

SUPPORTING INFORMATION

Quantitative Assessment of Protein Interaction with Methyl-Lysine Analoga by Hybrid Computational and Experimental Approaches

Daniel Seeliger,^{†,‡,||} Szabolcs Soeroes,^{‡,‡,¶} Rebecca Klingberg,[§] Dirk Schwarzer,[§] Helmut Grubmüller^{†,*}, and Wolfgang Fischle^{‡,*}

[†]Theoretische und computergestützte Biophysik, Max-Planck Institut für biophysikalische Chemie, Göttingen, Germany

[‡]Chromatin Biochemie, Max-Planck Institut für biophysikalische Chemie, Göttingen, Germany

[§]Protein Chemistry, Leibniz-Institut für molekulare Pharmakologie (FMP), Berlin, Germany

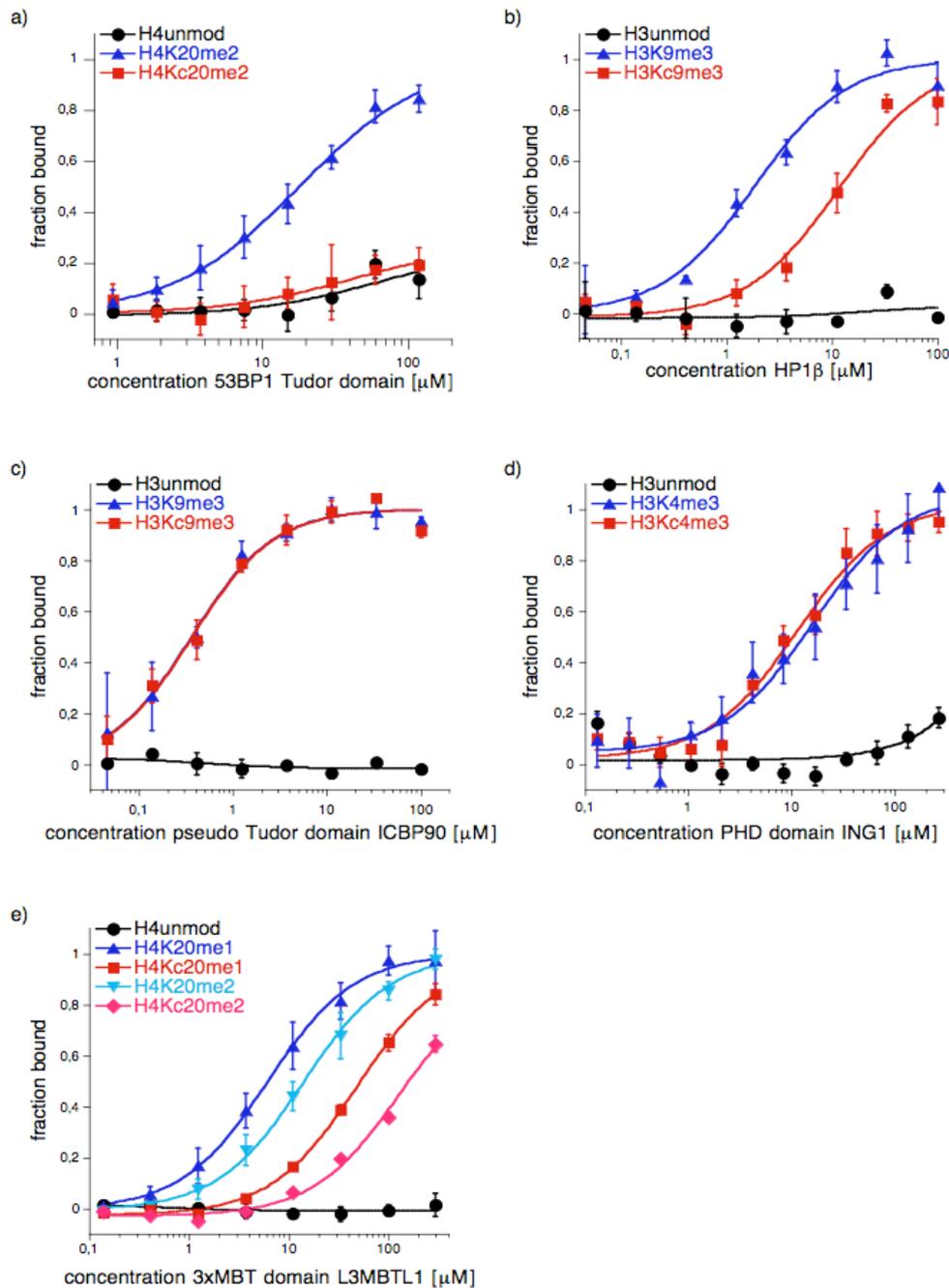


Figure S1. Analysis of different proteins binding to distinct methyl-lysine (Kme) or methyl-lysine analogs (K_Cme) residues in histones. Binding curve titrations using the indicated peptides and recombinant proteins or protein domains were performed using fluorescein labeled peptides. Averages from at least two independent experiments with three instrument readings each are blotted. Error bars correspond to standard deviation.

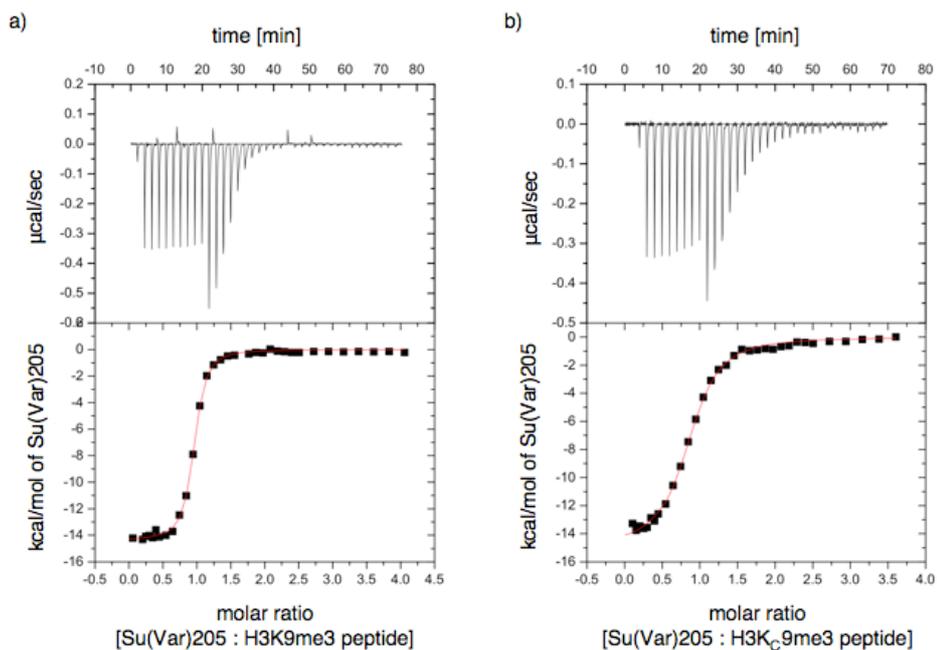
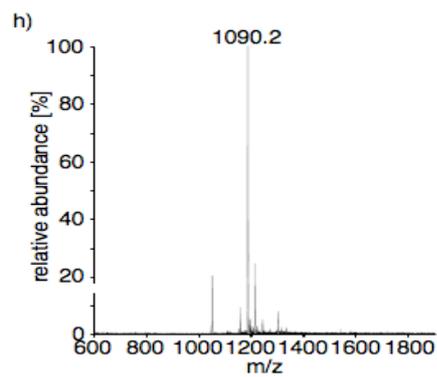
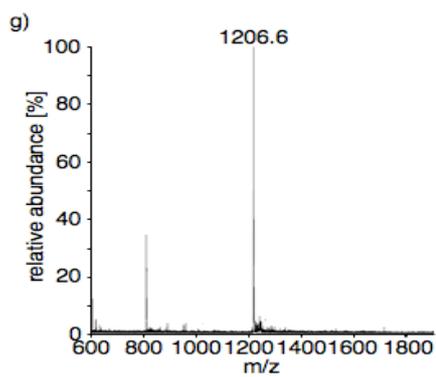
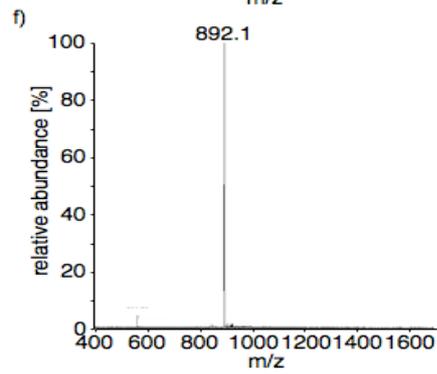
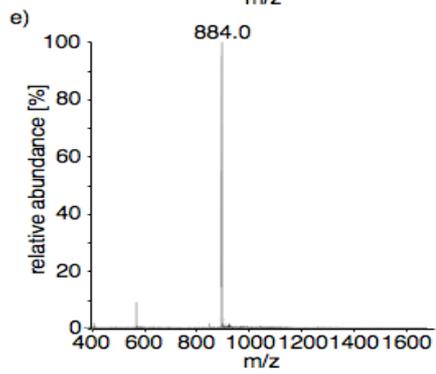
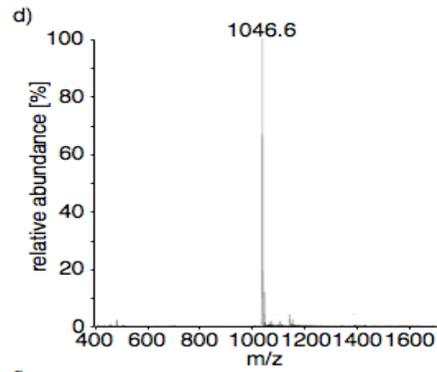
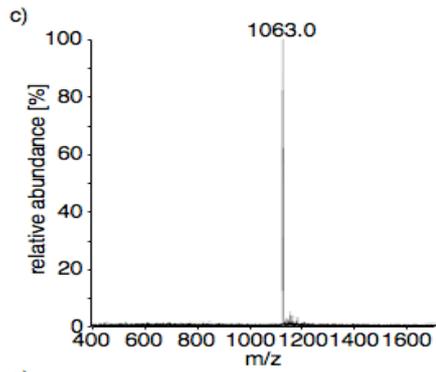
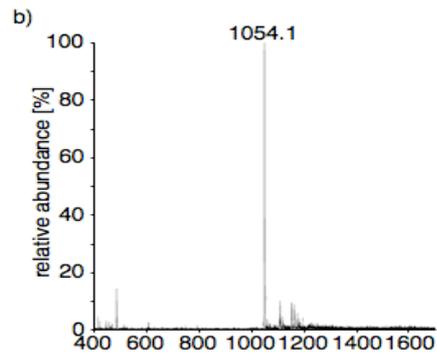
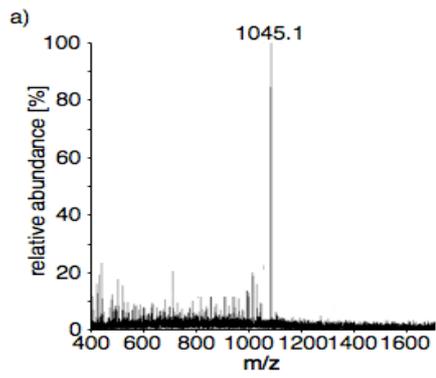


Figure S2. Isothermal titration calorimetric analysis of Su(Var)205 chromo domain binding affinity to (a) H3K9me3 methyl-lysine and (b) H3K_c9me3 methyl-lysine analog peptides. Raw data for injections of the Chromo domain into the peptide (upper panels). Integrated heats of injections and best fit of the data (lower panels).



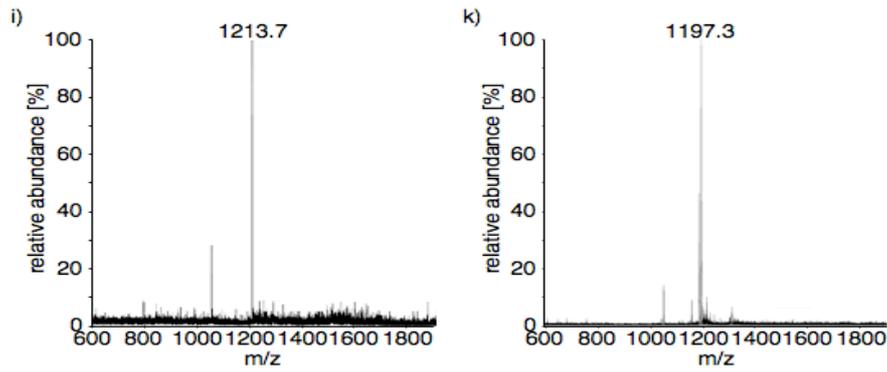


Figure S3. ESI-MS analysis of methyl-lysine (Kme) and methyl-lysine analog (K_Cme) containing histone peptides. Shown are the M+2 peaks of (a) H3K4me3-FI (calculated 1045.5 Da), (b) H3K_C4me3-FI (calculated 1053.5 Da), (c) FI-H3K9me3 (calculated 1062.5 Da), (d) FI-H3K_C9me3 (calculated 1046.0 Da), (e) H3K9me3 (calculated 884.5 Da), (f) H3K_C9me3 (calculated 892.5 Da), (g) FI-H4K20me1 (calculated 1206.0 Da), (h) FI-H4K_C20me1 (calculated 1190.0 Da), (i) FI-H4K20me2 (calculated 1213.0 Da), and (k) FI-H4K_C20me2 (calculated 1197 Da).