

# Predicting spectra of solutions

Use with utilities~calculate X-ray absorption parameters (SF) to ESTIMATE visibility of spectral features in aqueous solution, and from that, estimate the solution concentration and water thickness to target in sample preparation.

## Utilities~Calculate concentration

Aqueous solution concentration calculator

Update concentration      Update solute thickness

Concentration (mol/L)      Solute thickness (nm)      Solute density (g/cc)

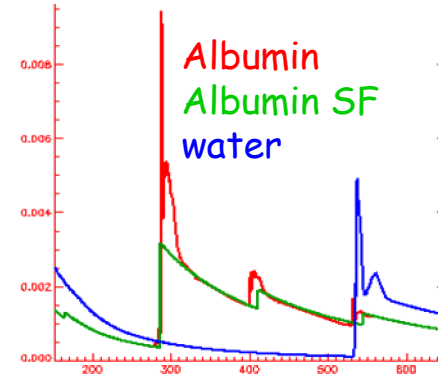
0.00300000      =      80.6008      ×      1.2

Dismiss      64480.67      ×      500.00

Solute molecular weight (g/mol)      Water thickness (nm)

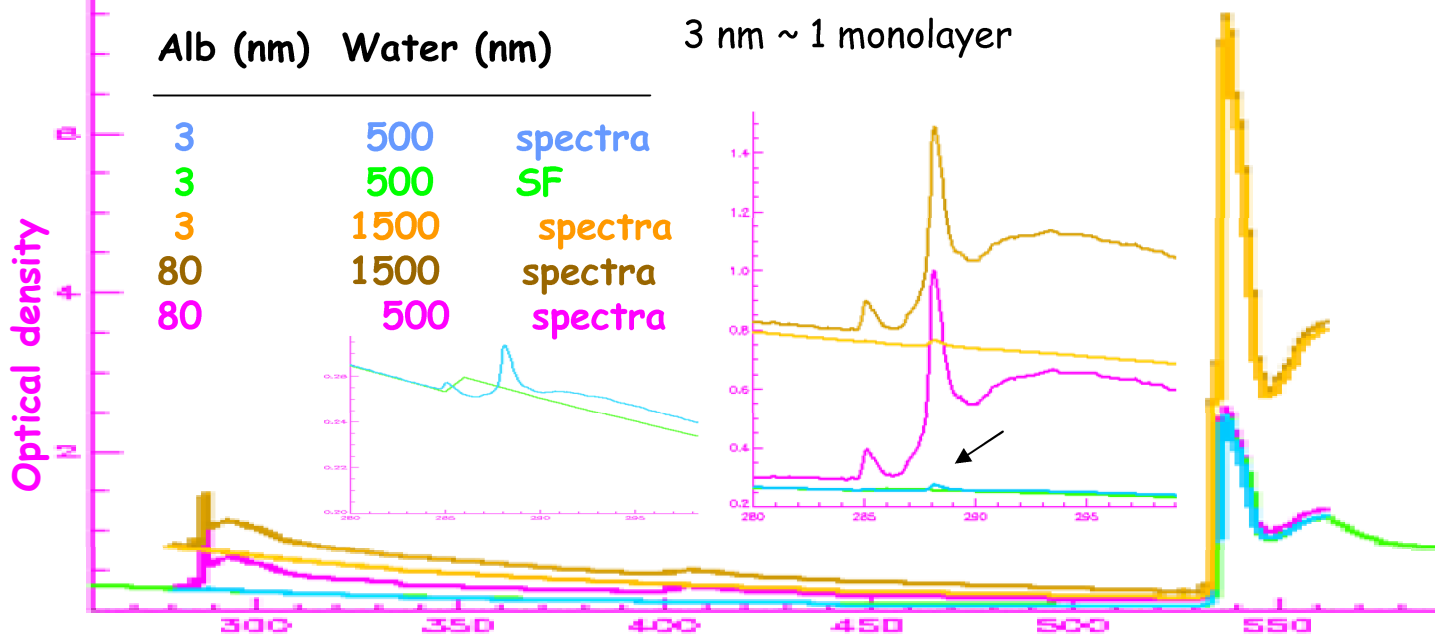
Molecular weightcalculator

## OD1 reference spectra



User enters solute Mol. weight, density, water thickness  
 enter solute thickness → update concentration  
 enter concentration → update solute thickness

**EXAMPLE** - can STXM measure 1 mL of protein in water ?  
 alb is human serum albumin



Data files: water-liq-od1-long.txt    alb-cno-od1.txt    alb-sf-od1.txt