Supplementary information

Supplementary Materials and methods

Molecular dynamics simulations followed a semi-isotropic NPT ensemble with a time step of 20fs. All systems were initially prepared using CHARMM-GUI web-based interface (Jo et al., 2008). The temperature was set at T=303.15K (Wu et al., 2014) and controlled by a V-rescale thermostat (Bussi et al., 2007) using a coupling constant of 1ps. The pressure was set at 1.0bar with a compressibility of to 3x10−4 bar−1, using the Parrinello-Rahman barostat (Parrinello and Rahman, 1981) with a 12ps time constant. Neighbor search used the Verlet cut-off scheme with a buffer tolerance of 0.005kJ/mol/ps and a 20 step update-frequency of the neighbor list. Periodic Boundary Conditions were used in all directions. Coulomb interactions used the reaction field method with a cut-off of 1.1nm. Van der Waals interactions used the cut-off scheme set to 1.1 nm.

Supplementary Figure legends

**Legend to Figure S1: (A)** FITC-PSA staining of SLO-permeabilized sperm. Gallery showing acrosomal staining of human sperm that have (asterisks) or have not (the rest) undergone AE. Shown are six representative fields.

**(B)** Dumbbell plot of the percentages of AE from 30 representative samples used for indirect AE assay experiments. The y-axis shows the sample number and the x-axis shows percentages of AE, with the dumbbell plot connecting the values from the basal control (open circles) to stimulated with calcium (positive control, closed circles) within a sample.

**Legend to Figure S2: specificity controls.** SLO permeabilized human sperm were treated for 15 min at 37 °C in the presence of 7.5 nM nonimmune rabbit IgG, 27.8 mM imidazole (the concentration present in purified 20 nM α-synuclein), 7.5 nM anti-α-synuclein antibodies-pretreated (anti-α-synuclein + α-synuclein) or not with 20 nM α-synuclein, 7.5 nM anti-complexin I/II antibodies (anti-cpx) or 20 nM α-synuclein before challenging with 0.5 mM CaCl2 for an additional 15 min. Treatment with 20 nM α-synuclein alone was also tested. Cells were fixed and acrosomal exocytosis was evaluated by FITC-PSA binding (indirect method). The data represent the mean ± SEM of at least three independent experiments. Different letters indicate statistical significance (p<0.001).

References

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Ref Type: Generic

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