

Supplementary Code: CPLOT Fitting Function

```
#define VERSION 5
#define NUM_XS 1 /* Num of independent variables */
#define MAXPAR 28 /* Num of parameters */
#define MAXPTS 500 /* Most points for fitting */
#define MAXPLT 500 /* Most for pg ps md mr sA */
#include <math.h>
#include <p_fitsize.h>

char *title = "Fits first 12 peaks from hexagonally bound MTs, single-ring tubulin FF, unified fit
BG";

char *comment = "";

void
setup() {
    set_prompt(0, "LINE");
    set_prompt(1, "line");
}

struct init_4 initial[] = {

/* Name      Deriv? Fit? Initial Limit? Low High */
{"G", 0, 1, 0, 1, 0, 1}, /* Coefficient for BG Guiner exp*/
{"Rg", 0, 0, 19000.0, 3, 10,20000}, /* Rg for Guiner exp */
{"B1", 0, 1, .05514, 1, 0, 0}, /* Coefficient for the low-q Porod region (mass
fractal)*/
{"Pwr1", 0, 1, 3.886, 3, 1, 4}, /* Power law for mass fractal*/
{"B2", 0, 1, .000530184, 1, 0, 0}, /* Coefficient for the high-q Porod region (surface
fractal)*/
{"Pwr2", 0, 1, 1.82616, 3, 1, 4}, /* Power law for surface fractal*/
{"y0", 0, 0, 0.42324, 3, 0, 15}, /* flat BG scattering */
{"Aring", 0, 0, 0e-9, 1, 0, 0}, /* Coefficient for Ring FF */
{"Lring", 0, 0, 38.5, 1, 0, 0}, /* L = length of ring */
{"W", 0, 0, 49, 3, 30, 50}, /* W = width of tubulin */
{"Rring", 0, 0, 162.98, 3, 75, 220}, /* Rring = inner radius of the tubulin ring */
{"q10", 0, 1, .0121360, 3, .008, .02}, /* q10 = q of Imax */
{"Rin", 0, 0, 94.41, 3, 90, 180}, /* Rin = inner radius of MT */
{"P1", 0, 1, 1.25645e-10, 3, 1e-20, 1e-6}, /* coefficient for peak 1 */
{"K", 0, 1, 0.00308035, 3, 0.001, 0.01}, /* K = 1.554*HWHM at peak 1*/
{"P2", 0, 1, 1.24528e-10, 3, 1e-20, 1e-6}, /* coefficient for peak 2 */
{"K2", 0, 0, 0.0035, 3, 0.001, 0.01}, /* K2 = 1.554*HWHM at peak 2*/
{"P3", 0, 0, 1.00e-11, 3, 1e-20, 1e-8}, /* coefficient for peak 3 */
{"K3", 0, 0, 0.0055, 3, 0.001, 0.01}, /* K3 = 1.554*HWHM at peak 3 */
{"P4", 0, 0, 1.01e-11, 3, 1e-20, 1e-8}, /* coefficient for peak 4 */
```

```
{"P5", 0, 0, 1.00e-11, 3, 1e-20, 1e-8}, /* coefficient for peak 5 */
{"P6", 0, 0, 1.00e-11, 3, 1e-20, 1e-8}, /* coefficient for peak 6 */
{"P7", 0, 0, 1.00e-11, 3, 1e-20, 1e-8}, /* coefficient for peak 7 */
{"P8", 0, 0, 1.00e-11, 3, 1e-20, 1e-8}, /* coefficient for peak 8 */
{"P9", 0, 0, 1.00e-11, 3, 1e-20, 1e-8}, /* coefficient for peak 9 */
{"P10", 0, 0, 1.00e-11, 3, 1e-20, 1e-8}, /* coefficient for peak 10 */
{"P11", 0, 0, 1.00e-11, 3, 1e-20, 1e-8}, /* coefficient for peak 11 */
{"P12", 0, 0, 1.00e-11, 3, 1e-20, 1e-8}, /* coefficient for peak 12 */
};
```

```
/* define the parameters */
```

```
#define G fpar[0].p_b
#define fG fpar[0].p_fit
#define dG fpar[0].p_p
```

```
#define Rg fpar[1].p_b
#define fRg fpar[1].p_fit
#define dRg fpar[1].p_p
```

```
#define B1 fpar[2].p_b
#define fB1 fpar[2].p_fit
#define dB1 fpar[2].p_p
```

```
#define Pwr1 fpar[3].p_b
#define fPwr1 fpar[3].p_fit
#define dPwr1 fpar[3].p_p
```

```
#define B2 fpar[4].p_b
#define fB2 fpar[4].p_fit
#define dB2 fpar[4].p_p
```

```
#define Pwr2 fpar[5].p_b
#define fPwr2 fpar[5].p_fit
#define dPwr2 fpar[5].p_p
```

```
#define y0 fpar[6].p_b
#define fy0 fpar[6].p_fit
#define dy0 fpar[6].p_p
```

```
#define Aring fpar[7].p_b
#define fAring fpar[7].p_fit
#define dAring fpar[7].p_p
```

```
#define Lring fpar[8].p_b
#define fLring fpar[8].p_fit
```

```
#define dLringfpar[8].p_p

#define W    fpar[9].p_b
#define fW   fpar[9].p_fit
#define dW   fpar[9].p_p

#define Rring    fpar[10].p_b
#define fRring   fpar[10].p_fit
#define dRring   fpar[10].p_p

#define q10    fpar[11].p_b
#define fq10   fpar[11].p_fit
#define d10    fpar[11].p_p

#define Rin    fpar[12].p_b
#define fRin   fpar[12].p_fit
#define dRin   fpar[12].p_p

#define P1    fpar[13].p_b
#define fP1   fpar[13].p_fit
#define dP1   fpar[13].p_p

#define K    fpar[14].p_b
#define fK   fpar[14].p_fit
#define dK   fpar[15].p_p

#define P2    fpar[15].p_b
#define fP2   fpar[15].p_fit
#define dP2   fpar[15].p_p

#define K2    fpar[16].p_b
#define fK2   fpar[16].p_fit
#define dK2   fpar[16].p_p

#define P3    fpar[17].p_b
#define fP3   fpar[17].p_fit
#define dP3   fpar[17].p_p

#define K3    fpar[18].p_b
#define fK3   fpar[18].p_fit
#define dK3   fpar[18].p_p

#define P4    fpar[19].p_b
#define fP4   fpar[19].p_fit
#define dP4   fpar[19].p_p
```

```
#define P5 fpar[20].p_b
#define fP5 fpar[20].p_fit
#define dP5 fpar[20].p_p
```

```
#define P6 fpar[21].p_b
#define fP6 fpar[21].p_fit
#define dP6 fpar[21].p_p
```

```
#define P7 fpar[22].p_b
#define fP7 fpar[22].p_fit
#define dP7 fpar[22].p_p
```

```
#define P8 fpar[23].p_b
#define fP8 fpar[23].p_fit
#define dP8 fpar[23].p_p
```

```
#define P9 fpar[24].p_b
#define fP9 fpar[24].p_fit
#define dP9 fpar[24].p_p
```

```
#define P10 fpar[25].p_b
#define fP10 fpar[25].p_fit
#define dP10 fpar[25].p_p
```

```
#define P11 fpar[26].p_b
#define fP11 fpar[26].p_fit
#define dP11 fpar[26].p_p
```

```
#define P12 fpar[27].p_b
#define fP12 fpar[27].p_fit
#define dP12 fpar[27].p_p
```

```
/*define the independent variables */
```

```
#define Q (M_flag? Make_x[0]:dp->d_xx[0])
```

```
double model(int deriv_flag)
```

```
{
```

```
    double q, Sfit, j, FFring=0, FFmt, SFmt, x, wt, L=20000, Wmt = 49;
```

```
    int i;
```

```
    q = Q;
```

```
    wt = M_PI/2048;
```

```
    for (i=1;i<2049;i++) {
```

```
        x = cos((2*i-1)*M_PI/(2*2048));
```

```

FFmt = pow(sin(q*x*L/2)/(q*q*x)*((Rin+Wmt)*j1(q*sqrt(1-x*x)*(Rin+Wmt))-
Rin*j1(q*sqrt(1-x*x)*Rin)),2)/sqrt(1-x*x);

```

```

SFmt = pow(P1/(K*K+(q*sqrt(1-x*x)-q10)*(q*sqrt(1-x*x)-q10)),
2)+pow(P2/(K2*K2+(q*sqrt(1-x*x)-sqrt(3)*q10)*(q*sqrt(1-x*x)-sqrt(3)*q10)),
2)+pow(P3/(pow(K3,2)+(q*sqrt(1-x*x)-2*q10)*(q*sqrt(1-x*x)-2*q10)),
2)+pow(P4/(pow(K3,2)+(q*sqrt(1-x*x)-sqrt(7)*q10)*(q*sqrt(1-x*x)-sqrt(7)*q10)),
2)+pow(P5/(pow(K3,2)+(q*sqrt(1-x*x)-3*q10)*(q*sqrt(1-x*x)-3*q10)),
2)+pow(P6/(pow(K3,2)+(q*sqrt(1-x*x)-sqrt(12)*q10)*(q*sqrt(1-x*x)-sqrt(12)*q10)),
2)+pow(P7/(pow(K3,2)+(q*sqrt(1-x*x)-sqrt(13)*q10)*(q*sqrt(1-x*x)-sqrt(13)*q10)),
2)+pow(P8/(pow(K3,2)+(q*sqrt(1-x*x)-4*q10)*(q*sqrt(1-x*x)-4*q10)),
2)+pow(P9/(pow(K3,2)+(q*sqrt(1-x*x)-sqrt(19)*q10)*(q*sqrt(1-x*x)-
sqrt(19)*q10)),2)+pow(P10/(pow(K3,2)+(q*sqrt(1-x*x)-sqrt(21)*q10)*(q*sqrt(1-x*x)-
sqrt(21)*q10)), 2)+pow(P11/(pow(K3,2)+(q*sqrt(1-x*x)-5*q10)*(q*sqrt(1-x*x)-5*q10)),
2)+pow(P12/(pow(K3,2)+(q*sqrt(1-x*x)-sqrt(27)*q10)*(q*sqrt(1-x*x)-sqrt(27)*q10)), 2);

```

```

FFring = pow(sin(q*x*Lring/2)/(q*q*x)*((Rring+W)*j1(q*sqrt(1-
x*x)*(Rring+W))-Rring*j1(q*sqrt(1-x*x)*Rring)),2)/sqrt(1-x*x);

```

```

Sfit = Sfit+Aring*FFring+FFmt*SFmt;

```

```

}
if (deriv_flag) {

```

```

}
Sfit = Sfit*wt+y0+G*exp(-1*q*q*Rg*Rg/3)+B2*pow(pow(erf(q*Rg/sqrt(6)),
3)/q,Pwr2)+B1*exp(-1*Rg*Rg*q/3)*pow(pow(erf(q*1e10/sqrt(6)), 3)/q,Pwr1);
return(Sfit);

```

```

}

```

```

int prefilter(), postfilter();

```

```

struct user_cmds {
    char c_one;
    char two;
    int (*c_func)();
} user_cmds[] = {
    {'n', 'm', postfilter},
    {'m', 'n', prefilter},
    0,
};
prefilter() {
}
postfilter() {
}

```

