

PROTEIN	UNIPROT ID	LENGTH	PDB/ALPHA ID	RES.	METHOD	INHIBITOR
HDAC1	Q13547	482	4BKX (B)	3.00	X-ray	Entinostat
HDAC2	Q92769	488	6WBW	1.46	X-ray	Mocetinostat
HDAC3	O15379	428	AF-O15379-F1		Alpha	Valproic acid
HDAC4	P56524	1084	AF-P56524-F1		Alpha	Romidepsin
HDAC5	Q9UQL6	1122	AF-Q9UQL6-F1		Alpha	LMK-235 or 19i or N-((6-(hydroxyamino)-6-oxohexyl)oxy)-3,5-dimethylbenzamide
HDAC6	Q9UBN7	1215	AF-Q9UBN7-F1		Alpha	Ricolinostat
HDAC7	Q8WUI4	952	AF-Q8WUI4-F1		Alpha	Tucidinostat
HDAC8	Q9BY41	377	3MZ7(A)	1.90	X-RAY	Resminostat
HDAC9	Q9UKV0	1011	AF-Q9UKV0-F1		Alpha	Panobinostat
HDAC10/ HDA10	Q969S8	669	AF-Q969S8-F1		Alpha	Belinostat
HDAC11/ HDA11	Q96DB2	347	AF-Q96DB2-F1		Alpha	Vorinostat

Table 1. Overview of structural data for 11 HDAC subtypes

PROTEIN	ACTIVE & BINDING SITE		
	UNIPROT	LITERATURE	PRANKWEB
1	141	His140, Asp176, and Asp264	
2	142,175,177,179,188, 223, 265,191,194,198,199	His145, Asp181, and His183	
3	135	His134, Asp166, and His168	
4	667, 669, 675, 751, 803	Asp183 and His184.	A_759 A_802 A_803 A_811 A_812 A_842 A_871 A_942 A_943 A_974 Probability:0.689
5	696,698,704,781, 833		A_1004 A_1006 A_789 A_830 A_833 A_841 A_842 A_872 A_901 A_972 A_973
6	216, 611, 1113,1115,1133,1136,1145,1148,1153,1160,1164,1176,1183,1186	Tyr345, His611, and Asp610	A_1083 A_1085 A_1086 A_1141 A_1143 A_1155 A_1161 A_1162 A_1166 A_1173 A_1182 A_1184 A_1189
7	533, 535, 541,618, 670, 843	Asp178, His180, and His183	A_254 A_841 A_709 A_678 A_679 A_667 Probability: 0.207
8	101, 143, 151,178,180, 267, 306	Asp178, His180	A_101 A_105 A_108 A_111 A_137 A_138 A_139 A_140 A_141 A_142 A_143 A_151 A_152 A_153 A_154 A_178 A_180 A_207 A_208 A_263 A_267 A_274 A_30 A_303
9	646, 648, 654, 731, 783	Asp181, His184, and His186	A_322 A_323 A_324 A_326 A_327 A_330 A_332 A_656 A_737 A_738 A_739 A_780 A_782 A_783 A_791 A_792 A_822 A_850 A_851 A_922 A_923 A_954 A_956 Probability: 0.823
10	20, 135, 172,174, 265, 272, 305	Asp172, His174, and His176.	
11	143		A_114 A_139 A_140 A_141 A_142 A_143 A_151 A_152 A_153 A_181 A_183 A_209 A_26 A_261 A_268 A_28 A_301 A_302 A_304 A_32 A_35 A_37 A_39 A_42 A_93 Probability sc: 0.857

Table2. Active &Binding sites from different resources, *Blue: publication, red: similarity