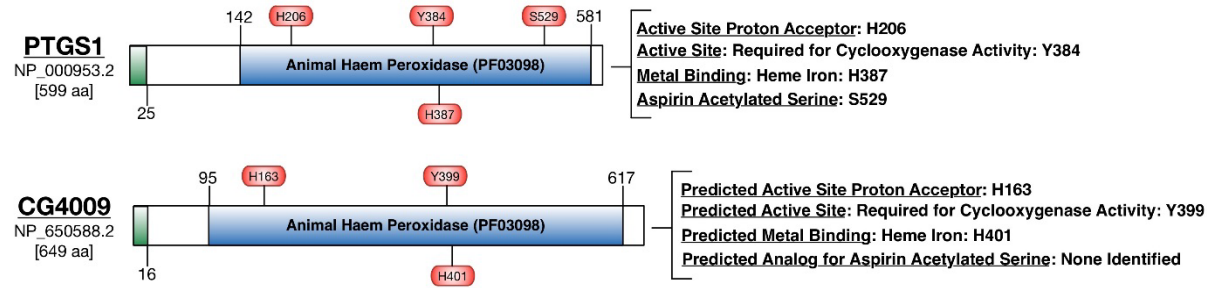
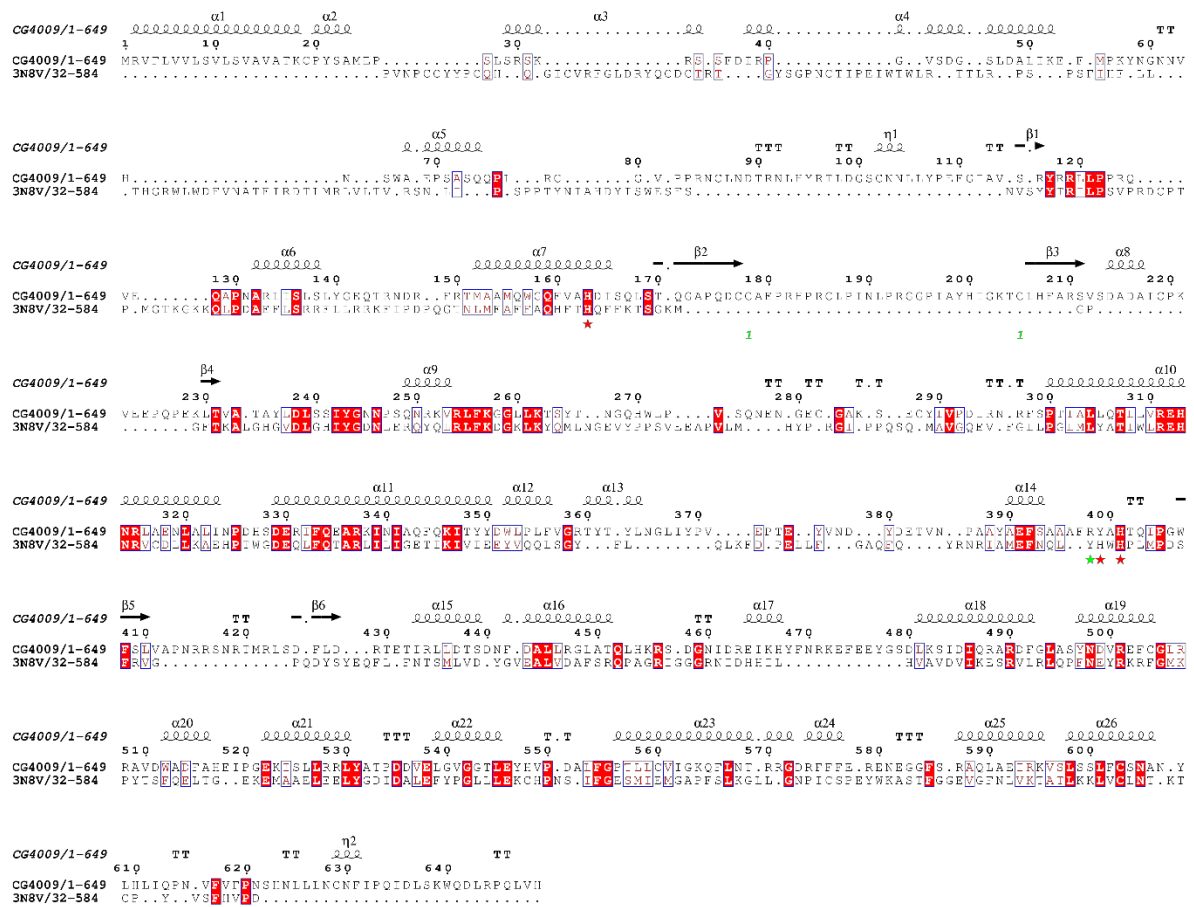


A.



B.



CG4009/1-649  
3N8V/32-584

1 - - - - - MRVFLVLVL SVLSVAVATKC EYSAMEPSL - SRS - - - - - KRSSFDIRP - - - - - G-41  
32 R V N P C C Y Y R - - - - - C Q H Q - - G I C V R F G L D R Y Q C - D C I R - T G Y S G P N C T I P E I W T W 77

CG4009/1-649  
3N8V/32-584

42 - - V S D G - - S L D A L I K E F M P K Y - - N G - - - - - N N V H N S W A - E F S A S Q Q P - - - - - L R C - - - - - 79  
78 L R - - - - - T T L - - R - - P S P S F I H F L L T H G R W L W D F V N A T F I R D T L M R L V L T - - V - - R S N - L I - - P S P P T Y N I A H D 135

CG4009/1-649  
3N8V/32-584

80 - - - - - G V - P P - R N C L N D T R N L H Y R T L D G S C N N L L Y P E F G I A V S - R Y R R L L P P R Q - - - - - V - - - - - E Q A P N A R L I S L 137  
136 Y I S W - E S F S N - - - - - V S Y T T R I L P S V R P D C P T M G T K G K K - Q L P D A E F L S R 179

CG4009/1-649  
3N8V/32-584

138 S L Y G E Q T R N D R - - F R T M A A M Q W G G F V A H D I S Q L S T - Q G A P Q D C C A E P R H P R C L P I N L P R G G P I A Y H T G K T C L H F A R S 211  
180 R F L L R R K F I P D P Q Q T N L M F A F F A Q H F T H Q F K T S G K M - - - - - Q 217

CG4009/1-649  
3N8V/32-584

212 V S D A D A I C P K V E E P Q P E K L T V A - T A Y L D L S H I Y G N N P S Q N R K V R L F K G G L L K T S Y T - N G O H W L P - - - - - V S - Q N E 272  
218 P - - - - - G T F K A L G H G V D L G H I Y G D N L E R Q Q L R L F K D G K L Y Q M L N G E V Y P P S V E E A P V L - M H - - - - - 278

CG4009/1-649  
3N8V/32-584

279 N G E - C G A K S - E C Y I V P D I R - - N R F S P T I A L L Q T L L V R E H N F L A E N L A L I N P D H S D E R I F C E A R K I N I A Q F Q K I T Y Y Q 351  
275 - Y P R - G I P P Q S M A V G Q E V F G - L - L P G M L Y A T I W L R E H N R V C D L L K A E H P T W G D Q L F T A R L L I L I G E T I K I V I E E 347

CG4009/1-649  
3N8V/32-584

352 W L P L F V G R - T Y T Y - - - - - L N G L I Y P E P T E - - Y - - V N D Y D - E T V N P A A Y A E F S A A F R Y A H T Q I P G W F S L V A P N R R 416  
348 Y V Q Q L S G Y F - - L Q L F K - - - - - D - P E L L F G A Q - - F Q Y R - - - N R I A M E F N Q - L - Y H W H P L M P D S F R V G - - - - - 398

CG4009/1-649  
3N8V/32-584

417 S N R T M R L S D - F L D - - R T E T I R L L D T S D N F D A L L R G L A T L H K R S - D G N I D R E K I Y F N R K E F E E Y G S D L K S I D I Q R 484  
399 - - - - - P Q D Y S Y E Q F L - F N T S M L V D Y G V A L V D A F S R P A G I I G G G R N I D H I L - - - - - H V A V D V I E K 454

CG4009/1-649  
3N8V/32-584

489 A R D F G L A S Y N D V E F C G L R R A V D W A D F A H E I P G E K I S L L R R L Y A T P D D V L E G V G G T L E Y H V - P D A L F G P T L L C V I G K 564  
455 S V L R L Q P F N E Y K R F G M K P Y T S Q E L T G - E K E M A A E L E E L Y G D I D A L E F Y P G L L L K E C H P N S - I F G E S M I E M G A P 528

CG4009/1-649  
3N8V/32-584

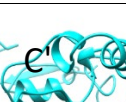
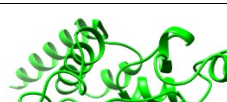
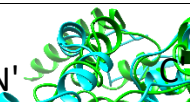
565 Q F L N T - R R G D R F F F - E R E N E G G F - S R A Q L A E I F K V S L S S L F C S N A - - N Y L H - - L I Q P N V F V F P N S H N L L L N C N F I P Q 634  
529 F S L K G L L - G N P I C S P E Y W K A S T F G G E V G E N L V A T A L K K L V G L N T K T - C P Y V - - - - - S F H V P D - - - - - 584

CG4009/1-649  
3N8V/32-584

635 I D L S K W Q D L R P Q L V H

649

Figure 1 consists of three panels. The left panel shows a 3D ribbon diagram of the protein structure, with the N' and C' termini labeled. The middle panel is a scatter plot of Z-score vs. Number of residues, showing a Z-score of -6.59. The right panel is a line plot of Z-score vs. Number of residues, showing a window size of 10 and 40.

PTGS1 Structure	<i>D. melanogaster</i> Model	Superimposed
		

F.	Length (AA)	Domain Architecture (Pfam, range)	Functional Residues (aligned matches in <i>D. melanogaster</i> )	Sequence ID%	Structural Overlap (RMSD)
Cyclooxygenase 1 (PTGS1, NP_000953.2, PDB: 3N8V)	599	Animal heme peroxidase domain (PF03098) 142-581	H207, Y385 and H388	14% ID 26% SIM	2.660 Å
Uncharacterized protein CG4009, NP_650588.2)	649	Animal heme peroxidase domain (PF03098) 95-617	H163, Y399, and H401		

**S14 Fig. Sequence and structural details of the modeled fly PTGS1 candidate.** A. Domain architecture of PTGS1 and CG4009 and known/predicted functional residues B. Pairwise alignment of CG4009 and 3N8V generated from structural superposition showing shared secondary structure elements and known/predicted functional residues (marked with red asterisk; the green asterisk marks the putative analog for Y384) C. Pairwise alignment of CG4009 and 3N8V generated from structural superposition with conserved residues highlighted using the physiochemical color scheme (CLUSTALX) D. Validation of the CG4009 model: ProQ2 quality score mapped to a 3D model of CG4009 (left); ProSA global quality score ranking (middle) and per-residue quality graph (right) E. PTGS1 (3N8V, cyan-blue) superimposed on the predicted structure of CG4009 (green-red) with potential matches for conserved functional residues highlighted F. Summary of features shared by PTGS1 and potential *D. melanogaster* ortholog CG4009.