PROTEIN SCIENCE

Supporting Information

Structural basis for acceptor-substrate recognition of UDP-glucose: anthocyanidin 3-*O*-glucosyltransferase from *Clitoria ternatea*

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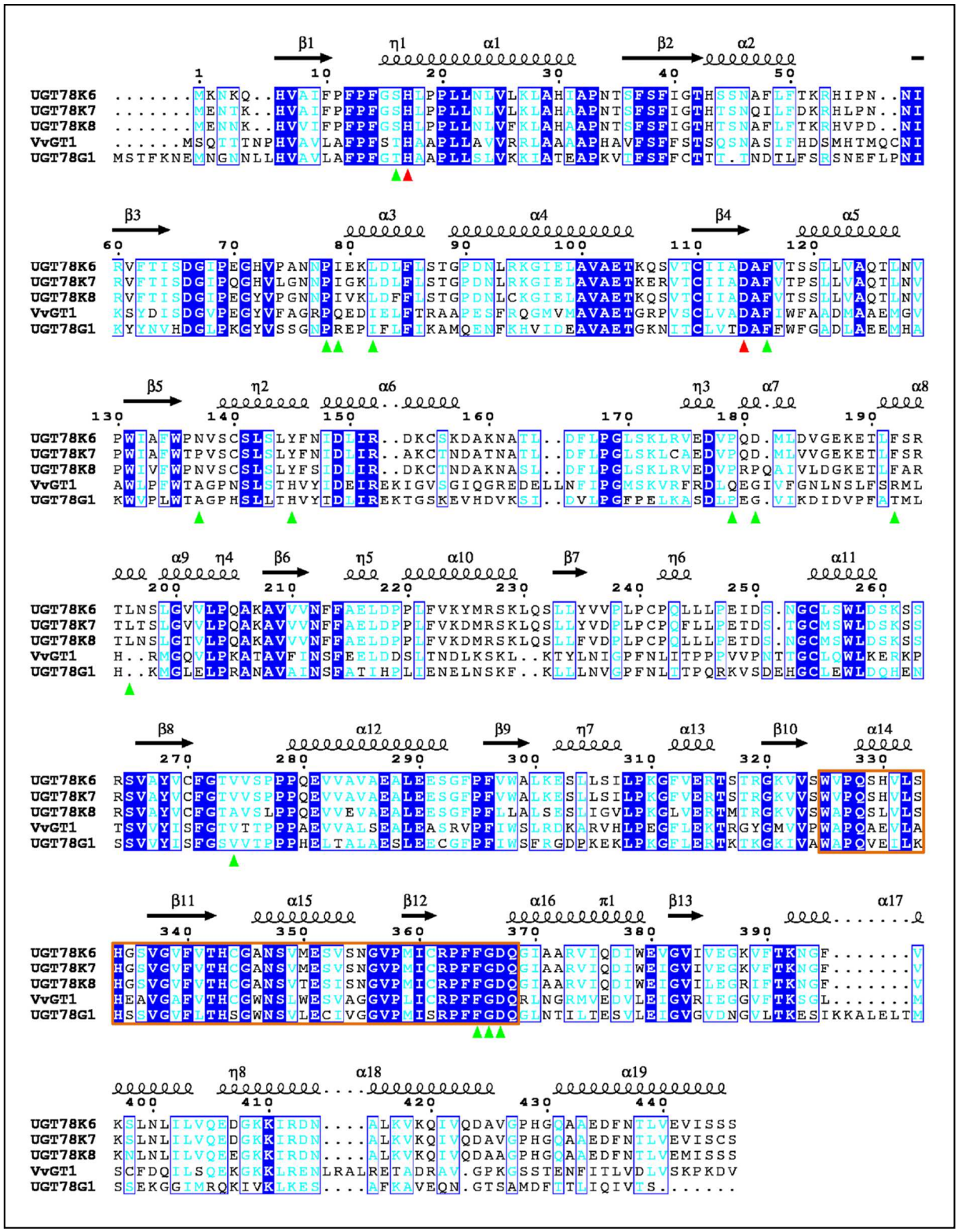

Figure S1. Amino acid sequence alignment of UGT78K6 with the homologous flavonoid UGTs. UGT78K7 (UDP-glucose: flavonoid 3-*O*-glucosyltransferase) and UGT78K8 (UDP-glucose: anthocyanin 3′,5′-*O*-glucosyltransferase) from *Clitoria ternatea*,[1] showing high sequence identities of 92% and 87% with UGT78K6, respectively, were added to the alignment. The homologous UGTs

detected by the Dali server[2] are as follows: *Vv*GT1 from *Vitis vinifera* (PDB ID: 2C1Z, a flavonoid UGT that functions in anthocyanin biosynthesis[3]) and UGT78G1 from *Medicago truncatula* (PDB ID: 3HBF, an (iso)flavonoid UGT in anthocyanin biosynthesis[4]). The secondary structure elements observed in the UGT78K6 structure are shown above the alignment. Identical residues in all sequences are highlighted in blue. Equivalent residues calculated considering their physic-chemical properties in each column are indicated in cyan letters and enclosed in blue boxes. The proposed His-Asp catalytic dyad and the residues involved in the acceptor binding in the delphinidin-bound form of UGT78K6 are indicated with red and green triangles, respectively. The UGT signature PSPG motif (residues 325-368) is indicated with orange boxes. The sequence alignment was performed by *CLUSTAL-W*[5], and represented with *ESPript*[6].

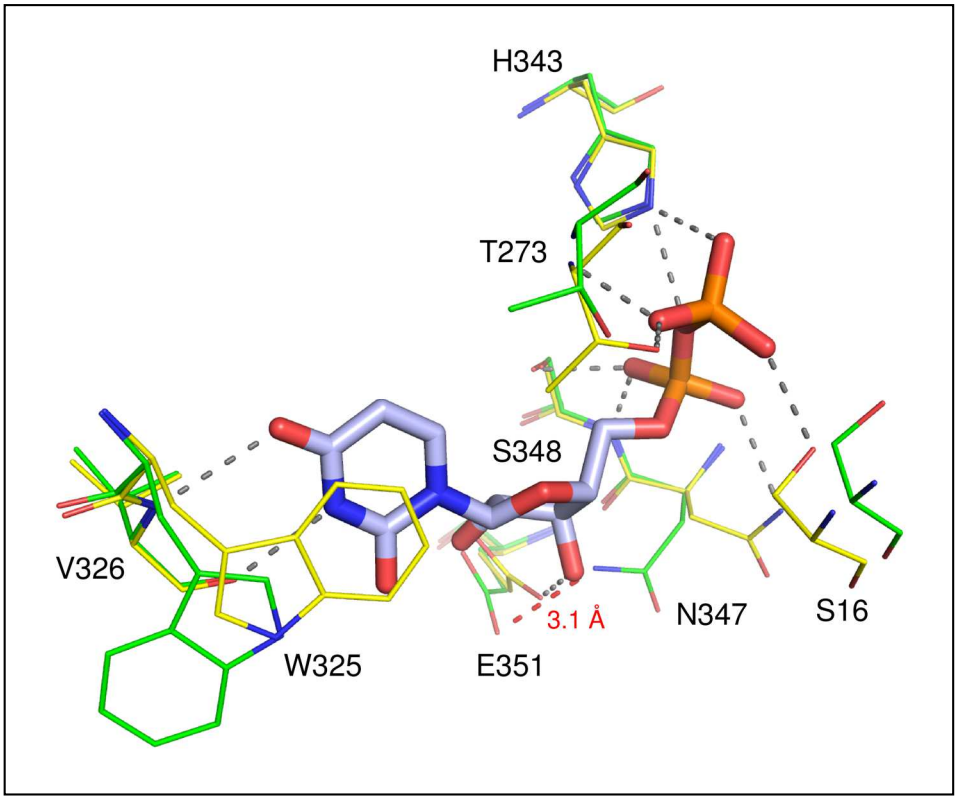

Figure S2. Superimposed structures of the unliganded form (green carbon) and the UDP-bound form (yellow carbon) of UGT78K6. The UDP moiety is shown as a stick model. Residues involved in the UDP binding are shown as lines and labeled. Hydrogen bonds are depicted with dotted lines. In particular, the hydrogen bond between the Oε1 oxygen of Glu351 and the Nδ2 nitrogen of Asn347 in the unligand form is colored in red.

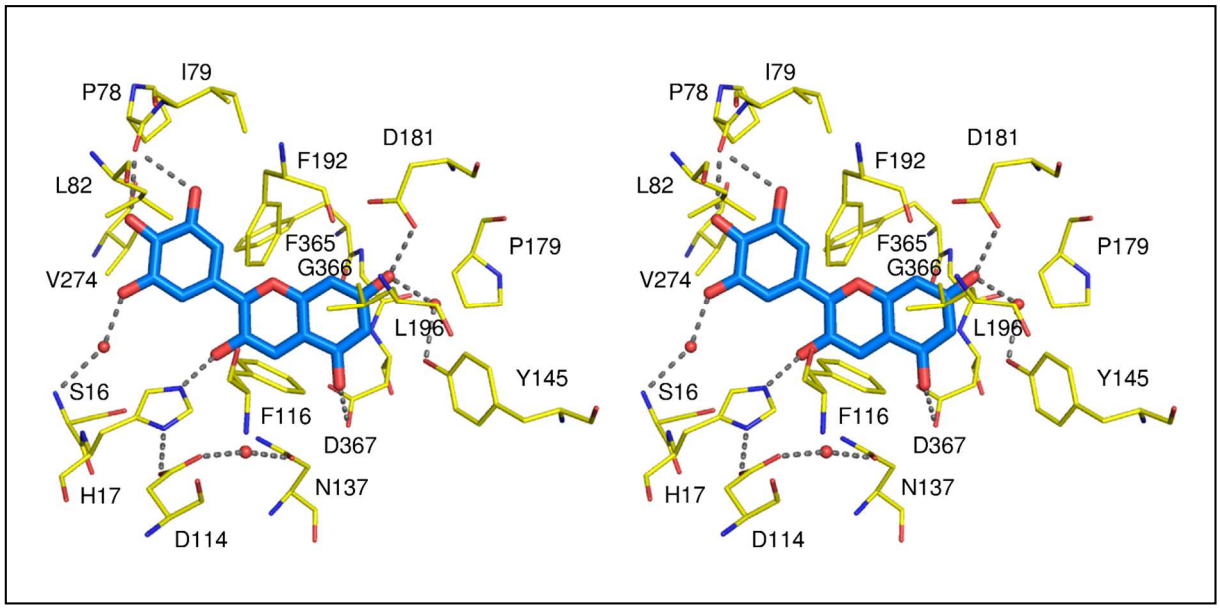

Figure S3. Stereo view of the acceptor-binding site in the delphinidin-bound form of UGT78K6. Residues within a distance of 4 Å around the acceptor substrate are shown as yellow lines and labeled. Hydrogen bonds are depicted with dotted lines.

References

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