</i> <i>isomer</i> | shoots | 2,44 | 230 | 579,1373 | | 579,1355 | 1,8 | 3,0 | C ₂₆ H ₂₇ O ₁₅ | 32 | [III] |
| | | | | | | | 489,1059 | 489,1039 | 2,0 | 4,1 | C ₂₃ H ₂₁ O ₁₂ | | |
| | | | | | | | 471,0947 | 471,0933 | 1,4 | 3,0 | C ₂₃ H ₁₉ O ₁₁ | | |

| | | | | | | | | | | | | | | |
|----|---|---|--------|------|-----|----------|----------|----------|----------|---|---|----|--------------------|---|
| | | | | | | 459,0948 | 459,0933 | 1,5 | 3,3 | C ₂₂ H ₁₉ O ₁₁ | | | | |
| | | | | | | 441,0835 | 441,0827 | 0,8 | 1,9 | C ₂₂ H ₁₇ O ₁₀ | | | | |
| | | | | | | 429,0845 | 429,0827 | 1,7 | 4,0 | C ₂₁ H ₁₇ O ₁₀ | | | | |
| | | | | | | 411,0741 | 411,0722 | 1,9 | 4,7 | C ₂₁ H ₁₅ O ₉ | | | | |
| | | | | | | 399,0729 | 399,0722 | 0,7 | 1,7 | C ₂₀ H ₁₅ O ₉ | | | | |
| | | | | | | 369,0630 | 369,0616 | 1,4 | 3,7 | C ₁₉ H ₁₃ O ₈ | | | | |
| | | | | | | 339,0514 | 339,0510 | 0,4 | 1,2 | C ₁₈ H ₁₁ O ₇ | | | | |
| 13 | Flavonoids (apigenin derivatives) | <i>Schaftoside isomer</i> | shoots | 2,66 | 230 | 563,1426 | | 563,1406 | 2,0 | 3,5 | C ₂₆ H ₂₇ O ₁₄ | 33 | [III] | |
| | | | | | | | | 503,1219 | 503,1195 | 2,4 | 4,8 | | | C ₂₄ H ₂₃ O ₁₂ |
| | | | | | | | | 473,1113 | 473,1089 | 2,3 | 4,9 | | | C ₂₃ H ₂₁ O ₁₁ |
| | | | | | | | | 443,1002 | 443,0984 | 1,9 | 4,2 | | | C ₂₂ H ₁₉ O ₁₀ |
| | | | | | | | | 425,0887 | 425,0878 | 0,9 | 2,0 | | | C ₂₂ H ₁₇ O ₉ |
| | | | | | | | | 413,0894 | 413,0878 | 1,6 | 3,8 | | | C ₂₁ H ₁₇ O ₉ |
| | | | | | | | | 383,0786 | 383,0772 | 1,4 | 3,7 | | | C ₂₀ H ₁₅ O ₈ |
| | | | | | | | | 353,0672 | 353,0667 | 0,5 | 1,4 | | | C ₁₉ H ₁₃ O ₇ |
| 16 | Hydroxycinnamic acids | 3-O- caffeoylquinic acid | shoots | 1,03 | 174 | 353,0885 | | 353,0878 | 0,7 | 2,0 | C ₁₆ H ₁₇ O ₉ | 13 | [IV, V] | |
| | | | | | | | | 339,0514 | 339,0510 | 0,4 | 1,2 | | | C ₁₈ H ₁₁ O ₇ |
| | | | | | | | | 191,0561 | 191,0561 | 0,0 | -0,2 | | | C ₇ H ₁₁ O ₆ |
| 17 | Hydroxycinnamic acids | <i>Caffeoylquinic acid isomer</i> | shoots | 1,60 | 177 | 353,0887 | | 353,0878 | 0,9 | 2,6 | C ₁₆ H ₁₇ O ₉ | 13 | [IV, V] | |
| | | | | | | | | 191,0561 | 191,0561 | 0,0 | -0,1 | | | C ₇ H ₁₁ O ₆ |
| 18 | Hydroxycinnamic acids | <i>Caffeoylquinic acid hexoside</i> | shoots | 0,62 | 231 | 515,1423 | | 515,1406 | 1,6 | 3,2 | C ₂₂ H ₂₇ O ₁₄ | 25 | [IV, V] | |
| | | | | | | | | 353,0891 | 353,0878 | 1,3 | 3,6 | | | C ₁₆ H ₁₇ O ₉ |
| | | | | | | | | 191,0562 | 191,0561 | 0,1 | 0,6 | | | C ₇ H ₁₁ O ₆ |
| 19 | Hydroxycinnamic acids | Caftaric acid | roots | 0,68 | 172 | 333,0224 | | 333,0252 | -2,8 | -8,4 | C ₁₅ H ₉ O ₉ | 14 | [V] | |
| 20 | Hydroxycinnamic acids | Icariside F2 | roots | 1,78 | 204 | 447,1520 | | 447,1508 | 1,2 | 2,8 | C ₁₉ H ₂₇ O ₁₂ * | 10 | [VI, VII, VIII] | |
| | | | | | | | | 402,1498 | 402,1531 | -3,4 | -8,3 | | | C ₁₈ H ₂₆ O ₁₀ |
| | | | | | | | | 401,1463 | 401,1453 | 0,9 | 2,3 | | | C ₁₈ H ₂₅ O ₁₀ |
| 21 | Hydroxycinnamic | Chicoric acid | roots | 2,77 | 204 | 473,0739 | | 473,0726 | 1,4 | 2,9 | C ₂₂ H ₁₇ O ₁₂ | 13 | [V] | |

| | | | | | | | | | | | | | |
|-------|----------|--|-------|------|--|----------|----------|----------|--|---|--|------------------------|------------------------|
| acids | | | | | 311,0414 | 311,0409 | 0,5 | 1,7 | C ₁₃ H ₁₁ O ₉ | | | | |
| | | | | | 293,0303 | 293,0303 | 0,0 | 0,1 | C ₁₃ H ₉ O ₈ | | | | |
| | | | | | 179,0347 | 179,0350 | -0,2 | -1,4 | C ₉ H ₇ O ₄ | | | | |
| | | | | | 149,0088 | 149,0092 | -0,4 | -2,6 | C ₄ H ₅ O ₆ | | | | |
| 26 | Lignans | (-)-Olivil 4'-O-beta-D-glucopyranoside | roots | 2,57 | 231 | 583,2041 | 583,2032 | 0,8 | 1,4 | C ₂₇ H ₃₅ O ₁₄ * | 12 | [IX, X, XI, XII, XIII] | |
| | | | | | | 538,2019 | 538,2056 | -3,7 | -6,9 | C ₂₆ H ₃₄ O ₁₂ | | | |
| | | | | | | 537,1984 | 537,1978 | 0,7 | 1,3 | C ₂₆ H ₃₃ O ₁₂ | | | |
| | | | | | | 375,1453 | 375,1449 | 0,3 | 0,9 | C ₂₀ H ₂₃ O ₇ | | | |
| 27 | Lignans | Olivil isomer 1 | roots | 1,64 | 238 | 583,2052 | 583,2032 | 2,0 | 3,4 | C ₂₇ H ₃₅ O ₁₄ | 19 | [IX, X, XI, XII, XIII] | |
| | | | | | | 507,1873 | 507,1872 | 0,1 | 0,3 | C ₂₅ H ₃₁ O ₁₁ | | | |
| | | | | | | 375,1459 | 375,1449 | 0,9 | 2,5 | C ₂₀ H ₂₃ O ₇ | | | |
| | | | | | | 357,1348 | 357,1344 | 0,4 | 1,3 | C ₂₀ H ₂₁ O ₆ | | | |
| | | | | | | 345,1347 | 345,1344 | 0,3 | 0,9 | C ₁₉ H ₂₁ O ₆ | | | |
| | | | | | | 315,1240 | 315,1238 | 0,2 | 0,8 | C ₁₈ H ₁₉ O ₅ | | | |
| 28 | Lignans | Olivil isomer 2 | roots | 2,63 | | | 297,1139 | 297,1132 | 0,7 | 2,2 | C ₁₈ H ₁₇ O ₄ | 17 | [IX, X, XI, XII, XIII] |
| | | | | | 223 | 583,2042 | 583,2032 | 1,0 | 1,6 | C ₂₇ H ₃₅ O ₁₄ | | | |
| | | | | | | 537,1998 | 537,1978 | 2,0 | 3,7 | C ₂₆ H ₃₃ O ₁₂ | | | |
| | | | | | | 375,1460 | 375,1449 | 1,0 | 2,7 | C ₂₀ H ₂₃ O ₇ | | | |
| | | | | | | 327,1248 | 327,1238 | 1,0 | 3,1 | C ₁₉ H ₁₉ O ₅ | | | |
| 29 | Lignans | Olivil isomer 3 | roots | 2,90 | | | 195,0663 | 195,0663 | 0,0 | 0,0 | C ₁₀ H ₁₁ O ₄ | 17 | [IX, X, XI, XII, XIII] |
| | | | | | 222 | 583,2050 | 583,2032 | 1,8 | 3,1 | C ₂₇ H ₃₅ O ₁₄ | | | |
| | | | | | | 537,1990 | 537,1978 | 1,2 | 2,3 | C ₂₆ H ₃₃ O ₁₂ | | | |
| | | | | | | 375,1457 | 375,1449 | 0,8 | 2,1 | C ₂₀ H ₂₃ O ₇ | | | |
| | | | | | | 327,1244 | 327,1238 | 0,6 | 1,7 | C ₁₉ H ₁₉ O ₅ | | | |
| | | | | | | 195,0661 | 195,0663 | -0,2 | -1,1 | C ₁₀ H ₁₁ O ₄ | | | |
| | | | | | | 179,0713 | 179,0714 | -0,1 | -0,4 | C ₁₀ H ₁₁ O ₃ | | | |
| | 165,0555 | 165,0557 | -0,2 | -1,1 | C ₉ H ₉ O ₃ | | | | | | | | |

| | | | | | | | | | | | | |
|----|---------|------------------------|-------|------|-----|----------|----------|------|------|---|----|-----------|
| 30 | Lignans | <i>Olivil isomer 4</i> | roots | 3,29 | 237 | 583,2019 | 583,2032 | -1,3 | -2,3 | C ₂₇ H ₃₅ O ₁₄ | 17 | [XIV, XV] |
| 32 | Lignans | <i>SMG isomer</i> | roots | 3,90 | 217 | 523,2191 | 523,2185 | 0,6 | 1,1 | C ₂₆ H ₃₅ O ₁₁ | 15 | [XIV,XV] |
| | | | | | | 361,1662 | 361,1657 | 0,5 | 1,4 | C ₂₀ H ₂₅ O ₆ | | |

* [M+HCOO]- adduct

Table S4: Identification of phenolics compounds in roots and shoots of flax seedlings by UPLC- HDMS^E.

| N | Family | Compounds | Part used | RT (min) | CCS (Å²) | [M-H] ⁻ precursor ion (m/z) | MS ^E fragment ions (m/z) | m/z (Expected) | Error (mDa) | Error (ppm) | Elemental Composition | References |
|----|-----------------------------------|-----------------------------------|---------------|----------|----------|--|-------------------------------------|----------------|-------------|-------------|---|------------|
| 1 | Cyanogenic glycoside | Linamarin | shoots, roots | 0,54 | 165 | 292,1035 | | 292,1038 | -0,3 | -1,0 | C ₁₁ H ₁₈ O ₈ N* | [I, II] |
| | | | | | | | 246,0979 | 246,0983 | -0,4 | -1,6 | C ₁₀ H ₁₆ O ₆ N | |
| 2 | Cyanogenic glycoside | Lotaustralin | shoots, roots | 0,81 | 169 | 306,1189 | | 306,1194 | -0,5 | -1,6 | C ₁₂ H ₂₀ O ₈ N* | [I, II] |
| | | | | | | | 260,1133 | 260,114 | -0,7 | -2,7 | C ₁₁ H ₁₈ O ₆ N | |
| 6 | Flavonoids (luteolin derivatives) | <i>Carlinoside isomer</i> | shoots | 2,44 | 230 | 579,1362 | | 579,1362 | 0 | 0,0 | C ₂₆ H ₂₇ O ₁₅ | [III] |
| | | | | | | | 489,1046 | 489,1038 | 0,8 | 1,6 | C ₂₃ H ₂₁ O ₁₂ | |
| | | | | | | | 459,0942 | 459,0927 | 1,5 | 3,3 | C ₂₂ H ₁₉ O ₁₁ | |
| | | | | | | | 429,0836 | 429,0827 | 0,9 | 2,1 | C ₂₁ H ₁₇ O ₁₀ | |
| | | | | | | | 399,0731 | 399,0722 | 0,9 | 2,3 | C ₂₀ H ₁₅ O ₉ | |
| | | | | | | | 369,0619 | 369,0616 | 0,3 | 0,8 | C ₁₉ H ₁₃ O ₈ | |
| | | | | | | | 339,0510 | 339,051 | 0 | 0,0 | C ₁₈ H ₁₁ O ₇ | |
| 13 | Flavonoids (apigenin derivatives) | <i>Schaftoside isomer</i> | shoots | 2,66 | 231 | 563,1403 | | 563,1406 | -0,3 | -0,5 | C ₂₆ H ₂₇ O ₁₄ | [III] |
| | | | | | | | 503,1206 | 503,1195 | 1,1 | 2,2 | C ₂₄ H ₂₃ O ₁₂ | |
| | | | | | | | 443,0982 | 443,0984 | -0,2 | -0,5 | C ₂₂ H ₁₉ O ₁₀ | |
| | | | | | | | 383,0767 | 383,0772 | -0,5 | -1,3 | C ₂₀ H ₁₅ O ₈ | |
| 16 | Hydroxycinnamic acids | 3-O-caffeoylquinic acid | shoots | 1,03 | 174 | 375,0697 | | 375,0692 | 0,5 | 1,3 | C ₁₆ H ₁₆ O ₉ Na** | [IV, V] |
| | | | | | | | 353,0880 | 353,0878 | 0,2 | 0,6 | C ₁₆ H ₁₇ O ₉ | |
| | | | | | | | 191,0558 | 191,0561 | -0,3 | -1,6 | C ₇ H ₁₁ O ₆ | |
| | | | | | | | 135,0448 | 135,0452 | -0,4 | -3,0 | C ₈ H ₇ O ₂ | |
| | | | | | | | 134,0366 | 134,0373 | -0,7 | -5,2 | C ₈ H ₆ O ₂ | |
| 17 | Hydroxycinnamic acids | <i>Caffeoylquinic acid isomer</i> | shoots | 1,6 | 177 | 375,0697 | | 375,0692 | 0,4 | 1,1 | C ₁₆ H ₁₆ O ₉ Na** | [IV, V] |
| | | | | | | | 353,0881 | 353,0878 | 0,3 | 0,8 | C ₁₆ H ₁₇ O ₉ | |
| | | | | | | | 191,0561 | 191,0561 | 0 | 0,0 | C ₇ H ₁₁ O ₆ | |

| | | | | | | | | | | | | |
|----|-----------------------|--|--------|------|-----|----------|----------|----------|------|------|--|------------------------|
| 18 | Hydroxycinnamic acids | <i>Caffeoylquinic acid hexoside</i> | shoots | 0,62 | 231 | 537,1230 | | 537,122 | 1 | 1,9 | C ₂₂ H ₂₆ O ₁₄ Na** | [IV, V] |
| | | | | | | | 515,1403 | 515,1403 | 0 | 0,0 | C ₂₂ H ₂₇ O ₁₄ | |
| 19 | Hydroxycinnamic acids | Caftaric acid | roots | 0,68 | 172 | 333,0224 | | 333,0228 | -0,4 | -1,2 | C ₁₃ H ₁₀ O ₉ Na** | [V] |
| | | | | | | | 311,0404 | 311,0409 | -0,5 | -1,6 | C ₁₃ H ₁₁ O ₉ | |
| | | | | | | | 135,0449 | 135,0452 | -0,3 | -2,2 | C ₈ H ₇ O ₂ | |
| | | | | | | | 134,0371 | 134,0373 | -0,2 | -1,5 | C ₈ H ₆ O ₂ | |
| 20 | Hydroxycinnamic acids | Icariside F2 | roots | 1,78 | 204 | 447,1512 | | 447,1508 | 0,4 | 0,9 | C ₁₉ H ₂₇ O ₁₂ * | [VI, VII, VIII] |
| | | | | | | | 401,1458 | 401,1453 | 0,5 | 1,2 | C ₁₈ H ₂₅ O ₁₀ | |
| 21 | Hydroxycinnamic acids | Chicoric acid | roots | 2,77 | 204 | 495,0550 | | 495,054 | 1 | 2,0 | C ₂₂ H ₁₆ O ₁₂ Na** | [V] |
| | | | | | | | 473,0734 | 473,0725 | 0,9 | 1,9 | C ₂₂ H ₁₇ O ₁₂ | |
| | | | | | | | 311,0408 | 311,0403 | 0,5 | 1,6 | C ₁₃ H ₁₁ O ₉ | |
| | | | | | | | 293,0303 | 293,0297 | 0,6 | 2,0 | C ₁₃ H ₉ O ₈ | |
| | | | | | | | 219,0297 | 219,0299 | -0,2 | -0,9 | C ₁₁ H ₇ O ₅ | |
| | | | | | | | 179,0346 | 179,035 | -0,4 | -2,2 | C ₉ H ₇ O ₄ | |
| | | | | | | | 149,0089 | 149,0092 | -0,3 | -2,0 | C ₄ H ₅ O ₆ | |
| | | | | | | | 135,0446 | 135,0452 | -0,6 | -4,4 | C ₈ H ₇ O ₂ | |
| 26 | Lignans | (-)-Olivil 4'-O-beta-D-glucopyranoside | roots | 2,57 | 231 | 583,2041 | | 583,2032 | 0,9 | 1,5 | C ₂₇ H ₃₅ O ₁₄ * | [IX, X, XI, XII, XIII] |
| | | | | | | | 537,1988 | 537,1978 | 1 | 1,9 | C ₂₆ H ₃₃ O ₁₂ | |
| | | | | | | | 375,1456 | 375,1449 | 0,7 | 1,9 | C ₂₀ H ₂₃ O ₇ | |
| 27 | Lignans | <i>Olivil isomer 1</i> | roots | 1,64 | 238 | 583,2040 | | 583,2032 | 0,8 | 1,4 | C ₂₇ H ₃₅ O ₁₄ | [IX, X, XI, XII, XIII] |
| | | | | | | | 537,1960 | 537,1978 | -1,8 | -3,4 | C ₂₆ H ₃₃ O ₁₂ | |
| 28 | Lignans | <i>Olivil isomer 2</i> | roots | 2,63 | 223 | 583,2032 | | 583,2032 | 0 | 0,0 | C ₂₇ H ₃₅ O ₁₄ | [IX, X, XI, XII, XIII] |
| | | | | | | | 537,1972 | 537,1978 | -0,6 | -1,1 | C ₂₆ H ₃₃ O ₁₂ | |
| 29 | Lignans | <i>Olivil isomer 3</i> | roots | 2,9 | 222 | 583,2029 | | 583,2032 | -0,3 | -0,5 | C ₂₇ H ₃₅ O ₁₄ | [IX, X, XI, XII, XIII] |
| | | | | | | | 537,1966 | 537,1978 | -1,2 | -2,2 | C ₂₆ H ₃₃ O ₁₂ | |

| | | | | | | | | | | | |
|----|---------|------------------------|-------|------|-----|----------|----------|------|------|---|------------------------|
| 30 | Lignans | <i>Olivil isomer 4</i> | roots | 3,29 | 237 | 583,2019 | 583,2032 | -1,3 | -2,2 | C ₂₇ H ₃₅ O ₁₄ | [IX, X, XI, XII, XIII] |
| 31 | Lignans | SMG | roots | 4,35 | 225 | 523,2185 | 523,2185 | 0 | 0,0 | C ₂₆ H ₃₅ O ₁₁ | [XIV, XV] |
| | | | | | 217 | 523,2189 | 523,2185 | 0,4 | 0,8 | C ₂₆ H ₃₅ O ₁₁ | |
| 32 | Lignans | <i>SMG isomer</i> | roots | 3,9 | | 361,1651 | 361,1657 | -0,6 | -1,7 | C ₂₀ H ₂₅ O ₆ | [XIV, XV] |
| | | | | | | 346,1410 | 346,1422 | -1,2 | -3,5 | C ₁₉ H ₂₂ O ₆ | |

* [M+HCOO]- adduct

** [M-2H+Na]- adduct

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