Biophysical Journal, Volume 96

**Supporting Material**

# Functional and Structural Characterization of Factor Xa Dimer In Solution

Rima Chattopadhyay, Roxana Iacob, Shalmali Sen, Rinku Majumder, Kenneth B. Tomer, and Barry R. Lentz

**Supplemental Material**

Table S1

| **Residue changes 3 mM $Ca^{+2}$ to 3 mM $Ca^{+2}$ + C6PS** | **Residue changes 5 mM $Ca^{+2}$ to 5 mM $Ca^{+2}$ + C6PS** | **Residue changes due to dimerization** |
|---|---|---|
| 9 → 9 | 9 → 9 | |
| 62 → 62 | 62 → 62 | |
| 79 → 79 | 79 → 79 | |
| 242 → 242 (62) | 242 → 242 | |
| 270 → 270 (90) | 270 → 270 | 270 |
| 276 → 276 (96) | 276 → 276 | |
| 289 → 289 (109) | 289 → 289 | |
| 317 → 317 (134) | 317 → 317 | |
| 330 → 330 (147) | 330 → 330 | |
| 338 → 338 (156) | 338 → 338 | |
| 351 → 351 (169) | 351 → 351 | |
| 388 → 388 (204) | 388 → 388 | |
| 406 → 406 (223) | 406 → 406 | |
| 408 → 408 (224) | 408 → 408 | |
| 414 → 414 (230) | 414 → 414 | 414 |
| 420 → 420 (236) | 420 → 420 | |
| 427 → 427 (243) | 427 → 427 | |

Table S2

| **Residue changes 3 mM $Ca^{+2}$ TO mM 5 $Ca^{+2}$** | **Residue changes 3 mM $Ca^{+2}$ + C6PS TO 5 mM $Ca^{+2}$ + C6PS** | **Residue changes due to dimerization** |
|---|---|---|
| **9 → 9** | **9 → 9** | |
| **62 → 62** | **62 → 62** | |
| **7 9 → 79** | **7 9 → 79** | |
| **242 → 242 (62)** | **242 → 242** | |
| **270 → 270 (90)** | **270 → 270** | **270** |
| **276 → 276 (96)** | **221 → 221** | |
| **289 → 289 (109)** | **289 → 289** | |
| **317 → 317 (134)** | **317 → 317** | |
| **330 → 330 (147)** | **330 → 330** | |
| **338 → 338 (156)** | **338 → 338** | |
| **351 → 351 (169)** | **351 → 351** | |
| **388 → 388 (204)** | **388 → 388** | |
| **406 → 406 (223)** | **406 → 406** | |
| **408 → 408 (224)** | **408 → 408** | |
| **414 → 414 (230)** | **414 → 414** | **414** |
| **420 → 420 (236)** | **420 → 420** | |
| **427 → 427 (243)** | **427 → 427** | |

**Table S: Change in Lys residues upon addition of C6PS and Calcium determined from Lys acetylation followed by mass spectrometry.** S1) Columns 1 and 2 show Lys residues that change upon addition of C6PS at 3 mM and 5 mM $Ca^{+2}$, respectively, S2) Columns 1 and 2 show Lys residues that change upon increase from 3 mM to 5 mM $Ca^{+2}$ in the absence and presence of 400 μM C6PS, respectively. Blue = residues accessible to both acetylation and enzymatic digestion, Green = residues not accessible to acetylation but observed after enzymatic digestion, Red = residues not observed at all. Numberings of the Lysine residues are according to Fung et al., Proceedings of the National Academy of Sciences, 1985, 82, 3591-3595. Parenthesis shows the chymotrypsin numbering for the amino acid residues in the catalytic domain. In Pedersen model Fung Numbering system is followed.