Supporting Information

Molecular Dynamics Simulations Indicate an Induced-Fit Mechanism for LSD1/CoREST-H3-Histone Molecular Recognition

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Figure-S1: Root-mean-square fluctuation (RMSF) of the H3-binding site. Only the C^{α} atoms of the H3-binding site were used for RMSF calculation. The RMSF for regions of the binding site are shaded as yellow, white and blue for residues 353-363, 370-391 and 529-564 respectively.

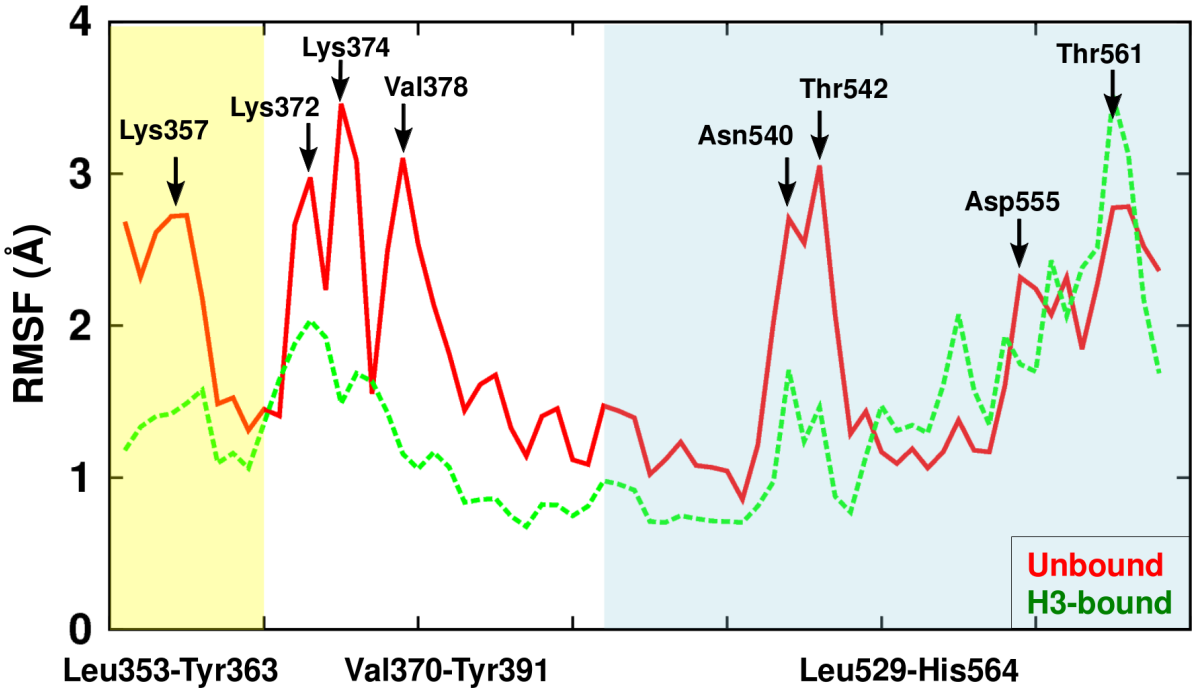

Table-S1: PCA rank for the three-selection scheme considered and corresponding relative contributions.

PC rank	Whole	AO domain	H3-binding site
	Percentage population (cumulative)		
1	37 (37)	55 (55)	71 (71)
2	31 (67)	16 (71)	9 (80)
3	19 (86)	13 (84)	7 (87)
4	5 (91)	5 (89)	3 (90)
5	4 (95)	4 (93)	2 (92)