

1 **Supplementary materials**

2 **Fig. S1** Secondary structure prediction by PSI-PRED **A)** mNalp3-NACHT domain, **B)** mNalp3-
3 LRR domain. Representation of helix, b-sheets and loops are shown in the legend. Amino acid
4 numbers depicted in the figure represents numbers 216-532 (mNalp3-NACHT) and 739-988
5 (mNalp3-LRR) in mouse Nalp3 protein

6 **Fig. S2** Secondary structure assignment as a function of MD simulation time. **A)** mNalp3-
7 NACHT domain, **B)** mNalp3-LRR domain. Legends of different structural elements are
8 presented. Amino acid numbers depicted in the figure represents numbers 216-532 (mNalp3-
9 NACHT) and 739-988 (mNalp3-LRR) in mouse Nalp3 protein

10 **Fig. S3** Validation reports of mNalp3-NACHT and LRR models by Ramachandran plot and
11 ProSA analysis

12 **Fig. S4** Secondary structure assignments of **A)** mNalp3-NACHT and **B)** LRR domains from their
13 3D-models by ProFunc program. Representation of secondary structural elements are given at
14 the right hand bottom corner

15 **Video**

16 The separation of walker A and B forming a wider space during the MD simulation was presented
17 in the video. The walker A and B regions were highlighted with dotted representation in VMD
18 program.

