Supporting Information

Exploring the Conformational and Binding Dynamics of HMGA2•DNA Complexes Using Trapped Ion Mobility Spectrometry – Mass Spectrometry

Kevin Jeanne Dit Fouque,¹ Sarah N. Sipe,² Alyssa Garabedian,¹ German Mejia,¹ Linjia Su,¹ Md Lokman Hossen,³ Prem P. Chapagain,^{3,4} Fenfei Leng,^{1,4} Jennifer S. Brodbelt,² and Francisco Fernandez-Lima^{1,4*}

¹ Department of Chemistry and Biochemistry, Florida International University, Miami, FL 33199, United States.

² Department of Chemistry, University of Texas, Austin, TX 78712 United States.

³ Department of Physics, Florida International University, Miami, FL 33199, United States.

⁴ Biomolecular Sciences Institute, Florida International University, Miami, FL 33199, United States.

Corresponding Author <u>fernandf@fiu.edu</u>

Table of Contents:

Figure S1. TIMS-MS instrument showing the convex electrode TIMS geometry and TIMS operation.

Figure S2. TIMS profiles as a function of the collision activation for the multiply protonated species of the free HMGA2 protein.

Figure S3. Typical native nESI MS profile of the HMGA2•DNA22 complexes with 1:3 excess DNA22 in solution.

Figure S4. TIMS profiles as a function of the collision activation for the multiply protonated species of the HMGA2•DNA₂₂ and HMGA2•DNA₂₂•HOE complexes.

Figure S5. TIMS profiles as a function of the collision activation for the multiply protonated species of the HMGA₂•DNA₅₀ and HMGA₂•DNA₅₀•HOE complexes.



Trapped Ion Mobility Spectrometry (TIMS)

Figure S1. TIMS-MS instrument showing the convex electrode TIMS geometry and TIMS operation.



Figure S2. TIMS profiles as a function of the collision activation for the multiply protonated species of the free HMGA2 protein (black traces).



Figure S3. Typical native nESI MS profile of the HMGA2•DNA₂₂ complexes with 1:3 excess DNA₂₂ in solution. Notice the absence of the 1:3 stoichiometry when DNA is in excess.



Figure S4. TIMS profiles as a function of the collision activation for the multiply protonated species of the HMGA2•DNA₂₂ (green traces) and HMGA2•DNA₂₂•HOE (purple traces) complexes.



Figure S5. TIMS profiles as a function of the collision activation for the multiply protonated species of the HMGA2•DNA₅₀ (blue traces) and HMGA2•DNA₅₀•HOE (magenta traces) complexes.