X-ray Standing Wave Investigation of Lipid Layers

Data evaluation software for X-ray standing waves investigation of element-specific density profiles in biomembranes

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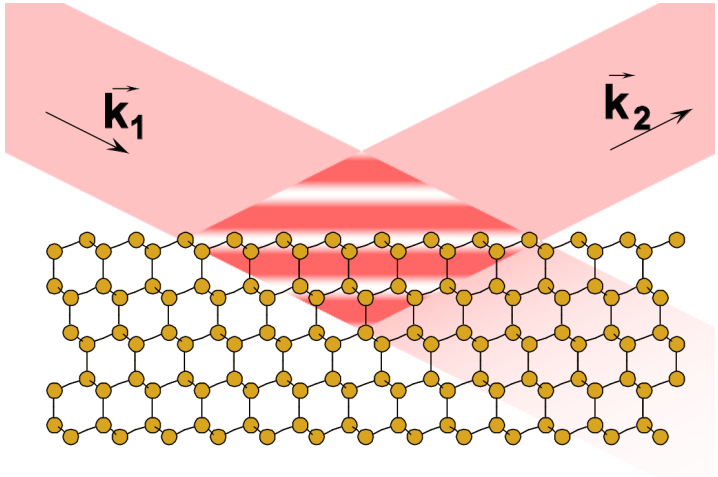
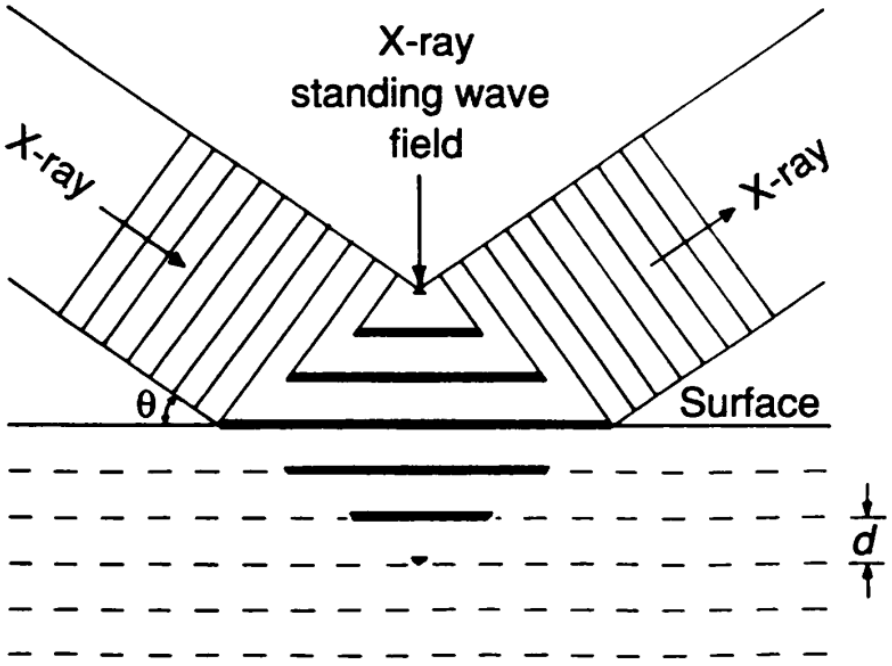
HELMHOLTZ ASSOCIATION

DESY

X-ray standing wave

- X rays (monochromatic, collimated)
- Periodic structure
- Bragg reflection





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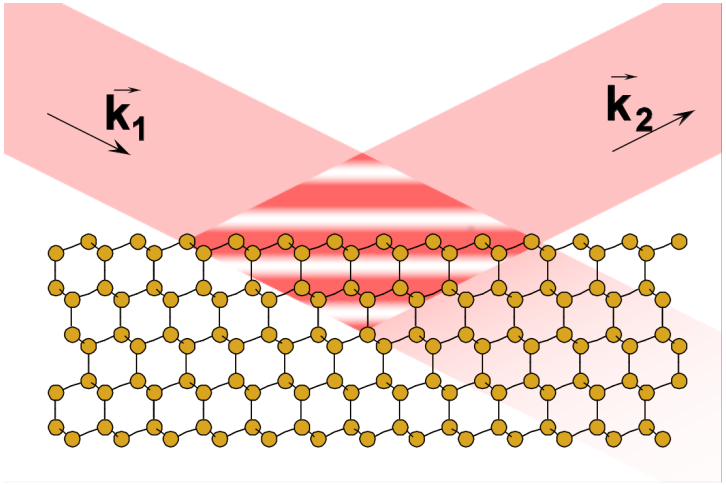
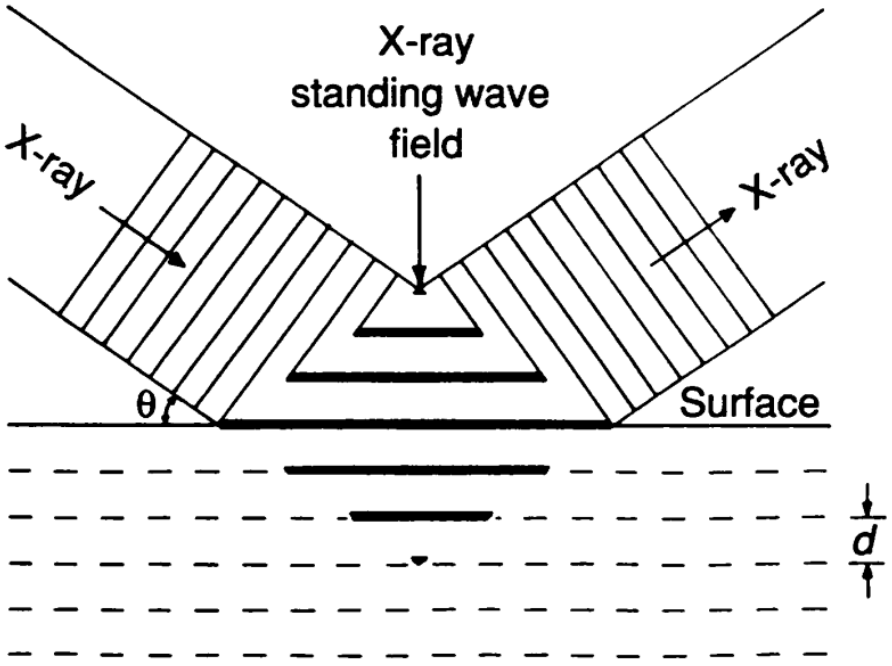
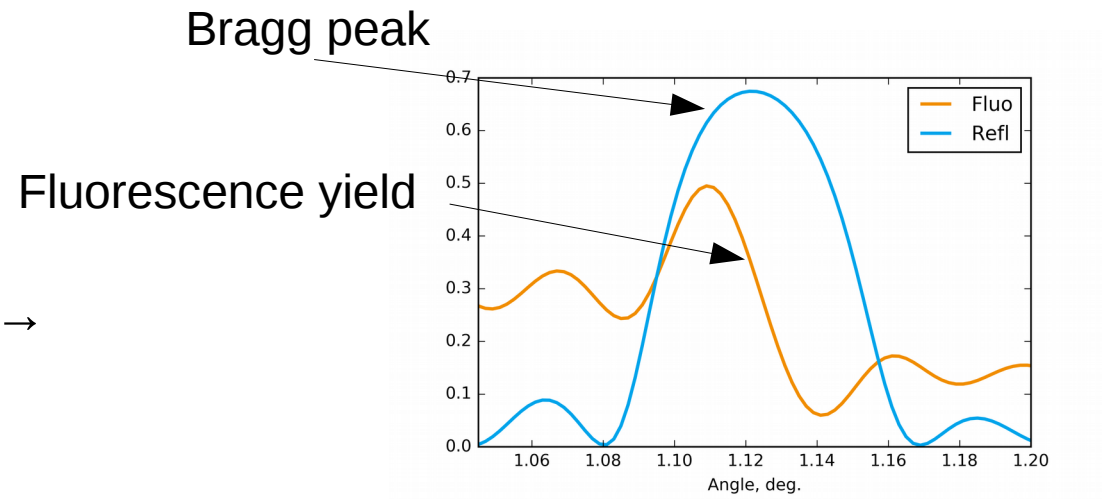
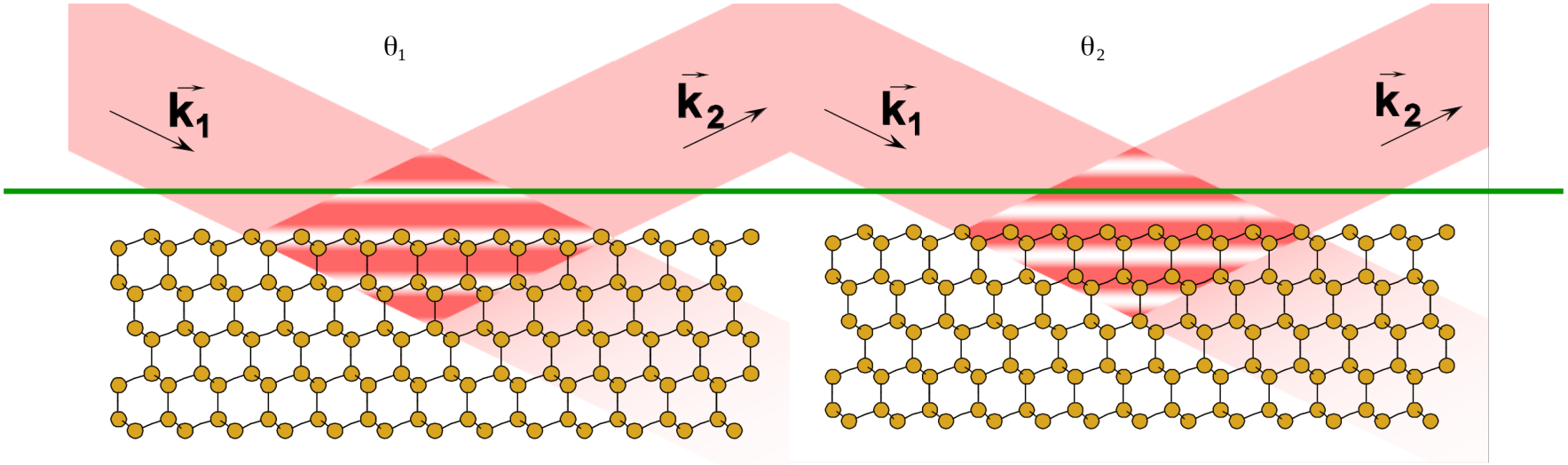




X-ray standing wave fluorescence

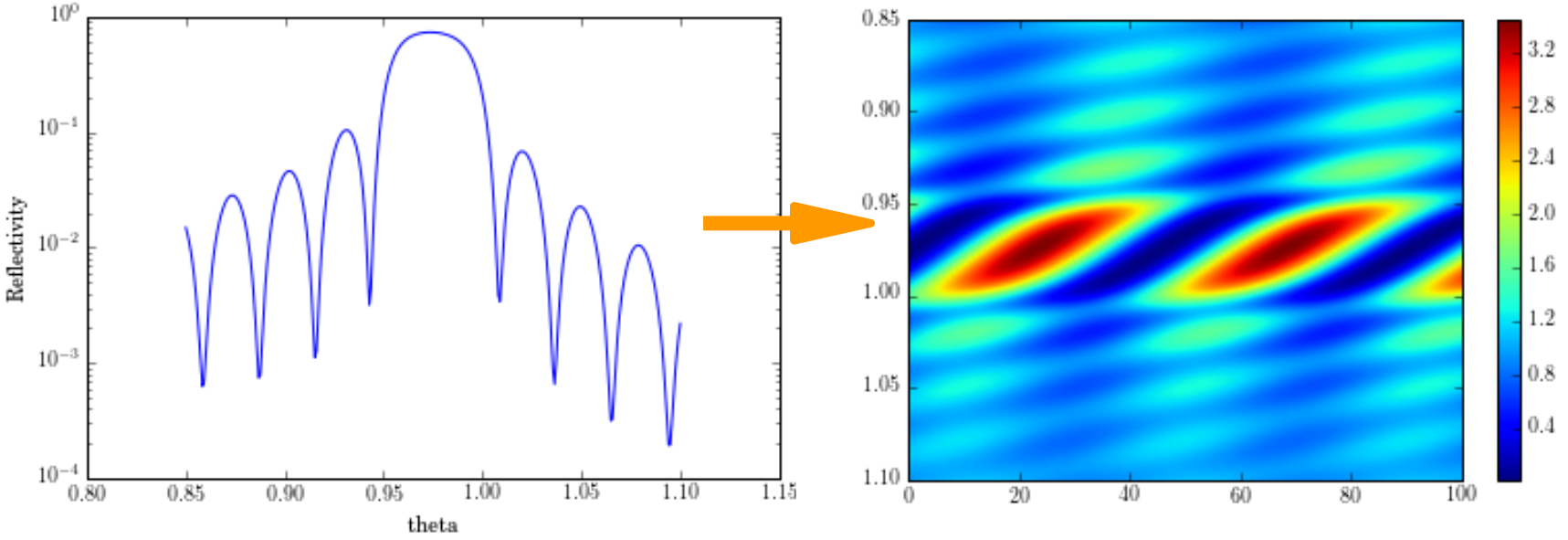
- Incident wave excites fluorescence
- Different peaks in fluorescence spectrum → chemical selectivity





We do know the standing wave!

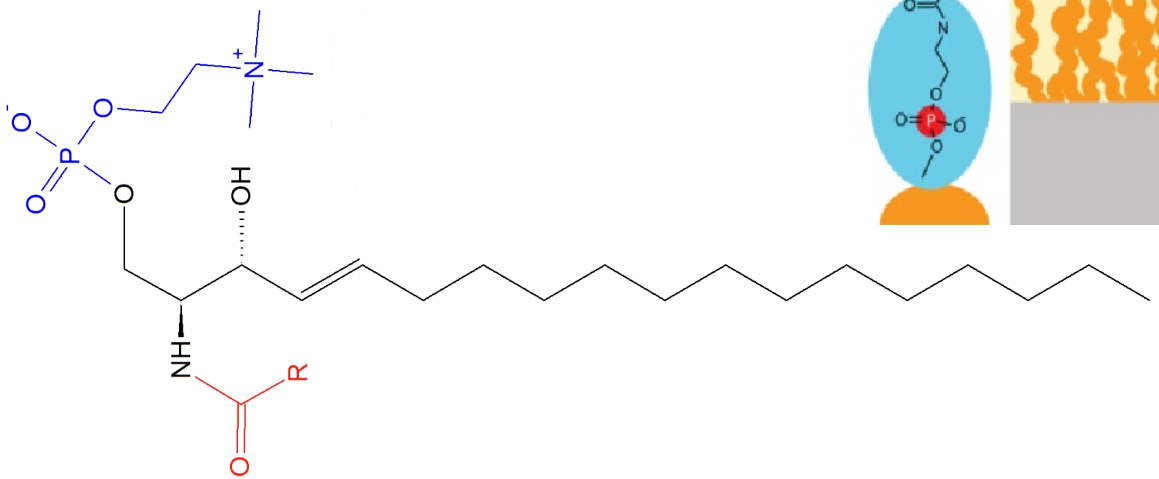
- Reflectivity measurements → ML characteristics
- ML characteristics → standing wave
- 2D-landscape: angle + coordinate

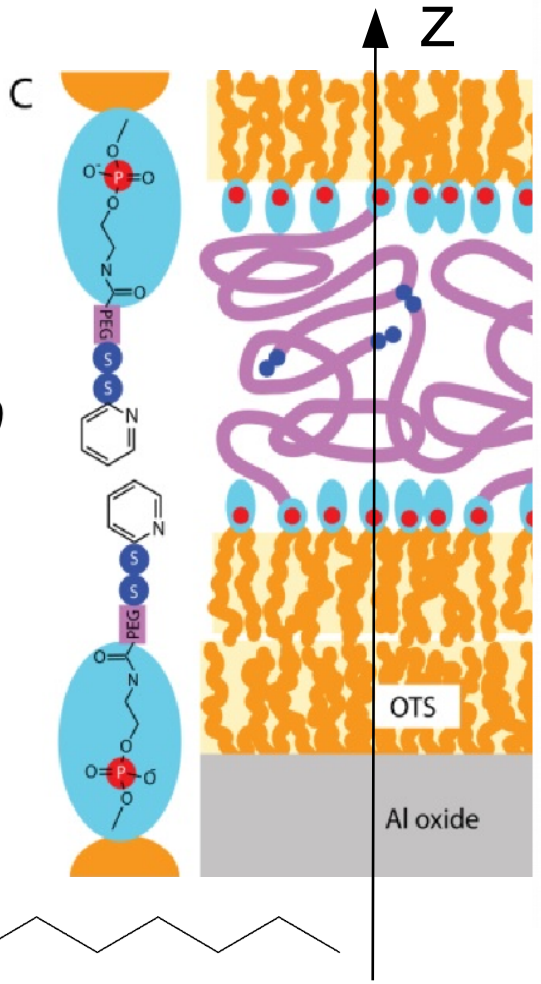


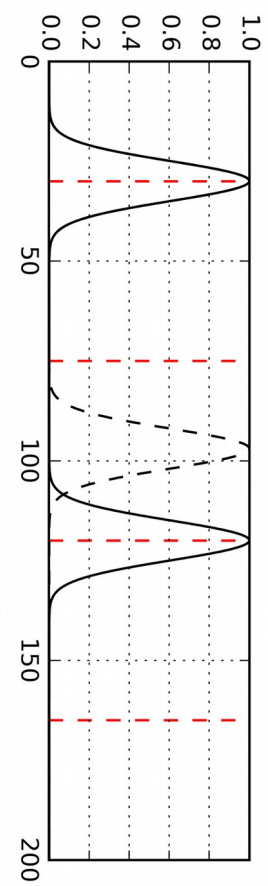
Sample: lipid bilayers

- Chemistry: H, C, N, O, P, S
- Mono- or bilayer → gaussian model

$$\rho(z,\theta) = c \cdot \exp\left(-\frac{(z-z_0)^2}{2\sigma^2}\right) + k\theta$$







Model fluorescence yield curve

- Known standing wave + model distribution = model curve
- Complex model → non-linear least-squares fitting

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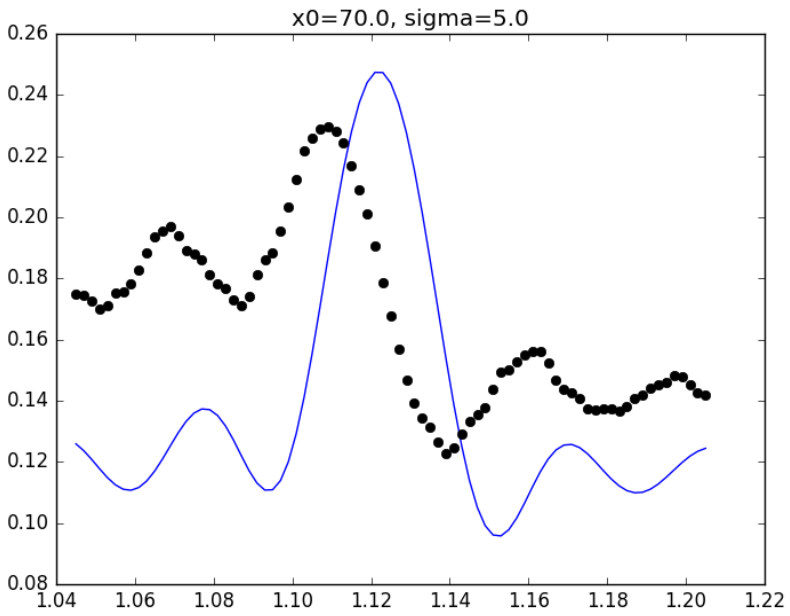
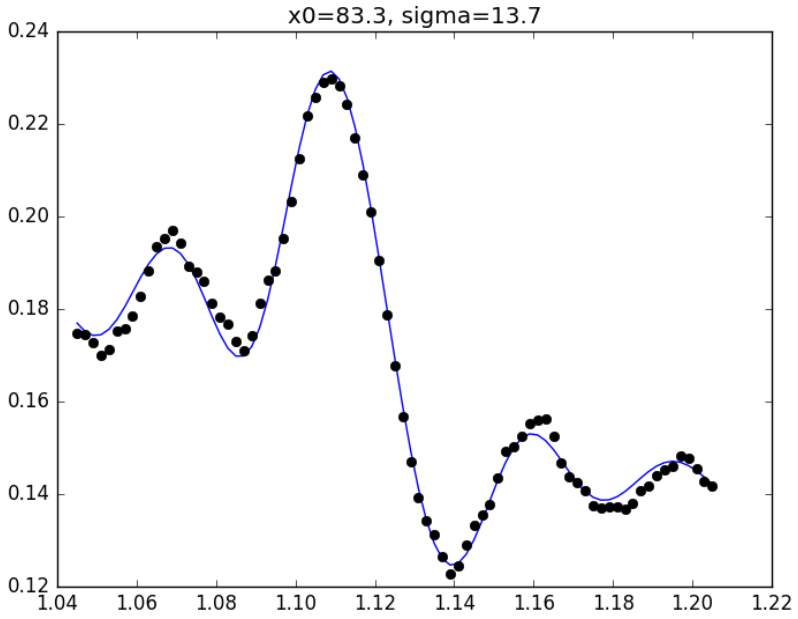
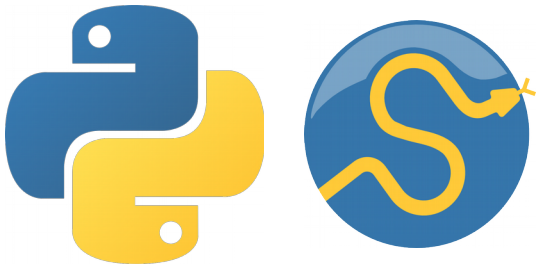




Software: Python 2, 3 + least-squares fitting

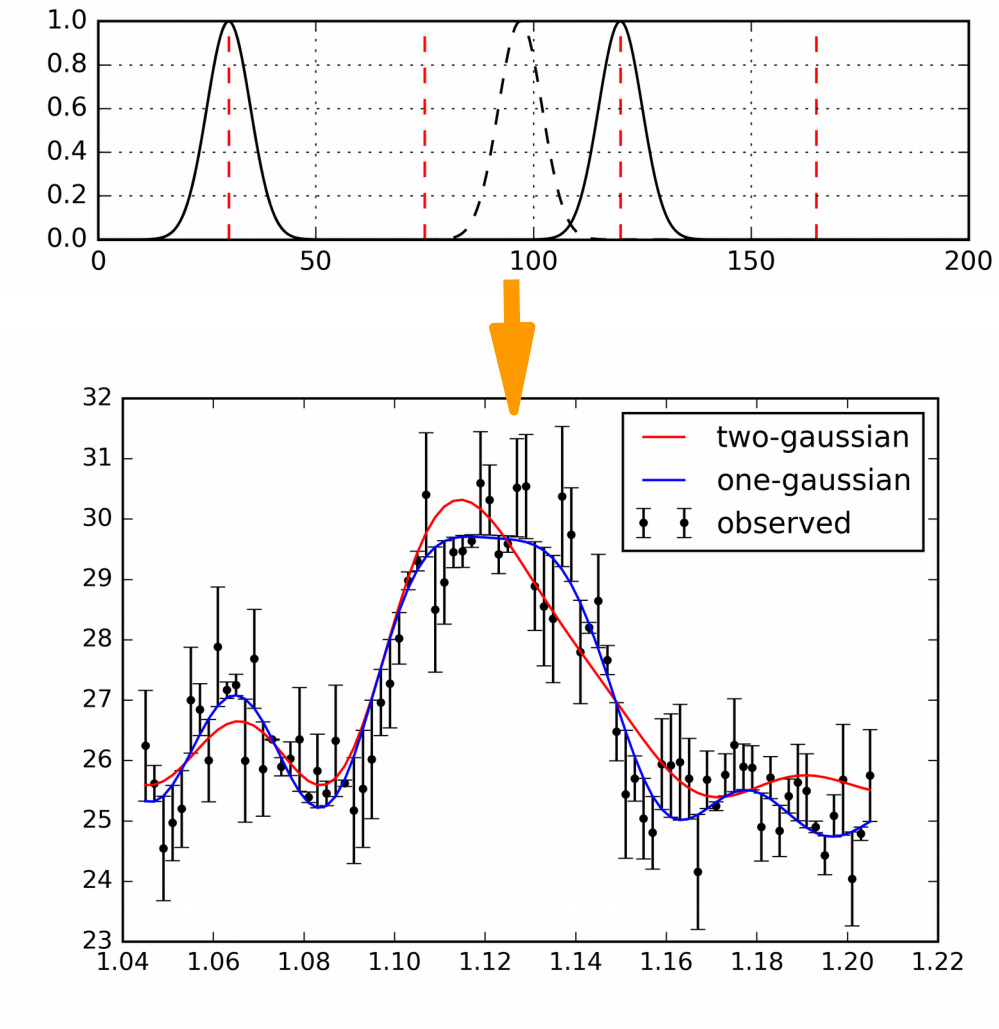
- Levenberg-Marquardt algorithm
- Python: lmfit, scipy.optimize
- Chi-square target function

$$\chi^2 = \frac{1}{L-p} \sum_{\theta_{min}}^{\theta_{max}} \left(\frac{I_{model} - I_{obs}}{\Delta_{obs}} \right)$$

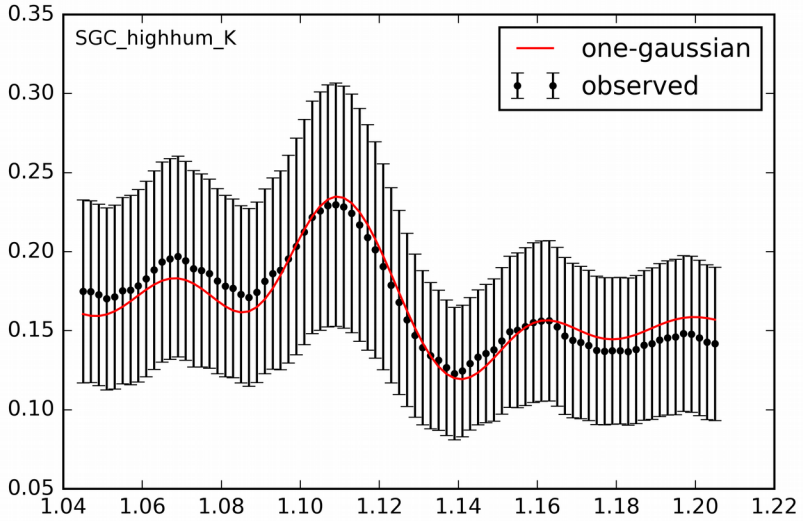


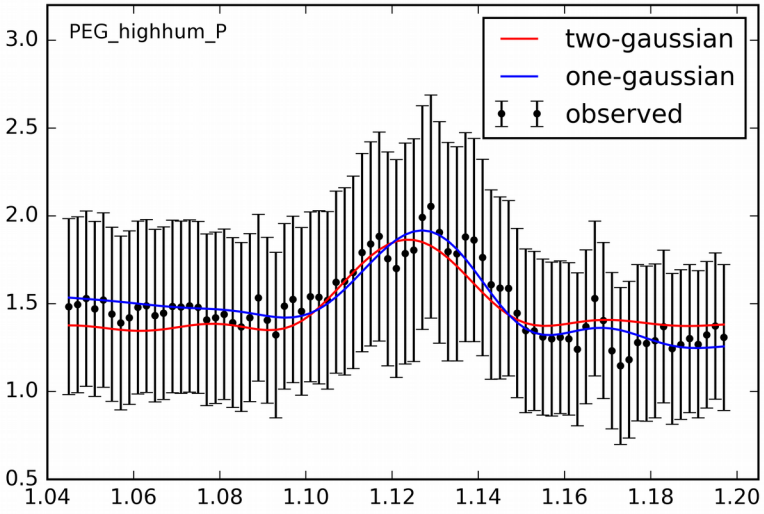
Model fluorescence yield curve: bimodal distribution

- Lipid bilayers → bimodal distribution
- Fitting algorithm reliably detects bimodal case



Real experimental data (ESRF ID10)





Dataset	$z_{0,fit}$	σ_{fit}	χ^2	R
SGC_highhum_K	36	8.0	0.026	0.046
PEG_highhum_P, 2-fit	23, 96	8.7, 9.4	0.028	0.043
PEG_highhum_P, 1-fit	60	13.0	0.030	0.046

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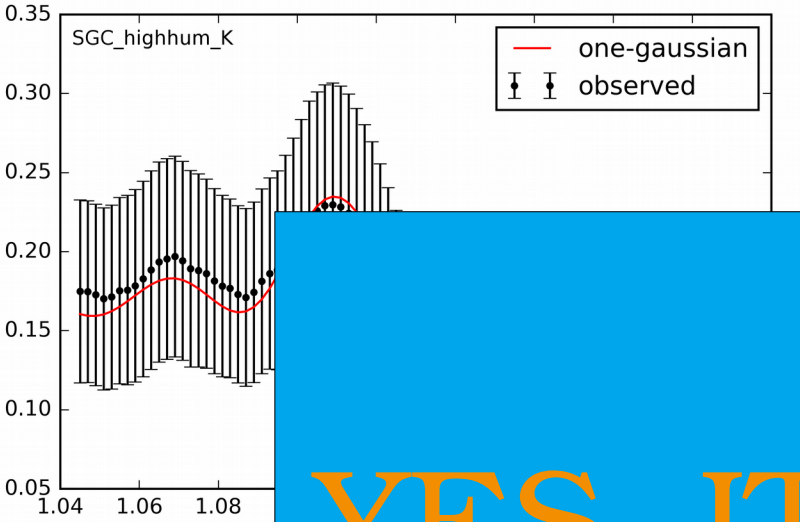

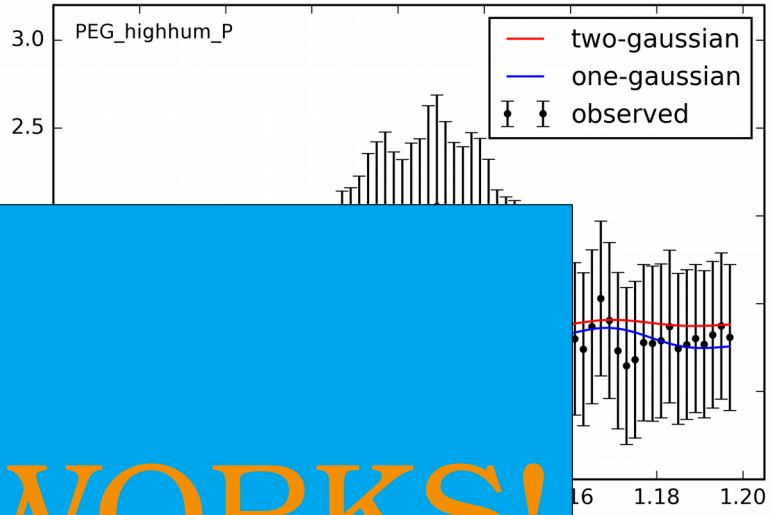

YES, IT WORKS!

Datase				R
SGC_hi				0.046
PEG_highhum_P, 2-fit	23, 96	8.7, 9.4	0.028	0.043
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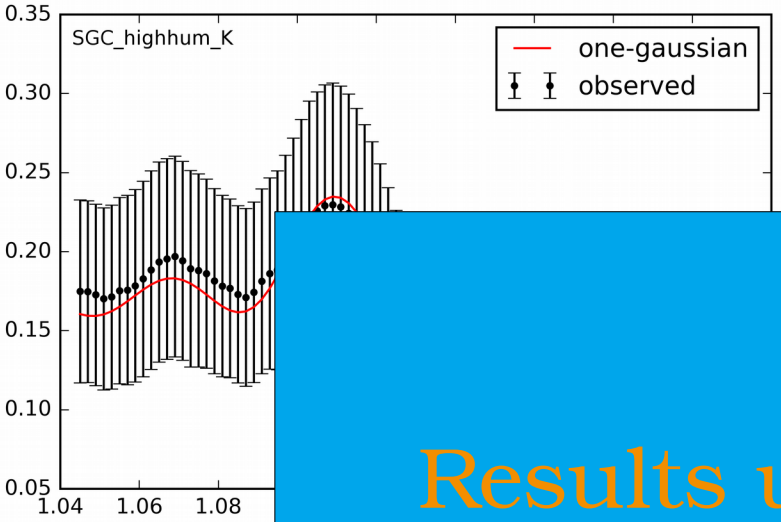

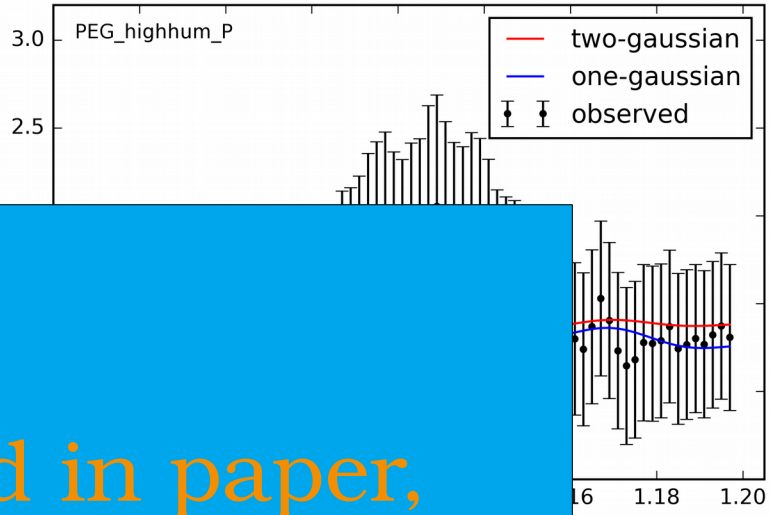

Results used in paper, submitted this week.

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