

Electronic supplementary information

Inhibitory properties of saponin from *Eleocharis dulcis* peel against α -glucosidase

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1. Supplementary Figure

Figure S1. ¹H NMR (A) and HPLC (B) analysis of Fr.3 and Fr.4 separated from silica gel column.

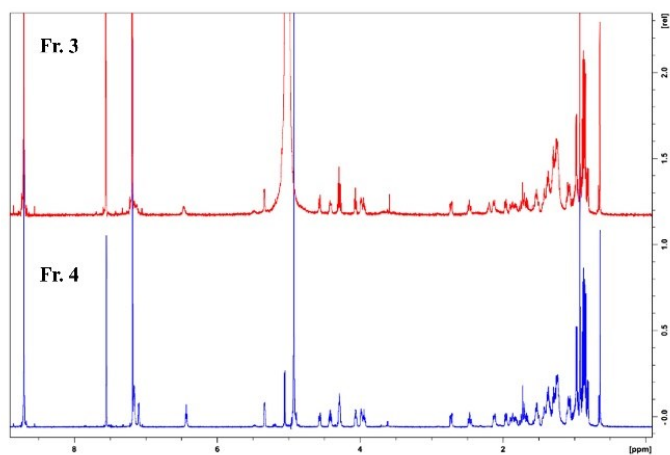
Figure S2. The chromatogram of saponin fraction by Prep LC System with the recycle mode.

Figure S3. Sequence alignment of the amino acid residue between α -glucosidase (GenBank: KZV11524.1) and isomaltase (PDB: 3AXI_A) from *Saccharomyces cerevisiae*.

2. ¹H and ¹³C NMR Chemical Shifts for Compounds 1-3

1. Supplementary Figure

A



B

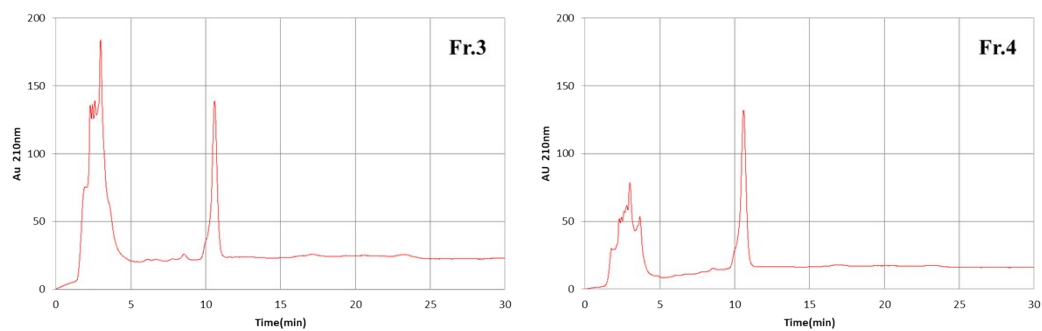


Figure S1. ^1H NMR (A) and HPLC (B) analysis of Fr.3 and Fr.4 separated from silica gel column.

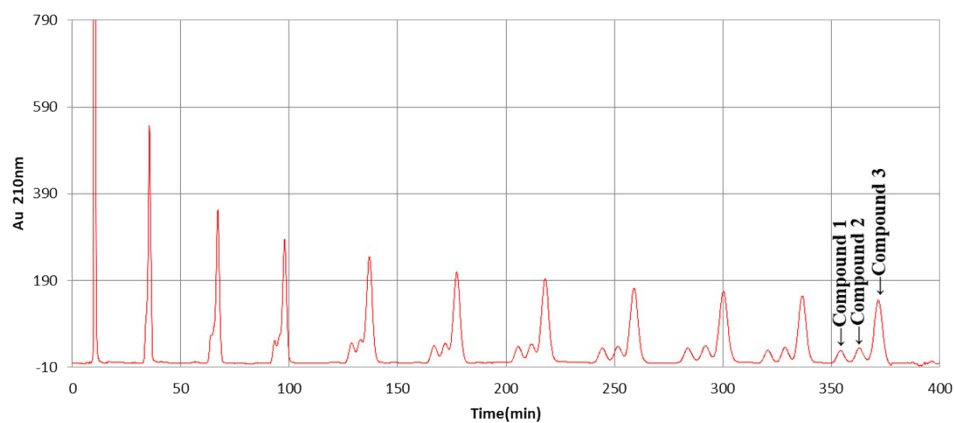


Figure S2. The chromatogram of saponin fraction by Prep LC System with the recycle mode.

| Score | Expect | Method | Identities | Positives | Gaps | | | |
|------------------|--|------------------------------|----------------------------|----------------|----------------|------------|------|-----|
| 1147 bits (2966) | 0.0 | Compositional matrix adjust. | 545/589 (93%) | 568/589 (96%) | 0/589 (0%) | | | |
| KZV11524.1 | MTISSAHPETEPKWWKEATVYQIYFASPKDSNDDGWDGDMKGI | SKLEYIKELGVD | DAIWISPFYDSPQDDMGYDIANYEKV | | 80 | | | |
| 3AXI_A | MTISSAHPETEPKWWKEATVYQIYFASPKDSNDDGWDGDMKGI | SKLEYIKELGVD | DAIWISPFYDSPQDDMGYDIANYEKV | | 80 | | | |
| Consensus | mtissahpetepkwwkeat yqiypasfkdsnddgwdmkgi skleyikelg daiwispfydspqddmgydianyekv | | | | | | | |
| KZV11524.1 | WPTYGTNEDCFALIEKTHKLGKRFITDLVINHCSEHEWFKESRSKTNPKRDWFFWRPPKGYIAEGKPIPPNNWKS YFG | | | | 160 | | | |
| 3AXI_A | WPTYGTNEDCFALIEKTHKLGKRFITDLVINHCSEHEWFKESRSKTNPKRDWFFWRPPKGYIAEGKPIPPNNWKS YFG | | | | 160 | | | |
| Consensus | wptygtnedcfaliekthklgmkrfitdlvinhcssehewfkesrsktnpkrdwffwrppkgydaegkpippnnwksyfg | | | | | | | |
| KZV11524.1 | GSAWTFDEKTOEFYLRFCSTQPDLNWENEDCRKAIYESAVGYWLDHGVDGFRIDVGSLSYKVVGLPLAEV | IIENSVWQS | | | 240 | | | |
| 3AXI_A | GSAWTFDEKTOEFYLRFCSTQPDLNWENEDCRKAIYESAVGYWLDHGVDGFRIDVGSLSYKVVGLPLAEV | IIENSVWQS | | | 240 | | | |
| Consensus | gsawtfdektqefylrlfcstqpdlnwenedcrkaiyesavgywldhgvdgfridvgslyskvvglplap d n s wqs | | | | | | | |
| KZV11524.1 | SDPYTLNGPRIHEFHQEMNQFIRNRVKDGREIMTVGMQHASDETKKLYTSASRHEL | ELFNFSHTDVGTSPLFRYNLVP | | | 320 | | | |
| 3AXI_A | SDPYTLNGPRIHEFHQEMNQFIRNRVKDGREIMTVGMQHASDETKKLYTSASRHEL | ELFNFSHTDVGTSPLFRYNLVP | | | 320 | | | |
| Consensus | sdpytlngprihefhqemnqfirnrvkdgreimtv gmqhasdetk lytsasrhel elfnfshtdvgtsplfrynlvp | | | | | | | |
| KZV11524.1 | FELKDWKIAIAELFRYINGTDCWSTIYLENHDQPRSITRFGDDSPKNRV | SGKLLS | LLVSLTGTLYYQGOELGQINFK | | 400 | | | |
| 3AXI_A | FELKDWKIAIAELFRYINGTDCWSTIYLENHDQPRSITRFGDDSPKNRV | SGKLLS | LLVSLTGTLYYQGOELGQINFK | | 400 | | | |
| Consensus | felkdwkiaiaelfryingtdcwstiylenhdqprsitrfgddspknrv sgklls ll ltgtl yqqqelgqinfk | | | | | | | |
| KZV11524.1 | NWVEKYEDVEIRNNYNAIKEE | GENSEEMKKFLE | IALVSRDHARTPMW | EPNAGFSGP | KPWFYLN | SFR | GIN | 480 |
| 3AXI_A | NWVEKYEDVEIRNNYNAIKEE | GENSEEMKKFLE | IALVSRDHARTPMW | EPNAGFSGP | KPWFYLN | SFR | GIN | 480 |
| Consensus | nw vekyedveirnny ikee genseemkkfle ial srdhartpm w epnagfsgp kpwfyl n sfr gin | | | | | | | |
| KZV11524.1 | VEBEGRNDSVLA | FWKFALE | FRRNHKDIEVGYDFE | FIDLDNKKLFSFTK | YNNKTLFAALNFSS | IATDFRIPND | SSFK | 560 |
| 3AXI_A | VEBEGRNDSVLA | FWKFALE | FRRNHKDIEVGYDFE | FIDLDNKKLFSFTK | YNNKTLFAALNFSS | IATDFRIPND | SSFK | 560 |
| Consensus | ve e k svl fwk al frk hkdi vygydf fidldnkklsftk ynnktlfaalnffssiatdfripnd ssfk | | | | | | | |
| KZV11524.1 | LEFGNYPKKEVIASSRTLKPWEGRITYI | | | | | | | 588 |
| 3AXI_A | LEFGNYPKKEVIASSRTLKPWEGRITYI | | | | | | | 588 |
| Consensus | lefgnypkkev d assrtlkpwegriyi | | | | | | | |

Figure S3. Sequence alignment of the amino acid residue between α -glucosidase (GenBank: KZV11524.1) and isomaltase (PDB: 3AXI_A) from *Saccharomyces cerevisiae*. ■: Identical sequence (homology=100%); ■: similar sequence (homology \geq 50%); □: different sequence (homology=0%).

2. ¹H and ¹³C NMR Chemical Shifts for Compounds 1-3

Compound 1: C₃₅H₅₈O₆, white amorphous powder. ¹H NMR (600 MHz, Pyridine-*d*₅): 5.34 (1H, dd, *J* = 4.8, 2.1 Hz, H-6), 5.19 (1H, dd, *J* = 15.2, 8.8 Hz, Ha-22), 4.58 (1H, ddd, *J* = 11.8, 5.7, 2.5 Hz, glc. Ha-6'), 4.43 (1H, m, glc. Hb-6'), 4.07 (1H, dd, *J* = 8.1, 3.5 Hz, glc. H-2'), 2.72 (1H, ddd, *J* = 13.4, 4.8, 2.3 Hz, Ha-4), 2.47 (1H, m, Hb-4), 1.91 (1H, dd, *J* = 12.5, 3.5 Hz, Ha-12), 0.89 (3H, d, *J* = 6.6 Hz, H-26), 0.84 (3H, d, *J* = 6.6 Hz, H-21), 1.05 (3H, d, *J* = 6.6 Hz, H-27), 0.86 (3H, t, *J* = 7.4 Hz, H-29), 0.92 (3H, s, H-19), 0.65 (3H, s, H-18); ¹³C NMR (600 MHz, Pyridine-*d*₅): 37.3 (C-1), 30.0 (C-2), 78.3 (C-3), 39.1 (C-4), 140.7 (C-5), 121.7 (C-6), 31.9 (C-7), 31.8 (C-8), 50.1 (C-9), 36.7 (C-10), 21.0 (C-11), 39.6 (C-12), 42.1 (C-13), 56.7 (C-14), 24.3 (C-15), 29.1 (C-16), 55.8 (C-17), 11.9 (C-18), 19.2 (C-19), 40.6 (C-20), 19.0 (C-21), 138.6 (C-22), 129.2 (C-23), 51.2 (C-24), 32.0 (C-25), 21.1 (C-26), 21.3 (C-27), 25.5 (C-28), 12.3 (C-29), 102.3 (C-1'), 75.1 (C-2'), 78.4 (C-3'), 71.5 (C-4'), 77.8 (C-5'), 62.6 (C-6').

Compound 2: C₃₄H₅₈O₆, white amorphous powder. ¹H NMR (600 MHz, Pyridine-*d*₅): 5.34 (1H, dd, *J* = 4.8, 2.1 Hz, H-6), 5.06 (1H, d, *J* = 7.7 Hz, glc. H-1'), 4.56 (1H, ddd, *J* = 11.8, 5.6, 2.5 Hz, glc. Ha-6'), 4.42 (1H, m, glc. Hb-6'), 4.06 (1H, dd, *J* = 8.5, 3.8 Hz, glc. H-2'), 2.73 (1H, ddd, *J* = 13.4, 4.8, 2.3 Hz, Ha-4), 2.47 (1H, m, Hb-4), 2.12, (1H, m, Ha-2), 1.96 (1H, dd, *J* = 12.7, 3.3 Hz, Ha-12), 0.95 (3H, d, *J* = 6.5 Hz, H-21), 0.92 (3H, s, H-19), 0.87 (3H, d, *J* = 6.8 Hz, H-27), 0.82 (3H, d, *J* = 6.8 Hz, H-26), 0.81 (3H, d, *J* = 6.5 Hz, H-28), 0.65 (3H, s, H-18); ¹³C NMR (600 MHz, Pyridine-*d*₅): 37.3 (C-1), 30.0 (C-2), 78.3 (C-3), 39.1 (C-4), 140.7 (C-5), 121.7 (C-6), 32.0 (C-7), 31.8 (C-8), 50.1 (C-9), 36.7 (C-10), 21.1 (C-11), 39.7 (C-12), 42.3 (C-13), 56.6 (C-14), 24.2 (C-15), 28.3 (C-16), 56.1 (C-17), 11.8 (C-18), 19.2 (C-19), 35.9 (C-20), 18.7 (C-21), 33.8 (C-22), 30.4 (C-23), 38.8 (C-24), 32.4 (C-25), 18.1 (C-26), 20.1 (C-27), 15.3 (C-28), 102.4 (C-1'), 75.1 (C-2'), 78.4 (C-3'), 71.5 (C-4'), 77.9 (C-5'), 62.6 (C-6').

Compound 3: C₃₅H₆₀O₆, white amorphous powder. ¹H NMR (600 MHz, Pyridine-*d*₅): 5.34 (1H, dd, *J* = 4.8, 2.1 Hz, H-6), 5.05 (1H, d, *J* = 7.7 Hz, glc. H-1'), 4.56 (1H, ddd, *J* = 11.8, 5.6, 2.5 Hz, glc. Ha-6'), 4.42 (1H, m, glc. Hb-6'), 4.06 (1H, dd, *J* = 8.0, 3.6

Hz, glc. H-2'), 2.72 (1H, ddd, $J = 13.4, 4.8, 2.3$ Hz, Ha-4), 2.47 (1H, m, Hb-4), 1.96 (1H, dd, $J = 12.5, 3.5$ Hz, Ha-12), 0.97 (3H, d, $J = 6.5$ Hz, H-21), 0.92 (3H, s, H-19), 0.88 (3H, t, $J = 7.4$ Hz, H-29), 0.87 (3H, d, $J = 6.8$ Hz, H-27), 0.85 (3H, d, $J = 6.8$ Hz, H-26), 0.65 (3H, s, H-18); ^{13}C NMR (600 MHz, Pyridine- d_5): 37.3 (C-1), 30.0 (C-2), 78.3 (C-3), 39.1 (C-4), 140.7 (C-5), 121.7 (C-6), 31.9 (C-7), 31.8 (C-8), 50.1 (C-9), 36.7 (C-10), 21.0 (C-11), 39.7 (C-12), 42.3 (C-13), 56.6 (C-14), 24.2 (C-15), 28.3 (C-16), 56.0 (C-17), 11.7 (C-18), 19.2 (C-19), 36.1 (C-20), 18.9 (C-21), 33.9 (C-22), 26.1 (C-23), 45.3 (C-24), 29.2 (C-25), 18.7 (C-26), 19.7 (C-27), 23.1 (C-28), 11.9 (C-29), 102.4 (C-1'), 75.1 (C-2'), 78.4 (C-3'), 71.5 (C-4'), 77.9 (C-5'), 62.6 (C-6').