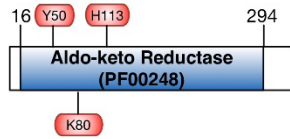


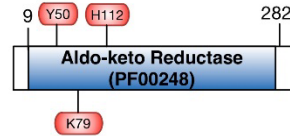
A.

**AKR1A1**  
NP\_006057.1  
[325 aa]



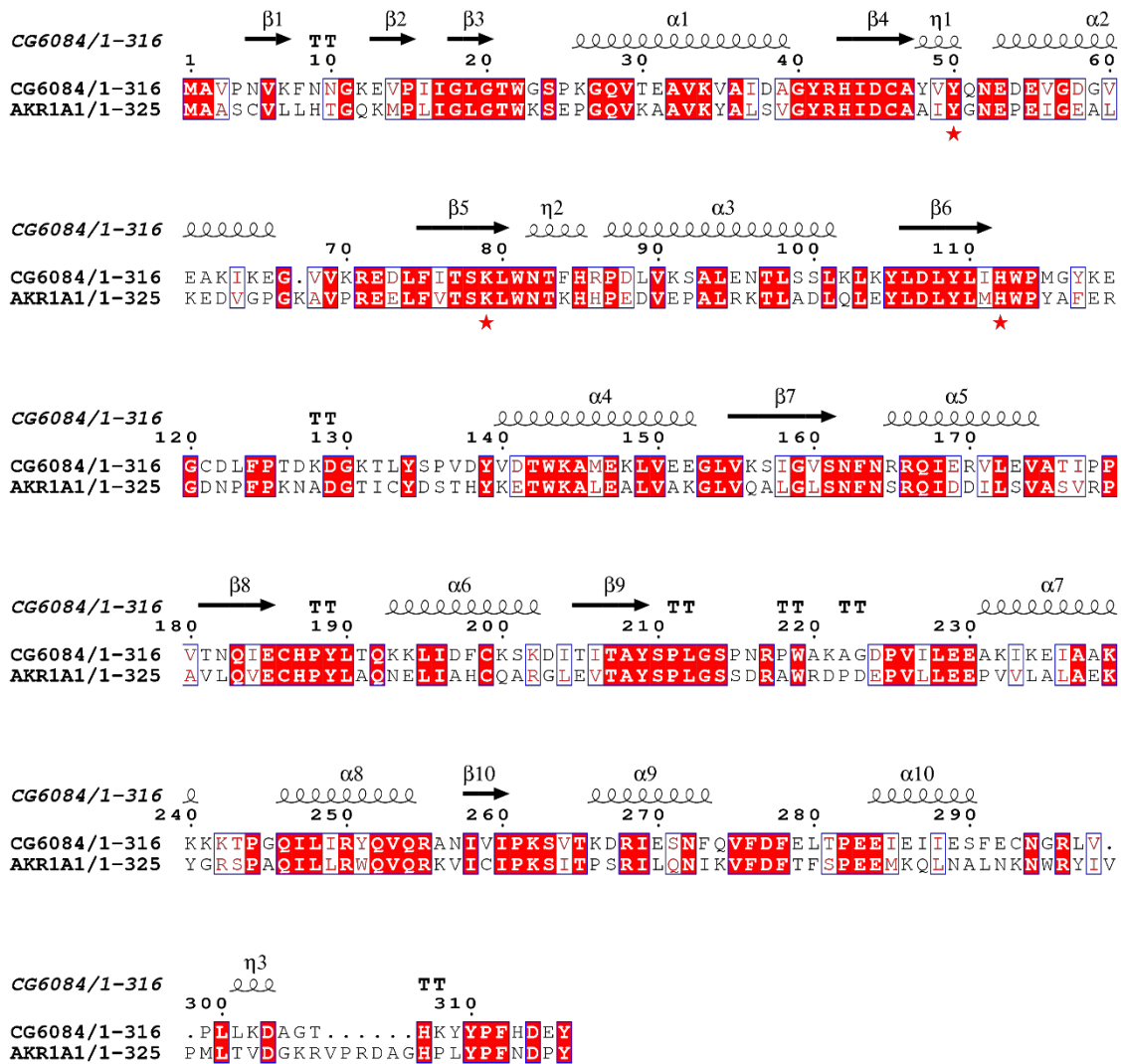
**Active Site Proton Donor: Y50**  
**Assists Catalysis** (lowers pKa of Active Site Tyrosine): K80  
**Important Residue:** (substrate binding): H113

**CG6084**  
NP\_001261717.1  
[316 aa]



**Predicted Active Site Proton Donor (Predicted): Y50**  
**Predicted Assists Catalysis** (lowers pKa of Active Site Tyrosine): K79  
**Predicted Important Residue** (substrate binding): H112

B.



C.

CG6084/1-316 1 --MAVNVKFNNGKEVP I IGLGTWGS PKGQVTEAVKVAIDAGYRHIDCAYVYQNEDEVGDGV EAKI ---KEG 67  
2ALR/1-324 1 AA ---SCVLLHTGQKMPL I IGLGTWKSEPGQVKAAYKYALSVGYRHIDCAA IYGN EPEIGEALKEDVGP G ---K 67

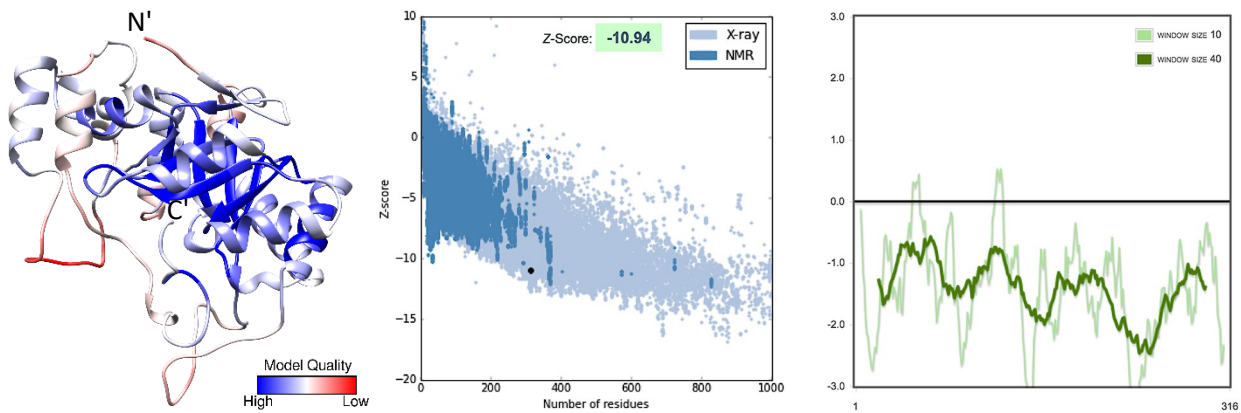
CG6084/1-316 68 VVKREDLFITSKLWNTFHRPDLVKSALENTLSSLKLKYLDLYLIHWP MG YKEGCDLFPTDKDGKTLYS PVDY 139  
2ALR/1-324 68 AVPREELFVTSKLWNTKHHPE DVEPALRKTLADLQLEYLDLYLMHWPYAFERGDNPF PKNADGTIC YDSTHY 139

CG6084/1-316 140 VDTWKAMEKLV E EGLVKS I GVS NFNRROI ERLV EAT I PPVTN QIECHPYLTQKKLIDFCKSKDITITAYSP 211  
2ALR/1-324 140 KETWKAL EALVAKGLVQALGLSNFSROI DDILSVASVRPAVLQVECHPYLAQNELIAHCQARGLEVITAYSP 211

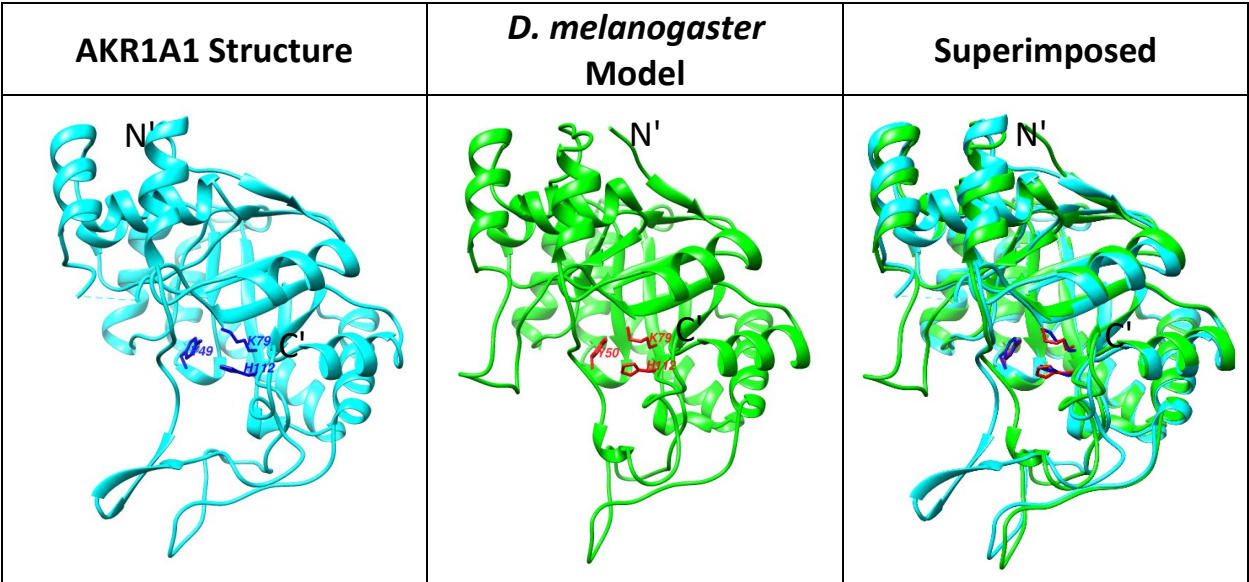
CG6084/1-316 212 LG -----SPNRPWAKAGDPVILEEAKI KEIAAKKKKTPGQILIRYQVQRANIVIPKSVTKDR IES 271  
2ALR/1-324 212 LGSSDRAWRPDEP-----V LLEEPVVLALAEKYGRSPAQILLRWQVQRKVICIPKSITPSR ILQ 271

CG6084/1-316 272 NFQVDFELTPEEIE I IESFECNGRLVPL -----LNQYGHPPHPFEKDEY 316  
2ALR/1-324 272 NIKVDFDTFSP EEMKQLNALNKNWR Y IVPMLTV DGRVPRDAGHPLYPFND -PY 324

D.



E.



F.	Length (AA)	Domain Architecture (Pfam, range)	Functional Residues (aligned matches in <i>D. melanogaster</i> )	Sequence ID%	Structural Overlap (RMSD)
Prostacyclin F synthase (AKR1B1, NP_001619.1)	316	Aldo/keto reductase family (PF00248) 4-289	Y49, K78, H111	48% ID 62% SIM	0.847 Å
Uncharacterized protein (CG6084, NP_648484.1)	316	Aldo/keto reductase family (PF00248) 9-282	Y50, K79, H112		

**S3 Fig. Sequence and structural details of the modeled fly Prostacyclin F synthase candidate.** A. Domain architecture of AKR1A1 and CG6084 and known/predicted functional residues B. Pairwise alignment of CG6084 and 2ALR generated from structural superposition showing shared secondary structure elements and known/predicted functional residues (marked with a red asterisk) C. Pairwise alignment of CG6084 and 2ALR generated from structural superposition with conserved residues highlighted using the physiochemical color scheme (CLUSTALX) D. Validation of the CG6084 model: ProQ2 quality score mapped to a 3D model of CG6084 (left); ProSA global quality score ranking (middle) and per-residue quality graph (right) E. AKR1A1 (2ALR, cyan-blue) superimposed on the predicted structure of CG6084 (green-red). RMSD: 0.847 Å with potential matches for conserved functional residues highlighted F. Summary of features shared by Prostacyclin F synthase and potential *D. melanogaster* ortholog CG6084.