Table S1. Phenolic composition and levels in cereals and in cereal-based products

| Cereals/ cereal products | Polyphenol class | Compound (mg/100g, edible portion) | Technique | Data source | | Reference |
|---|---|---|---|---|---|---|
| | | | | Phenol-explorer | USDA | |
| ***Cereal grains and flour*** | | | | | | |
| Wheat (*Triticum aestivum* L. ssp. *aestivum*), whole grain flour | Flavones | Apigenin 6,8-C-arabinoside-C-glucoside (30.47); Apigenin 6,8-C-galactoside-C-arabinoside (46.82) | HPLC | √ | | *Asenstorfer et al. (2006)* |
| | Hydroxycinnamic acids | Caffeic acid (0.04); Ferulic acid (0.15); p-Coumaric acid (0.03); Sinapic acid (0.01) | HPLC | √ | | *Weidner et al. (1999)* |
| | Alkylphenols | 5-Heneicosenylresorcinol (16.78) | HPLC | √ | | *Mullin et al. (1992)* |
| | | 5-Heneicosenylresorcinol (19.29); | GC-MS | | | *Gohil et al. (1988)* |
| | | 5-Heptadecylresorcinol (1.80); | HPLC | | | *Mullin et al. (1992)* |
| | | 5-Nonadecenylresorcinol (2.80); | HPLC | | | *Mattila et al. (2005)* |
| | | 5-Nonadecylresorcinol (14.51); | HPLC | | | *Mullin et al. (1992)* |
| | | 5-Pentacosenylresorcinol (1.71); | HPLC | | | *Mullin et al. (1992)* |
| | | 5-Pentacosylresorcinol (0.59); | HPLC | | | *Mattila et al. (2005)* |
| | | 5-Pentadecylresorcinol (0.18); | HPLC | | | *Ross et al. (2003)* |
| | | 5-Tricosenylresorcinol (3.43); | HPLC | | | *Mullin et al. (1992)* *Ross et al. (2003)* |

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|---|---|---|---|---|---|---|
| | | 5-Tricosylresorcinol (3.05) | HPLC | | | |
| Wheat, purple | Anthocyanidins | Cyanidin (11.07); Delphinidin (3.20); Malvidin (4.02); Pelargonidin (3.41); Peonidin (1.81); Petunidin (2.34) | UPLC/MS/MS | | ⌂ | *Hosseinian et al. (2008)* |
| Wheat (*Triticum aestivum* L. ssp. *aestivum*), refined flour | Hydroxybenzoic acids | Syringic acid (0.37)<br>Vanillic acid (0.32) | GLC-MS | √ | | *Sosulski et al. (1982)* |
| | Hydroxycinnamic acids | Ferulic acid (5.31)<br>Trans-Ferulic acid (5.72) | GLC-MS | √ | | *Sosulski et al. (1982)* |
| | Lignans | Lariciresinol (0.18)<br>Matairesino (2.14e-04)<br>Pinoresinol (9.00e-03)<br>Secoisolariciresinol (0.02) | LC-MS | √ | | *Milder et al. (2005)*<br>*Penalvo et al. (2008)* |
| Hard wheat (*Triticum durum* Desf.), whole grain flour | Hydroxycinnamic acids | Ferulic acid (72.21) | HPLC | √ | | *Lempereur et al. (1997)* |
| | Alkylphenols | 5-Heneicosylresorcinol (23.82)<br>5-Heptadecylresorcinol (0.24)<br>5-Nonadecylresorcinol (5.90)<br>5-Pentacosylresorcinol (2.82)<br>5-Pentadecylresorcinol (0.45)<br>5-Tricosylresorcinol (8.69) | HPLC | √ | | *Landberg et al. (2006)* |
| Hard wheat (*Triticum durum* Desf.), semolina | Hydroxycinnamic acids | 5-5'-Dehydrodiferulic acid (4.49)<br>5-8'-Benzofuran dehydrodiferulic acid (8.23)<br>5-8'-Dehydrodiferulic acid (6.13)<br>8-O-4'-Dehydrodiferulic acid (11.02)<br>Cis-Ferulic acid (0.11) | HPLC | √ | | *Lempereur et al. (1998)*<br>*Peyron et al. (2002)* |

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|---|---|---|---|---|---|---|
| | | Ferulic acid (64.04)<br>Sinapic acid (0.33)<br>Trans-Ferulic acid (1.03) | | | | |
| | Lignans | Secoisolariciresinol (2.00e-03) | LC-MS | √ | | *Kuhnle et al. (2009)* |
| Maize (*Zea mays* L.), whole grain | Hydroxycinnamic acids | Ferulic acid (0.53) | HPLC | √ | | *Adom et al. (2002)* |
| Maize (*Zea mays* L.), refined flour | Hydroxybenzoic acids | 4-Hydroxybenzoic acid (0.02)<br>Protocatechuic acid (0.09)<br>Syringic acid (0.09)<br>Vanillic acid (0.08) | GLC-MS | √ | | *Sosulski et al. (1982)* |
| | Hydroxycinnamic acids | Caffeic acid (0.04)<br>Cis-Ferulic acid (0.06)<br>p-Coumaric acid (0.33)<br>Trans-Ferulic acid (0.34) | GLC-MS | √ | | *Sosulski et al. (1982)* |
| | Hydroxyphenylacetic acids | 4-Hydroxyphenylacetic acid (0.09) | GLC-MS | √ | | *Sosulski et al. (1982)* |
| Barley (*Hordeum vulgare* L. ssp. *vulgare)*, whole grain flour | Flavanols | (+)-Catechin (1.23)<br>(+)-Catechin (1.23)<br>Procyanidin dimer B3 (10.90)<br>Prodelphinidin dimer B3 (23.07) | HPLC | √<br><br>√ | ⌂ | *Madigan et al. (1994)* Holtekjølen et al. (2006) |
| | Alkylphenols | 5-Heneicosylresorcinol (1.18)<br>5-Heptadecylresorcinol (0.19)<br>5-Nonadecylresorcinol (0.71)<br>5-Pentacosylresorcinol (1.65)<br>5-Pentadecylresorcinol (0.01)<br>5-Tricosylresorcinol (0.77) | HPLC | √ | | *Ross et al. (2003)* |

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|---|---|---|---|---|---|
| Oat (*Avena sativa* L.), whole grain flour | Hydroxybenzoic acids | 4-Hydroxybenzoic acid (0.45)<br>Vanillic acid (0.27) | HPLC | √ | *Emmons et al. (1999)* |
| | Hydroxycinnamic acids | Avenanthramide 2c (3.85)<br>Avenanthramide 2f (2.65)<br>Avenanthramide 2p (2.70)<br>Avenanthramide K (1.95)<br>Caffeic acid (0.16)<br>Ferulic acid (0.19)<br>p-Coumaric acid (0.16)<br>Sinapic acid (0.04) | HPLC | √ | *Dimberg et al. (1996)*<br>*Emmons et al. (1999)* |
| | Hydroxybenzaldehydes | 4-Hydroxybenzaldehyde (0.12)<br>Vanillin (0.21) | HPLC | √ | *Dimberg et al. (1996)*<br>*Emmons et al. (1999)* |
| Oat (*Avena sativa* L.), refined flour | Hydroxybenzoic acids | 4-Hydroxybenzoic acid (0.06)<br>Protocatechuic acid (0.04)<br>Syringic acid (0.20)<br>Vanillic acid (0.06) | GLC-MS | √ | *Sosulski et al. (1982)* |
| | Hydroxycinnamic acids | Avenanthramide 2f (8.12)<br>Caffeic acid (0.04)<br>p-Coumaric acid (0.06)<br>Trans-Ferulic acid (0.21) | GLC-MS | √ | *Sosulski et al. (1982)* |
| | Hydroxyphenylacetic acids | 4-Hydroxyphenylacetic acid (0.03) | GLC-MS | √ | *Sosulski et al. (1982)* |
| Rice (*Oryza sativa* L.) whole grain | Hydroxybenzoic acids | 4-Hydroxybenzoic acid (0.07)<br>Syringic acid (0.03)<br>Vanillic acid (0.13) | GC | √ | *Kato et al. (1983)* |
| | Hydroxycinnamic acids | Caffeic acid (0.05)<br>Ferulic acid (0.10)<br>p-Coumaric acid (0.02) | GC | √ | *Kato et al. (1983)* |

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|---|---|---|---|---|---|
| Rice (*Oryza sativa* L.) parboiled and refined* | Hydroxybenzoic acids | 4-Hydroxybenzoic acid (0.08/0.17*)<br>Syringic acid (0.01)<br>Vanillic acid (0.29/0.11*) | GC | √ | *Kato et al. (1983)* |
| | Hydroxycinnamic acids | Caffeic acid (0.34)<br>Ferulic acid (0.17/0.02*)<br>p-Coumaric acid (0.19/0.11*)<br>Trans-Ferulic acid (0.21*) | GC | √ | *Kato et al. (1983)* |
| Rye (*Secale cereale* L.), whole grain flour | Hydroxycinnamic acids | Caffeic acid (0.20)<br>Ferulic acid (0.45)<br>p-Coumaric acid (0.23)<br>Sinapic acid (0.21) | HPLC | √ | *Weidner et al. (1999)* |
| | Alkylphenols | 5-Heneicosylresorcinol (16.17)<br>5-Heptadecylresorcinol (15.11)<br>5-Nonadecenylresorcinol (3.55)<br>5-Nonadecylresorcinol (20.41)<br>5-Pentacosylresorcinol (5.21)<br>5-Pentadecylresorcinol (1.64)<br>5-Tricosylresorcinol (7.01) | HPLC | √ | *Mattila et al. (2005)*<br>*Ross et al. (2003)* |
| Rye (*Secale cereale* L.), refined flour | Alkylphenols | 5-Heneicosylresorcinol (2.40)<br>5-Heptadecylresorcinol (2.13)<br>5-Nonadecylresorcinol (3.11)<br>5-Pentacosylresorcinol (0.44)<br>5-Tricosylresorcinol (0.80) | HPLC | √ | *Chen et al. (2004)* |
| Sorghum (*Sorghum bicolor* L.), whole grain | Hydroxybenzoic acids | Protocatechuic acid (2.55) | HPLC | √ | *Beta et al. (1999)* |

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|---|---|---|---|---|---|---|
| Sorghum, grain, red | Flavanones | Eriodictyol (0.29)<br>Naringenin (1.67) | HPLC | | ⌂ | *Dykes et al. (2009)* |
| | Flavones | Apigenin (2.54)<br>Luteolin (3.93) | HPLC | | ⌂ | *Dykes et al. (2009)* |
| ***Bread*** | | | | | | |
| Bread, wheat, whole grain flour | Alkylphenols | 5-Heneicosylresorcinol (10.87)<br>5-Heptadecylresorcinol (1.53)<br>5-Nonadecylresorcinol (9.57)<br>5-Pentacosylresorcinol(0.89)<br>5-Tricosylresorcinol (1.85) | HPLC | √ | | *Ross et al. (2003)* |
| Bread, wheat, refined flour | Lignans | Lariciresinol (0.01)<br>Matairesinol (1.23e-03)<br>Pinoresinol (0.01)<br>Secoisolariciresinol (7.19e-03)<br>Syringaresinol (0.04) | MS | √ | | *Milder et al. (2005)*<br>*Thompson et al. (2006)* |
| Bread, rye, whole grain flour | Hydroxybenzoic acids | Vanillic acid (0.57) | HPLC | √ | | *Mattila et al. (2002)* |
| | Hydroxycinnamic acids | Caffeic acid (0.77)<br>Ferulic acid (3.90) | HPLC | √ | | *Mattila et al. (2002)* |
| | Alkylphenols | 5-Heneicosylresorcinol (14.63)<br>5-Heptadecylresorcinol (14.05)<br>5-Nonadecenylresorcinol (2.30)<br>5-Nonadecylresorcinol (20.03)<br>5-Pentacosylresorcinol (4.64)<br>5-Tricosylresorcinol (6.29) | HPLC | √ | | *Ross et al. (2003)* |
| ***Breakfast cereals*** | | | | | | |

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|---|---|---|---|---|---|
| Breakfast cereals, bran | Alkylphenols | 5-Heneicosenylresorcinol (81.52)<br>5-Heneicosylresorcinol (92.76)<br>5-Heptadecylresorcinol (8.93)<br>5-Nonadecylresorcinol (48.31)<br>5-Pentacosenylresorcinol (7.84)<br>5-Pentacosylresorcinol (7.13)<br>5-Tricosenylresorcinol (19.55)<br>5-Tricosylresorcinol (19.62) | HPLC | √ | *Mullin et al. (1992)* |
| Breakfast cereals, corn | Lignans | Matairesinol (1.67e-03)<br>Secoisolariciresinol (5.50e-03) | LC-MS | √ | *Kuhnle et al. (2009)* |
| Breakfast cereals, muesli | Alkylphenols | 5-Heneicosylresorcinol (5.71)<br>5-Heptadecylresorcinol (1.54)<br>5-Nonadecylresorcinol (3.99)<br>5-Pentacosylresorcinol (0.61)<br>5-Tricosylresorcinol (1.41) | HPLC | √ | *Chen et al. (2004)* |
| Breakfast cereals, oat, wholemeal | Lignans | Matairesinol (0.06)<br>Secoisolariciresinol (0.02) | LC-MS | √ | *Kuhnle et al. (2009)* |
| ***Pasta*** | | | | | |
| Pasta, whole grain | Alkylphenols | 5-Heneicosylresorcinol (11.94)<br>5-Heptadecylresorcinol (0.25)<br>5-Nonadecylresorcinol (3.83)<br>5-Pentacosylresorcinol (1.46) | HPLC | √ | *Landberg et al. (2006)* |

| 5-Tricosylresorcinol (4.37) |
|---|

Data source: Phenol Explorer √; USDA vers. 3.2 ⌂.

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