Supplementary Table 1. Fatty acid composition, the content of storage compounds and seed viability of 42 oilseed rape accessions multiplied in 1983 and maintained since at 7±3°C, 6±2% seed moisture content. Counts were conducted for %NS and %TG in 1983, 1990, 1993, 2009 and 2014. The germination data are given as the arithmetic mean, along with the standard deviation (SD) and range (minimum (Min) to maximum (Max)) derived from four replicates per accession. The fatty acid composition and storage compound data represent the mean of three replicates. TSW: thousand seed weight. Least significant difference (LSD5%) is given between genotypes.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Trait** | **Test Year** | **Mean** | **SD** | **Min** | **Max** | **LSD5%** |
|  | TSW | 2009 | 4.45 | 0.64 | 3.00 | 5.70 |  |
| **Germination** | %TG | 1983 | 94.71 | 5.37 | 80.00 | 100.00 |  |
| %TG | 1990 | 92.97 | 4.64 | 83.00 | 100.00 |  |
| %TG | 1993 | 79.10 | 12.48 | 57.00 | 99.00 |  |
| %TG | 2009 | 65.67 | 14.23 | 41.75 | 98.00 | 15.81 |
| %NS | 2009 | 21.11 | 24.00 | 0.00 | 90.00 | 11.19 |
| %TG | 2014 | 35.10 | 28.67 | 2.00 | 97.00 | 7.23 |
| %NS | 2014 | 13.11 | 25.28 | 0.00 | 87.00 | 4.52 |
| **Fatty Acids** | 14:0 Myristic acid in % | 2014 | 0.05 | 0.01 | 0.04 | 0.06 | 0.00 |
| 16:0 Palmitic acid in % | 2014 | 4.63 | 0.30 | 4.00 | 5.18 | 0.20 |
| 16:1 Palmitoleic acid in % | 2014 | 0.28 | 0.02 | 0.22 | 0.32 | 0.02 |
| 18:0 Stearic acid in % | 2014 | 1.44 | 0.12 | 1.23 | 1.80 | 0.10 |
| 18:1 Oleic acid in % | 2014 | 57.41 | 6.79 | 33.72 | 64.43 | 1.66 |
| 18:2 Linoleic acid in % | 2014 | 19.46 | 1.73 | 15.69 | 22.52 | 0.44 |
| 18:3 α-Linolenic acid in % | 2014 | 9.36 | 1.11 | 7.16 | 11.10 | 0.26 |
| 20:0 Arachidic acid in % | 2014 | 0.52 | 0.04 | 0.46 | 0.61 | 0.00 |
| 20:1 Eicosenoic acid in % | 2014 | 3.13 | 2.91 | 1.09 | 12.48 | 0.62 |
| 20:2 Eicosadienoic acid in % | 2014 | 0.12 | 0.09 | 0.06 | 0.43 | 0.02 |
| 22:0 Behenic acid in % | 2014 | 0.31 | 0.03 | 0.25 | 0.37 | 0.00 |
| 22:1 Erucic acid in % | 2014 | 3.18 | 5.75 | 0.05 | 23.14 | 1.33 |
|  | 24:0 Lignoceric acid in % | 2014 | 0.13 | 0.02 | 0.10 | 0.16 | 0.00 |
|  | 24:1 Nervonic acid in % | 2014 | 0.20 | 0.08 | 0.13 | 0.43 | 0.03 |
|  | Total Saturated Acids | 2014 | 7.03 | 0.35 | 6.39 | 7.72 | 0.18 |
|  | Total Unsaturated Acids | 2014 | 92.96 | 0.35 | 92.26 | 93.26 | 0.19 |
| **NIRS** | Oil in % | 2014 | 44.61 | 1.91 | 41.10 | 48.17 | 0.69 |
| Glucosinolates in µmol | 2014 | 56.63 | 26.84 | 9.13 | 85.10 | 3.53 |
| Protein in % | 2014 | 24.24 | 1.92 | 19.13 | 27.03 | 0.42 |
| Protein i.S. in % | 2014 | 43.74 | 2.53 | 36.93 | 47.20 | 0.44 |
| H2O in % | 2014 | 5.05 | 0.31 | 4.40 | 5.77 | 0.18 |

Supplementary Table 2. Overview for different network settings for three best combination methods and %TG 2014 as target value. Values in brackets indicate the parameter for the neural network method, e.g. five centers for RBF.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Method** | **Lignoceric acid** | | **Nervonic acid** | | **Glucosinolates** | |
| **in %** | | **in %** | | **in µmol** | |
| **Neural Network** | **r** | **R²** | **r** | **R²** | **r** | **R²** |
| PLS [5], 10-fold | 0.97 | -0.03 | 0.91 | 0.33 | 0.69 | -0.18 |
| RBF [3], 10-fold | NaN | 0.00 | NaN | 0.00 | NaN | 0.00 |
| RBF [5], 10-fold | NaN | -0.05 | NaN | -0.01 | NaN | -0.21 |
| RBF [7], 10-fold | NaN | -0.02 | NaN | -0.01 | NaN | 0.00 |
| RBF [10], 10-fold | NaN | 0.00 | NaN | -0.01 | NaN | -0.02 |
| MLP [5], 10-fold | 0.71 | 0.10 | 0.46 | 0.09 | 0.96 | 0.58 |
| MLP [10], 10-fold | 0.46 | -0.22 | 0.84 | 0.57 | 0.59 | 0.20 |
| MLP [5 3], 10-fold | -0.82 | -0.87 | 0.88 | 0.69 | 0.86 | 0.52 |

Supplementary Table 3. Multivariate regression reveals correlation coefficients for %NS 2014 for a combination of fatty acids and compounds. Values for r represent best fit for all networks with p<0.01. Compounds include oil, glucosinolates, protein and H2O content. Fatty acids include all individual fatty acids.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Additional Input Values** | **TSW** | | **%NS 2009** | | **TSW and %NS 2009** | |
| **Method** | **r** | **R²** | **r** | **R²** | **r** | **R²** |
| Fatty acids | 0.86 | 0.60 | 0.90 | 0.73 | 0.91 | 0.62 |
| Compounds | 0.93 | 0.26 | 0.95 | 0.67 | 0.99 | 0.29 |
| Fatty acids and compounds | 0.99 | 0.05 | 0.73 | 0.32 | 0.99 | 0.73 |
| 14:0 Myristic acid in % | 0.97 | 0.46 | 0.94 | 0.86 | 0.99 | 0.77 |
| 16:0 Palmitic acid in % | 0.99 | 0.76 | 0.97 | 0.89 | 0.96 | 0.86 |
| 16:1 Palmitoleic acid in % | 0.98 | 0.63 | 0.96 | 0.91 | 0.89 | 0.60 |
| 18:0 Stearic acid in % | 0.86 | 0.70 | 0.99 | 0.79 | 0.99 | 0.83 |
| 18:1 Oleic acid in % | 0.91 | 0.65 | 0.98 | 0.87 | 0.94 | 0.87 |
| 18:2 Linoleic acid in % | 0.76 | 0.16 | 0.90 | 0.62 | 0.99 | 0.87 |
| 18:3 α-Linolenic acid in % | 0.98 | 0.42 | 0.99 | 0.82 | 0.97 | 0.87 |
| 20:0 Arachidic acid in % | 0.90 | 0.76 | 0.92 | 0.71 | 0.94 | 0.74 |
| 20:1 Eicosenoic acid in % | 0.87 | 0.75 | 0.98 | 0.83 | 0.97 | 0.79 |
| 20:2 Eicosadienoic acid in % | 0.80 | 0.34 | 1.00 | 0.79 | 0.99 | 0.87 |
| 22:0 Behenic acid in % | 0.96 | 0.59 | 1.00 | 0.89 | 0.56 | 0.19 |
| 22:1 Erucic acid in % | 0.95 | 0.61 | 0.98 | 0.91 | 0.98 | 0.74 |
| 24:0 Lignoceric acid in % | 0.95 | 0.69 | 0.97 | 0.80 | 0.88 | 0.66 |
| 24:1 Nervonic acid in % | 0.99 | 0.47 | 0.94 | 0.85 | 0.99 | 0.59 |
| Oil in % | 0.99 | 0.92 | 0.92 | 0.63 | 0.94 | 0.83 |
| Glucosinolates in µmol | 0.80 | 0.63 | 0.99 | 0.89 | 0.95 | 0.86 |
| Protein in % | 1.00 | 0.63 | 0.92 | 0.60 | 1.00 | 0.72 |
| H2O in % | 1.00 | 0.68 | 0.96 | 0.80 | 0.97 | 0.91 |
| Stearic, Linoleic, Arachidic, Eicosadienoic and Erucic acid in %, Glucosinolates in µmol | 1.00 | 0.77 | 0.93 | 0.78 | 0.97 | 0.92 |
| Oleic, α-Linolenic, Arachidic, Eicosenoic and Eicosadienoic acid in %, Glucosinolates in µmol | 0.99 | 0.89 | 0.79 | 0.49 | 0.97 | 0.93 |
| α-Linolenic acid in %, Oil in % and Glucosinolates in µmol | 0.90 | 0.54 | 0.84 | 0.50 | 0.99 | 0.59 |
| Myristic, Stearic, Oleic, α-Linolenic, Arachidic, Eicosenoic, Eicosadienoic, Erucic, Lignoceric and Nervonic acid in % | 0.87 | 0.56 | 0.96 | 0.91 | 0.85 | 0.72 |
| Myristic, Stearic, Oleic, α-Linolenic, Arachidic, Eicosenoic, Eicosadienoic, Erucic, Lignoceric and Nervonic acid in %, Oil in %, Glucosinlates in µmol | 0.68 | 0.45 | 0.99 | 0.54 | 0.88 | 0.64 |
| Myristic, Stearic, Oleic, α-Linolenic, Arachidic, Eicosenoic, Eicosadienoic, Erucic, Lignoceric and Nervonic acid in %, Oil, Proteins and H2O in %, Glucosinolates in µmol | 0.82 | 0.55 | 0.81 | 0.63 | 0.89 | 0.73 |

Supplementary Table 4. Multivariate regression reveals correlation coefficients for %TG 2014 for a combination of fatty acids and compounds. Values for r represent best fit for all networks with p<0.01. Compounds include oil, glucosinolates, protein and H2O content. Fatty acids include all individual fatty acids.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Additional Input Values** | **TSW** | | **%TG 1983, 1990, 1993, 2009** | | **TSW and % TG 1983, 1990, 1993, 2009** | |
| **Method** | **r** | **R²** | **r** | **R²** | **r** | **R²** |
| Fatty acids | 0.52 | 0.16 |  |  |  |  |
| Compounds | 0.97 | 0.20 |  |  |  |  |
| Fatty acids and compounds | 0.77 | 0.19 | 0.86 | 0.70 | 0.94 | 0.86 |
| 14:0 Myristic acid in % | 0.87 | 0.69 | 0.88 | 0.73 | 0.90 | 0.78 |
| 16:0 Palmitic acid in % | 0.83 | 0.34 | 0.90 | 0.75 | 0.74 | 0.44 |
| 16:1 Palmitoleic acid in % | 0.95 | 0.88 | 0.89 | 0.78 | 0.92 | 0.75 |
| 18:0 Stearic acid in % | 0.95 | 0.81 | 0.79 | 0.58 | 0.98 | 0.77 |
| 18:1 Oleic acid in % | 0.89 | 0.50 | 0.87 | 0.73 | 0.93 | 0.02 |
| 18:2 Linoleic acid in % | 0.93 | 0.83 | 0.92 | 0.59 | 0.98 | 0.96 |
| 18:3 α-Linolenic acid in % | 0.96 | 0.32 | 0.93 | 0.86 | 0.96 | 0.90 |
| 20:0 Arachidic acid in % | 0.78 | 0.21 | 0.80 | 0.61 | 0.99 | 0.85 |
| 20:1 Eicosenoic acid in % | 0.78 | 0.59 | 0.94 | 0.56 | 0.83 | 0.73 |
| 20:2 Eicosadienoic acid in % | 0.79 | 0.50 | 0.98 | 0.92 | 0.96 | 0.66 |
| 22:0 Behenic acid in % | 0.77 | 0.58 | 0.97 | 0.30 | 0.98 | 0.95 |
| 22:1 Erucic acid in % | 0.94 | 0.35 | 0.84 | 0.57 | 0.95 | 0.84 |
| 24:0 Lignoceric acid in % | 0.75 | 0.49 | 0.88 | 0.76 | 0.98 | 0.91 |
| 24:1 Nervonic acid in % | 0.78 | 0.42 | 0.98 | 0.77 | 1.00 | 0.91 |
| Oil in % | 0.95 | 0.26 | 0.98 | 0.89 | 0.90 | 0.78 |
| Glucosinolates in µmol | 0.94 | 0.71 | 0.92 | 0.83 | 0.99 | 0.82 |
| Protein in % | 0.92 | 0.64 | 0.95 | 0.87 | 0.90 | 0.56 |
| H2O in % | 0.87 | 0.52 | 0.97 | 0.89 | 0.98 | 0.67 |
| Stearic, Linoleic, Arachidic, Eicosadienoic and Erucic acid in %, Glucosinolates in µmol | 0.93 | 0.84 | 0.98 | 0.53 | 0.98 | 0.79 |
| Oleic, α-Linolenic, Arachidic, Eicosenoic and Eicosadienoic acid in %, Glucosinolates in µmol | 0.91 | 0.56 | 0.77 | 0.57 | 0.96 | 0.92 |
| α-Linolenic acid in %, Oil in % and Glucosinolates in µmol | 0.96 | 0.00 |  |  |  |  |
| Myristic, Stearic, Oleic, α-Linolenic, Arachidic, Eicosenoic, Eicosadienoic, Erucic, Lignoceric and Nervonic acid in % | 0.86 | 0.19 |  |  |  |  |
| Myristic, Stearic, Oleic, α-Linolenic, Arachidic, Eicosenoic, Eicosadienoic, Erucic, Lignoceric and Nervonic acid in %, Oil in %, Glucosinlates in µmol | 0.71 | 0.33 |  |  |  |  |
| Myristic, Stearic, Oleic, α-Linolenic, Arachidic, Eicosenoic, Eicosadienoic, Erucic, Lignoceric and Nervonic acid in %, Oil, Proteins and H2O in %, Glucosinolates in µmol | 0.71 | 0.34 |  |  |  |  |

 







**Supplementary Figure 1.** Distribution of fatty acids and seed components in 37 oilseed rape accessions measured after >30 years of storage. Fatty acid compositions are given as percentage (%) of the total fatty acid content. Saturated and unsaturated acids were calculated by adding up fatty acids having single or at least one double bond, respectively.