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**Supporting information for article:**

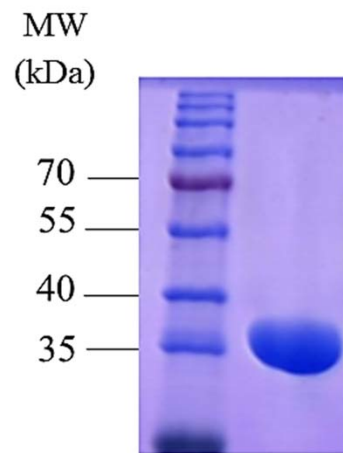
**Structure–function study of AKR4C14, an aldo-keto reductase from Thai Jasmine rice (*Oryza sativa* L. ssp. Indica cv. KDML105)**

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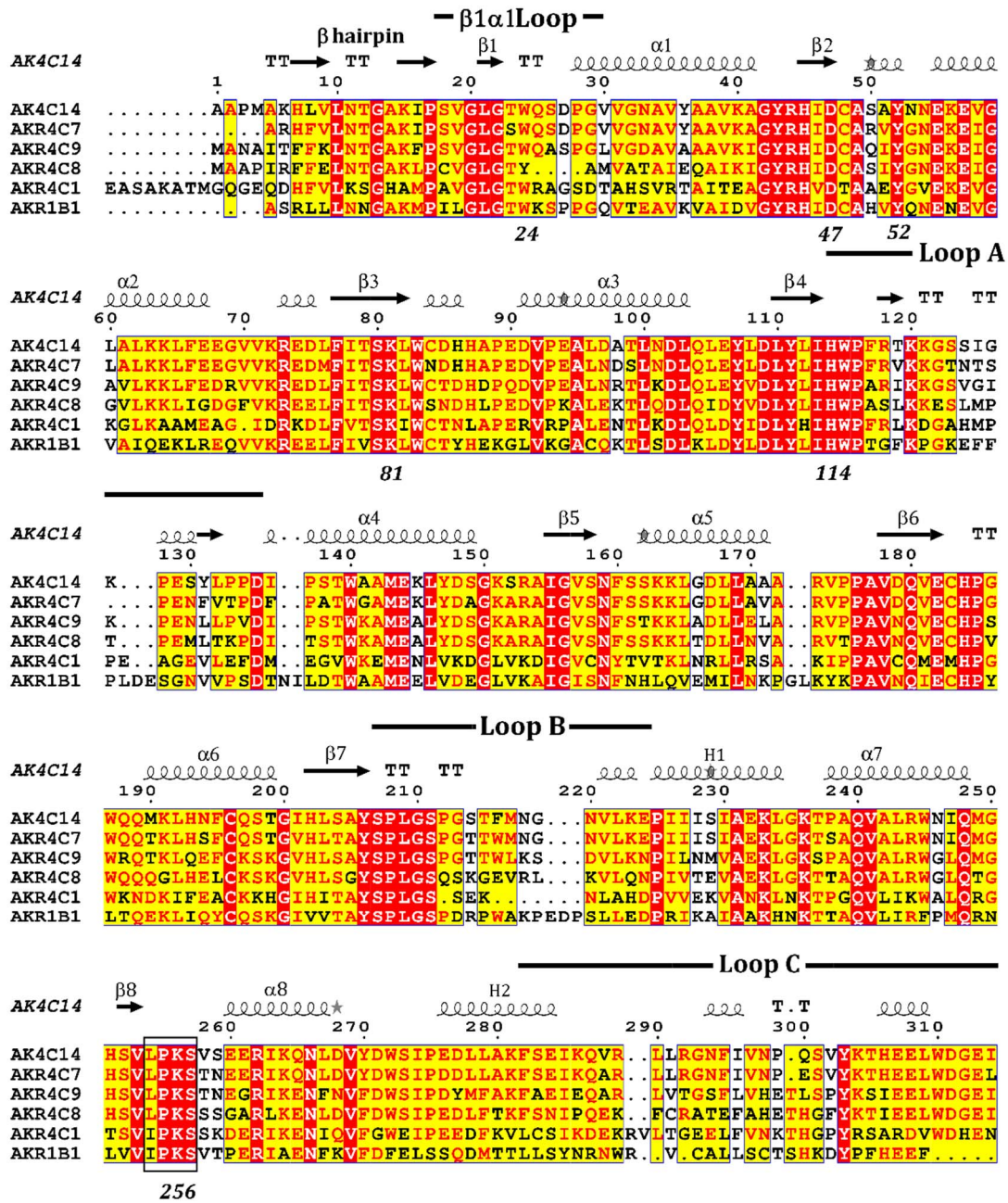
**Table S1** Three-dimensional AKR structures

AKRs	Common Name		PDB code	
			<i>Apo</i> form	<i>Holo</i> form
AKR1A1	Human	aldehyde reductase	2ALR (el-Kabbani <i>et al.</i> , 1994)	-
AKR1A2	Porcine	aldehyde reductase	-	1CWN (el-Kabbani <i>et al.</i> , 1996)
AKR1B1	Human	aldehyde reductase	1XGD (Bohren <i>et al.</i> , 2005)	1ADS (Wilson <i>et al.</i> , 1992) 2ACS (Harrison <i>et al.</i> , 1994)
AKR1B6	Porcine	aldehyde reductase	-	1AH4 (Urzhumtsev <i>et al.</i> , 1997)
AKR1B8	Mouse	F fibroblast growth factor-induced protein	-	1FRB (Wilson <i>et al.</i> , 1995)
AKR1B9	Chinese hamster	ovary reductase	-	1C9W (Ye <i>et al.</i> , 2000)
AKR1C9	Rat	3 $\alpha$ -hydroxysteroid/dihydrodiol dehydrogenase	1RAL (Hoog <i>et al.</i> , 1994)	1LWI (Bennett <i>et al.</i> , 1996)
AKR2B5	Xylose reductase from		1JEZ (Kavanagh <i>et al.</i> , 2002)	1K8C (Kavanagh <i>et al.</i> , 2002)
AKR4C1	Barley	aldose reductase	2BGQ (Olsen <i>et al.</i> , 2008)	2BGS (Olsen <i>et al.</i> , 2008)
AKR4C7	Maize	aldose reductase	5JH1 (Giuseppe <i>et al.</i> , 2016)	5JH2 (Giuseppe <i>et al.</i> , 2016)
AKR4C8	Aldo-keto reductase from	<i>Arabidopsis thaliana</i>	-	3H7R (Simpson <i>et al.</i> , 2009)
AKR4C9	Aldo-keto reductase from	<i>Arabidopsis thaliana</i>	-	3H7U (Simpson <i>et al.</i> , 2009).
AKR4C14	Aldo-keto reductase from	<i>indica rice</i>	6KBL (This work)	-
AKR5C	Corynebacterium	2,5-diketo-D-gluconic acid reductase	1HW6 (Sanli & Blaber 2001)	1A80 (Khurana <i>et al.</i> , 1998)



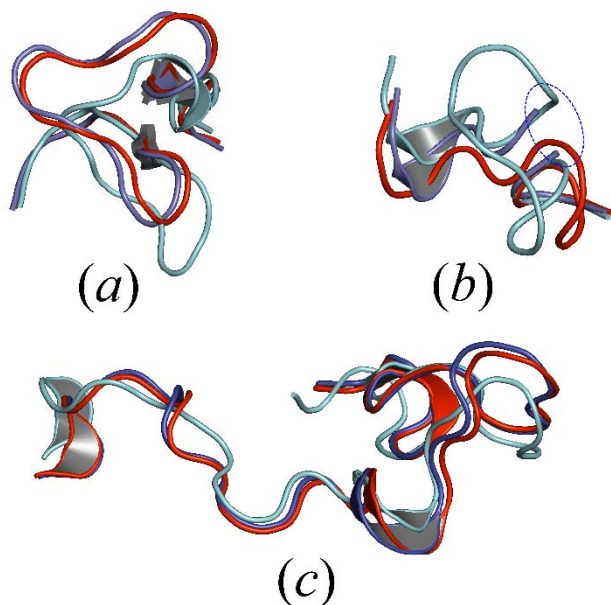


**Figure S2** SDS-PAGE analysis of purified AKR4C14. The protein marker is labelled in kDa.

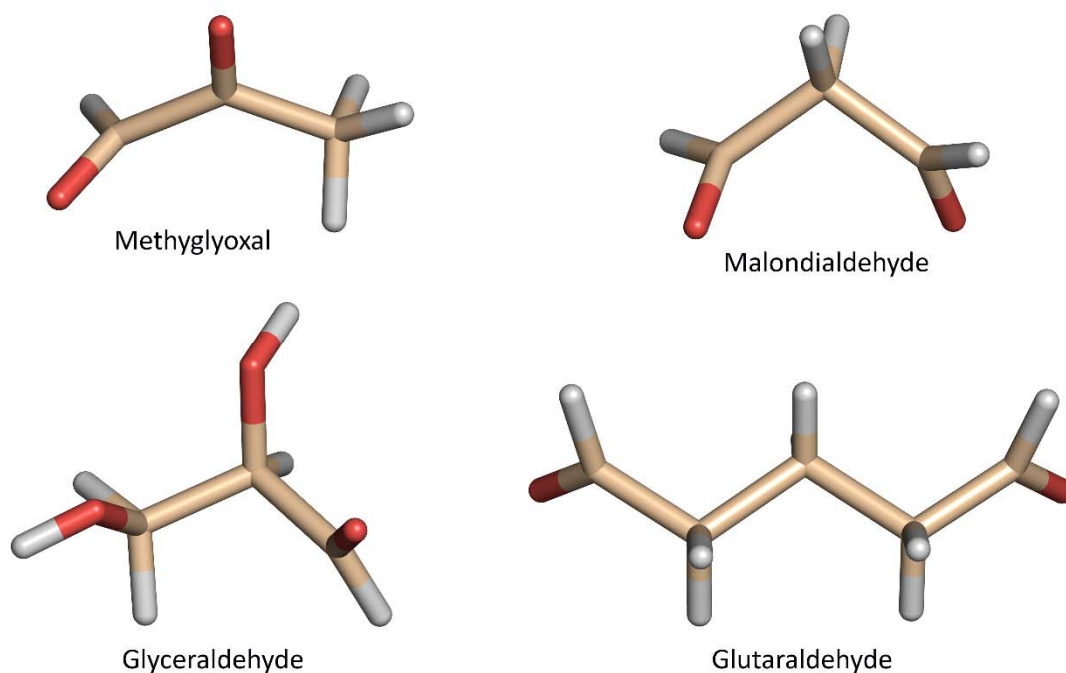


**Figure S3** Sequence and secondary structure comparison of AKR proteins. The amino acid sequence of rice AKR4C14 (PDB code 6KBL) was aligned with maize AKR4C7 (PDB code 5JH1), *Arabidopsis* AKR4C9 (PDB code 3H7U), *Arabidopsis* AKR4C8 (PDB code 3H7R), barley AKR4C1 (PDB code 2BGQ) and human AKR1B1 (PDB code 2ACS). The secondary structure of rice AKR4C14 is displayed as a diagram above the alignment and its catalytic residues and amino acids contributing to the cofactor-binding site are also marked in italics, according to the sequence numbering of AKR4C14. Black boxes enclose the highly conserved sequences, with an additional black box around the highly conserved motif among aldose reductases (Leu/Ile<sub>254</sub> -Ser<sub>257</sub>). The  $\alpha$  helices and  $\beta$  strands are displayed as squiggles and arrows, respectively. TT indicates strict  $\beta$ -turn.

Grey stars displayed in the secondary structure line above residues marks residue with alternate conformations. Residues printed as white characters in red frames are strictly conserved. Residues marked as red characters are designated as similar. Residues belonging to all loops mentioned are marked.



**Figure S4** The superposed structures of rice AKR4C14 (PDB code 6KBL, cyan), *apo* form of barley AKR4C1 (PDB code 2BGQ, blue) and *holo* form of barley AKR4C1 (PDB code 2BGS, red) shown as ribbon representation. (a) Loop A. (b) Loop B. The blue circle dash line highlights the partial disorder of loop B in the *apo* form of AKR4C1 (PDB code 2BGQ, blue). (c) Loop C.



**Figure S5** Structures of aldehyde substrates; Methyglyoxal (2-oxopropanal); *Malondialdehyde* (propanedial); Glyceraldehyde (2,3-dihydroxypropanal) and Glutaraldehyde (pentanedial).

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