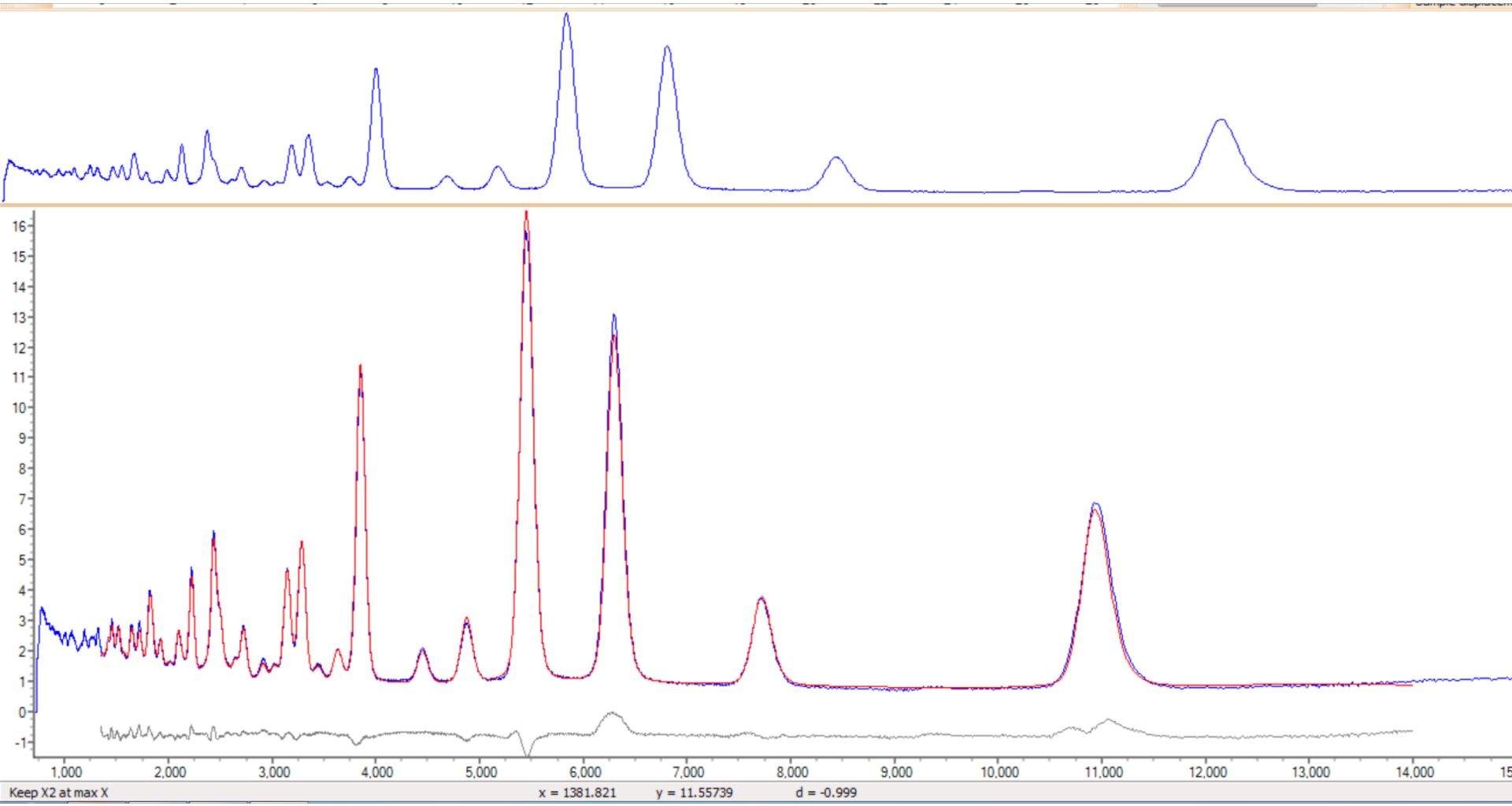
Get a good Rietveld fitting



Rietveld -> LeBail Step-1

```
1
2  '------------------------------------------------------------------------------#
3  iters 100000 → 0
4  chi2_convergence_criteria 0.000001
5  'Auto_T(2)                                                  ' simulated annealing
6  do_errors
7  no_LIMIT_warnings
8  'continue_after_convergence
9  r_wp  4.59913937 r_exp  0.436003648 r_p  4.19709076 r_wp_dash  5.57778862 r_p_dash  6.9788
10 '------------------------------------------------------------------------------#
```

Rietveld To LeBail Step-2

```
'------------------------------------------------------------------------------------------ ### Main refinemer
#ifdef Si_NOMAD_bank2
xdd "NOM_Sn1Fe3_10_K-1.xye"
r_wp  4.37533342 r_exp  0.786626218 r_p  3.86891702 r_wp_dash  5.8107804 r_p_dash  7.41848766 r_exp_dash  1.04

    NeutronDiffraction                                          ' TOF neutron diffraction data
    local alpha0 -52.16841` min -200 max 200      ' GSAS back to back function
    local alpha1  30.76918` min -200 max 200
    local beta0  -10.09696` min -200 max 200
    local beta1  -1.37726` min -200 max 200


    local !Lpath 21.125                          ' Using Lobanov absoprtion funciton for TOF neutron. Details i
    local !two_theta 31
    local mu  0.00000`_0.00728 min 0 max 1
    Abs_Lobanov

    scale_pks = D_spacing^4;                ' Scale peak intensity as d^4
    bkg @  1.00304645`_0.0106173269 -0.256080107`_0.0167168543  0.222906868`_0.0148364912 -0.109785986`_0.0139
    start_X 1350
    finish_X 14000
    TOF_x_axis_calibration(!t02_90, 11.99445_2.51045 , !difc2_90, 2846.73760_6.81217, difa2_90,  3.13577`_0.74

    str
        phase_name "Sn1Fe3"
        space_group Pm-3m
        Phase_LAC_1_on_cm( 0.00000)
        Phase_Density_g_on_cm3( 7.68237`_0.01072)
        Cubic(a  3.796212`_0.001766)
        site Sn x  0 y  0 z  0 occ Sn 0.25 beq beqSn  4.50516`_0.47911
        site Fe1 x  0 y  0 z  0 occ Fe 0.75 beq beqFe1  0.03003`_0.03336 min=0.03;
        site Fe2 x  0.5 y  0.5 z  0 occ Fe  1 beq beqFe2  0.55681`_0.01820
        site N  x  0.5 y  0.5 z  0.5 occ N  1 beq beqN  0.72681`_0.02106
        scale scale_nuclear  1.73489387`_0.03059

        TOF_PV(@, 2451.96911`_21.41087,@ , 0.289921927`_0.022908466, difc2_90)

        'TOF_Exponential (a21, 60.08496_10.50278, a22, 35.28298_10.89156, 4, difc2_90, +)

        moderator_mic_NOMAD(two_theta,31,tspow2, 1.50000`_19.78177,alph02, 0.43663`_0.44200,alph12, 0.01000`_0

#endif
```

To be replaced

To Keep

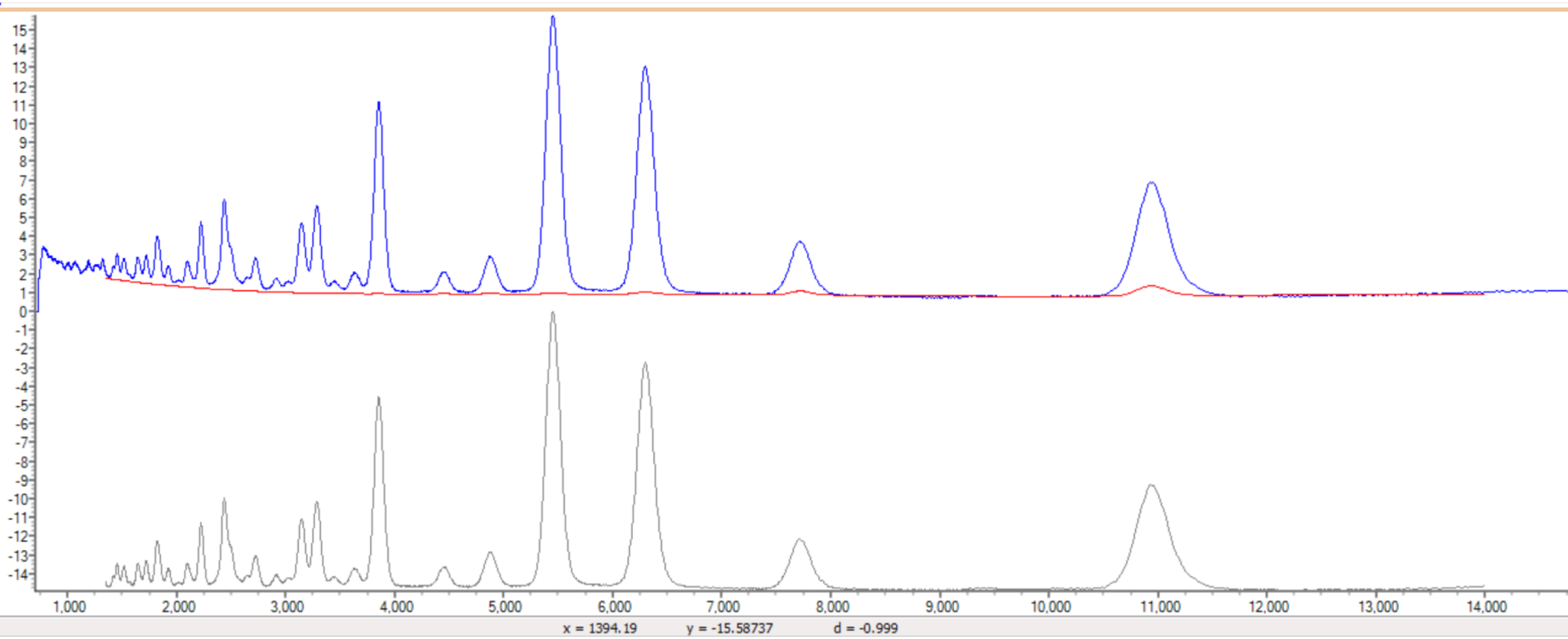
Rietveld To LeBail Step-2

```
'------------------------------------------------------------------------------------------ ### Main refinemer
#ifdef Si_NOMAD_bank2
xdd "NOM_Sn1Fe3_10_K-1.xye"
r_wp  4.37488743 r_exp  0.786626218 r_p  3.8712888 r_wp_dash  5.81021557 r_p_dash  7.42334527 r_exp_dash  1.04

    NeutronDiffraction                                          ' TOF neutron diffraction data
    local alpha0 -52.16841` min -200 max 200      ' GSAS back to back function
    local alpha1  30.76918` min -200 max 200
    local beta0  -10.09696` min -200 max 200
    local beta1  -1.37726` min -200 max 200


    local !Lpath 21.125                          ' Using Lobanov absoprtion funciton for TOF neutron. Details i
    local !two_theta 31
    local mu  0.00000`_0.00729 min 0 max 1
    Abs_Lobanov

    scale_pks = D_spacing^4;                ' Scale peak intensity as d^4
    bkg @  1.0031498`_0.0106137501 -0.256190597`_0.0167118208  0.22309758`_0.0148336004 -0.11012634`_0.013952
    start_X 1350
    finish_X 14000
    TOF_x_axis_calibration(!t02_90, 11.99445_2.51045 , !difc2_90, 2846.73760_6.81217, difa2_90,  3.13731`_0.74

    hkl_Is
        phase_name "Sn1Fe3"
        Phase_LAC_1_on_cm( 0.00000)
        Phase_Density_g_on_cm3( 0.00000)
        MVW( 0.000, 54.778, 0.000)
        space_group "Pm-3m"
        Cubic(3.796226)
        scale 1

        TOF_PV(@, 2452.34193`_21.32188,@ , 0.289724397`_0.0229157273, difc2_90)

        'TOF_Exponential (a21, 60.08496_10.50278, a22, 35.28298_10.89156, 4, difc2_90, +)

        moderator_mic_NOMAD(two_theta,31,tspow2, 1.50000`_19.52490,alph02, 0.43752`_0.44406,alph12, 0.01000`_0

#endif
```

New LeBail Section

Peak Profile from Rietveld

Run LeBail for 0 time



Since we change the iteration number to 0, Topas then just run once without any fitting. The LeBail intensities will be initialized to be 1 and the calculation is then far away from the experiment, as can be seen in the picture above. However, this DOES NOT matter since we are only going to extract the peak profiles where we will anyway set the intensity of each hkl peak to 1. The reason we want to force 0 LeBail run is that we don't want the already refined peak profiles from the Rietveld refinement to be changed in the LeBail running. In that case, we have inconsistency introduced, which is probably not we want in principle.