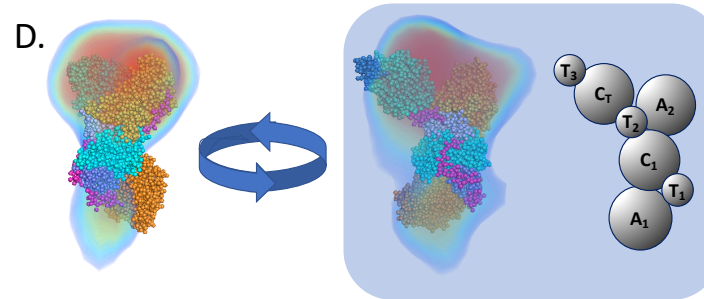
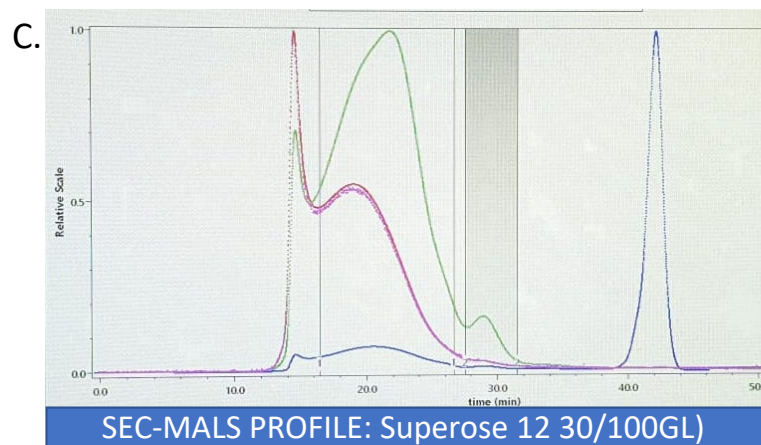
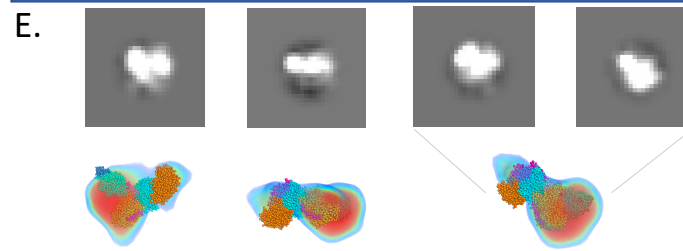


M.D. Simulation overlay with SAXS envelope



Preliminary 2D Classification from ns-EM



**A. Purification of GliP** Final stock of 236kDa GliP on 10% SDS-PAGE, (right) chromatography profile from SEC with Superdex200

**B. GliP Domain Architecture and Reaction** GliP catalyzes the diketopiperazine scaffold for Gliotoxin

**C. SEC-MALS Profile for GliP** Illustrates equilibrium of oligomeric states, small green monomer peak highlighted

**D. Molecular Dynamics Model for GliP** overlaid with envelope from SAXS Red represents region of domain flexibility for execution of catalysis

**E. 2D Classification with RELION** ns-EM imaging with 120keV Tecnai TEM at Max Planck Florida Institute. 1000 particles were. picked manually from 50 micrographs. (bottom) Comparison of representative class averages with *in silico* model from MD and SAXS envelope