Fig S1. MPRSS and UPLC-ESI-Q-TOF of the five anthocyanins we used in our study.
Figure S2. The structure for the five anthocyanins. The first row represents the structure for mono-glucoside, the second row represents the structure of di-glycoside, and the third row represent the poly-glycoside anthocyanins.
Table S1. Molecular interaction of different anthocyanins active sties with β-Lg-subunits.

<table>
<thead>
<tr>
<th>Mixtures</th>
<th>Binding energy (Kcal mol⁻¹)</th>
<th>H-bonds</th>
<th>Van der Waals bonds</th>
<th>Hydrophobic bonds</th>
<th>Others</th>
<th>ANs-involved groups</th>
</tr>
</thead>
</table>
Table S2. Partition coefficient for octanol water mixture (ClogP), molecular weight, number of H-bonds donor or acceptor, volume, and polar surface area for the five different anthocyanins (SYBYL-X 2.0).

<table>
<thead>
<tr>
<th>Anthocyanins</th>
<th>CLogP</th>
<th>Molecular weight</th>
<th>Donor count</th>
<th>Acceptor count</th>
<th>Volume</th>
<th>Polar surface area</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pt-3G</td>
<td>-1.75</td>
<td>433.39</td>
<td>7</td>
<td>10</td>
<td>1050.80</td>
<td>313.07</td>
</tr>
<tr>
<td>D-3G</td>
<td>-3.01</td>
<td>465.38</td>
<td>9</td>
<td>12</td>
<td>1101.04</td>
<td>382.34</td>
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<tr>
<td>D-3S</td>
<td>-4.50</td>
<td>597.50</td>
<td>11</td>
<td>16</td>
<td>1330.81</td>
<td>399.58</td>
</tr>
<tr>
<td>C-3S</td>
<td>-3.87</td>
<td>611.53</td>
<td>11</td>
<td>16</td>
<td>1360.64</td>
<td>445.19</td>
</tr>
<tr>
<td>Pt-Gl</td>
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<td>917.84</td>
<td>12</td>
<td>22</td>
<td>2241.70</td>
<td>505.43</td>
</tr>
</tbody>
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