**Supplementary file**

**A computational study of the interactions between anthocyans and cyclodextrins**

The obtained inclusion complex (for the best binding affinity) for each anthocyan species and cyclodextrins are depicted in figures below:

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| Figure S1. Interaction between cy-3-rutinoside (flavylium cation) and α-cyclodextrin |
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| Figure S2. Interaction between cy-3-rutinoside (hemiketal form) and α-cyclodextrin | Figure S3. Interaction between dp-3-rutinoside (hemiketal form) and α-cyclodextrin |

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|  |
| Figure S4. Interaction between dp-3-rutinoside (1st quinonoidal structure) and α-cyclodextrin |
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| Figure S5. Interaction between cy-3-rutinoside (2nd quinonoidal structure) and α-cyclodextrin | Figure S6. Interaction between dp-3-rutinoside (2nd quinonoidal structure) and α-cyclodextrin |

|  |  |
| --- | --- |
|  |  |
| Figure S7. Interaction between mv-3-glucoside (flavylium cation) and β-cyclodextrin | Figure S8. Interaction between cy-3-rutinoside (hemiketal form) and β-cyclodextrin |
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| Figure S9. Interaction between mv-3-glucoside (1st quinonoidal structure) and β-cyclodextrin | Figure S10. Interaction between cy-3-rutinoside (1st quinonoidal structure) and β-cyclodextrin |

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|  |
| Figure S11. Interaction between dp-3-rutinoside (2nd quinonoidal structure) and β-cyclodextrin |

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|  |
| Figure S12. Interaction between dp-3-rutinoside (flavylium cation) and γ-cyclodextrin |

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|  |
| Figure S13. Interaction between dp-3-rutinoside (hemiketal form) and γ-cyclodextrin |
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| Figure S14. Interaction between dp-3-rutinoside (1st quinonoidal structure) and γ-cyclodextrin |

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| --- | --- |
|  |  |
| Figure S15. Interaction between dp-3-rutinoside (2nd quinonoidal structure) and γ-cyclodextrin | Figure S16. Interaction between mv-3-rutinoside (2nd quinonoidal structure) and γ-cyclodextrin |

Table 1S. Vina docking scores for the six anthocyans (flavylium cations) with α-cyclodextrin for nine conformations (kcal/mol)

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Compound | E1 | E2 | E3 | E4 | E5 | E6 | E7 | E8 | E9 | E\* |
| c (Cy-3-glucoside) | -4.9 | -4.8 | -4.7 | -4.6 | -4.6 | -4.6 | -4.5 | -4.5 | -4.5 | -4.6 |
| m (Dp-3-glucoside) | -5.0 | -4.8 | -4.7 | -4.7 | -4.6 | -4.5 | -4.5 | -4.5 | -4.4 | -4.6 |
| o (Mv-3-glucoside) | -4.6 | -4.5 | -4.4 | -4.2 | -4.2 | -4.1 | -4.1 | -4.1 | -4.1 | -4.3 |
| A (Cy-3-rutinoside) | -5.3 | -5.2 | -5.1 | -5.0 | -5.0 | -4.9 | -4.9 | -4.8 | -4.8 | ***-5.0*** |
| T (Dp-3-rutinoside) | -5.1  | -5.0 | -4.9 | -4.8 | -4.7 | -4.7 | -4.7 | -4.7 | -4.6 | -4.8 |
| P (Mv-3-rutinoside) | -4.6 | -4.5 | -4.5 | -4.5 | -4.4 | -4.3 | -4.3 | -4.2 | -4.2 | -4.4 |

Table 2S. Vina docking scores for the six anthocyans (flavylium cations) with β-cyclodextrin for nine conformations (kcal/mol)

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Compound | E1 | E2 | E3 | E4 | E5 | E6 | E7 | E8 | E9 | E\* |
| c (Cy-3-glucoside) | -6.5 | -6.4 | -6.2 | -6.1 | -6.1 | -6.1 | -6.1 | -5.8 | -5.7 | -6.1 |
| m (Dp-3-glucoside) | -6.7 | -6.7 | -6.6 | -6.5 | -6.3 | -6.2 | -6.1 | -6.0 | -5.9 | -6.3 |
| o (Mv-3-glucoside) | -6.9 | -6.9 | -6.8 | -6.7 | -6.7 | -6.7 | -6.6 | -6.6 | -6.6 | ***-6.7*** |
| A (Cy-3-rutinoside) | -6.4 | -6.4 | -6.3 | -6.3 | -6.2 | -6.2 | -6.2 | -6.2 | -6.1 | -6.3 |
| T (Dp-3-rutinoside) | -6.6 | -6.5 | -6.5 | -6.4 | -6.4 | -6.3 | -6.3 | -6.3 | -6.3 | -6.4 |
| P (Mv-3-rutinoside) | -6.5 | -6.5 | -6.4 | -6.4 | -6.4 | -6.4 | -6.1 | -6.0 | -5.8 | -6.3 |

Table 3S. Vina docking scores for the six anthocyans (flavylium cations) with γ-cyclodextrin for nine conformations (kcal/mol)

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Compound | E1 | E2 | E3 | E4 | E5 | E6 | E7 | E8 | E9 | E\* |
| c (Cy-3-glucoside) | -6.5 | -6.4 | -6.3 | -6.3 | -6.2 | -6.2 | -6.0 | -5.9 | -5.8 | -6.2 |
| m (Dp-3-glucoside) | -6.8 | -6.8 | -6.6 | -6.4 | -6.3 | -6.3 | -6.2 | -6.2 | -6.1 | -6.4 |
| o (Mv-3-glucoside) | -6.6 | -6.5 | -6.5 | -6.3 | -6.3 | -6.2 | -6.2 | -6.2 | -6.1 | -6.3 |
| A (Cy-3-rutinoside) | -6.6 | -6.6 | -6.4 | -6.3 | -6.3 | -6.3 | -6.2 | -6.2 | -6.2 | -6.3 |
| T (Dp-3-rutinoside) | -7.2 | -7.1 | -7.1 | -7.0 | -7.0 | -6.9 | -6.9 | -6.9 | -6.9 | ***-7.0*** |
| P (Mv-3-rutinoside) | -6.9 | -6.9 | -6.8 | -6.8 | -6.7 | -6.7 | -6.7 | -6.7 | -6.6 | -6.8 |

Table 4S. Vina docking scores for the six anthocyans (1st quinonoidal structure) with α-cyclodextrin for nine conformations (kcal/mol)

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Compound | E1 | E2 | E3 | E4 | E5 | E6 | E7 | E8 | E9 | E\* |
| c (Cy-3-glucoside) | -5.3 | -5.0 | -4.9 | -4.9 | -4.9 | -4.8 | -4.8 | -4.7 | -4.7 | ***-4.9*** |
| m (Dp-3-glucoside) | -5.0 | -5.0 | -4.8 | -4.7 | -4.5 | -4.5 | -4.4 | -4.4 | -4.4 | -4.6 |
| o (Mv-3-glucoside) | -4.6 | -4.6 | -4.4 | -4.3 | -4.3 | -4.2 | -4.2 | -4.1 | -4.1 | -4.3 |
| A (Cy-3-rutinoside) | -5.0 | -5.0 | -4.9 | -4.9 | -4.8 | -4.8 | -4.7 | -4.7 | -4.7 | -4.8 |
| T (Dp-3-rutinoside) | -5.3 | -5.3 | -5.1 | -5.1 | -5.0 | -5.0  | -4.9 | -4.9 | -4.9 | -5.1 |
| P (Mv-3-rutinoside) | -4.8 | -4.6 | -4.6 | -4.6 | -4.5 | -4.5 | -4.5 | -4.5 | -4.4 | -4.6 |

Table 5S. Vina docking scores for the six anthocyans (1st quinonoidal structure) with β-cyclodextrin for nine conformations (kcal/mol)

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Compound | E1 | E2 | E3 | E4 | E5 | E6 | E7 | E8 | E9 | E\* |
| c (Cy-3-glucoside) | -6.8 | -6.7 | -6.7 | -6.7 | -6.6 | -6.6 | -6.5 | -6.5 | -6.4 | -6.6 |
| m (Dp-3-glucoside) | -7.0 | -7.0 | -6.9 | -6.8 | -6.7 | -6.7 | -6.7 | -6.5 | -6.4 | -6.7 |
| o (Mv-3-glucoside) | -7.0 | -7.0 | -6.9 | -6.9 | -6.9 | -6.9 | -6.9 | -6.8 | -6.8 | ***-6.9*** |
| A (Cy-3-rutinoside) | -7.3 | -7.1 | -7.1 | -7.0 | -6.9 | -6.9 | -6.9 | -6.6 | -6.4 | ***-6.9*** |
| T (Dp-3-rutinoside) | -7.1 | -7.0 | -6.9 | -6.8 | -6.7 | -6.7 | -6.6 | -6.4 | -6.4 | -6.7 |
| P (Mv-3-rutinoside) | -6.9 | -6.9 | -6.8 | -6.7 | -6.7 | -6.5 | -6.5 | -6.5 | -6.5 | -6.7 |

Table 6S. Vina docking scores for the six anthocyans (1st quinonoidal structure) with γ-cyclodextrin for nine conformations (kcal/mol)

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Compound | E1 | E2 | E3 | E4 | E5 | E6 | E7 | E8 | E9 | E\* |
| c (Cy-3-glucoside) | -7.1 | -6.8 | -6.6 | -6.5 | -6.4 | -6.4 | -6.3 | -6.3 | -6.1 | -6.5 |
| m (Dp-3-glucoside) | -7.5 | -6.9 | -6.7 | -6.6 | -6.5 | -6.5 | -6.4 | -6.4 | -6.3 | -6.6 |
| o (Mv-3-glucoside) | -6.8 | -6.8 | -6.6 | -6.5 | -6.4 | -6.3 | -6.3 | -6.2 | -6.2 | -6.5 |
| A (Cy-3-rutinoside) | -7.0 | -6.8 | -6.7 | -6.6 | -6.5 | -6.5 | -6.5 | -6.4 | -6.4 | -6.6 |
| T (Dp-3-rutinoside) | -7.3 | -7.3 | -7.1 | -6.9 | -6.9 | -6.8 | -6.7 | -6.6 | -6.6 | ***-6.9*** |
| P (Mv-3-rutinoside) | -6.7 | -6.7 | -6.7 | -6.7 | -6.6 | -6.5 | -6.4 | -6.4 | -6.4 | -6.6 |

Table 7S. Vina docking scores for the six anthocyans (hemiketal structure) with α-cyclodextrin for nine conformations (kcal/mol)

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Compound | E1 | E2 | E3 | E4 | E5 | E6 | E7 | E8 | E9 | E\* |
| c (Cy-3-glucoside) | -4.7 | -4.6 | -4.6 | -4.6 | -4.6 | -4.5 | -4.4 | -4.4 | -4.3 | -4.5 |
| m (Dp-3-glucoside) | -4.8 | -4.7 | -4.6 | -4.6 | -4.6 | -4.6 | -4.6 | -4.6 | -4.5 | -4.6 |
| o (Mv-3-glucoside) | -4.6 | -4.6 | -4.3 | -4.3 | -4.2 | -4.1 | -4.1 | -4.1 | -4.1 | -4.3 |
| A (Cy-3-rutinoside) | -5.0 | -4.9 | -4.8 | -4.8 | -4.7 | -4.7 | -4.6 | -4.5 | -4.5 | -4.7 |
| T (Dp-3-rutinoside) | -5.4 | -5.2 | -5.2 | -5.1 | -5.1 | -5.0 | -5.0 | -5.0 | -5.0 | ***-5.1*** |
| P (Mv-3-rutinoside) | -4.8 | -4.5 | -4.5 | -4.5 | -4.5 | -4.3 | -4.2 | -4.2 | -4.2 | -4.4 |

Table 8S. Vina docking scores for the six anthocyans (hemiketal structure) with β-cyclodextrin for nine conformations (kcal/mol)

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Compound | E1 | E2 | E3 | E4 | E5 | E6 | E7 | E8 | E9 | E\* |
| c (Cy-3-glucoside) | -6.6 | -6.5 | -6.3 | -6.2 | -6.2 | -6.1 | -6.0 | -6.0 | -6.0 | -6.2 |
| m (Dp-3-glucoside) | -6.5 | -6.4 | -6.3 | -6.1 | -6.0 | -6.0 | -5.9 | -5.8 | -5.7 | -6.1 |
| o (Mv-3-glucoside) | -6.6 | -6.5 | -6.5 | -6.5 | -6.4 | -6.4 | -6.4 | -6.3 | -6.3 | -6.4 |
| A (Cy-3-rutinoside) | -7.0 | -7.0 | -6.9 | -6.4 | -6.4 | -6.3 | -6.3 | -6.2 | -6.1 | ***-6.5*** |
| T (Dp-3-rutinoside) | -6.7 | -6.7 | -6.6 | -6.4 | -6.4 | -6.3 | -6.2 | -6.2 | -6.2 | -6.4 |
| P (Mv-3-rutinoside) | -6.7 | -6.7 | -6.6 | -6.6 | -6.5 | -6.5 | -6.5 | -5.9 | -5.9 | -6.4 |

Table 9S. Vina docking scores for the six anthocyans (hemiketal structure) with γ-cyclodextrin for nine conformations (kcal/mol)

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Compound | E1 | E2 | E3 | E4 | E5 | E6 | E7 | E8 | E9 | E\* |
| c (Cy-3-glucoside) | -6.5 | -6.3 | -6.2 | -6.2 | -6.0 | -5.9 | -5.9 | -5.8 | -5.8 | -6.1 |
| m (Dp-3-glucoside) | -6.5 | -6.4 | -6.4 | -6.3 | -6.1 | -6.0 | -5.9 | -5.9 | -5.8 | -6.1 |
| o (Mv-3-glucoside) | -6.5 | -6.5 | -6.2 | -6.0 | -6.0 | -5.9 | -5.9 | -5.8 | -5.8 | -6.1 |
| A (Cy-3-rutinoside) | -6.7 | -6.7 | -6.6 | -6.6 | -6.6 | -6.6 | -6.5 | -6.5 | -6.5 | ***-6.6*** |
| T (Dp-3-rutinoside) | -6.9 | -6.8 | -6.7 | -6.6 | -6.6 | -6.6 | -6.6 | -6.5 | -6.5 | ***-6.7*** |
| P (Mv-3-rutinoside) | -6.3 | -6.3 | -6.2 | -6.2 | -6.2 | -6.2 | -6.2 | -6.1 | -6.1 | -6.2 |

Table 10S. Vina docking scores for the six anthocyans (2nd quinonoidal structure) with α-cyclodextrin for nine conformations (kcal/mol)

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Compound | E1 | E2 | E3 | E4 | E5 | E6 | E7 | E8 | E9 | E\* |
| c (Cy-3-glucoside) | -4.8 | -4.8 | -4.7 | -4.5 | -4.5 | -4.4 | -4.4 | -4.4 | -4.4 | -4.5 |
| m (Dp-3-glucoside) | -4.8 | -4.7 | -4.7 | -4.7 | -4.6 | -4.5 | -4.5 | -4.5 | -4.4 | -4.6 |
| o (Mv-3-glucoside) | -4.6 | -4.6 | -4.4 | -4.3 | -4.1 | -4.1 | -4.1 | -4.0 | -4.0 | -4.2 |
| A (Cy-3-rutinoside) | -5.4 | -5.1 | -5.0 | -4.9 | -4.9 | -4.9 | -4.8 | -4.8 | -4.8 | ***-5.0*** |
| T (Dp-3-rutinoside) | -5.4 | -5.2 | -5.0 | -5.0 | -4.9 | -4.9 | -4.8 | -4.8 | -4.8 | ***-5.0*** |
| P (Mv-3-rutinoside) | -4.9 | -4.9 | -4.9 | -4.9 | -4.8 | -4.8 | -4.8 | -4.6 | -4.6 | -4.8 |

Table 11S. Vina docking scores for the six anthocyans (2nd quinonoidal structure) with β-cyclodextrin for nine conformations (kcal/mol)

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Compound | E1 | E2 | E3 | E4 | E5 | E6 | E7 | E8 | E9 | E\* |
| c (Cy-3-glucoside) | -6.9 | -6.8 | -6.8 | -6.7 | -6.6 | -6.6 | -6.5 | -6.5 | -6.5 | -6.7 |
| m (Dp-3-glucoside) | -7.3 | -7.3 | -7.2 | -7.2 | -7.2 | -7.1 | -7.1 | -7.0 | -7.0 | ***-7.2*** |
| o (Mv-3-glucoside) | -7.0 | -7.0 | -7.0 | -6.9 | -6.9 | -6.9 | -6.9 | -6.9 | -6.9 | -6.9 |
| A (Cy-3-rutinoside) | -7.1 | -7.0 | -6.8 | -6.8 | -6.7 | -6.6 | -6.5 | -6.4 | -6.3 | -6.7 |
| T (Dp-3-rutinoside) | -7.0 | -7.0 | -6.7 | -6.6 | -6.3 | -6.3 | -6.3 | -6.3 | -6.2 | -6.5 |
| P (Mv-3-rutinoside) | -6.9 | -6.8 | -6.8 | -6.7 | -6.7 | -6.6 | -6.5 | -6.3 | -6.3 | -6.6 |

Table 12S. Vina docking scores for the six anthocyans (2nd quinonoidal structure) with γ-cyclodextrin for nine conformations (kcal/mol)

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Compound | E1 | E2 | E3 | E4 | E5 | E6 | E7 | E8 | E9 | E\* |
| c (Cy-3-glucoside) | -6.8 | -6.7 | -6.4 | -6.4 | -6.1 | -6.0 | -6.0 | -6.0 | -6.0 | -6.3 |
| m (Dp-3-glucoside) | -6.9 | -6.9 | -6.5 | -6.4 | -6.4 | -6.2 | -6.1 | -6.0 | -6.0 | -6.4 |
| o (Mv-3-glucoside) | -6.8 | -6.7 | -6.6 | -6.5 | -6.4 | -6.3 | -6.1 | -6.1 | -6.1 | -6.4 |
| A (Cy-3-rutinoside) | -6.8 | -6.6 | -6.4 | -6.3 | -6.3 | -6.2 | -6.1 | -5.9 | -5.9 | -6.3 |
| T (Dp-3-rutinoside) | -6.9 | -6.8 | -6.6 | -6.6 | -6.5 | -6.3 | -6.3 | -6.3 | -6.2 | ***-6.5*** |
| P (Mv-3-rutinoside) | -6.9 | -6.6 | -6.6 | -6.5 | -6.5 | -6.4 | -6.4 | -6.4 | -6.3 | ***-6.5*** |

\*E represents the mean value of the nine binding energies 1-9.