Summary of Sirtuin Structures.

Protein(+small molecule)	PDB ID	Major Findings	Reference
Sir2Af1 + NAD^+ (ADPR observed)	1ICI	Overall sirtuin fold and NAD^+ binding site	Xu group, Cell 2001
hSIRT2 apo	1J8F	Overall sirtuin fold	Pavletich group, NSMB 2001
Sir2Af2 + p53K382Ac	1MA3	Mode of p53 substrate binding	Wolberger group, Mol Cell 2002
Sir2Af1 + NAD^+ (ADPR observed)	1M2G	Overall sirtuin fold	Cho group, J Biol Chem 2002
Sir2Af1(S24A) + NAD^+ (ADPR observed)	1M2H	Local conformation change around S24A	
Sir2Af1(H80N) + NAD^+ (ADPR observed)	1M2J	Local conformation change around H80N	
Sir2Af1(F159A) + NAD^+ (ADPR observed)	1M2K	F159 is proposed to participate in substrate binding	
Sir2Af1(D102G, F159A, R170A) + NAD^+	1M2N	2'-O-Ac-ADP-ribose product observed after the crystal was incubated with N-acetyl lysine	
yHst2, full length	1Q14	Overall Hst2 fold. C- and N-terminal extensions interact with NAD+ and acetyllysine binding sites, respectively to autoinhibit the enzyme	Marmorstein group, NSMB 2003
yHst2 + NAD^+ (ADPR observed)	1Q17	Cofactor binding loop becomes ordered compared to apo structure	Marmorstein group, Structure 2003
yHst2 + NAD^+ (2'-O-Ac-ADPR observed) +H4K16Ac peptide	1Q1A	Model for 2'-O-Ac-ADP-ribose product and acetyllysine substrate binding in the same structure	
CobB (E. Coli) +H4K16Ac peptide	1S5P	Model of acetyllysine peptide substrate binding	Marmorstein group, J Mol Biol 2004
Sir2Af2 + NAD^+	1S7G	Active NAD^+ binding with nicotinamide moiety ound in the C pocket	Wolberger group, Mol Cell 2004
yHst2 + H4K16Ac peptide + carba-NAD^+ (non-hydrolyzable analogue)	1S7C	Nicotinamide moiety binds in C pocket; N-ribose planar to acetyllsine supporting an S_N1 catalytic mechanism	Marmorstein group, PNAS 2004
yHst2 +ADPR+H4K16Ac peptide	1SZD	Model of ADPR binding and proposal of a D pocket for free nicotinamdie binding	
Sir2Af2 + NAD+ + NAM	1YC2	Free nicotinamdie binding observed in the C pocket	Wolberger group, Mol Cell 2005
Sir2Tm +p53K382Ac peptide + NAM	1YC5	Free nicotinamide binding observed in the C pocket	
Sir2Tm + polypropylene glycol	2H2I	Approximation of the apoenzyme	Wolberger group, Biochemistry 2006
Sir2Tm +p53K382Ac peptide	2H2D	Residues at -1 and +2 positions of the peptide make side chain interactions with Sir2Tm	
Sir2Tm +p53K382 peptide	2H2F	Residues at -1 and +2 positions of the peptide make side chain interactions with Sir2Tm	
Sir2Tm +H4K79Ac peptide	2H2H	Residues at -1 and +2 positions of the peptide make side chain interactions with Sir2Tm	
Sir2Tm +H4K115Ac peptide	2H2G	Residues at -1 and +2 positions of the peptide make side chain interactions with Sir2Tm	
SirTm + NAD^+ +p53K382Ac peptide	2H4F	Putative Michaelis complex suggesting an S_N2 catalytic mechanism	Wolberger group, Structure 2006
SirTm(H116Y) + NAD^+ +p53K382Ac peptide	2H4H	Identical to wild type and NAD+ orientation is not dependent on contacts with the His116 general base	
(Sir2Tm + p53K382Ac peptide) crystal soaked with NAD+	2H4J	Deacetylated p53 observed	
Sir2Tm(H116A) + NAD^++p53K382Ac peptide	2H59	3'-O-Ac-ADP-ribose +p53K382 observed in one molecule	
yHst2+ADP-HPD + H4K16Ac peptide	2OD7	Binding model of an oxocarbenium intermediate mimic	Marmorstein group, Mol Cell 2007
yHst2+ADP-HPD + H4K16Ac peptide +NAM	2OD9	Nicotinamide is observed to bind in the D pocket (valid issues were raised regarding the crystallographic evidence)	
yHst2(I117F) + carba-NAD^++H4K16Ac peptide	2OD2	Isomorphous to wild type; I117 is proposed to participate in nicotinamdie binding in D pocket	
hSIRT5 +NAD^+ (ADPR observed)	2B4Y	Sirtuin fold	Plotnikov group, Structure 2007
hSIRT5 + suramin	2NYR	Suramin binding model	

Sir2Tm +DADMe-NAD^+ +p53K382Ac peptide	3D4B	Binding model of a dissociative intermediate	Wolberger group, Structure 2008
Sir2Tm + S-alkylamidate	3D81	Binding model of an O-alkylamidate intermediate mimic	
Sir2Tm + p53 peptide(K_{Ac}XXR)	3JR3	Putative nucleophilic attack from Arg at +2 of acetyllysine peptide for ADP-ribosylation	Wolberger group, J Biol Chem 2009
hSIRT3 apo	3GLS	Sirtuin fold	Perni group, J Biol Chem 2009
hSIRT3 + AceCS2-K_{Ac}	3GLR	Model of acetyllysine binding	
hSIRT3 +AceCS2-$K_{S\text{-}Ac}$-ADPR	3GLT	Binding model of an S-alkylamidate intermediate	
hSIRT3+AceCS2-K	3GLU	Binding of a dethioacetylated AceCS2 peptide	
hSIRT5+H3K9 (thioacetyl) peptide	3RIG	Binding model of an Succinyl-lysine peptide	Lin group, Science 2011
hSIRT5 +NAD++H3K9 (N-succinyl) peptide	3RIY		
Sir2Tm + p53K382 (propionyl) peptide)	3PDH	Binding model of propionyl-lysine	Wolberger group, Protein Sci 2011
hSIRT6 +NAD^+ (ADPR observed)	3K35	Sirtuin fold(lacks the helical module in the smaill domain); ADPR binding	Denu group, J Boil Chem 2011
hSIRT6 + ADPR	3PKI		
hSIRT6+2'-N-acetyl-ADP-ribose	3PKJ	Sirtuin bound to 2'-N-acetyl-ADP-ribose, a non-hydrolyzable analog of O-acetyl-ADP-ribose	

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