Correlated mutations select misfolded from properly folded proteins

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*Centre for Molecular and Biomolecular Informatics, Radboud University Medical Centre,
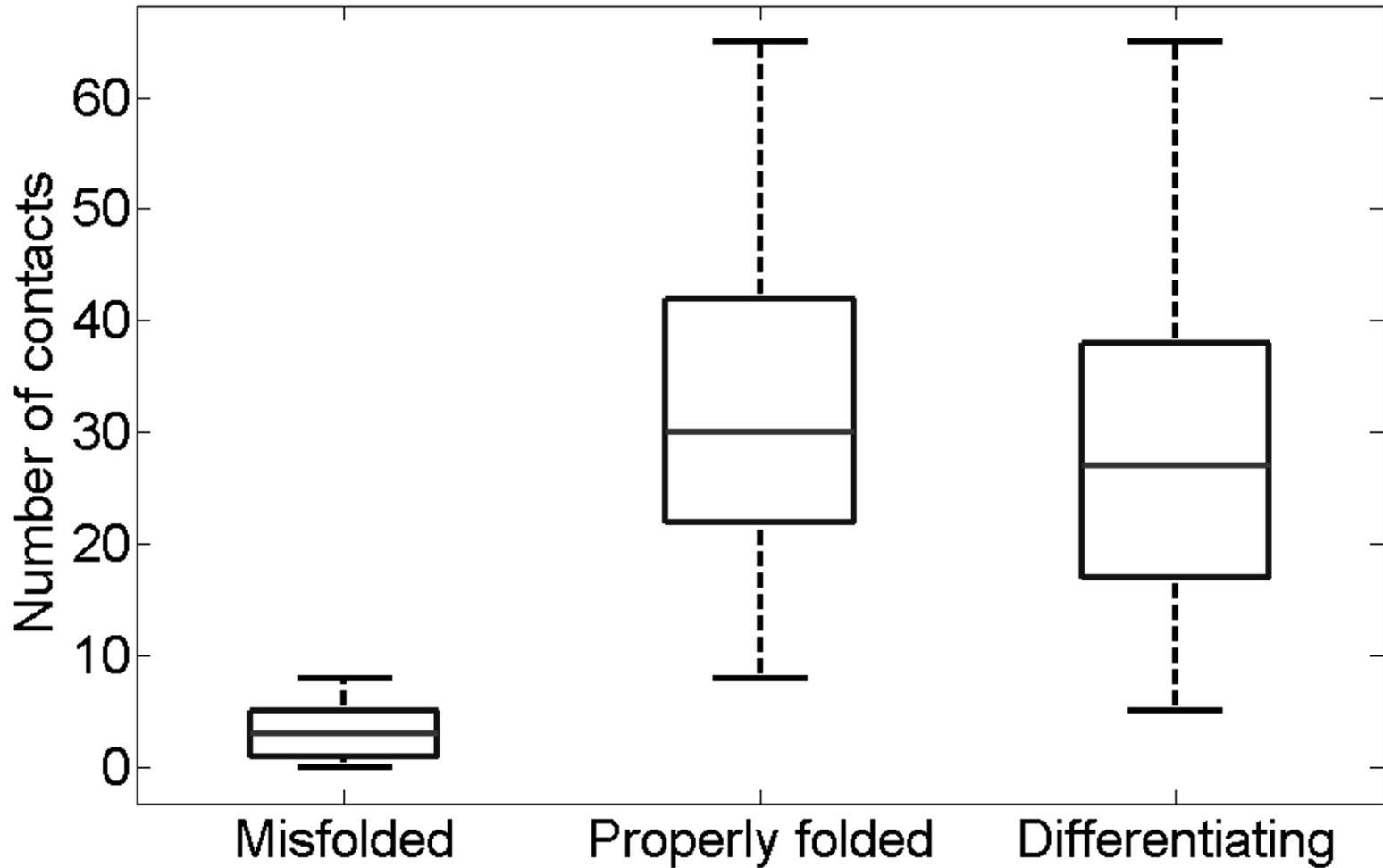Nijmegen, the Netherlands*

Residue-residue contact definition

Created in PyMOL

8 Å

5 aa

DCA

Data

- 26 protein pairs

- RMSD > 1.1 Å, TM-score < 0.9

- only X-ray (22)

DECOYS 'R' US

R. Samudrala, M. Levitt, *Decoys 'R' Us: A database of incorrect protein conformations to improve protein structure prediction*, **2000**, Protein Science 9: 1399-1401.
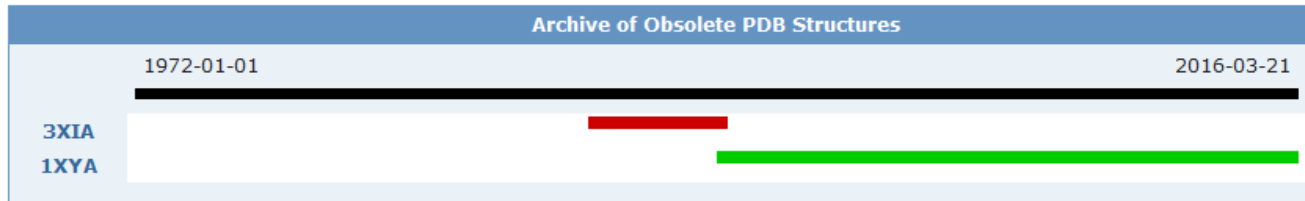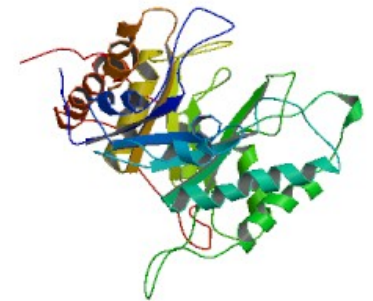
Native vs. Misfolds

Data

- 2421 „obsolete-successor" protein pairs

- RMSD > 1.1 Å, TM-score < 0.9

- divided on NMR (110) i X-ray (42)

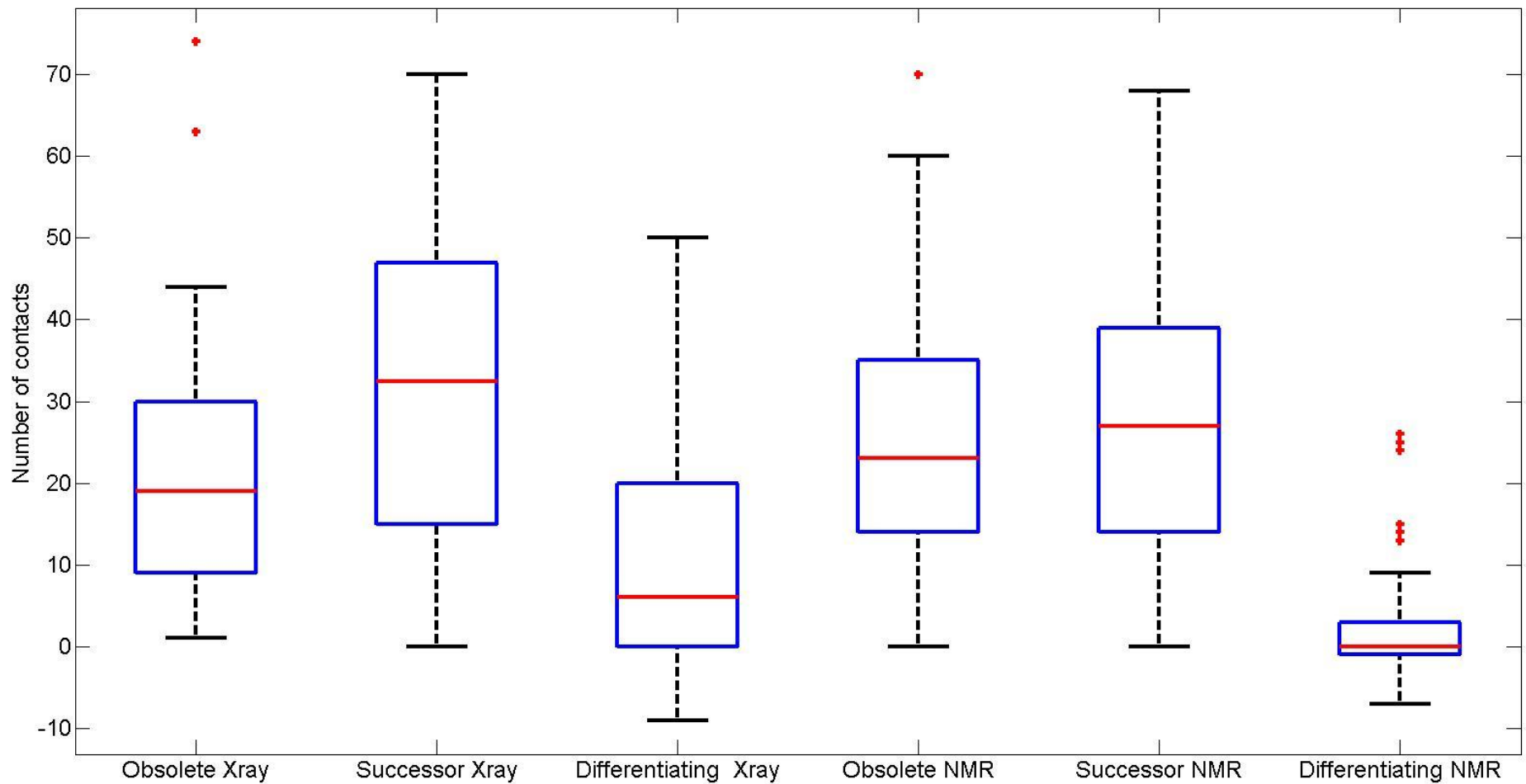**3XIA** was obsoleted on 1994-05-31 and superseded by **1XYA**

Archive of Obsolete PDB Structures

1972-01-01		2016-03-21
3XIA		
1XYA		

Note: Mouse over colored bars for date info, mouse over PDB IDs for file download or Structure Explorer link.

Image of 3XIA

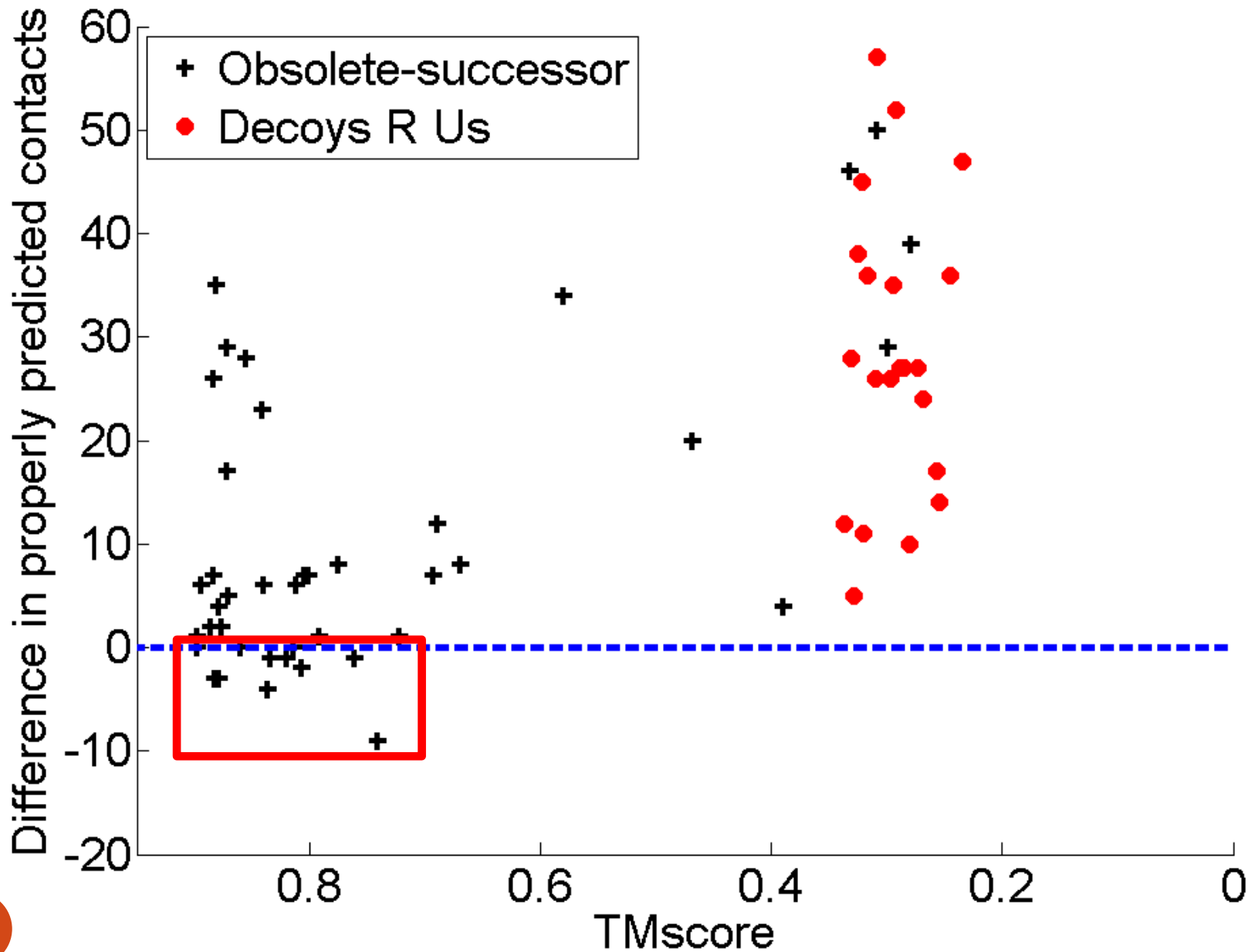| **Textual Comparison**		
	3XIA	**1XYA**
Title ⓘ	CRYSTALLOGRAPHIC STUDIES OF THE MECHANISM OF XYLOSE ISOMERASE	X-RAY CRYSTALLOGRAPHIC STRUCTURES OF D-XYLOSE ISOMERASE-SUBSTRATE COMPLEXES POSITION THE SUBSTRATE AND PROVIDE EVIDENCE FOR METAL MOVEMENT DURING CATALYSIS
Authors ⓘ	Farber, G., Petsko, G.	Lavie, A., Allen, K.N., Petsko, G.A., Ringe, D.
Residues per chain ⓘ	n	A: 386, B: 386
Number of Atoms ⓘ	2966	6550
Non-polymer entities ⓘ	none	MG, OH
Source ⓘ	Polymer 1: n/a	Polymer 1: Streptomyces olivochromogenes
Exp. Method ⓘ	X-RAY DIFFRACTION	X-RAY DIFFRACTION

Y. Zhang, J. Skolnick, *TM-align: A protein structure alignment algorithm based on TM-score*, **2005**, Nucleic Acids Research, 33: 2302-2309.

Obsolete vs. Successors

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