Supporting Online material for "X+ : A Comprehensive, Computationally Accelerated, Structural Analysis Tool of Solution X-ray Scattering from Supramolecular Self-Assemblies"

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S1 Form Factor Expressions

S1.1 Rectangular cuboid with a uniform electron density

The solution scattering intensity of a rectangular cuboid with a uniform electron density contrast, $\Delta\rho_0$, and dimensions ω, τ and μ, in the x, y and z directions, respectively, is:

$$I(q) = \frac{8\Delta\rho_0^2}{q^6}\int_0^{2\pi} d\phi_q \int_0^{\pi} \left\{ \begin{array}{c} [1-\cos(q\sin\theta_q\cos\phi_q\omega)]\times \\ [1-\cos(q\sin\theta_q\sin\phi_q\tau)]\times \\ [1-\cos(q\cos\theta_q\mu)]\times \\ \sin^{-3}\theta_q\cos^{-2}\phi_q\sin^{-2}\phi_q\cos^{-2}\theta_q \end{array} \right\} d\theta_q. \tag{1}$$

S1.2 Layered structures

Stack of infinite flat uniform slabs with varying electron density N is the number of infinite flat slabs. τ_i and τ_{i-1} are the start and end points of the ith slab, along the z direction. The electron density contrast of the ith slab is defined as $\Delta\rho_i = \rho_i - \rho_{solvent}$, where $\rho_{solvent}$ is the solvent electron density and ρ_i is the uniform slab electron density. The scattering intensity in solution is:

$$I(q) = \frac{8\pi^2 S}{q^4}\sum_{i=1}^{N}\sum_{j=1}^{N}\Delta\rho_j\Delta\rho_i \left\{ \begin{array}{c} \cos[q(\tau_j-\tau_i)]- \\ 2\cos[q(\tau_{j-1}-\tau_i)]+ \\ \cos[q(\tau_{j-1}-\tau_{i-1})] \end{array} \right\}, \tag{2}$$

where S is a correction prefactor with units of area.

Stack of infinite flat slabs having a Gaussian electron density profile along the normal direction It is useful to consider a stack of N infinite flat layers that have a uniform electron density contrast in the xy plane, but their electron-density contrast profile along the z direction is given by a sum of N Gaussian functions where the maximum of the electron density contrast, $\Delta\rho_i$, of the ith layer is centered at $z = z_i$ and the full width at half maximum (FWHM) of the ith layer is τ_i . In this case :

$$I(q) = \frac{2\pi^3 S}{q^2\ln 2}\sum_{i=1}^{N}\sum_{j=1}^{N} \left\{ \begin{array}{c} \Delta\rho_j\Delta\rho_i\tau_j\tau_i\cdot \\ e^{-\frac{q^2\left(\tau_i^2+\tau_j^2\right)}{16\ln 2}}\cdot \\ \cos[q(z_i-z_j)] \end{array} \right\}. \tag{3}$$

S1.3 Spherical structures

Multiple uniform spherical shells with varying electron density We now consider the case of a sequence of N shells. The uniform electron density contrast of the ith shell is $\Delta\rho_i$, its core radius is R_{i-1} and its outer shell radius is R_i, where $R_0 \equiv 0$. In this case:

$$I(q) = 4\pi\left|\frac{4\pi}{q^2}\left\{ \begin{array}{c} \sum_{i=1}^{N-1}(\Delta\rho_i-\Delta\rho_{i+1})\left[\cos(qR_i)R_i - \frac{\sin(qR_i)}{q}\right] \\ -\Delta\rho_N\left[\cos(qR_N)R_N - \frac{\sin(qR_N)}{q}\right] \end{array} \right\}\right|^2. \tag{4}$$

Multiple spherical shells with Gaussian electron density profiles along the radial direction A more realistic situation of multiple spherical shells is when each layer has a Gaussian electron density profile along the radial direction, r. The center of the ith layer is located at r_i, its FWHM is τ_i and its electron density contrast at r_i is $\Delta\rho_i$. In this case we get:

$$I(q)=4\pi\left|\frac{\pi^{3/2}}{2q}\sum_{i=1}^{N}\Delta\rho_i\tau_i e^{-\frac{\tau_i^2q^2}{16\ln 2}}\left[\begin{array}{c}-\frac{2r_i\sin(qr_i)}{\sqrt{\ln 2}}-\frac{\tau_i^2q\cos(r_iq)}{4\ln 2\sqrt{\ln 2}}+\\ +\int_0^1\left(\begin{array}{c}e^{\left(\frac{\tau_i^2q^2}{16\ln 2}-\frac{4\ln 2r_i^2}{\tau_i^2}\right)y^2}\times\\ \left\{\begin{array}{c}\left(\frac{4r_i^2}{\tau_i}-\frac{\tau_i^3q^2}{16\ln^2 2}\right)\sin\left[r_iq\left(y^2-1\right)\right]\\ -\frac{r_i\tau_iq}{\ln 2}\cos\left[r_iq\left(y^2-1\right)\right]\end{array}\right\}\end{array}\right)dy\end{array}\right]\right|^2, \tag{5}$$

where y is an integration variable.

S1.4 Cylindrical structures

Concentric uniform hollow cylinders with varying electron density The intensity of N concentric hollow cylinders that each has a uniform electron density contrast, $\Delta\rho_i$, shell radius, R_i, core radius, R_{i-1}, and height, $2h$, is:

$$I(q)=\frac{(4\pi)^3}{q^4}\int_0^1\left\{\begin{array}{c}\frac{\sin^2[qhx]}{x^2(1-x^2)}\times\\ \sum_{i,j=1}^{N-1}\left[\begin{array}{c}\left(\Delta\rho_i-\Delta\rho_{i+1}\right)R_iJ_1\left(q\sqrt{1-x^2}R_i\right)\times\\ \left(\Delta\rho_j-\Delta\rho_{j+1}\right)R_jJ_1\left(q\sqrt{1-x^2}R_j\right)\end{array}\right]\\ +2\sum_{i=1}^{N-1}\left[\begin{array}{c}R_N\Delta\rho_NJ_1\left(q\sqrt{1-x^2}R_N\right)\times\\ \left(\Delta\rho_i-\Delta\rho_{i+1}\right)R_iJ_1\left(q\sqrt{1-x^2}R_i\right)\end{array}\right]\\ +R_N^2\Delta\rho_N^2J_1^2\left(q\sqrt{1-x^2}R_N\right)\end{array}\right\}dx, \tag{6}$$

where $x=\cos\theta_q$.
If the concentric cylinders are infinitely long the measured intensity in solution is:

$$I(q)=\frac{\left(16\pi^4\right)L}{q^3}\left\{\begin{array}{c}\sum_{i,j=1}^{N-1}\left[\begin{array}{c}\left(\Delta\rho_i-\Delta\rho_{i+1}\right)R_iJ_1\left(qR_i\right)\times\\ \left(\Delta\rho_j-\Delta\rho_{j+1}\right)R_jJ_1\left(qR_j\right)\end{array}\right]\\ +2\sum_{i=1}^{N-1}\left[\begin{array}{c}R_N\Delta\rho_NJ_1\left(qR_N\right)\times\\ \left(\Delta\rho_i-\Delta\rho_{i+1}\right)R_iJ_1\left(qR_i\right)\end{array}\right]\\ +R_N^2\Delta\rho_N^2J_1^2\left(qR_N\right)\end{array}\right\}, \tag{7}$$

where L is a correction prefactor with units of length.

Concentric hollow cylinders with Gaussian electron density profiles along the radial projection A more realistic situation is when each cylindrical layer has a Gaussian electron density profile along its radial projection, $r_\perp$. The center of the ith layer is located at r_i, its FWHM is τ_i and its electron density contrast at r_i is $\Delta\rho_i$. The intensity of this model is:

$$I(q)=\frac{32\pi^3}{q^2}\int_0^\pi\left\{\begin{array}{c}\left[\frac{\sin(q\cos\theta_qh)}{\cos\theta_q}\right]^2\sin\left(\theta_q\right)\times\\ \left|\sum_{i=1}^{N}\Delta\rho_i\int_0^\infty e^{-\frac{4\ln 2\left(r_\perp-r_i\right)^2}{\tau_i^2}}r_\perp J_0\left(q\sin\theta_qr_\perp\right)dr_\perp\right|^2\end{array}\right\}d\theta_q. \tag{8}$$

For infinitely long cylinders the measured intensity in solution is:

$$I(q)=\frac{64\pi^4L}{q}\left|\sum_{i=1}^{N}\Delta\rho_i\int_0^\infty e^{-\frac{4\ln 2\left(r_\perp-r_i\right)^2}{\tau_i^2}}r_\perp J_0\left(qr_\perp\right)dr_\perp\right|^2. \tag{9}$$

Concentric hollow cylindroids with varying electron density A cylindroid is a rod with an elliptical cross section that is defined by its radii, a and b along the x- and y-axes. The scattering intensity from N concentric hollow cylindroids that each has a uniform electron density contrast $\Delta\rho_i$, shell radii a_i and b_i, along the x and y directions, respectively, and the corresponding core radii, a_{i-1} and b_{i-1} and height $2h$ is:

$$I(q)=\int_0^{2\pi}d\phi_q\left[\int_0^\pi\left|\int_0^{2\pi}\left(\begin{array}{c}\frac{2\sin(q\cos\theta_qh)}{q\cos\theta_q}\cdot\\ \sum_{i=1}^{N-1}\left\{\begin{array}{c}\left(\Delta\rho_i-\Delta\rho_{i+1}\right)e^{-iq\sin\theta_q\frac{b_i\cos\left(\phi_r-\phi_q\right)}{\sqrt{1-\varepsilon_i^2\cos^2\phi_r}}}\\ \times\left[\begin{array}{c}\frac{b_i}{-iq\sin\theta_q\cos\left(\phi_r-\phi_q\right)\sqrt{1-\varepsilon_i^2\cos^2\phi_r}}+\\ \frac{1}{q^2\sin^2\theta_q\cos^2\left(\phi_r-\phi_q\right)}\end{array}\right]\end{array}\right\}\\ +\left\{\begin{array}{c}\Delta\rho_Ne^{-iq\sin\theta_q\frac{b_N\cos\left(\phi_r-\phi_q\right)}{\sqrt{1-\varepsilon_N^2\cos^2\phi_r}}}\times\\ \left[\begin{array}{c}\frac{b_N}{-iq\sin\theta_q\cos\left(\phi_r-\phi_q\right)\sqrt{1-\varepsilon_N^2\cos^2\phi_r}}+\\ \frac{1}{q^2\sin^2\theta_q\cos^2\left(\phi_r-\phi_q\right)}\end{array}\right]\end{array}\right\}\\ -\frac{\Delta\rho_1}{q^2\sin^2\theta_q\cos^2\left(\phi_r-\phi_q\right)}\end{array}\right)d\phi_r\right|^2d\theta_q\right], \tag{10}$$

where $\varepsilon_i\left(a_i,b_i\right)\equiv\sqrt{1-\left(\frac{b_i}{a_i}\right)^2}$ is the eccentricity of the ith elliptical cross section.
For infinitely long cylindroids the measured intensity in solution is:

$$I\left(q\right)=\frac{2\pi L}{q}\int_0^{2\pi}\left|\int_0^{2\pi}\left[\begin{array}{c}\sum_{i=1}^{N-1}\left\{\begin{array}{c}\left(\Delta\rho_i-\Delta\rho_{i+1}\right)e^{-iq\frac{b_i\cos\left(\phi_r-\phi_q\right)_r}{\sqrt{1-\varepsilon_i^2\cos^2\phi_r}}}\times\\ \left[\frac{b_i}{-iq\cos\left(\phi_r-\phi_q\right)\sqrt{1-\varepsilon_i^2\cos^2\phi_r}}+\frac{1}{q^2\cos^2\left(\phi_r-\phi_q\right)}\right]\end{array}\right\}\\ +\left\{\begin{array}{c}\Delta\rho_N e^{-iq\frac{b_N\cos\left(\phi_r-\phi_q\right)}{\sqrt{1-\varepsilon_N^2\cos^2\phi_r}}}\times\\ \left[\frac{b_N}{-iq\cos\left(\phi_r-\phi_q\right)\sqrt{1-\varepsilon_N^2\cos^2\phi_r}}+\frac{1}{q^2\cos^2\phi_r}\right]\end{array}\right\}\\ -\frac{\Delta\rho_1}{q^2\cos^2\left(\phi_r-\phi_q\right)}\end{array}\right]d\phi_r\right|^2d\phi_q, \tag{11}$$

where L is a correction prefactor with units of length.

S1.5 Coaxial helical structures

A series of coaxial shifted infinitely long thick helices with a uniform electron density We look at k infinitely long thick coaxial helices or radius R, pitch P, each of electron density $\Delta\rho_i$ and cross section radius R_{cs}^i. The helices are displaced along a common z axis by amounts Δ_j from the first helix. The solution scattering intensity is:

$$I\left(q\right)=\frac{8\pi^3L}{q^3}\sum_{h=0}^{h_{\max}}\left|\begin{array}{c}\left(\sum_{j=0}^{k-1}\left(\frac{J_1\left(qR_{cs}^j\sqrt{1-\left(\frac{2\pi h}{qP}\right)^2}\right)R_{cs}^j}{\sqrt{1-\left(\frac{2\pi h}{qP}\right)^2}}\right)\Delta\rho_j\exp\left[i\frac{2\pi h}{P}\Delta_j\right]\right)\times\\ J_h\left(qR\sqrt{1-\left(\frac{2\pi h}{qP}\right)^2}\right)\end{array}\right|^2, \tag{12}$$

where h_{max} is a function of q and is given by: $h_{\max}=floor\left(\frac{qP}{2\pi}\right)$.

A series of coaxial shifted finite length thick helices with a uniform electron density When the helices have a finite length $l=NP$:

$$I\left(q\right)=\frac{2\pi P^2}{q^2}\int_{-1}^{1}\left|\begin{array}{c}\left[\sum_{j=0}^{k-1}\left(\frac{J_1\left(qR_{cs}^j\sqrt{1-x^2}\right)R_{cs}^j}{\sqrt{1-x^2}}\right)\Delta\rho_j\exp\left(iqx\Delta_j\right)\right]\times\\ \left\{\int_0^{2\pi}\exp\left[i\left(qR\sqrt{1-x^2}\cos\varphi+\frac{qxP\varphi}{2\pi}\right)\right]d\varphi\right\}\\ \times\frac{\sin\left(Nqx\frac{P}{2}\right)}{\sin\left(qx\frac{P}{2}\right)}\end{array}\right|^2dx, \tag{13}$$

where $x=\cos\theta_q$.

A series of coaxial shifted finite length helices composed of discrete spheres with a uniform electron density We now consider the case of N coaxial discrete helices of radius R_{helix} and pitch P. The jth helix is displaced from the first helix by Δ_j and composed of $N_{spheres}$ spheres of radius R_j and uniform electron density contrast $\Delta\rho_j$. The gap between two spheres along the helix is δ_w and the projection of the distance between the centers of two adjacent spheres on the z-axis is given by: $\delta_z^j\equiv\frac{P(2R_j+\delta_w)}{2\pi R_{Helix}}$. The scattering intensity in solution is:

$$I\left(q\right)=\\ \sum_{j,j'=1}^{N}\left\{\int_0^1\sum_{n,n'=1}^{N_{spheres}}dxJ_0\left[2q\sqrt{1-x^2}R_{helix}\sin\left(\frac{\pi\left(n\delta_z^j-n'\delta_z^{j'}+\Delta_j-\Delta_{j'}\right)}{P}\right)\right]\cos\left(qx\left(n\delta_z^j-n'\delta_z^{j'}\right)\right)\right\}\times\\ \frac{32\pi^2}{q^6}\Delta\rho_j\Delta\rho_{j'}\left[\sin\left(qR_j\right)-\cos\left(qR_j\right)qR_j\right]\left[\sin\left(qR_{j'}\right)-\cos\left(qR_{j'}\right)qR_{j'}\right], \tag{14}$$

where $x=\cos\theta_q$.

S2 Peak Centers and Phases

The 3D reciprocal lattice vectors (see section 2.3.2 of the paper for parameter definitions) are given by (Als-Nielsen & McMorrow, 2001):

$$\vec{a}_1^*=\frac{2\pi\vec{a}_2\times\vec{a}_3}{\vec{a}_1\cdot\left(\vec{a}_2\times\vec{a}_3\right)},\vec{a}_2^*=\frac{2\pi\vec{a}_3\times\vec{a}_1}{\vec{a}_1\cdot\left(\vec{a}_2\times\vec{a}_3\right)},\vec{a}_3^*=\frac{2\pi\vec{a}_1\times\vec{a}_2}{\vec{a}_1\cdot\left(\vec{a}_2\times\vec{a}_3\right)}. \tag{15}$$

If $\vec{a}_1=\left(x_1,y_1,z_1\right)$, $\vec{a}_2=\left(x_2,y_2,z_2\right)$ and $\vec{a}_3=\left(x_3,y_3,z_3\right)$, then:

$$v_c = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) = \\ x_1 (y_2 z_3 - y_3 z_2) + y_1 (x_3 z_2 - x_2 z_3) + z_1 (x_2 y_3 - x_3 y_2) \tag{16}$$

and we get that:

$$\vec{a}_1^* = \frac{2\pi}{v_c} (\hat{x} (y_2 z_3 - y_3 z_2) - \hat{y} (x_2 z_3 - x_3 z_2) + \hat{z} (x_2 y_3 - x_3 y_2)) \tag{17}$$

$$\vec{a}_2^* = \frac{2\pi}{v_c} (\hat{x} (y_3 z_1 - y_1 z_3) - \hat{y} (x_3 z_1 - x_1 z_3) + \hat{z} (x_3 y_1 - x_1 y_3)) \tag{18}$$

$$\vec{a}_3^* = \frac{2\pi}{v_c} (\hat{x} (y_1 z_2 - y_2 z_1) - \hat{y} (x_1 z_2 - x_2 z_1) + \hat{z} (x_1 y_2 - x_2 y_1)) \tag{19}$$

2D crystals can be represented in the $x-y$ plane by two basis vectors: $\vec{a}_1 = (x_1, y_1)$, $\vec{a}_2 = (x_2, y_2)$ and each lattice point in real space is given by $\vec{R}_{n_1,n_2} = n_1\vec{a}_1 + n_2\vec{a}_2$ where n_1 and n_2 are integers. In reciprocal space $\vec{a}_1^* = \frac{2\pi}{s} (\hat{x} (y_2) - \hat{y} (x_2))$ and $\vec{a}_2^* = \frac{2\pi}{s} (\hat{x} (-y_1) + \hat{y} (x_1))$, where $s = x_1 y_2 - y_1 x_2$.
In the case of 1D crystals the lattice points in real space are given by: $\vec{R}_{n_1} = n_1\vec{a}_1$ where $\vec{a}_1 = a\hat{x}$. In reciprocal space we get: $\vec{a}_1^* = \frac{2\pi\vec{a}_1}{|\vec{a}_1|^2} = \frac{2\pi}{a}\hat{x}$.
1D crystals are therefore represented only by the length a of their repeat unit and $\vec{G}_h = \frac{2\pi h}{a}\hat{x}$. In solution scattering we only get the magnitude of the Bragg scattering vectors: $\left|\vec{G}_h\right| = \frac{2\pi h}{a}$. From the peak positions we only need to find the index h and repeat distance a.
2D crystals can be represented by two basis vectors of lengths a and b and the angle between them γ. Those parameters determine the type of lattice we get. If $\gamma = \frac{\pi}{2}$ we get a rectangular lattice. If $\gamma = \frac{\pi}{4}$ we get a centered rectangular lattice. If $\gamma \neq \frac{\pi}{2}, \frac{\pi}{4}$ we get an oblique lattice. If $\gamma = \frac{\pi}{2}$ and $a = b$ we get a square lattice. If $\gamma = \frac{2\pi}{3}$ and $a = |\vec{a}_1| = |\vec{a}_2| = b$ we get a hexagonal lattice.
We can always rotate the lattice so that $\vec{a}_1$ is along the $\hat{x}$ direction and is given by:

$$\vec{a}_1 = a(1, 0). \tag{20}$$

$\vec{a}_2$ is then given by:

$$\vec{a}_2 = b (\cos\gamma, \sin\gamma) . \tag{21}$$

Therefore:

$$\vec{a}_1^* = \frac{2\pi}{a}(1, \frac{-\cos\gamma}{\sin\gamma}), \tag{22}$$

and

$$\vec{a}_2^* = \frac{2\pi}{b\sin\gamma}(0, 1), \tag{23}$$

$$\vec{G}_{h,k} = h\vec{a}_1^* + k\vec{a}_2^* = \left(\frac{2\pi h}{a}, \frac{2\pi}{\sin\gamma}\left(\frac{k}{b} - \frac{h\cos\gamma}{a}\right)\right). \tag{24}$$

In solution we only measure the absolute values:

$$\left|\vec{G}_{h,k}\right| = 2\pi\sqrt{\left(\frac{h}{a}\right)^2 + \frac{1}{\sin^2\gamma}\left(\frac{k}{b} - \frac{h\cos\gamma}{a}\right)^2} \tag{25}$$

We need to fit a, b, γ and the indexes h and k of each peak.
In 3D we can select a plane use the 2D vectors as above and add a third vector $\vec{a}_3$ defined by it length c and two more angles α and β, where the former is between the vectors $\vec{a}_1$ and $\vec{a}_3$, and the latter is between the vectors $\vec{a}_2$ and $\vec{a}_3$. In real space the basis vectors are given by:

$$\vec{a}_1 = (a, 0, 0), \tag{26}$$

$$\vec{a}_2 = (b\cos\gamma, b\sin\gamma, 0) , \tag{27}$$

$$\vec{a}_3 = \left(c\cos\alpha, c\zeta, c\sqrt{\sin^2\alpha - \zeta^2}\right), \tag{28}$$

where

$$\zeta = \frac{(\cos\beta - \cos\alpha\cos\gamma)}{\sin\gamma}$$

and in reciprocal space:

$$\vec{a}_1^* = \left(\frac{2\pi}{a}, \frac{-2\pi\cos\gamma}{a\sin\gamma}, \frac{2\pi\left(\zeta\cos\gamma - \cos\alpha\sin\gamma\right)}{a\sin\gamma\sqrt{\sin^2\alpha - \zeta^2}} \right), \tag{29}$$

$$\vec{a}_2^* = \left(0, \frac{2\pi}{b\sin\gamma}, \frac{-2\pi\left(\cos\beta - \cos\alpha\cos\gamma\right)}{b\sin^2\gamma\sqrt{\sin^2\alpha - \zeta^2}} \right), \tag{30}$$

$$\vec{a}_3^* = \left(0, 0, \frac{2\pi}{c\sqrt{\sin^2\alpha - \zeta^2}} \right). \tag{31}$$

The Bragg scattering vector amplitudes are:

$$\left|\vec{G}_{h,k,l}\right| = |h\vec{a}_1^* + k\vec{a}_2^* + l\vec{a}_3^*| = \tag{32}$$

$$\frac{2\pi}{ab\sin\gamma}\sqrt{\frac{\left(hb\sin\gamma\right)^2 + \left(ka - hb\cos\gamma\right)^2 + \frac{\left(hbc(\cos\gamma\cos\beta - \cos\alpha) - kac\zeta\sin\gamma + lab\sin^2\gamma\right)^2}{c^2(\sin^2\gamma - \cos^2\alpha - \cos^2\beta + 2\cos\beta\cos\alpha\cos\gamma)}}{}}. \tag{33}$$

Here there is also classification of special cases. The general lattice is triclinic: $a \neq b \neq c$ and $\alpha \neq \beta \neq \gamma$. There are 2 monoclinic lattices: $a \neq b \neq c$ and $\alpha = \gamma = 90 \neq \beta$, 4 orthorhombic lattices, for which $a \neq b \neq c$ and $\alpha = \beta = \gamma = 90$, 2 tetragonal lattices $a = b \neq c$ and $\alpha = \beta = \gamma = 90$, 3 cubic lattices $a = b = c$ and $\alpha = \beta = \gamma = 90$, a trigonal lattice $a = b = c$ and $\alpha = \beta = \gamma < 120, \neq 90$, and a hexagonal lattice $a = b \neq c$ and $\alpha = \beta = 90, \gamma = 120$.

S3 Algorithms

Algorithm 1 Automatic Baseline Detection

Start the baseline from a given point (q_{min}), end the baseline at the global minimum of the data
Interpolate a line between the beginning and the end of the baseline with zero slope and an intercept at the global minimum
while baseline end-point is larger than the start-point **do**
    while baseline does not intersect the data **do**
        Increase line slope by ε and interpolate the start and end points
    end while
    Decrease line slope by the exact amount so that the lines don't intersect
    Interpolate the start and end points
    Set the end-point of the baseline to the leftmost intersection point
end while

Algorithm 2 Automatic Peak Detection

Divide $[I(q) - B(q)]$ by $FF(q)$ and set to $SF_o(q)$
Divide data points into segments according to σ
Calculate Goodness of Fit (GOF, see below) between SF_c and SF_o, set to χ^2
for each segment **do**
    Calculate GOF of SF_c and SF_o in the segment
    Sum the difference between SF_c and SF_o for all points in the segment
    if sum is not positive **then**
        Continue to the next segment
    end if
    if GOF of the segment is greater than or equal to $\tau \cdot \chi^2$ **then**
        Flag a peak to be added
    end if
    if the previous segment's GOF is greater than the current segment's GOF (we've passed the peak's maximum), and a peak is flagged to be added **then**
        Find the local maximum in this segment and the previous one, set to peak center
        Set the amplitude to the difference between SF_0 and SF_c at the peak center
        From amplitude, center and SF_0, deduce FWHM and add the peak to SF_c
        Clear the "add peak" flag
    end if
end for

S4 Additional Features

S4.1 Goodness of Fit Criteria

The fitting procedure requires a signal-model difference measure, or Goodness of Fit. In order to calculate it, several approaches may be taken. We allow the user to choose between the Coefficient of Determination, R^2, and Weighted Sum of Squared Residuals, χ^2 We use $w(q) = \sqrt{q} + 1$ as the weight function for χ^2, as to give significantly more weight to the higher q-range values.

S4.2 Instrument Resolution

In order to simulate the finite instrument resolution of a measurement we use a Gaussian weighted moving average on the theoretical model. Each point is averaged with the points around it with Gaussian weights of width σ:

$$I^{'}(q_i) = \frac{\sum_n I(q_n) \cdot e^{-\frac{(q_i - q_n)^2}{2\sigma^2}}}{\sum_n e^{-\frac{(q_i - q_n)^2}{2\sigma^2}}},$$

The limits on the index n are determined by a cutoff of $\pm 3\sigma$ around q_i. The points closer to the edge have the Gaussian function cropped on either side so that it remains symmetrical.

S5 Running X+ on Linux

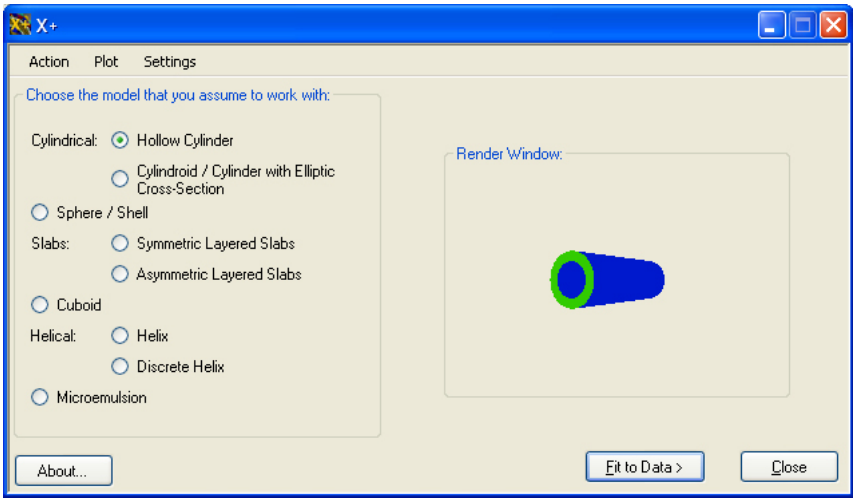
X+ is built for Windows, but can be run under Linux using Wine. A few additional programs must be installed under Wine. The following is the full set of commands required to get X+ up and running. If any of the programs are installed, skip the relevant command.

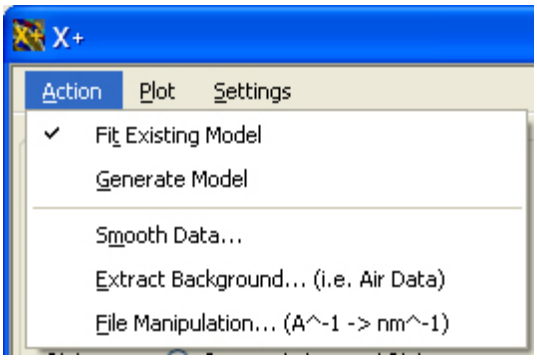
```
# apt-get install wine
$ wget http://winezeug.googlecode.com/svn/trunk/winetricks
$ sh winetricks corefonts dotnet20
$ sh winetricks vcrun2008
$ sh winetricks gdiplus
```

Run X+:

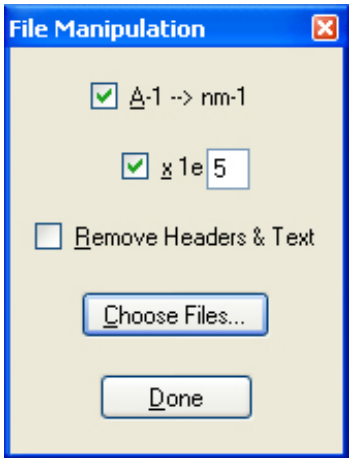
```
$ wine X+.exe
```

S6 Screenshots and short explanations



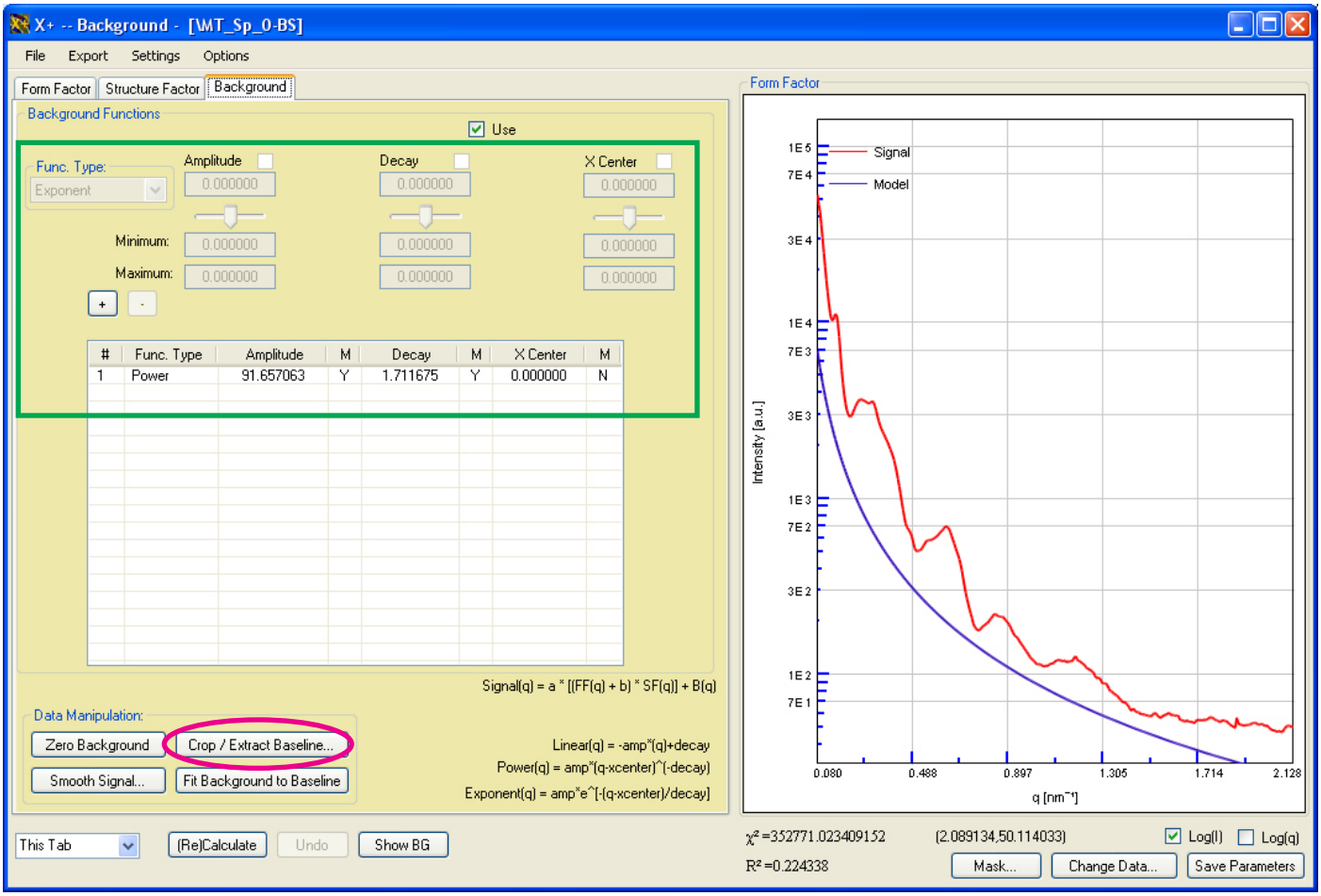


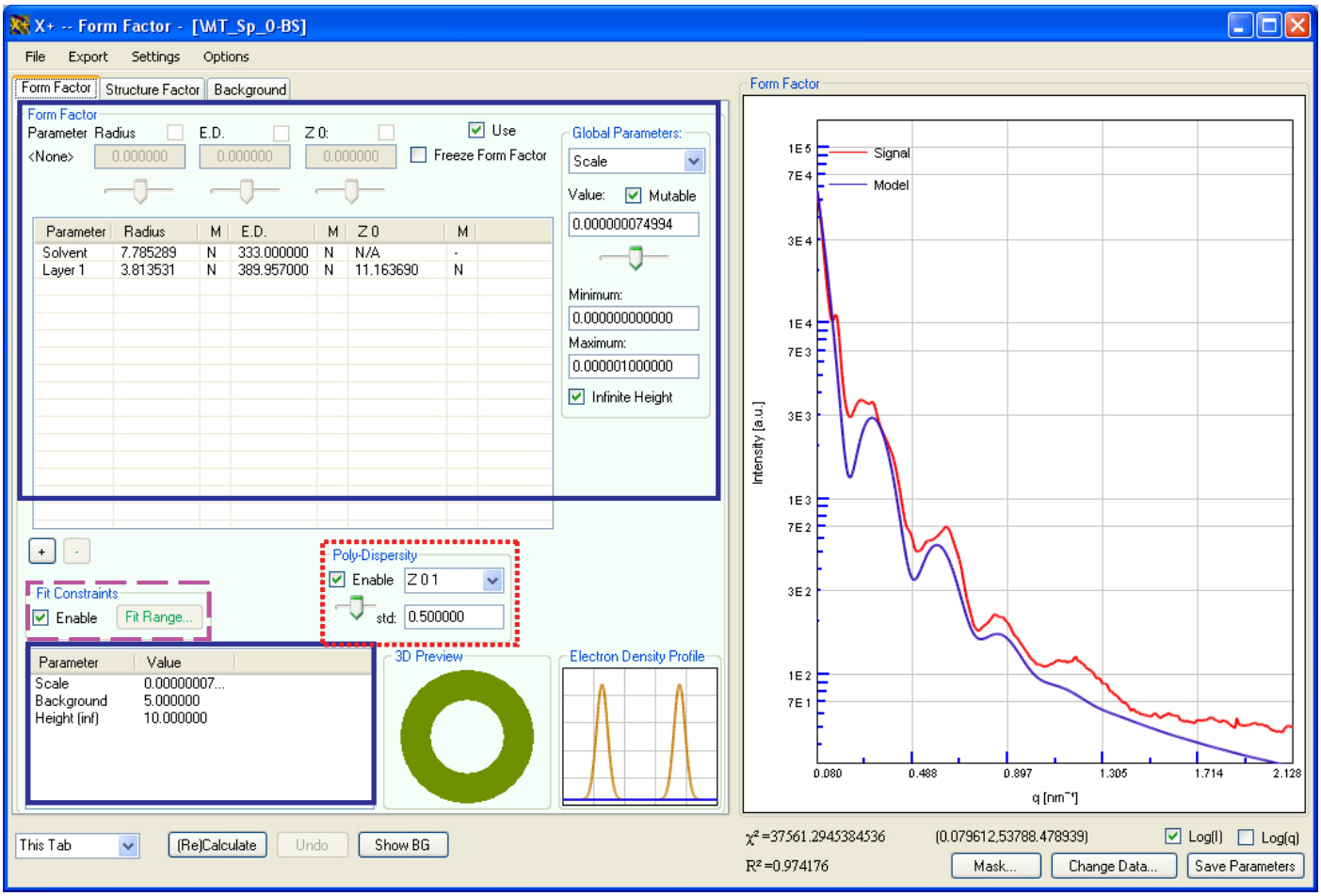
The opening window. In this screen, the desired geometric model can be chosen. In addition, under the Action menu, there are options for background subtraction (Extract Background…) and File Manipulation.



The File Manipulation window allows the manipulation of multiple files with one click. The options are to convert the file from inverse Angstroms to inverse nm; scale the entire signal; and to strip all headers and text from the files. New files are written to a new subdirectory.

The background pane. The Extract Baseline button (pink oval) opens a new window where a baseline can be generated. Another option is to add functions representing the background (green box).





The Form Factor pane. The model's parameters are entered in the areas surrounded by the blue boxes. Polydispersity of a parameter is controlled in the red dotted box. Constraints and linked parameters are defined in the area surrounded by the dashed pink box.

The Structure Factor pane. In the solid blue box peaks can be added. They can also be drawn on the graph itself with the mouse. Selected peaks can be moved to the Phase fitter (dotted pink box, follow the green arrows). There, the phase parameters can be fit to the peak centers. The iterative fitting can be chosen in the red oval.