

Figure 1.
Java frontend

CMWP fit control - All-users/Frontend/Zirc2_2-3dpa_250C/zirc2_2_3dpa_250C

CUBIC:	<input type="checkbox"/>	HEXAGONAL:	<input checked="" type="checkbox"/>	ORTHOROMBIC:	<input type="checkbox"/>
lat_a (CUB HEX ORT) [nm]:	.3232	lat_b (ORT) [nm]:		lat_c (HEX ORT) [nm]:	.515
Burgers vector [nm]:	.3232	Wavelength [nm]:	.0825634	Ch00 or Chk0:	0.255
Don't include size effect:	<input type="checkbox"/>	Use ellipsoidal size func.:	<input type="checkbox"/>	Use individual C factors:	<input type="checkbox"/>
Include St. Faults effect:	<input type="checkbox"/>	stacking.dat file:		<input type="button" value="Browse"/>	
Use weights:	<input checked="" type="checkbox"/>	Weighting algorithm (1-4):	1	Disable coinc. g ² code:	<input checked="" type="checkbox"/>
Use instrum. profiles:	<input checked="" type="checkbox"/>	Instrum. profiles dir.:	All-users/AAManchester-2016/Dia	<input type="button" value="Browse"/>	
Fit peak int.:	<input checked="" type="checkbox"/>	Fit peak pos.:	<input checked="" type="checkbox"/>	Use 2 W.f. asymmetry:	<input type="checkbox"/>
Fit in K instead of 2*theta:	<input type="checkbox"/>	Clone peak-index.dat file:	<input type="checkbox"/>	Clone bg-spline.dat file:	<input type="checkbox"/>
FT limit (if no instr. eff.):		Use FFT:	<input checked="" type="checkbox"/>	FFT cutting parameter (0-1):	0.25
Profile cutting parameter:	4	N1:	1024	N2:	1024
Min. 2*theta/K:	15	Max. 2*theta/K:	43	Use Groma-Csikor strain f.:	<input type="checkbox"/>
init_W:		init_X:		init_Y:	
init_a (q, CUB):		init_a1 (HEX ORT):	-0.563314	init_a2 (HEX ORT):	-0.32201
a_fixed:	<input type="checkbox"/>	a1_fixed:	<input type="checkbox"/>	a2_fixed:	<input type="checkbox"/>
init_a3 (ORT):		init_a4 (ORT):		init_a5 (ORT):	
a3_fixed:	<input type="checkbox"/>	a4_fixed:	<input type="checkbox"/>	a5_fixed:	<input type="checkbox"/>
init_epsilon:	1.0	epsilon_fixed:	<input type="checkbox"/>	Rc:	1
init_b (m):	1422.73	b_fixed:	<input type="checkbox"/>	rhoIGS:	
init_c (sigma):	0.173652	c_fixed:	<input type="checkbox"/>	<input type="button" value="Set Satellite parameters"/>	<input type="button" value="Set fit parameters"/>
init_d (Rho14):	86.1294	d_fixed:	<input type="checkbox"/>	<input type="button" value="Update peak-index.dat"/>	
init_e (M*):	0.0705582	e_fixed:	<input type="checkbox"/>	<input type="button" value="Edit phase No:"/>	
init_st_pr:		st_pr_fixed:	<input type="checkbox"/>	<input type="button" value="Clone INI files"/>	<input type="button" value="Save INI files"/>
Use Satellites:	<input type="checkbox"/>	<input type="button" value="Set Satellite parameters"/>		<input type="button" value="Set fit parameters"/>	<input type="button" value="Update peak-index.dat"/>
Number of phases:	3	Fit ONLY phase No:		<input type="button" value="Edit phase No:"/>	
<input type="button" value="Call MKSpline"/>	<input type="button" value="Call MKSpline2"/>	<input type="button" value="Index peaks"/>	<input type="button" value="Set individ. C values"/>	<input type="button" value="Clone INI files"/>	<input type="button" value="Save INI files"/>
<input type="button" value="(Re)Start FIT"/>	<input type="button" value="Stop FIT"/>	<input type="button" value="Update Params"/>	<input type="button" value="View Solutions"/>	<input type="button" value="View FIT"/>	<input type="button" value="Exit"/>

Figure 2.
 "Set fit parameters" pop-up window

CMWP fit fit_params_control - All-users/Frontend/Zirc2_2-3dpa_250C/zirc2_2_3dpa_250C

min_a_cubic:	-10	max_a_cubic:	3
min_a_other:	-5	max_a_other:	5
min_b:	0.1	max_b:	2000
min_c:	0.05	max_c:	2
min_d:	0.01	max_d:	1000
min_e:	0.000001	max_e:	3
min_epsilon:	0.01	max_epsilon:	1
min_st_pr:	0.01	max_st_pr:	10
min_C_i:	0.01	max_C_i:	10
Use MC:	<input checked="" type="checkbox"/>	Use ML:	<input checked="" type="checkbox"/>
		Use NR ML:	<input type="checkbox"/>
ML fit limit:	1e-5	ML max. iter.:	25
MC min. steps:	3000	MC max. steps:	9000
MC max. Delta:	0.4	MC min. Delta:	0.02
MC max. Delta steps:	3000	MC min. Delta steps:	6000
MC value of p [%]:	3.5	MC min. pstat:	100
MC clear pstat over:	1e-4	MC extended minimum scan:	<input type="checkbox"/>
MC cycle num.:			
Replot WSSR rel. change:		Replot interval:	
Save		Exit	

Figure 3.
"Set satellite parameters" pop-up-window

CMWP fit control - All-users/Frontend/Zirc2_2-3dpa_250C/zirc2_2_3dpa_250C

S1_l:	.01	S1_wl:	.8		
S1_eta:	.8	S1_s0:	.02		
S1_fit:	2	S1_al:	-.5	S1_a2:	-.2
S2_l:	.000000001	S2_wl:			
S2_eta:		S2_s0:			
S2_fit:	0	S2_al:		S2_a2:	
S3_l:	.000000001	S3_wl:			
S3_eta:		S3_s0:			
S3_fit:	0	S3_al:		S3_a2:	
S4_l:	.01	S4_wl:	.8		
S4_eta:	.8	S4_s0:	.02		
S4_fit:	2	S4_al:	-.5	S4_a2:	-.2
		Save and Exit		Exit without saving	

Figure 4.
"Call MKSpline" pop-up window

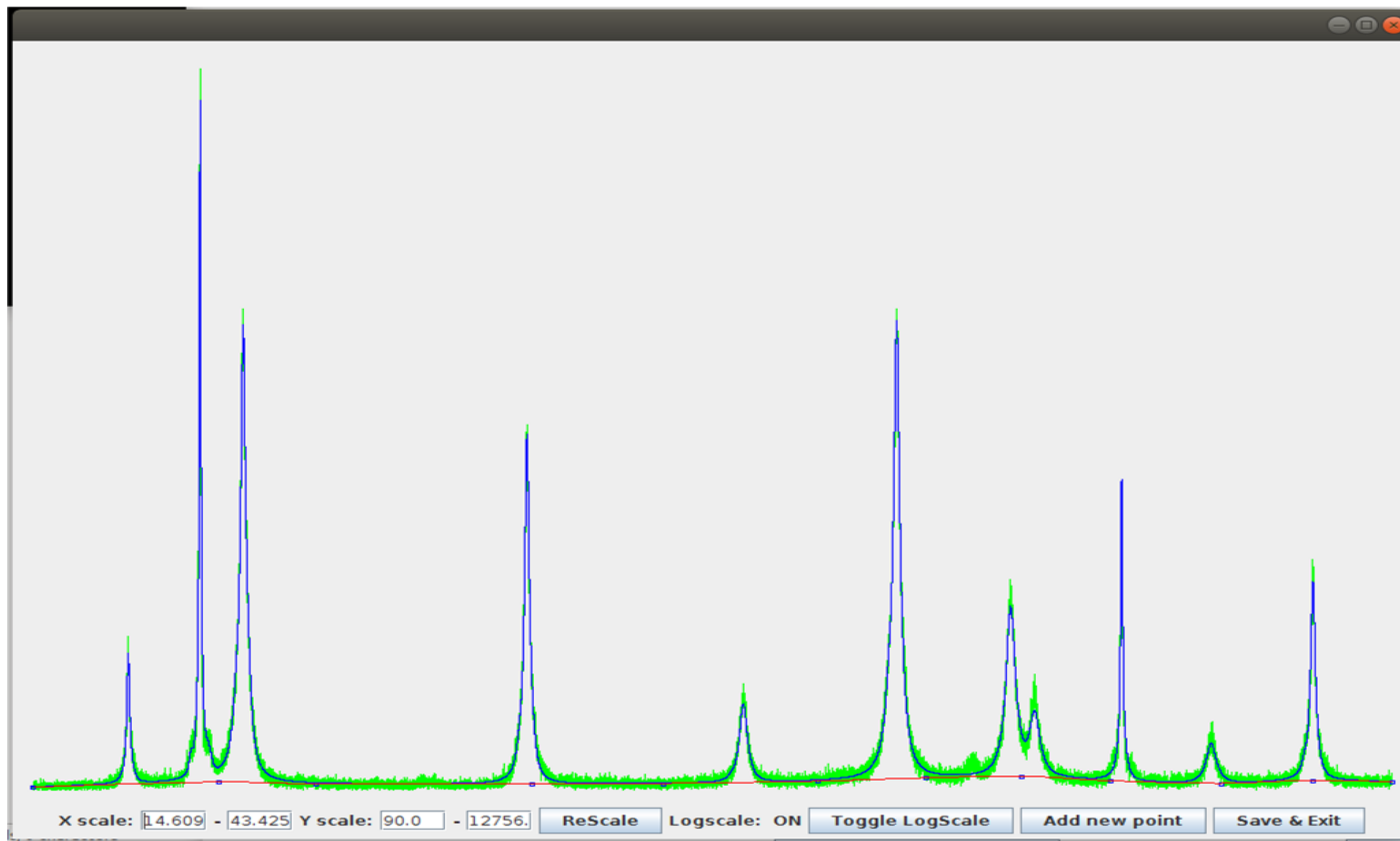


Figure 5.
Zoomed intensity scale of "Call MKSpline" pop-up window

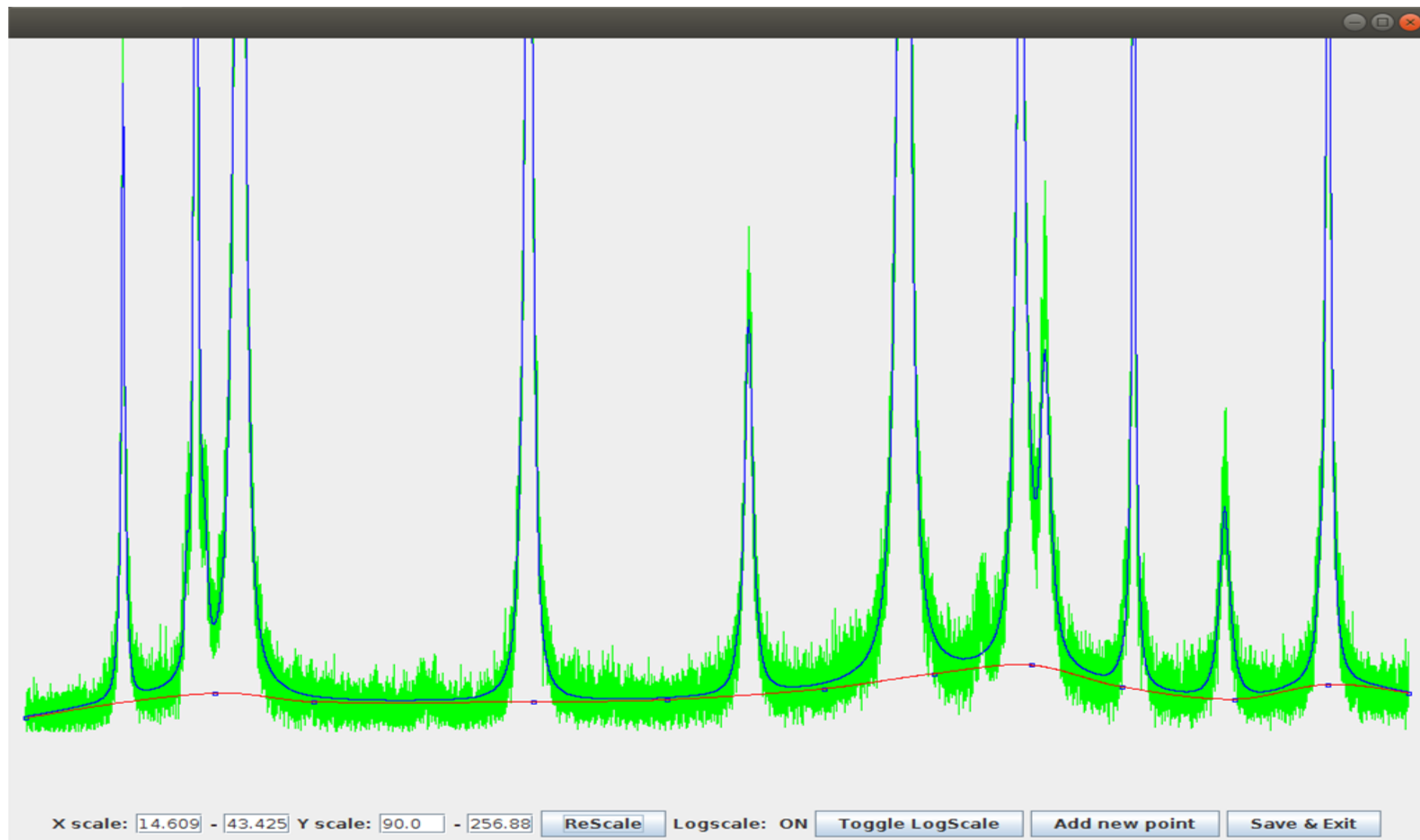


Figure 6.
Zoomed horizontal scale of "Call MKSpline" pop-up window

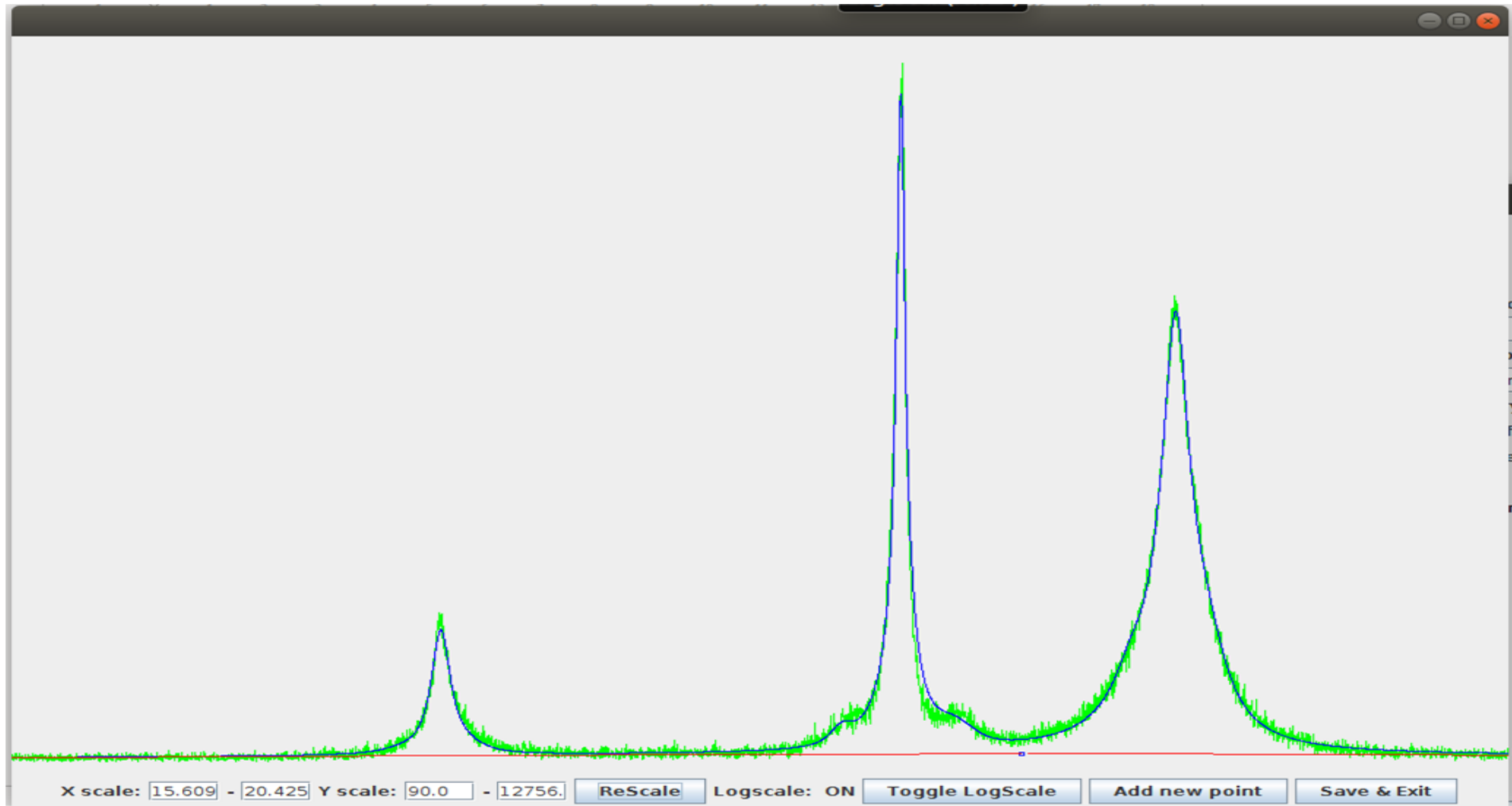


Figure 7.

Gnuplot image of fitting along with satellites (dash blue lines) available from the output files once the fitting procedure was done. (Note that the satellite peaks are added to the background spline.)

