Supporting Information

Allosteric Mechanism of Human Mitochondrial Phenylalanyl-

tRNA Synthetase: an Atomistic MD Simulation and Mutual

Information-based Network Study

Qi Shao[†], Zhongjie Han[†], Jingmin Cheng, Qiankun Wang, Weikang Gong, Chunhua Li^{*}

Faculty of Environmental and Life Sciences, Beijing University of Technology, Beijing 100124, China.

The authors state no conflict of interest.

[†]Qi Shao and Zhongjie Han contribute equally to this work.

*Correspondence to Chunhua Li. E-mail: chunhuali@bjut.edu.cn

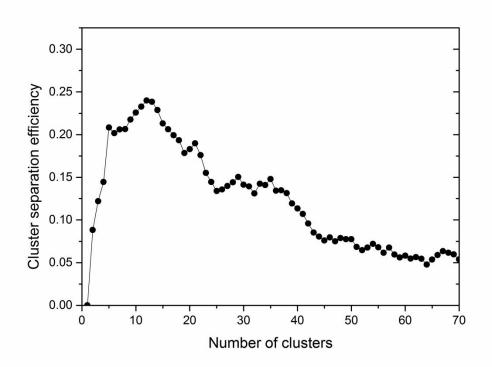


Figure S1. Change of the cluster separation efficiency (*SE*) as a function of the number of clusters.

No.	Amount
1	134
2	108
3	81
4	43
5	43
6	30
7	28
8	16
9	8
10	5
11	5
12	4

Table S1. Number of allosteric pathways in each cluster when 12 clusters are selected.