Supporting information

Identification, quantification and Chrastil modelling of wheat straw wax extraction using supercritical carbon dioxide

Table S1: Identification and quantification of wheat straw wax extracted under scCO2 conditions and heptane soxhlet extraction

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Identification |  | Calculated KI | Literature KI | µg.g-1 of wheat straw | |
| Supercritical extraction @ 373 K/40 MPa*a*  (4 h extraction) | Heptane soxhlet  (4 h extraction) |
| Tetradecanoic acid |  | 1750 | 1751 [[27](#_ENREF_27)] | 78 ± 12 | 134 ± 34 |
| Hexadecanoic acid |  | 1951 | 1950 [[28](#_ENREF_28)] | 476 ± 13 | 925 ± 54 |
| Octadecadienoic acid |  | 2126 | 2132 [[29](#_ENREF_29)] | 142 ± 16 | 70 ± 13 |
| Octadecenoic acid |  | 2128 | 2137 [[30](#_ENREF_30)] | 271 ± 23 | 224 ± 27 |
| Octadecanoic acid |  | 2148 | 2168 [[31](#_ENREF_31)] | 58 ± 9 | 133 ± 32 |
| **Total fatty acids** |  | **-** | **-** | **1026** ± 73 | **1485 ± 160** |
| Heptacosane |  | 2685 | 2700[[22](#_ENREF_22)] | 109 ± 10 | 116 ± 31 |
| Nonacosane |  | 2884 | 2900[[22](#_ENREF_22)] | 280 ± 18 | 318 ± 19 |
| Hentriacontane |  | 3083 | 3100[[22](#_ENREF_22)] | 1214*b* ± 45 | 500 ± 26 |
| Triatriacontane |  | 3282 | 3300[[22](#_ENREF_22)] | *Tr* | *114 ± 32* |
| **Total alkanes** |  | - | - | **1603** ± 73 | **1048 ± 108** |
| Campesterol |  | 3238 | 3193*c* | 153 ± 13 | 65 ± 13 |
| Stigmasterol |  | 3272 | 3249 [[32](#_ENREF_32)] | 191 ± 16 | 77 ± 14 |
| β-sitosterol |  | 3334 | 3408 [[33](#_ENREF_33)] | 401 ± 34 | 186 ± 38 |
| Sterol 1*c* |  | 3400 | - | 72 ± 7 | 52 ± 4 |
| β-sitosterone |  | 3476 | - | 313 ± 8 | 142 ± 32 |
| Sterol 2*c* |  | 3636 | - | *Tr* | *Tr* |
| **Total sterols** |  | - | - | **1130** ± 78 | **522 ± 101** |
| 14,16 hentriacontanedione |  | 3377 | 3375*d* | 1505 ± 56 | 814 ± 21 |
| 16,18 triatriacontanedione |  | 3581 | - | 195 ± 16 | 116 ± 11 |
| **Total β-diketones** |  | - | - | **1700** ± 72 | **930 ± 32** |
| Tetracosanyl hexadecanoate |  | 4137 | - | 113 ± 11 | 157 ± 32 |
| Hexacosanyl hexadecanoate |  | 4335 | - | 274 ± 15 | 291 ± 19 |
| Octacosanyl hexadecanoate |  | 4513 | - | 1160 ± 45 | 1064 ± 70 |
| Octacosanyl octadecanoate |  | 4699 | - | 630 ± 25 | 588 ± 11 |
| Octacosanyl eicosanoate |  | 4953 | - | 438 ± 33 | 520 ± 23 |
| Octacosanyl docosanoate |  | e | - | 378 ± 31 | 473 ± 19 |
| Octacosanyl tetracosanoate |  | e | - | 137 ± 13 | 134 ± 15 |
| Octacosanyl hexacosanoate |  | e | - | 72 ± 11 | 65 ± 15 |
| Octacosanyl octacosanoate |  | e | - | *Tr* | *Tr* |
| **Total wax esters** |  | **-** | **-** | **3203** ± 184 | **3291 ± 204** |
| Octacosanol |  | 3083 | 3118*c* | 1570*b* ± 78 | 444 ± 36 |
| **Total fatty alcohol** |  | - | - | **1570** ± 78 | **444 ± 36** |
| Octacosanal |  | 3024 | - | 108 ± 6 | 117 ± 13 |
| **Total aldehyde** |  | - | - | **108** ± 6 | **117 ± 13** |
| **Total identified** |  | **-** | **-** | **8873** ± 564 | **7837 ± 654** |
| a CO2 flow rate of 0.04 kgmin-1 for 4 hours, b Co-elution of hentriacontane and octacosanol showed total of both compounds, c Literature KI: DB-1 GC column, d Estimated non-polar retention index (n-alkane scale) from NIST library 2008, e Hexacontane: no clear peak so no KI calculated Tr = Trace level with limit of quantification approximately < 0.1 mgmL-1 | | | | | |