# Electronic Supplementary Information

## Metal Ions Provide Structural Stability and Compactness to Tetrameric Purothionin

Swagata Das, Uttam Pal and Nakul Chandra Maiti*

Structural Biology & Bioinformatics Division, CSIR-Indian Institute of Chemical Biology, 4, Raja S.C. Mullick Road, Kolkata 700032, India

***Corresponding author:** Nakul Chandra Maiti. Telephone: +91-33-2499-5940, +91-33-2499-5886; Fax: 12 +91-33-2473-5197. Email: ncmaiti@iicb.res.in

**Fig S1. SDS PAGE of 1mg/ml purothionin solution.**

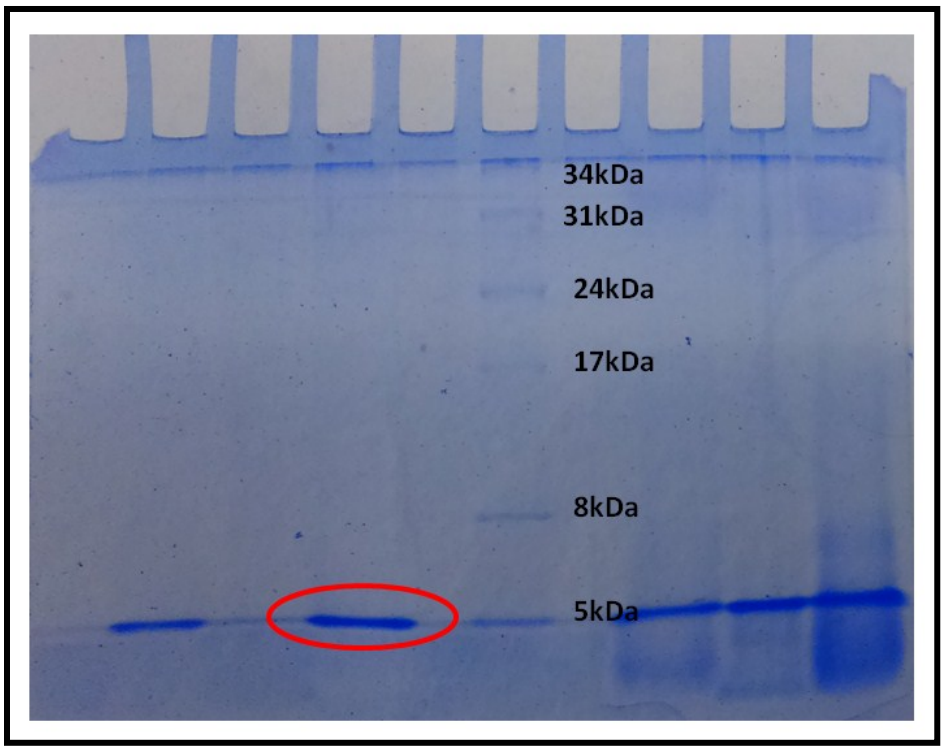

**Fig S2. MALDI TOF Analysis of purothionin.**

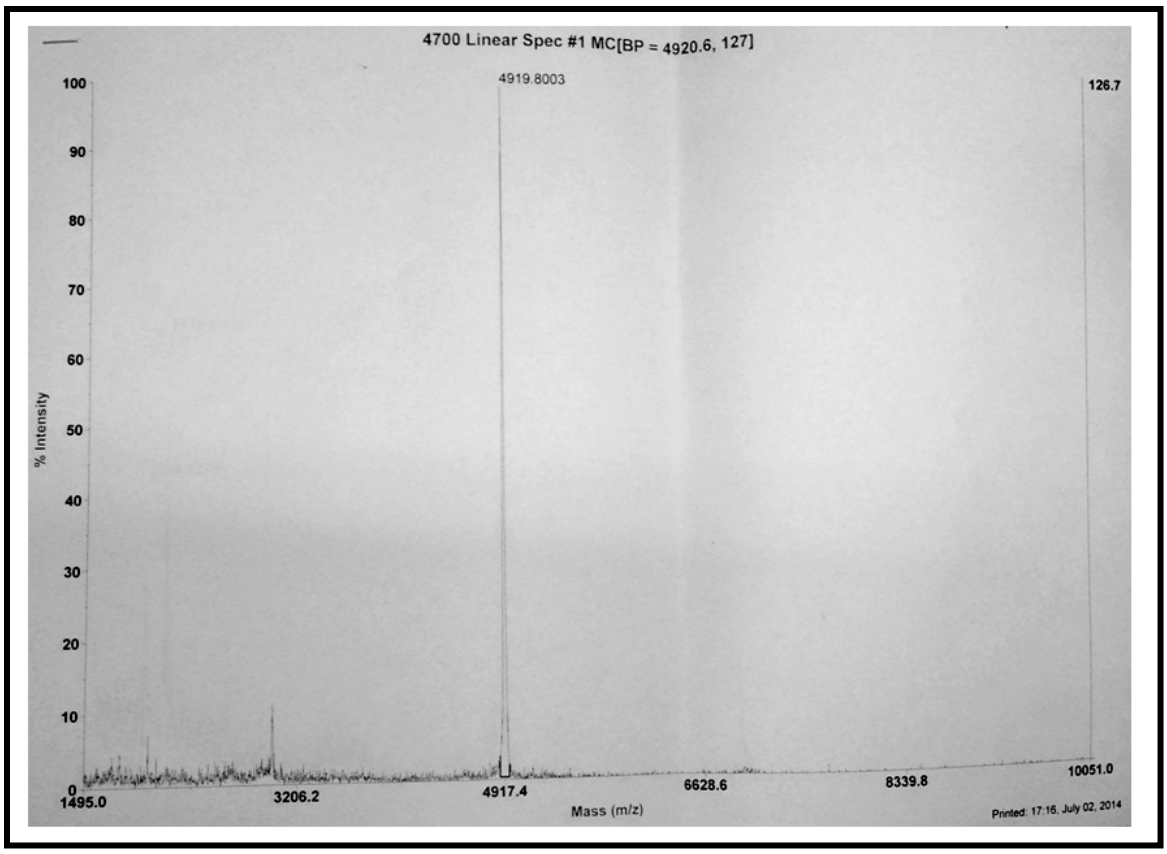

**Fig S3. Changes in the secondary structural components such as coils, turns and sheets w.r.t. to the simulation time scale (left panel) and the residue-wise analyses (right panel) are shown in the absence of ions (first from top) followed by in the presence of $Ca^{2+}$ and $Mg^{2+}$. Green color, in absence of ions; Orange color, in presence of $Ca^{2+}$ and blue color, in presence of $Mg^{2+}$. In the right panel, the four subunits are indicated by the red dotted grid lines.**

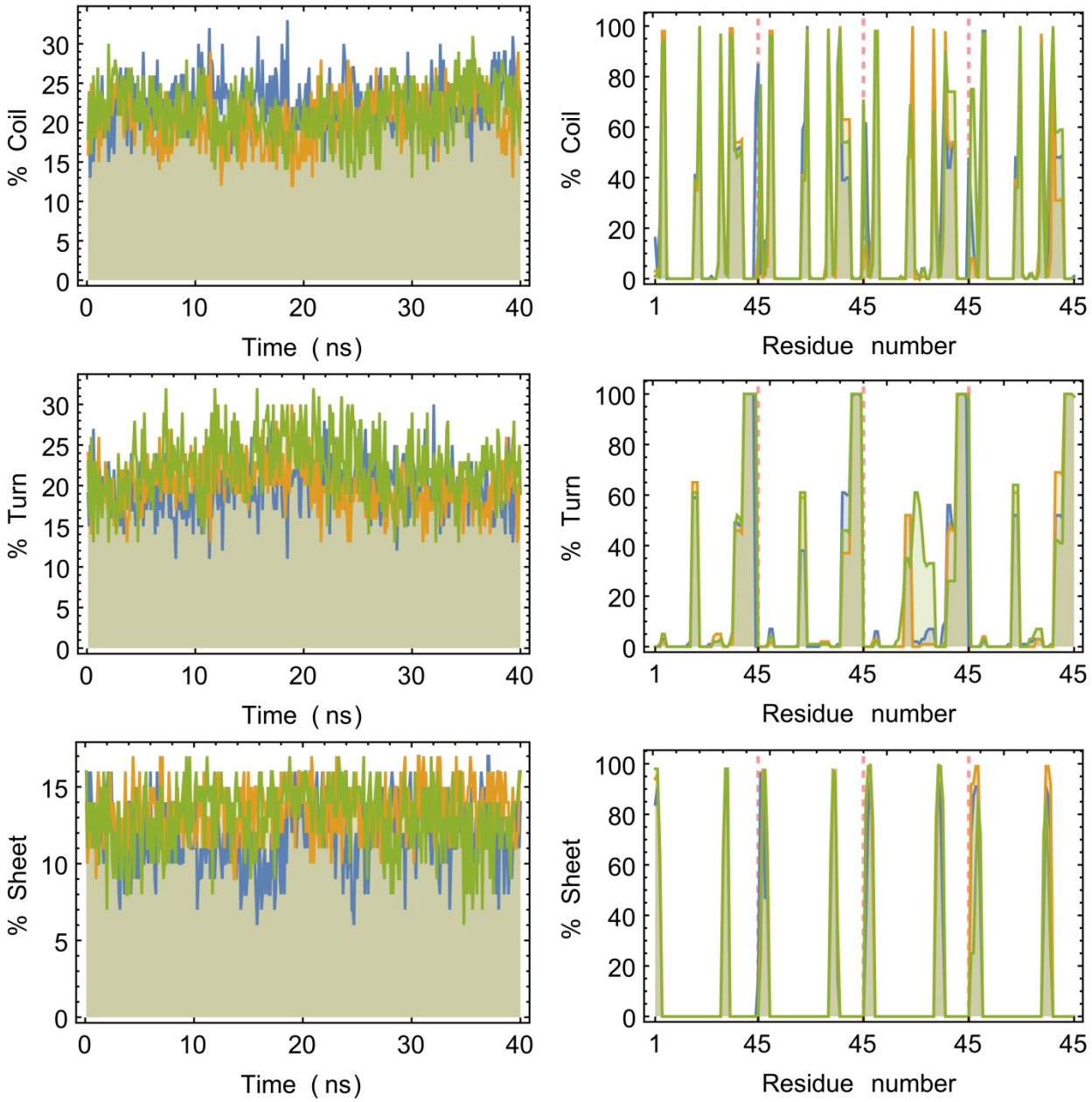

**Fig S4. Solid state FT-IR spectra of purothionin (range 600-2000cm$^{-1}$).**

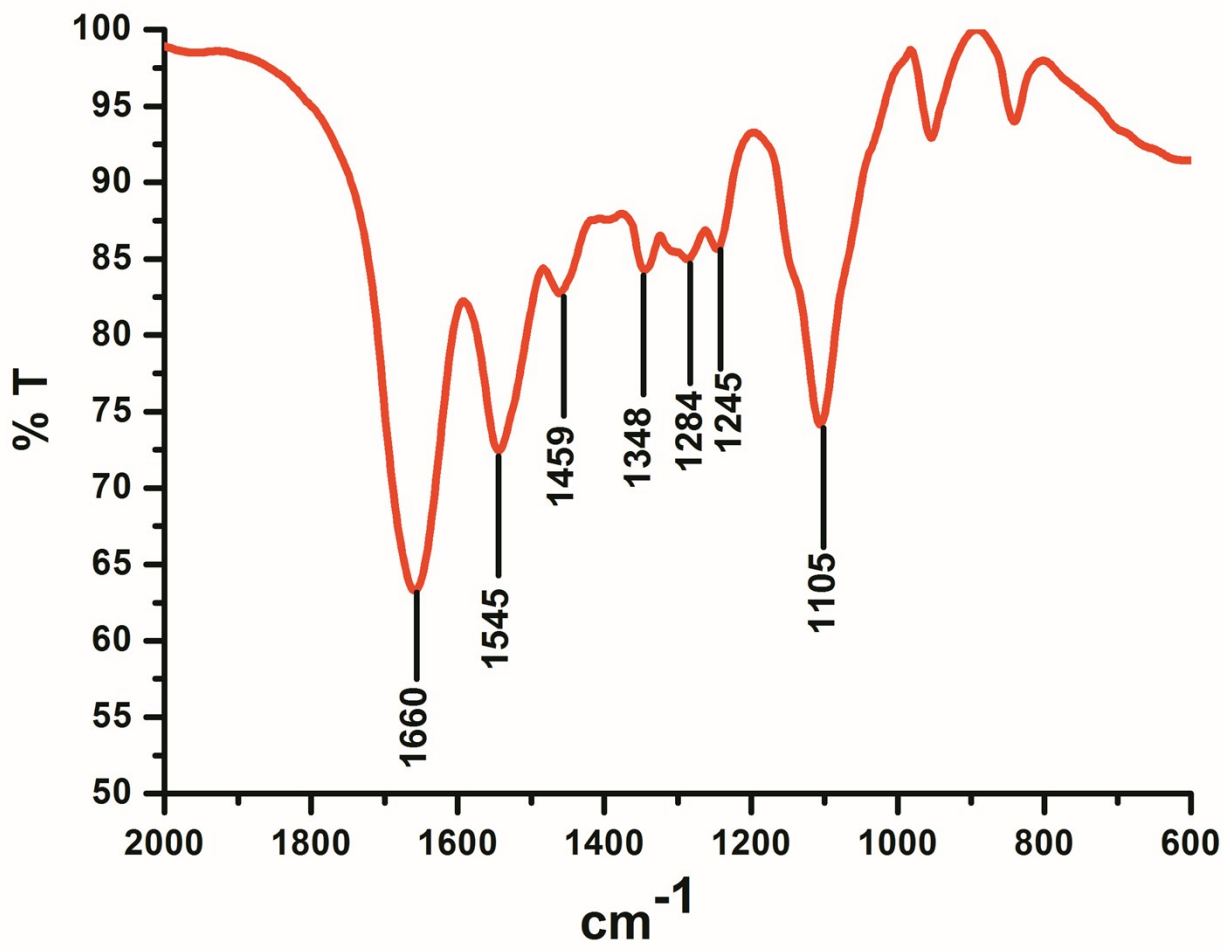

**Fig S5. Solution state FT-IR of purothionin in the presence of buffer (range 600-2000cm$^{-1}$).**

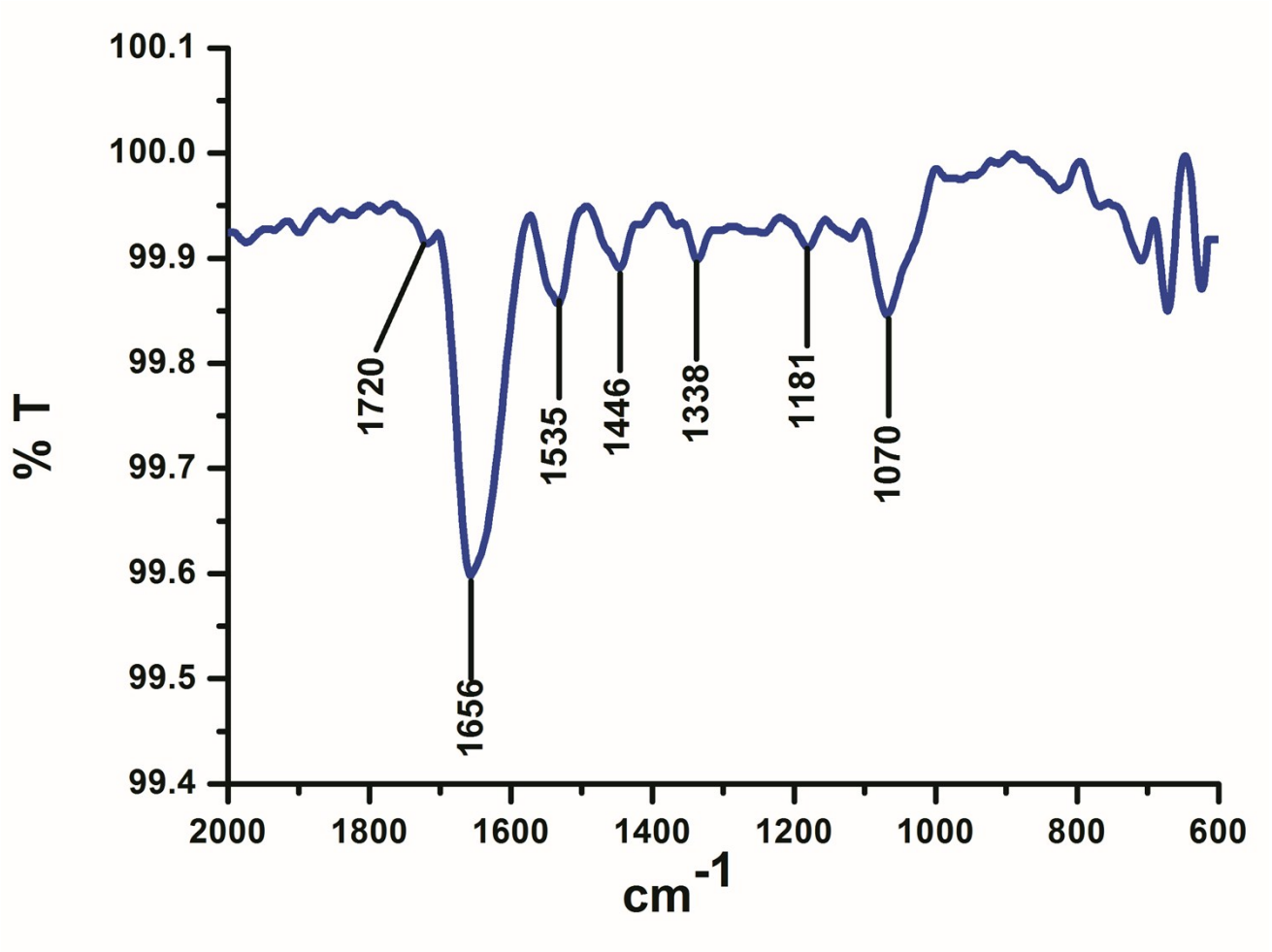

**Fig S6. Solution state FT-IR of purothionin in the presence of $Ca^{2+}$ (range 600-2000$cm^{-1}$).**

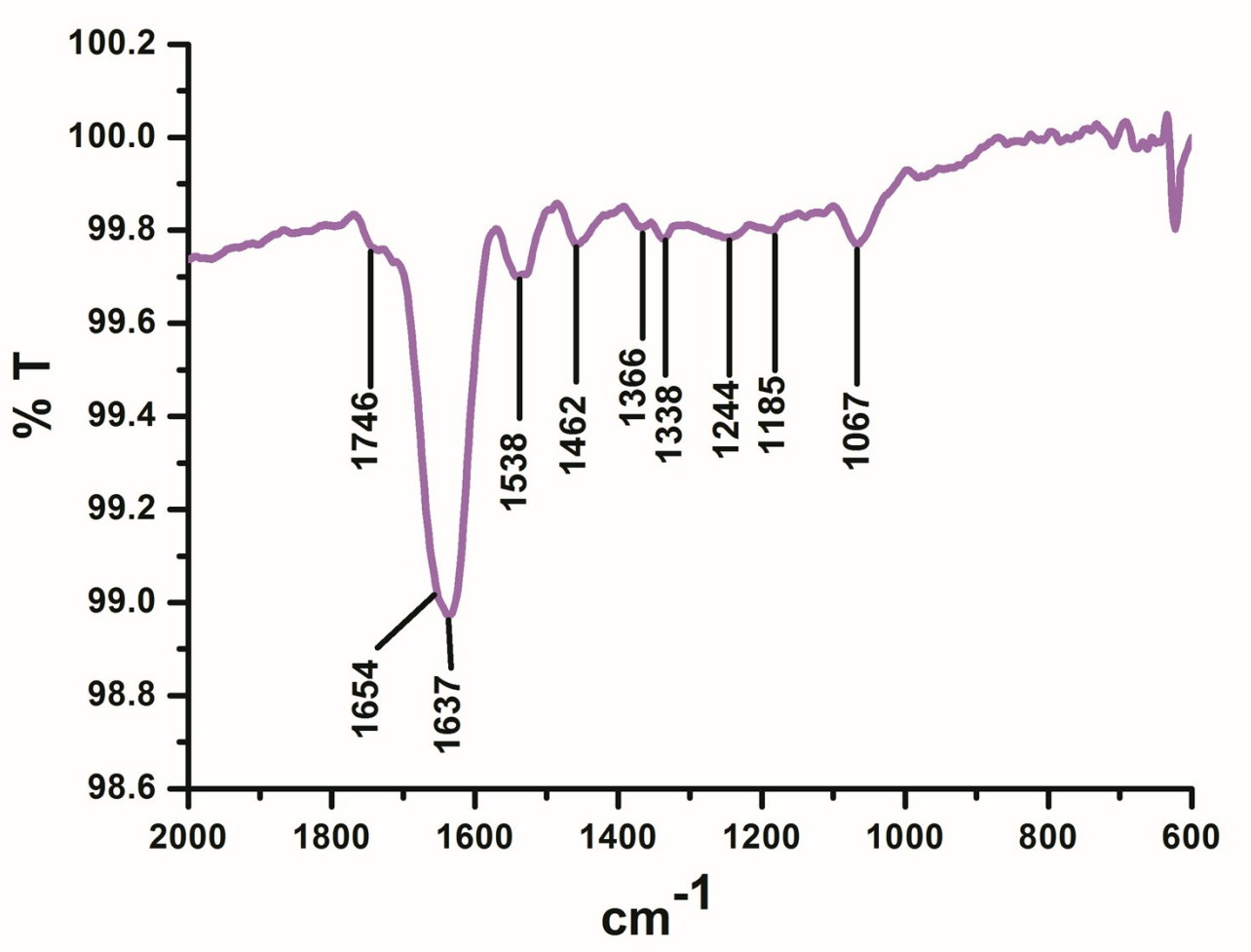

**Fig S7. Solution state FT-IR of purothionin in the presence of $Mg^{2+}$ (range 600-2000$cm^{-1}$).**

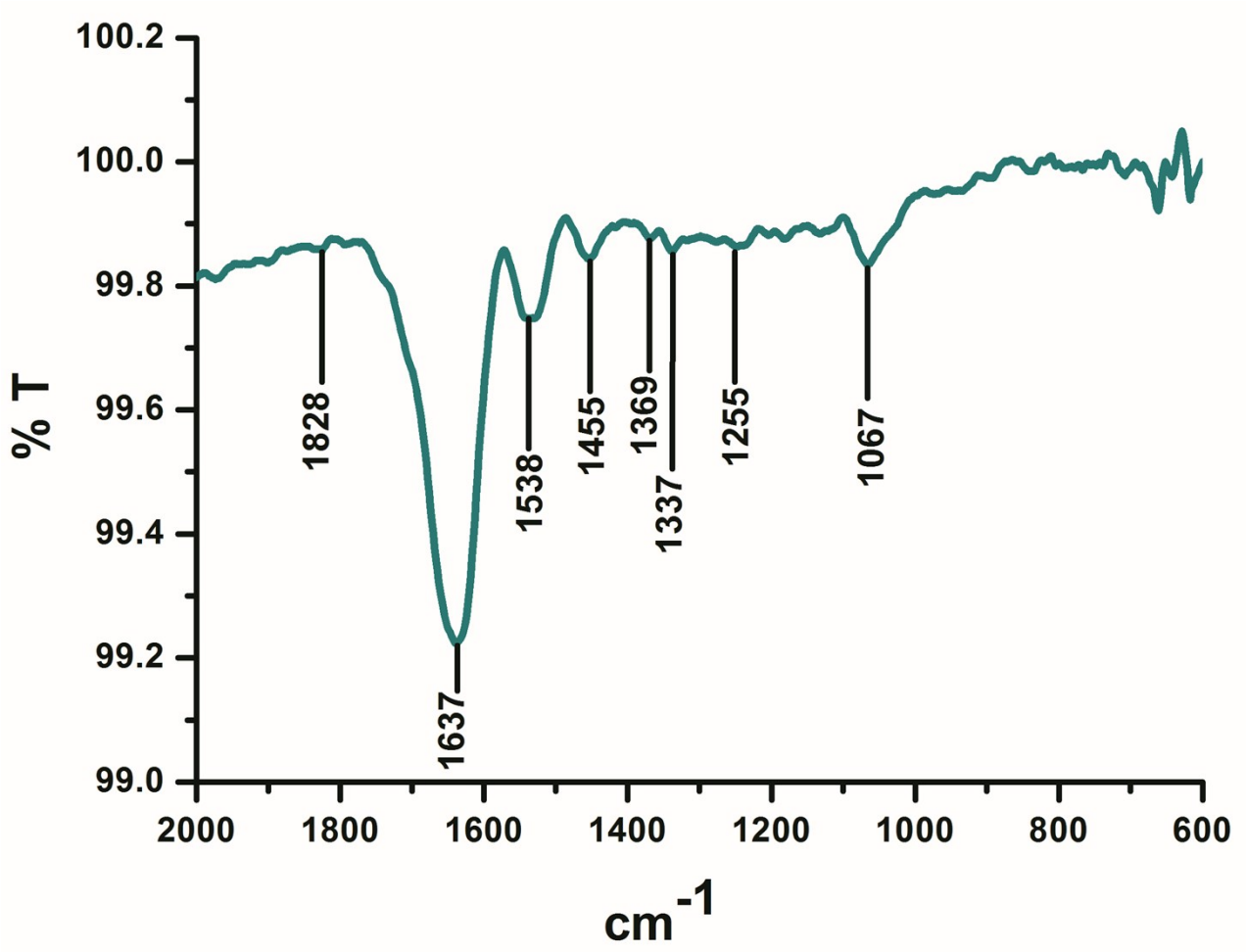

**Table S1. Overall secondary structural components computed over the complete MD trajectories**

| Secondary structural components | No salt | $Ca^{2+}$ | $Mg^{2+}$ |
|---|---|---|---|
| Alpha | 41 | 43 | 43 |
| Coil | 22 | 23 | 21 |
| Turn | 22 | 20 | 20 |
| Beta | 13 | 12 | 14 |
| Others ($3_{10}$ helix etc.) | 2 | 2 | 2 |