

## **Supplementary Data**

### **Extending MeCP2 interactome: Canonical nucleosomal histones interact with MeCP2**

David Ortega-Alarcon<sup>1</sup>, Rafael Claveria-Gimeno<sup>2</sup>, Sonia Vega<sup>1</sup>, Ladan Kalani<sup>3</sup>, Olga C. Jorge-Torres<sup>4</sup>, Manel Esteller<sup>4,5,6,7</sup>, Juan Ausio<sup>3\*</sup>, Olga Abian<sup>1,8,9,10\*</sup>, and Adrian Velazquez-Campoy<sup>1,8,9,10\*</sup>

<sup>1</sup> Institute of Biocomputation and Physics of Complex Systems (BIFI), Joint Unit GBsC-CSIC-BIFI, Universidad de Zaragoza, Zaragoza, 50018, Spain

<sup>2</sup> Certest Biotec S.L., 50840, Zaragoza, Spain

<sup>3</sup> Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC V8W 2Y2, Canada

<sup>4</sup> Josep Carreras Leukaemia Research Institute (IJC), 08916, Badalona, Barcelona, Spain

<sup>5</sup> Centro de Investigación Biomédica en Red Cáncer (CIBERONC), 28029, Madrid, Spain

<sup>6</sup> Institucio Catalana de Recerca i Estudis Avançats (ICREA), 08010, Barcelona, Spain

<sup>7</sup> Physiological Sciences Department, School of Medicine and Health Sciences, University of Barcelona (UB), 08907, l'Hospitalet de Llobregat, Barcelona, Spain

<sup>8</sup> Instituto de Investigación Sanitaria Aragón (IIS Aragón), 50009, Zaragoza, Spain

<sup>9</sup> Centro de Investigación Biomédica en Red en el Área Temática de Enfermedades Hepáticas y Digestivas (CIBERehd), 28029, Madrid, Spain

<sup>10</sup> Departamento de Bioquímica y Biología Molecular y Celular, Universidad de Zaragoza, 50009, Zaragoza, Spain

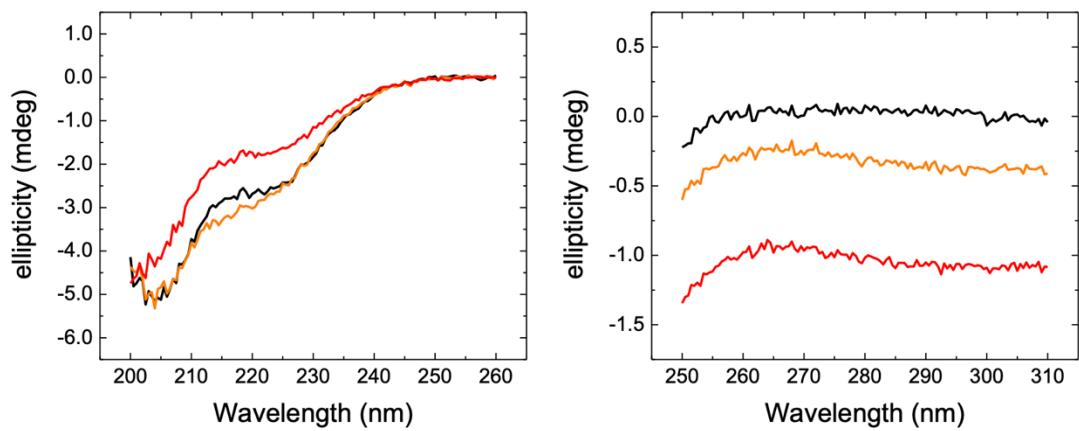
\* To whom correspondence should be addressed:

Adrian Velazquez-Campoy, Institute BIFI – University of Zaragoza, Mariano Esquillor s/n, 50018, Zaragoza, Spain, Email: adrianvc@unizar.es

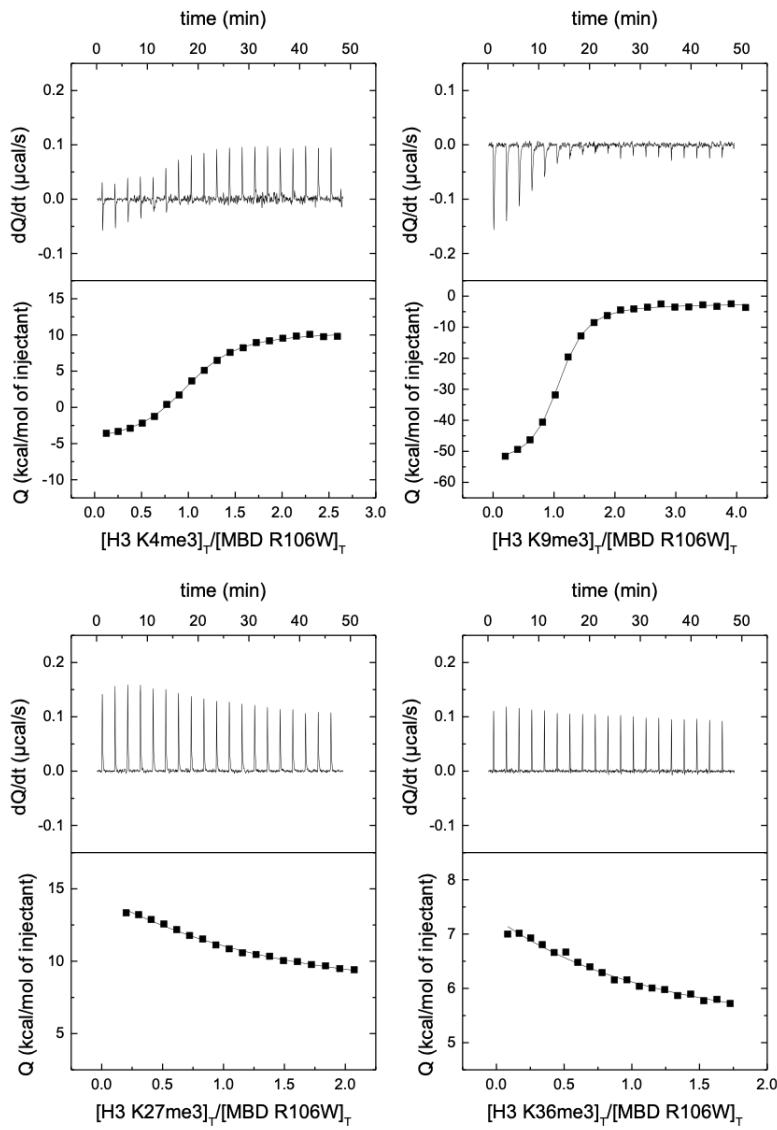
Correspondence may also be addressed to:

Olga Abian, Instituto de Investigación Sanitaria Aragón (IIS Aragon), San Juan Bosco 13, 50009, Zaragoza, Spain, Email: oabifra@unizar.es

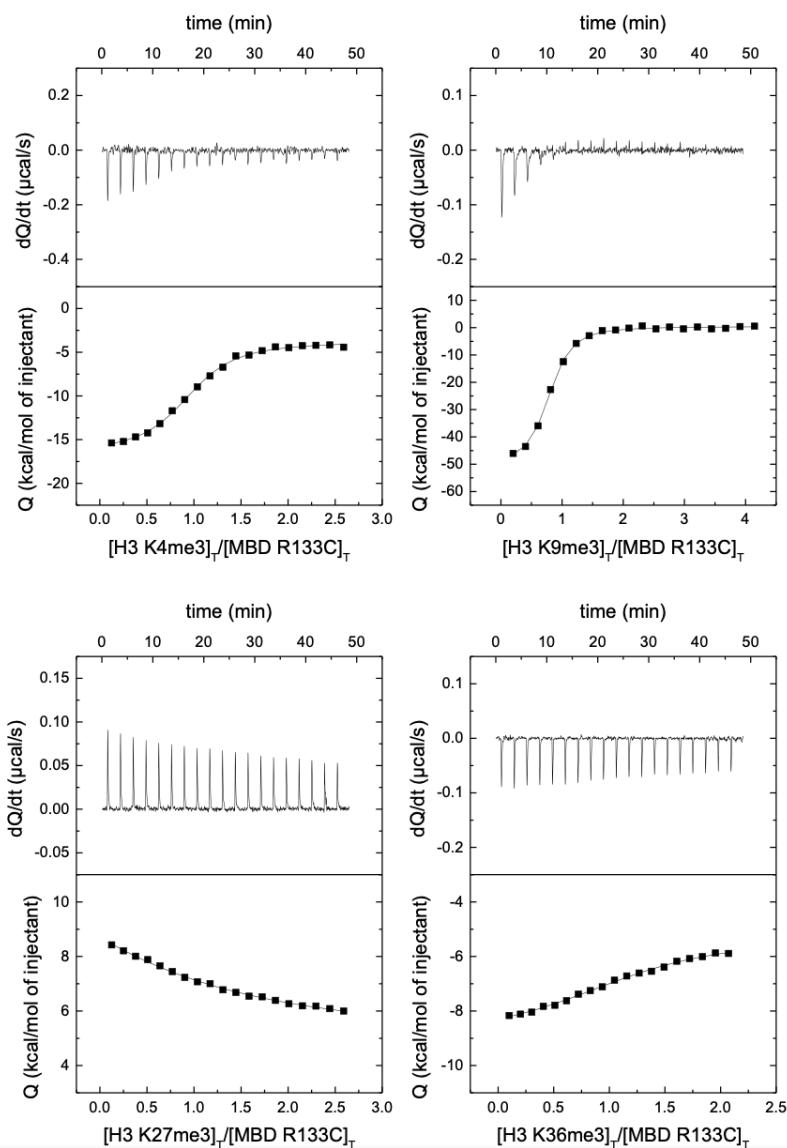
Juan Ausio, University of Victoria, 9882 Ring Rd, BC V8W 2Y2, Victoria, Canada, Email: jausio@uvic.ca



**Figure S1. Trimethylation induces small structural effects on H3.** Far-UV circular dichroism spectra for H3 (black), H3 K27C (orange), and H3 K27me3 (red). The substitution of K2 of a cysteine in K27 position required for the trimethylation procedure did not perturb much the structure of H3, whereas the trimethylation somewhat perturbed the structure of H3.



**Figure S2. MeCP2 R106W interaction with trimethylated H3 by ITC.** Calorimetric titrations of MBD R133C interacting with H3 trimethylated at K4, K9, K27, and K36. The upper panels show the thermograms (thermal power as a function of time to maintain the same temperature in the sample cell with respect to the reference cell), and the lower panels show the binding isotherms (ligand-normalized heat effect per injection as a function of the molar ratio in the sample cell). The continuous lines correspond to the non-linear least-squares fitting according to a single binding site model.



**Figure S3. MeCP2 R133C interaction with trimethylated H3 by ITC.** Calorimetric titrations of MBD R133C interacting with H3 trimethylated at K4, K9, K27, and K36. The upper panels show the thermograms (thermal power as a function of time to maintain the same temperature in the sample cell with respect to the reference cell), and the lower panels show the binding isotherms (ligand-normalized heat effect per injection as a function of the molar ratio in the sample cell). The continuous lines correspond to the non-linear least-squares fitting according to a single binding site model.