Supporting Information for

Probing Structural Features of Alzheimer's β-Amyloid Pores in Bilayers Using Site-Specific Amino Acid Substitutions

Ricardo Capone,[1,] Hyunbum Jang,[2,*] Samuel A. Kotler,[1,*] Bruce L. Kagan,[3] Ruth Nussinov,[2,4,#] and Ratnesh Lal[1,#]*

[1]Departments of Bioengineering and of Mechanical and Aerospace Engineering and Material Science Program, University of California, San Diego, La Jolla, CA 92093, USA

[2]Center for Cancer Research Nanobiology Program, SAIC-Frederick, Inc., NCI-Frederick, Frederick, MD 21702, USA

[3]Department of Psychiatry, David Geffen School of Medicine, Semel Institute for Neuroscience & Human Behavior,University of California, Los Angeles, CA 90024, USA

[4]Department of Human Molecular Genetics and Biochemistry, Sackler School of Medicine, Tel Aviv University, Tel Aviv 69978, Israel

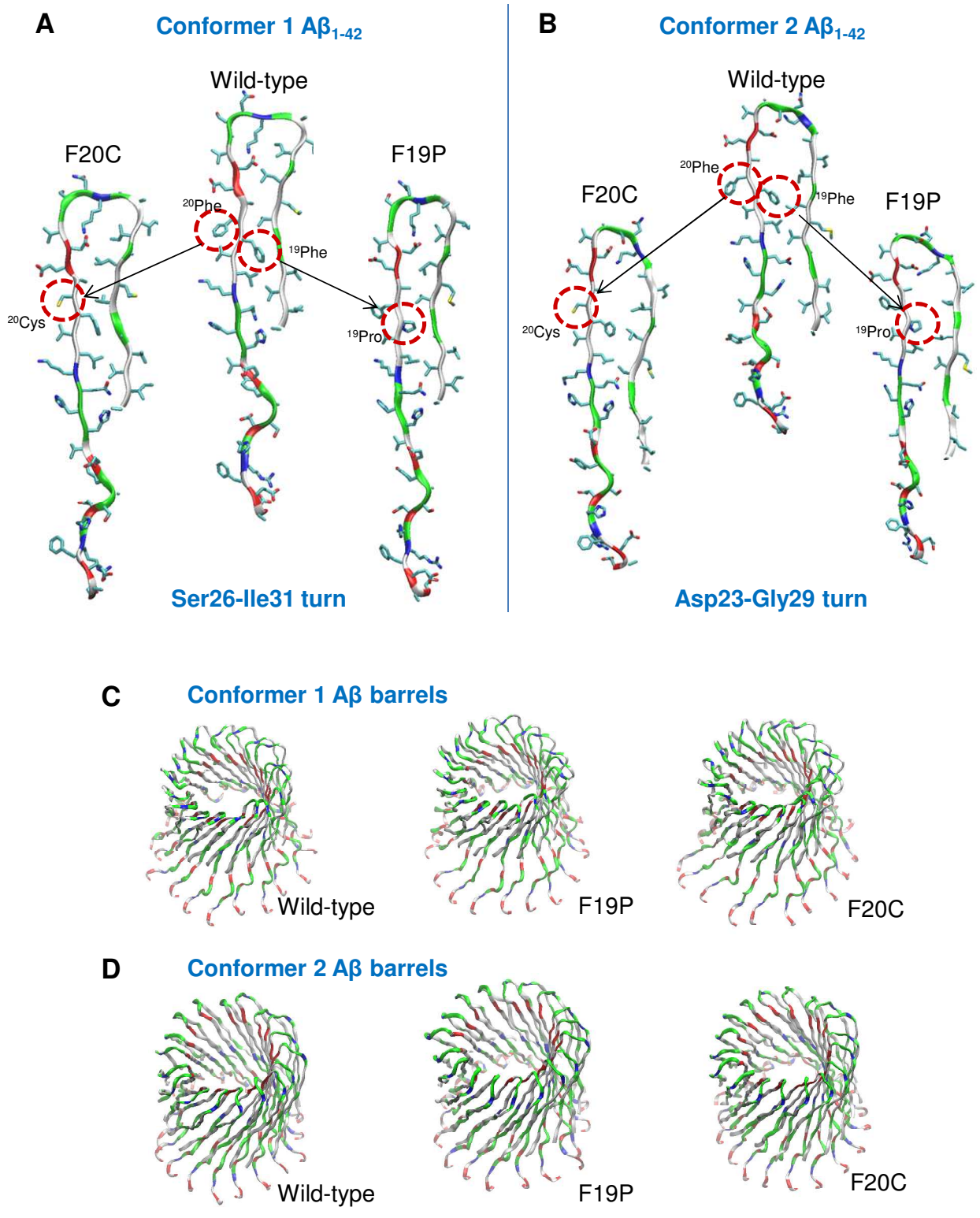

Figure S1. Monomer conformations of $A\beta_{1-42}$ wild-type, F19P and F20C mutants with different turns at (A) Ser26-Ile31 (conformer 1) and (B) Asp23-Gly29 (conformer 2). The angle views

without lipid for the starting points of MD simulations for (C) conformer 1 and (D) conformer 2 $A\beta_{1\text{-}42}$ barrels with two different mutants. In the peptide ribbon, hydrophobic residues are shown in white, polar and Gly residues are shown in green, positively charged residues are shown in blue, and negatively charged residues are shown in red.

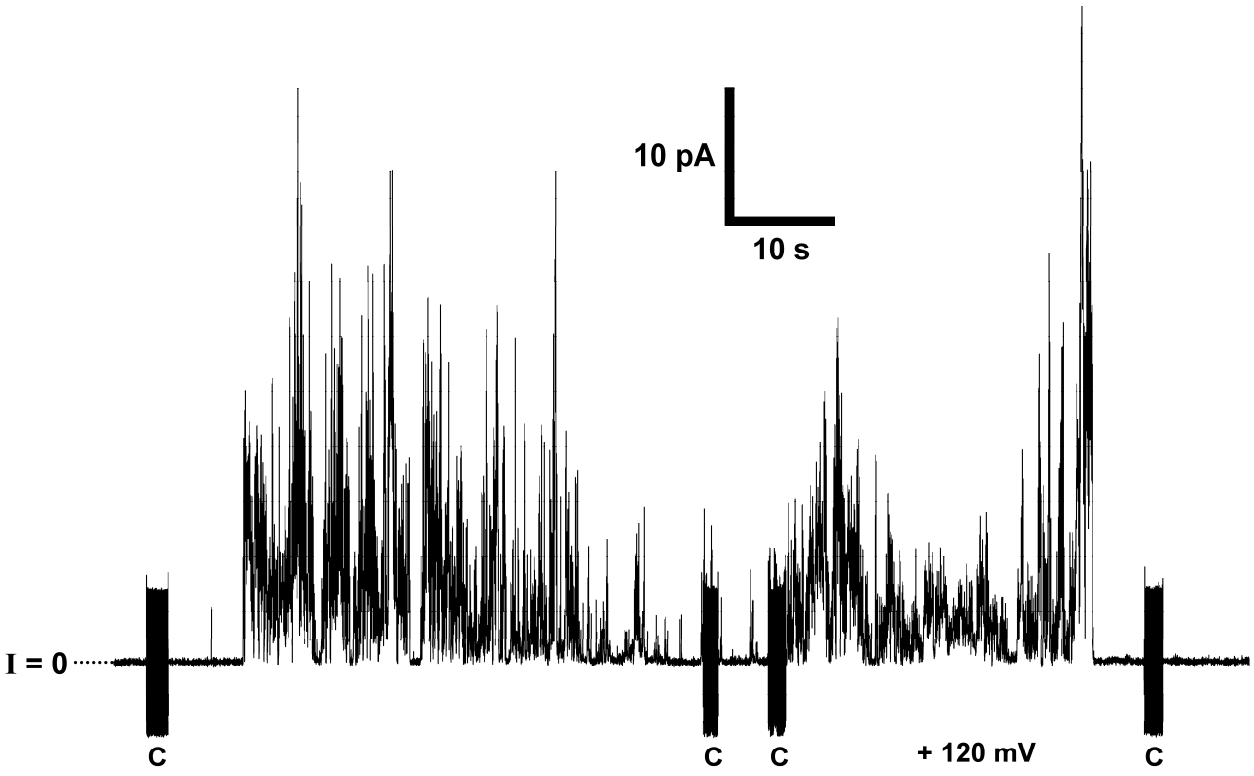

Figure S2. Current vs. time trace of channel-like activity of $A\beta_{1-42}$ F20C mutant. Channels formed by F20C predominantly exhibited spiky and bursting activity with conductance as high as 420 pS; however, there are well defined channel openings and closings noticeable among the bursts. The vertical lines marked with **C** indicate capacitance measurements during the recording. Electrolyte solution used contained 150 mM KCl, 10 mM Hepes pH 7.4, and 1 mM $MgCl_2$. The bilayer was composed of 1:1 $^{w}/_{w}$ DOPS:DOPE.