Supplementary Table S3. Predicted residue-level contacts in the MTOR–dauricine docking complex.

Interacting residue	Chain	Closest protein atom	Closest ligand atom	Minimum heavy-atom distance /Å	Predicted contact type
SER2036	B	OG	O	2.91	Polar contact / potential hydrogen-bond-related contact
TRP2102	B	CZ3	O	2.98	Aromatic-associated / van der Waals contact
GLU2033	B	OE1	C	3.35	van der Waals / polar-associated contact
PHE2109	B	CZ	C	3.37	Hydrophobic / aromatic-associated contact
ARG2037	B	N	O	3.41	Polar contact / potential hydrogen-bond-related contact
TYR2106	B	CB	O	3.43	van der Waals / aromatic-associated contact
PHE2040	B	CD2	C	3.46	Hydrophobic / aromatic-associated contact
GLY2041	B	CA	O	3.48	van der Waals contact
LEU2032	B	O	C	3.89	van der Waals / hydrophobic contact

Note: This table summarizes the predicted residue-level contacts between dauricine and MTOR in the best-scoring docking pose. The binding pocket corresponds to the MTOR FRB-domain-associated pocket. Distances represent the minimum heavy-atom distances between dauricine and the corresponding MTOR residues. Contact types were assigned based on spatial proximity and atom types and should be interpreted as predicted non-covalent contacts. The distance labels displayed in Figure 6 represent visualized interaction distances, whereas the distances listed in this table represent calculated minimum heavy-atom distances; therefore, the two values may not be numerically identical.