

# Revealing Allosteric Mechanism of Amino Acid Binding Proteins from Open to Closed State

Quanshan Shi <sup>1,2,3,†</sup>, Ling Liu <sup>1,2,†</sup>, Huaichuan Duan <sup>3,†</sup>, Yu Jiang <sup>2</sup>, Wenqin Luo <sup>2</sup>, Guangzhou Sun <sup>2,3</sup>, Yutong Ge <sup>2</sup>, Li Liang <sup>2</sup>, Wei Liu <sup>2</sup>, Hubing Shi <sup>3</sup> and Jianping Hu <sup>2,\*</sup>

- <sup>1</sup> Department of Thoracic Oncology, Affiliated Cancer Hospital, Guizhou Medical University, Guiyang 550025, China; sqs\_715@163.com (Q.S.); yzh2602023@163.com (L.L.)
- <sup>2</sup> Key Laboratory of Medicinal and Edible Plants Resources Development of Sichuan Education Department, School of Pharmacy, Chengdu University, Chengdu 610106, China; jy94940514@163.com (Y.J.); m13568453654@163.com (W.L.); s19196482291@163.com (G.S.); 13111153368@163.com (Y.G.); liangli\_cdu@163.com (L.L.); liuwe@cdu.edu.cn (W.L.)
- <sup>3</sup> Laboratory of Integrative Medicine, Clinical Research Center for Breast, State Key Laboratory of Biotherapy, West China Hospital, Sichuan University and Collaborative Innovation Center, Chengdu 610041, China; sumdhc@163.com (H.D.); shihb@scu.edu.cn (H.S.)
- \* Correspondence: hjpcdu@163.com
- † These authors contributed equally to this work.

**Table S1.** The shortest pathway of crucial residues to I-Loop in the AABPs-open and AABPs-closed systems.

Systems	Possible shortest pathways		
<b>GlnBP-open</b>	(1) D10→Y123→V154→V176→G171→A96; G68→Y123→V154→V176→G171→A96; (4) <b>K115→Y143→N170→G171→A96</b> ; (5) G119→L155→G177→G171→A96; (6) D157→V154→V176→G171→A96	(2) A67→L180→G177→G171→A96;	(3)
<b>HisJ-open</b>	(1) D11→K201→Q79→Q141→D149→V114→I102; L52→Q79→Q141→D149→V114→I102; (4) S69→E202→D53→Q79→Q141→D149→V114→I102; (5) <b>L117→Q79→Q141→D149→V114→I102</b>	(2) Y14→Q79→Q141→D149→V114→I102;	(3)
<b>LAOBP-open</b>	(1) D11→D32→K44→C45→K62→D91→A96→E123→K98; S70→S184→K188→D75→N129→E123→K98 (4) S72→S184→K188→D75→N129→E123→K98; <b>L117→R93→E123→A96→K98</b>	(2) F52→A96→E123→K98;	(3)
<b>GlnB-closed</b>	(1) D10→K125→T130→K110→V104→V176→A96; (2) A67→A126→T130→K110→V104→V176→A96 (3) G68→A126→T130→K110→V104→V176→A96; (4) <b>K115→T130→K110→G171→V176→A96</b> (5) G119→K129→K110→G171→V176→A96; (6) D157→T130→K110→G171→V176→A96		
<b>HisJ-closed</b>	(1) D11→C38→Q44→T43→P57→Q79→K189→K186→P104→E107→G134→F159→I102 (2) Y14→G168→E162→P183→T105→E107→G134→F159→I102; L52→R77→K189→K186→P104→E107→G134→F159→I102 (4) S69→C38→Q44→T43→P57→Q79→K189→K186→P104→E107→G134→F159→I102; <b>L117→R93→P104→E107→G134→F159→I102</b>		(3)
<b>LAOBP-closed</b>	(1) D11→G34→G9→I27→K229→K225→D232→K176→K98; (2) F52→I8→I27→K229→K225→D232→K176→K98; (3) <b>L117→Q78→K189→E177→K98</b> ; (4) S70→K60→D21→Y223→Q219→D232→K176→K98; (5) S72→A66→I27→K229→K225→D232→K176→K98; (6) R77→D75→K189→E177→K98		