

**The Physics of X rays
interacting in Ceramics,
Glasses, Soils and
predominantly Silica
material such as “Rocks “**

X rays interact with Si /Ca based materials in 4 different ways;

1. X rays are absorbed by the bound electrons in the atoms that make up the material . Then those atoms emit characteristic x rays based on the electron energy level and resulting electron transition in the atom that absorbed the x ray. This is the process that leads to the term x ray fluorescence.
2. The incoming and out going x rays maybe scattered elastically. This is known as Raleigh scattering. In this case the direction of the x ray is changed but there is no loss in energy.
3. The incoming and out going x rays maybe scattered inelastically. This is known as Compton scattering. In this case the direction of the x ray is changed and there is a loss in energy. For the Tracer system the geometry is such that those x rays that are coming from the tube that are inelastically scattered back into the detector always lose about 5% of their energy. This is because the energy that the detector can detect is defined by geometry of source, sample and detector and that remains constant in the Tracer. This will be shown experimentally below.
4. The fourth x ray interaction is only present when the material being measured has large scale atomic ordering like in a quartz crystal. This is called coherent or Bragg Scattering.

Note for the materials discussed in this paper elastic and inelastic scatter of x rays above 18 keV occurs with about equal probability. This will be shown experimentally below. Also it is very unlikely that one will see Bragg scattering as almost all the materials are not atomically ordered on a large scale, indeed they are generally very amorphous.

1. X rays are absorbed by the bound electrons in the atoms that make up the material . Then those atoms emit characteristic x rays based on the electron energy level and resulting electron transition in the atom that absorbed the x ray. This is the process that leads to the term x ray fluorescence.

When an incoming x ray is close to, but just above, the binding energy of the bound K or L shell electron in a given atom there is a high probability that the electron in the atom will absorb the incoming x ray and cause the electron /x ray pair to leave the atom. After this the electron from a level above the missing electron in the atom moves down into the vacant spot and the electron that moves down then emits the energy difference between the levels as an x ray.

So there are 3 very important bits of physics that must go on before we detect such an emitted x ray from our sample.

1. First the incoming x ray must be of the right energy to get absorbed
2. Second it must be able to reach the atom of interest in the sample
3. And finally the resulting emitted x ray must make it back out of the sample into the detector for us to detect it and count it.

We have described how the first item above occurs but how does item 2 happen? Again physics takes over and the answer gets complicated. The first question is how deep is the atom in the sample and what is the binding energy of the bound electron we are trying to move. Let us use Y for example. The binding energy of its K shell electron is 17.04 keV. So the incoming x ray must be above this. That is the first important fact. Now what material is the Y atom in. Let us assume it is glass (80.6% [SiO₂](#), 12.6% [B₂O₃](#), 4.2% [Na₂O](#), 2.2% [Al₂O₃](#), 0.04% [Fe₂O₃](#), 0.1% [CaO](#), 0.05% [MgO](#), and 0.1% [Cl](#)). How deep the incoming x ray gets then depends on the energy of that x ray. The mass attenuation coefficient is a function of both the material (glass) and the energy of the incoming x ray. Something slightly above 17.04 keV. The higher the energy above this the deeper the incoming x ray can go into the material. This parameter is denoted by μ . In the equation below. A narrow beam of monoenergetic photons with an incident intensity I_0 , penetrating a layer of material with mass thickness x and density ρ , emerges with intensity I given by the exponential attenuation law

$$I/I_0 = \exp[-(\mu/\rho)x] .$$

Note that the mass thickness is defined as the mass per unit area, and is obtained by multiplying the thickness t by the density ρ i.e., $x = \rho t$.

So let us use this equation for 2 energies in “glass” above 17.04 keV. We will use 20 keV and 30 keV and we will calculate the depth at which all but 1% of the x rays are stopped i.e. we will assume that I / I_0 is 0.01. Solving for t in the above equation gives

t = thickness of material attenuating x rays

$$t = -\ln(I/I_0) / ((\mu/\rho) \rho)$$

(μ/ρ) = Mass attenuation coefficient read off the chart for a given material and a given x ray energy

ρ = density of the material that the x ray are going through

I = Beam intensity with attenuation

I_0 = Beam intensity without attenuation

Use a value of .01 for the ratio I/I_0 to assume that all but 1% of x rays have been stopped

Glass, Borosilicate ("Pyrex")

HTML table format

μ/ρ

Energy in MeV

1.03542E-03	2.887E+03
1.07210E-03	2.634E+03
1.07210E-03	2.800E+03
1.50000E-03	1.152E+03
1.55960E-03	1.037E+03
1.55960E-03	1.079E+03
1.69350E-03	8.629E+02
1.83890E-03	6.883E+02
1.83890E-03	1.776E+03
2.00000E-03	1.500E+03
3.00000E-03	5.123E+02
3.60740E-03	3.098E+02
3.60740E-03	3.133E+02
4.00000E-03	2.355E+02
5.00000E-03	1.260E+02
6.00000E-03	7.500E+01
8.00000E-03	3.269E+01
1.00000E-02	1.705E+01
1.50000E-02	5.217E+00
2.00000E-02	2.297E+00
3.00000E-02	7.987E-01

This data is taken from
this website

[http://physics.nist.gov/
PhysRefData/
XrayMassCoef/ComTab/
pyrex.html](http://physics.nist.gov/PhysRefData/XrayMassCoef/ComTab/pyrex.html)

$$t = -\ln(I/I_0) / ((\mu/\rho) \rho *)$$

So the intensity ratio is .01

The *Density* = 2.23 g/cm³.

And the attenuation coefficient at 20 keV is 2.3

And the attenuation coefficient at 30 keV is 0.8

And the attenuation coefficient at 14 keV is 76.0

So plugging these numbers in gives a thickness of .9 cm for 20 keV and 1.1 cm.

And to answer item 3 above: the resulting emitted x ray must make it back out of the sample into the detector for us to detect it and count it. The Sr x ray coming out of the glass at 14 keV can go through only .027 cm.

So from the above we have learned that the depth the incoming x rays needed to excite a given atom to fluorescence far exceeds the depth from which the fluorescence for that atom can escape. When measuring Sr and the atoms on the periodic table about it; Nb, Y, Zr and Nb we are measuring to a depth of about 3 mm, because this is the depth that the x rays from those atoms can get out of the silica material .

Using the same equations and the attenuation coefficient for the Si K alpha emission of 1.74 keV we find that in glass we measure Si to a depth of .03 mm. Or 1/100 the depth to which one can measure Sr!

So when measuring ceramic material that are relatively fine grain with the Tracer for the elements of Nb, Sr, Y, Zr and Nb one is measuring a 3 by 4 by (oval spot area of the Tracer) 3 mm (depth) volume!. If the material is uniform on this scale which most unglazed ceramics are then one gets a very good average content analysis.

Thus powdering the sample would not give one a different answer for the ratio of these elements.

This is not true of the lower mass elements like Si, because when measuring them we are measuring just the surface. Because of the use of slip, dirt, weathering and general use, the surface of the ceramic can be very different that the inner materials

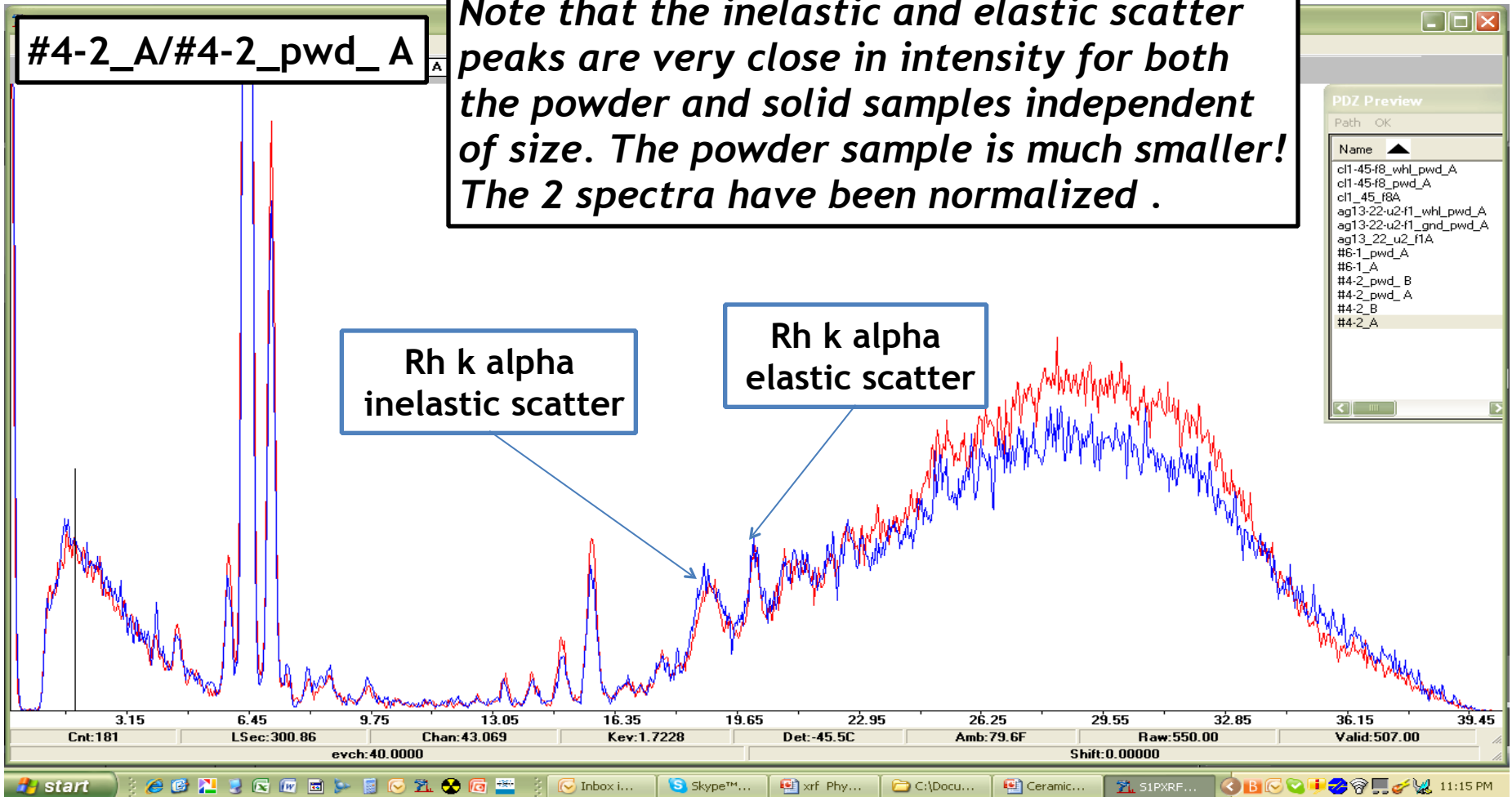
Note for the materials discussed in this paper, elastic and inelastic scatter of x rays above 18 keV occurs with about equal probability.

Note that the inelastic and elastic scatter peaks are very close in intensity for both the powder and solid samples independent of size. The powder sample is much smaller! The 2 spectra have been normalized.

#4-2_A/#4-2_pwd_A

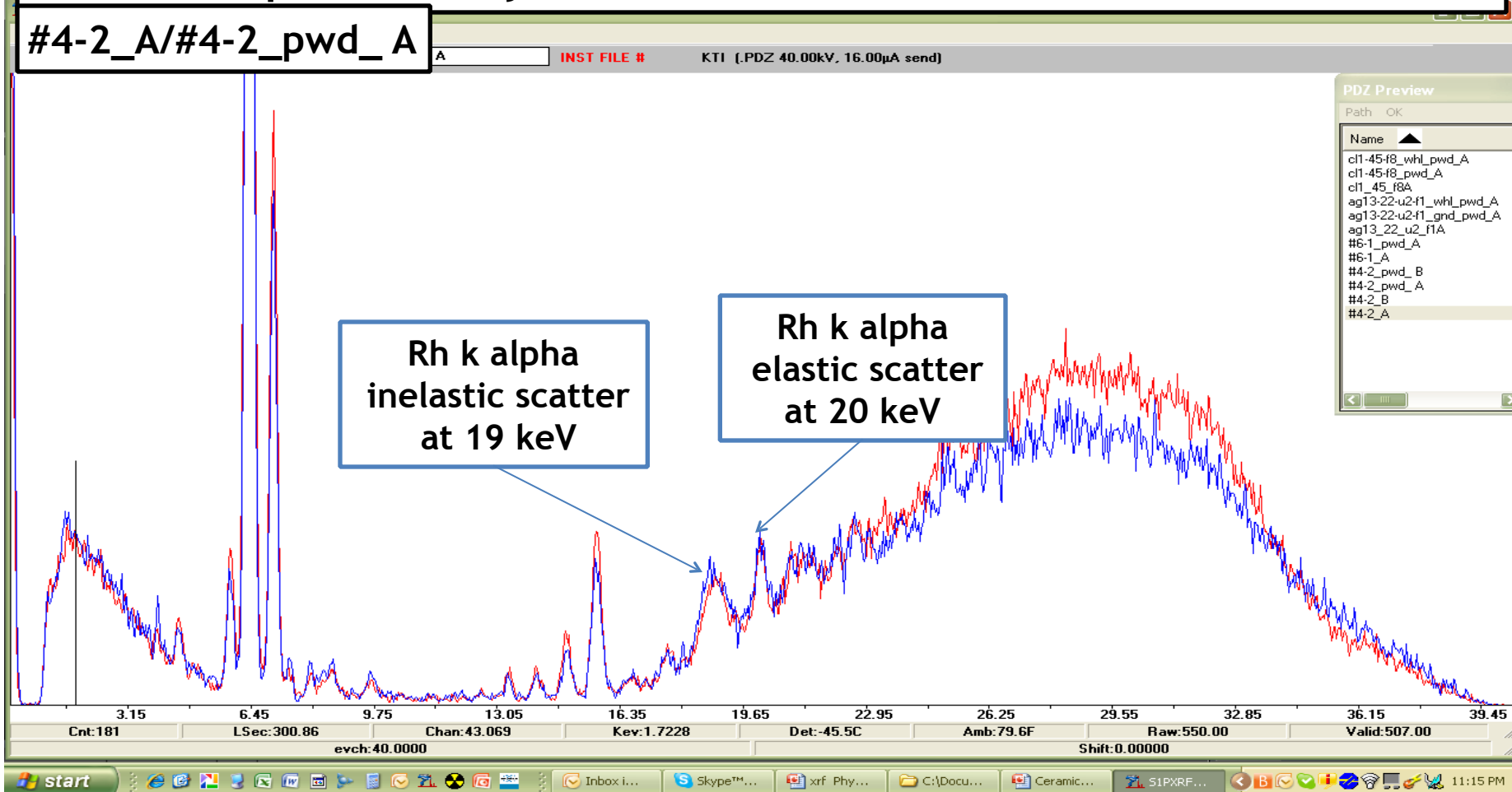
Rh k alpha
inelastic scatter

Rh k alpha
elastic scatter



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#4-2_A/#4-2_pwd_A



Experimental results

**The following
experiment validates
this theoretical
analysis**

Study of the Effect on Elemental Analysis of Converting Sherds From Solid to Powder

It is clear from the plots and the numbers in the charts below that there is no statistical difference **on Elemental Analysis of Converting Sherds From Solid to Powder**. This is true even when one must correct for the sample size difference, when it is not possible to make a powder sample as “thick” as the solid sample, as was done in this case. Note in all cases in the NORMALIZED overlaid plots of the solid and powdered samples below the key elements in the analysis directly overlap with in the statistics of the analysis.

To correct for sample size difference, the data sets were normalized to the signal from Zr or Sr, depending on which was in the sample in significant quantity. This removes the most of the effects of sample size. The relative net area under the elemental lines of interest were then compared and found to not be statistical different, also the entire raw spectrum was overlaid and also showed there to be no statistical difference between the powder and the solid sample when normalized to the key elements.

Rh backscatter was not used in this case because of the very large difference in the powder to solid sample sizes, and the fact that backscatter is caused by very different physics than xrf; so it is best not to use backscatter normalization in this case. Also, one can use the actual fluorescence of a given element in this case, since one is determining if the relative amount of the other elements within solid sample is the same, or different than the powdered sample, as a result of the converting it from a solid to a powder.

Net elemental peak area Normalized to Zr Ka

	Ba K12	Fe K12	Mn K12	Nb K12	Rb K12	Sr K12	Y K12	Zr K12	<u>Zr Norm</u>
#4-2_A@290610_074525	1184	20832	737	55	185	259	440	1268	<u>Zr Norm</u>
#4-2_pwd_A@290610_074525	1078	22116	824	114	124	233	368	1268	<u>Zr Norm</u>
									-
									-
#4-2_B@290610_074525	948	20862	896	121	113	207	347	1268	<u>Zr Norm</u>
#4-2_pwd_B@290610_074525	1010	19861	701	79	166	187	286	1268	<u>Zr Norm</u>
									-
									-
#6-1_A@290610_074525	1683	29651	348	25	114	1712	363	1268	<u>Zr Norm</u>
#6-1_pwd_A@290610_074525	643	26925	345	61	149	1560	307	1268	<u>Zr Norm</u>
									-
									-
NO Zr in Cl1 45 f8A must use Sr									-
cl1_45_f8A@290610_074525	1345	9789	49	16	105	9737	33	1268	<u>Zr Norm</u>
cl1-45-f8_pwd_A@290610_074525	3346	17646	53	93	0	16743	86	1268	<u>Zr Norm</u>
cl1-45-f8_whl_pwd_A@290610_074525	900	6309	52	24	0	5732	7	1268	<u>Zr Norm</u>
									-
cl1_45_f8A@290610_074525	36	260	1	0	3	259	1	34	<u>Sr NORM</u>
cl1-45-f8_pwd_A@290610_074525	52	273	1	1	0	259	1	20	<u>Sr NORM</u>
cl1-45-f8_whl_pwd_A@290610_074525	41	285	2	1	0	259	0	57	<u>Sr NORM</u>
									-
									-
ag13_22_u2_f1A@290610_074525	1919	6988	68	26	93	7447	57	1268	<u>Zr Norm</u>
ag13-22-u2-f1_whl_pwd_A@290610_074525	2131	8570	100	69	27	9855	55	1268	<u>Zr Norm</u>
ag13-22-u2-f1_gnd_pwd_A@290610_074525	2709	12127	184	53	0	11220	109	1268	<u>Zr Norm</u>

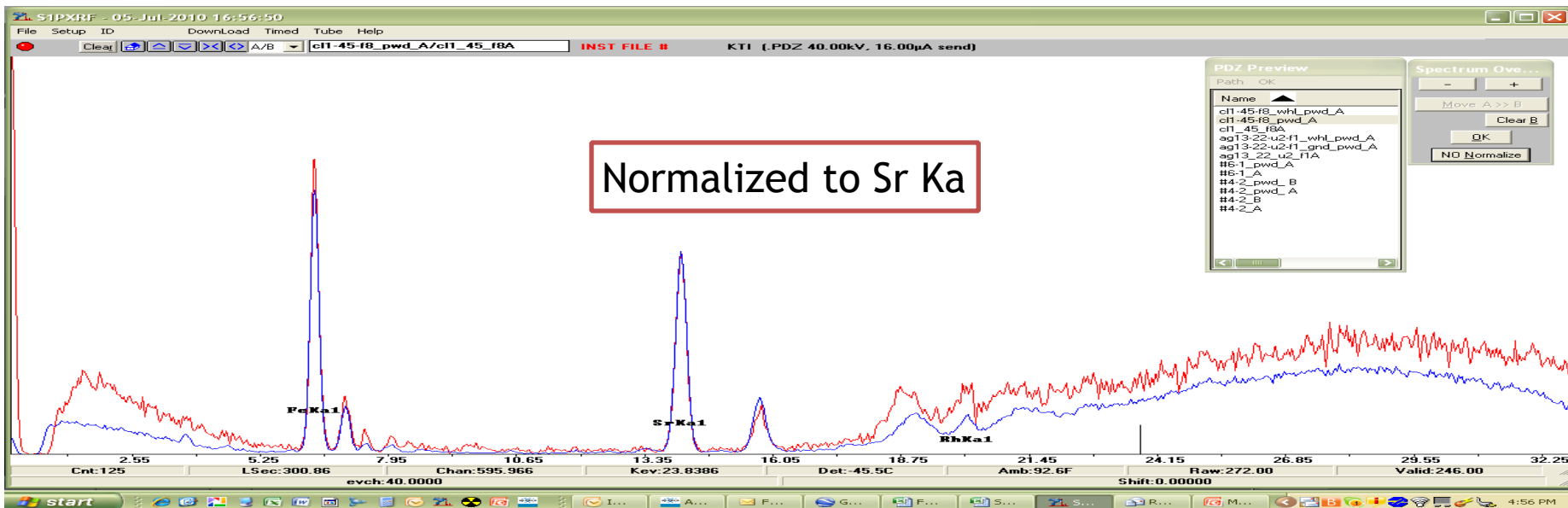
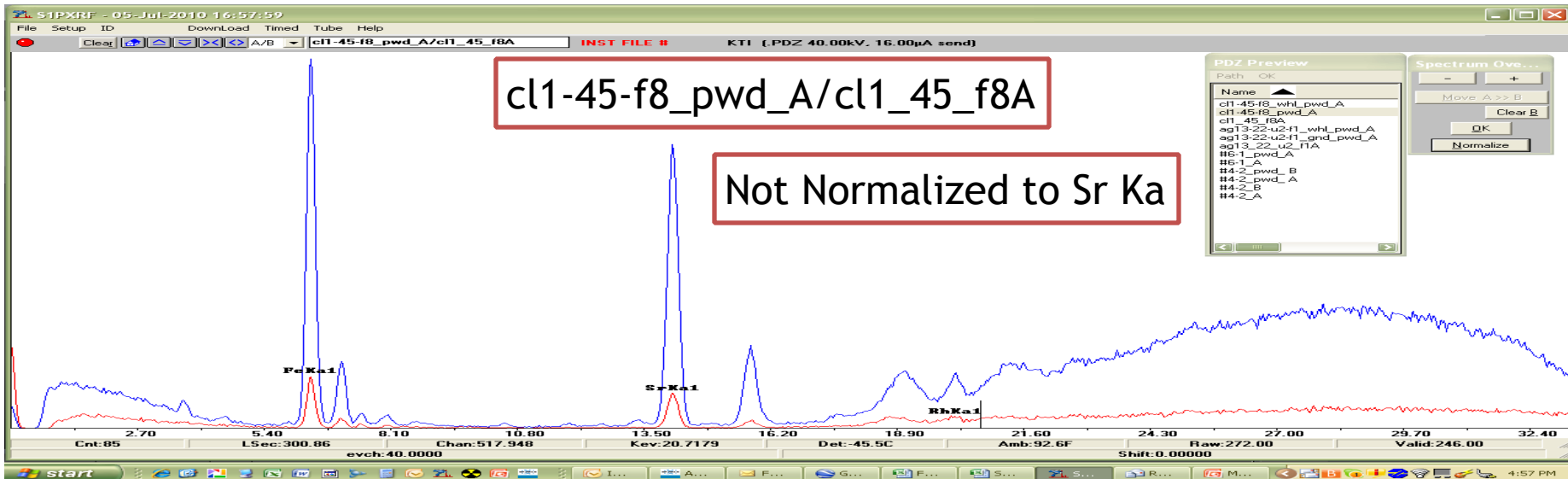
Net elemental peak area Normalized to Sr Ka

	Ba K12	Fe K12	Mn K12	Nb K12	Rb K12	Sr K12	Y K12	Zr K12	
#4-2_A@290610_074525	1184	20832	737	55	185	259	440	1268	Sr NORM
#4-2_pwd_A@290610_074525	1200	24620	917	127	138	259	410	1412	Sr NORM
#4-2_B@290610_074525	1188	26144	1123	152	142	259	435	1589	Sr NORM
#4-2_pwd_B@290610_074525	1398	27478	970	110	230	259	396	1754	Sr NORM
#6-1_A@290610_074525	255	4486	53	4	17	259	55	192	Sr NORM
#6-1_pwd_A@290610_074525	107	4470	57	10	25	259	51	210	Sr NORM
cl1_45_f8A@290610_074525	36	260	1	0	3	259	1	34	Sr NORM
cl1-45-f8_pwd_A@290610_074525	52	273	1	1	0	259	1	20	Sr NORM
cl1-45-f8_whl_pwd_A@290610_074525	41	285	2	1	0	259	0	57	Sr NORM
ag13_22_u2_f1A@290610_074525	67	243	2	1	3	259	2	44	Sr NORM
ag13-22-u2-f1_whl_pwd_A@290610_074525	56	225	3	2	1	259	1	33	Sr NORM
ag13-22-u2-f1_gnd_pwd_A@290610_074525	63	280	4	1	0	259	3	29	Sr NORM

Normalized to Sr
Ka

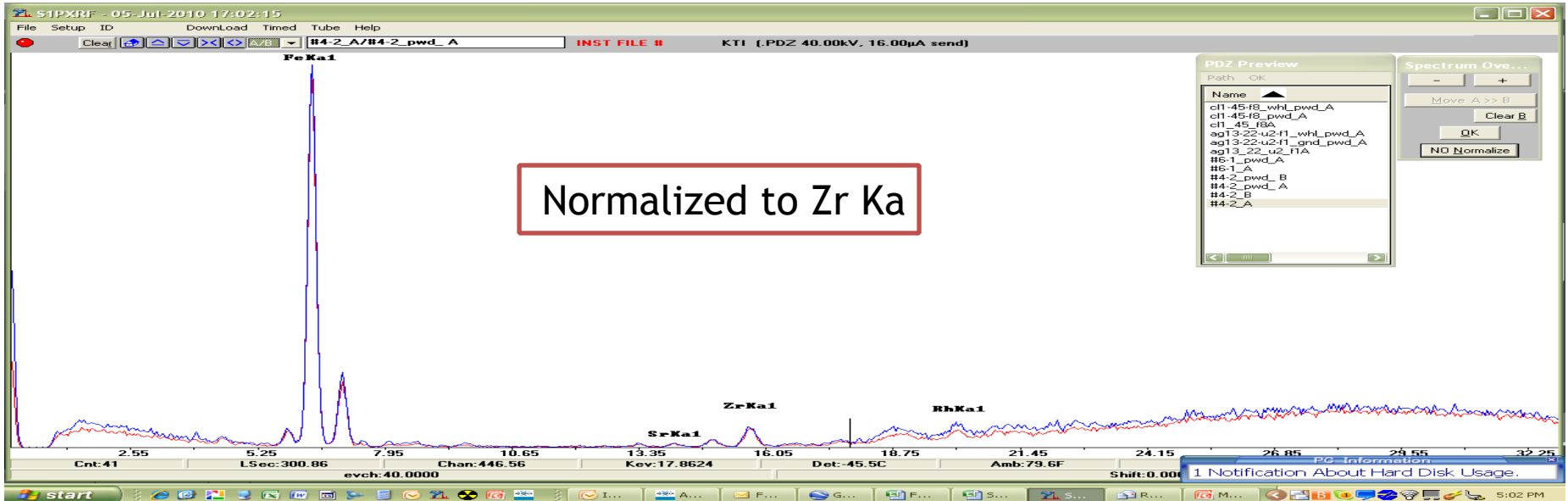
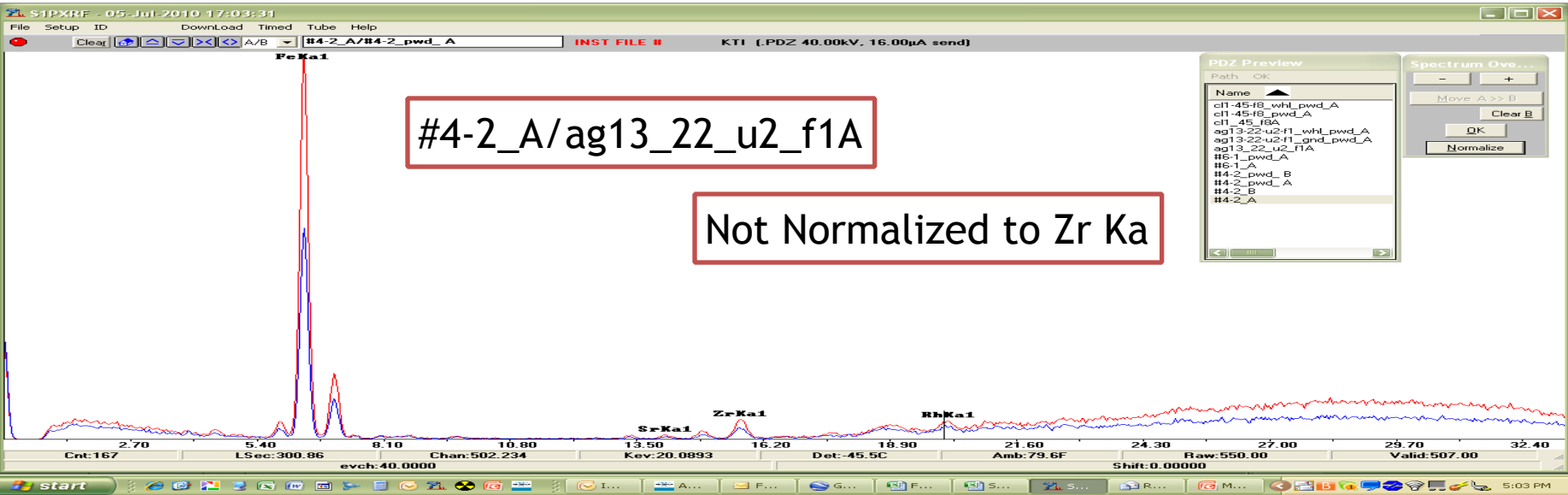
Ba K12	Fe K12	Mn K12	Nb K12	Rb K12	Sr K12	Y K12	Zr K12
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10_074525	36	260	1	0	3	259	1	34	Sr NORM
cl1-45-f8_pwd_A@290610_074525	52	273	1	1	0	259	1	20	Sr NORM
cl1-45-f8_whl_pwd_A@290610_074525	41	285	2	1	0	259	0	57	Sr NORM



Normalized to Zr Ka

Ba K12	Fe K12	Mn K12	Nb K12	Rb K12	Sr K12	Y K12	Zr K12
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1078	22116	824	114	124	233	368	1268

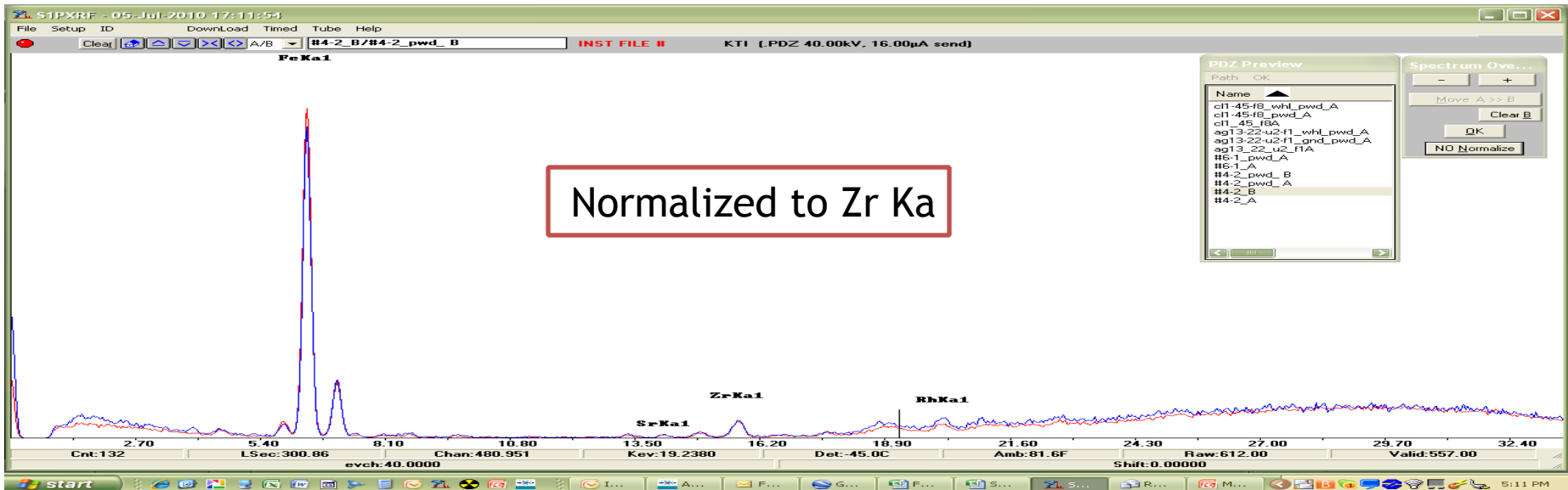
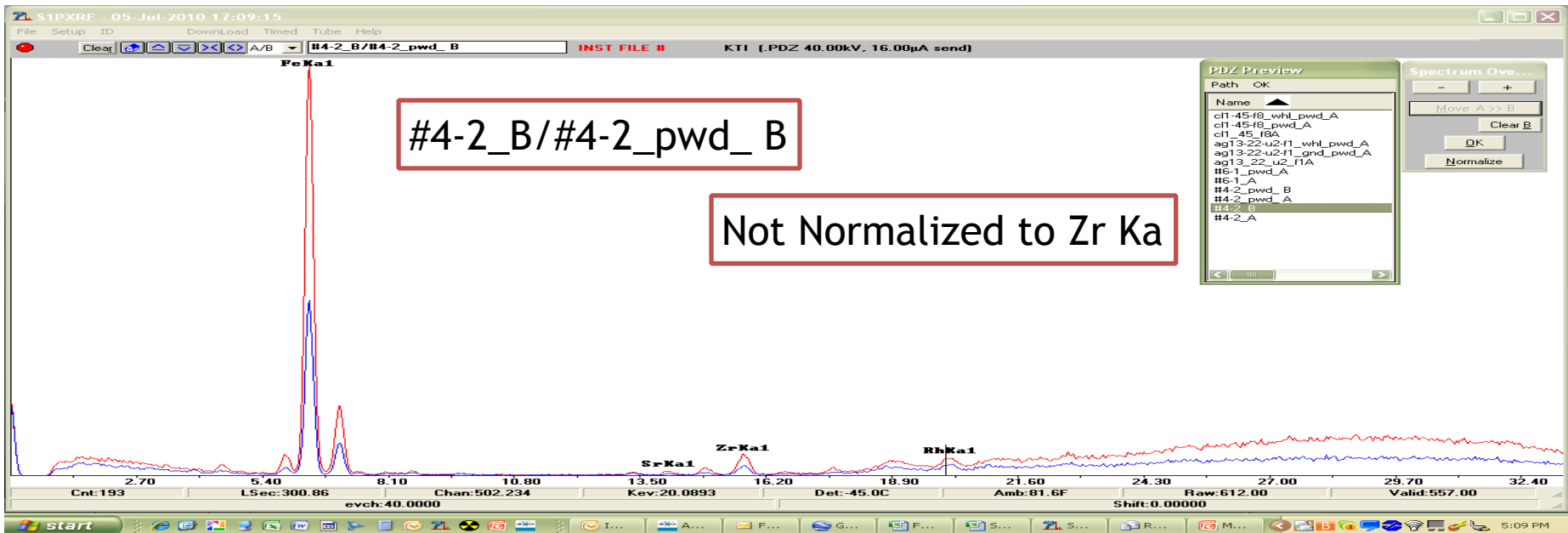


Normalized to Zr Ka

Ba K12	Fe K12	Mn K12	Nb K12	Rb K12	Sr K12	Y K12	Zr K12
948	20862	896	121	113	207	347	1268
1010	19861	701	79	166	187	286	1268

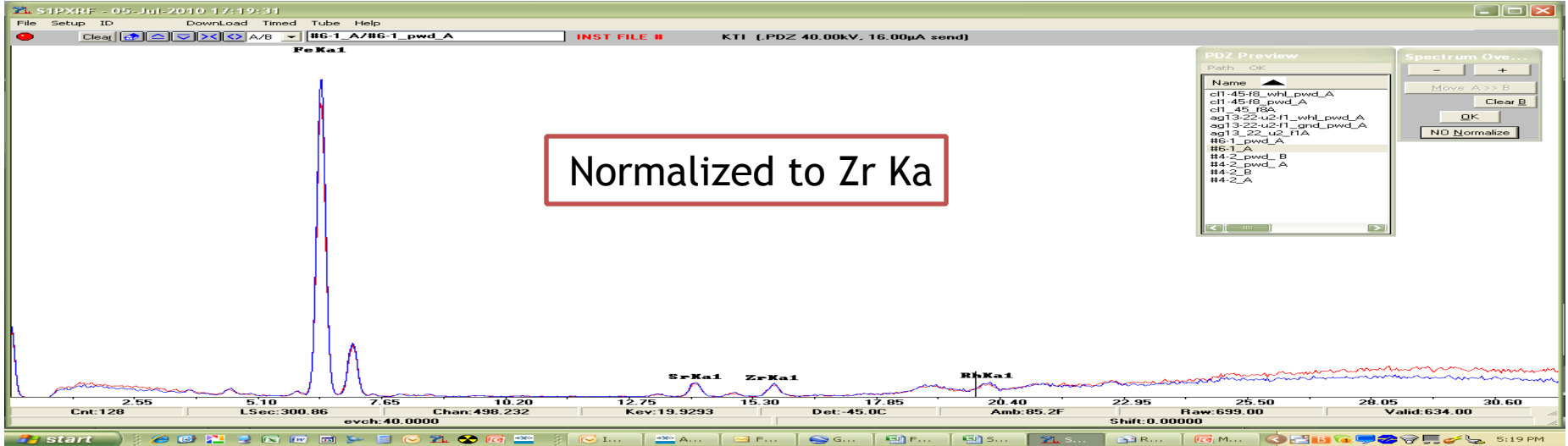
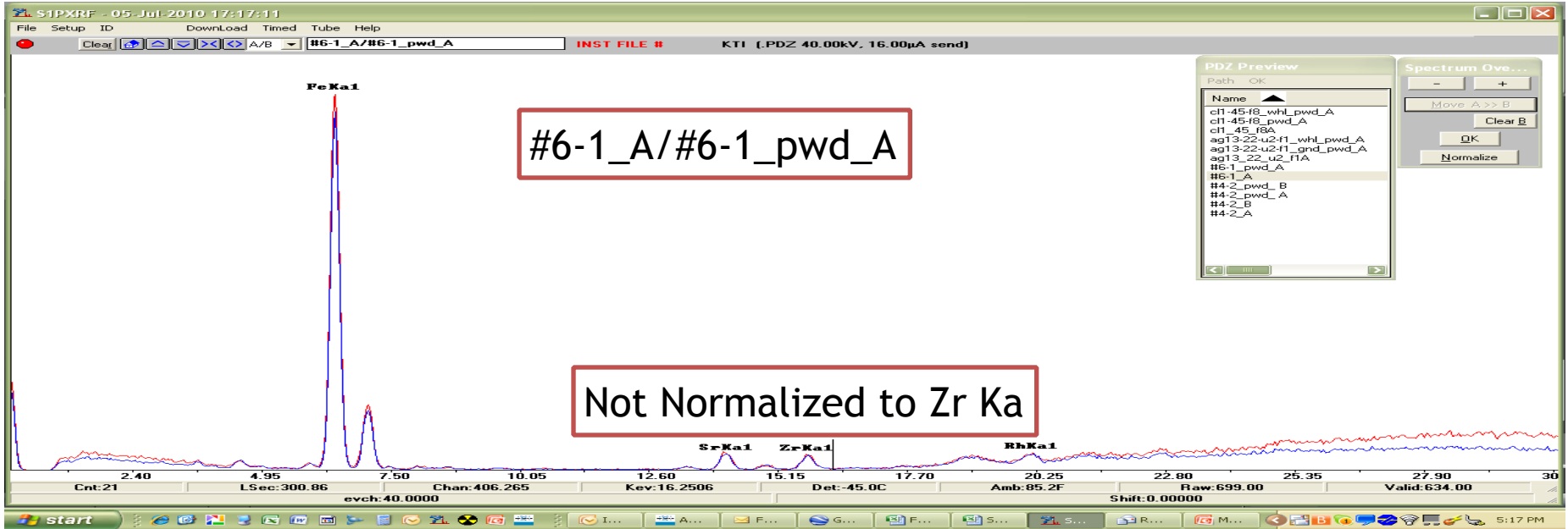
#4-2_pwd_B@290610_074525

#4-2_pwd_B@290610_074525



Ba K12	Fe K12	Mn K12	Nb K12	Rb K12	Sr K12	Y K12	Zr K12
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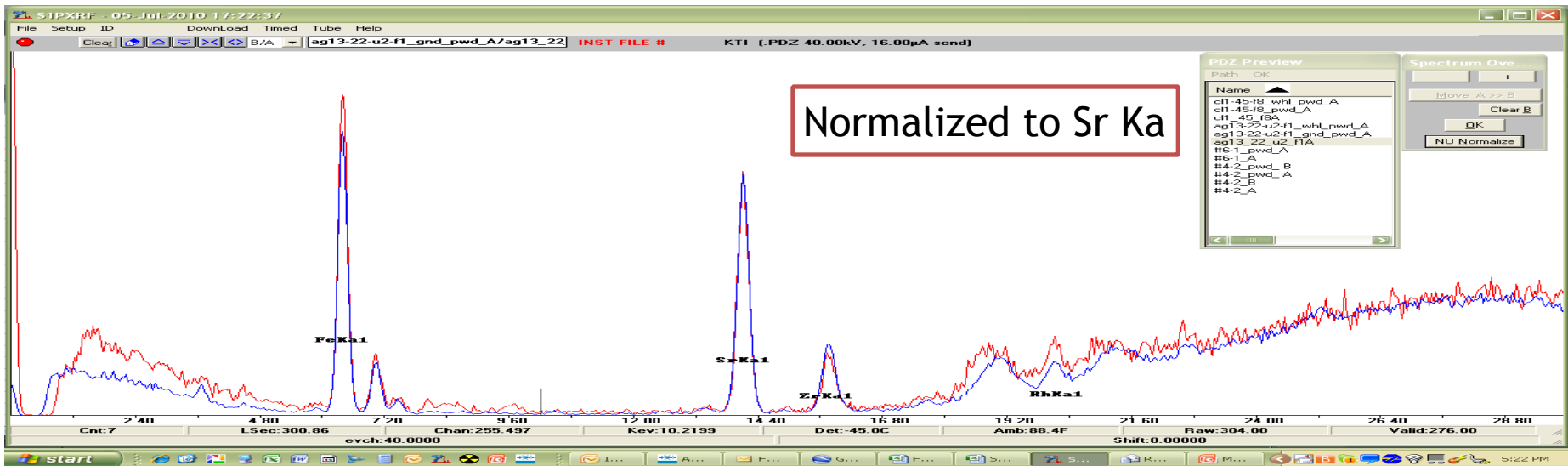
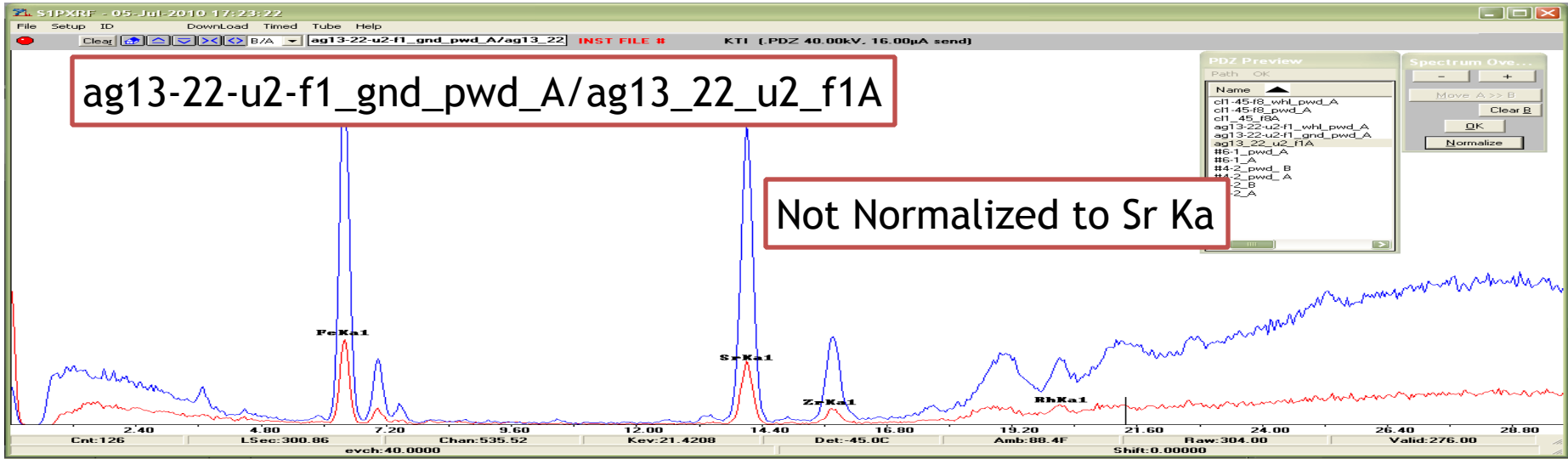
#6-1_A@290610_074525	1683	29651	348	25	114	1712	363	1268
#6-1_pwd_A@290610_074525	643	26925	345	61	149	1560	307	1268



Normalized to Sr

	Ba K12	Fe K12	Mn K12	Nb K12	Rb K12	Sr K12	Y K12	Zr K12
ag13_22_u2_f1A@290610_074525	67	243	2	1	3	259	2	44
ag13-22-u2-f1_whl_pwd_A@290610_074525	56	225	3	2	1	259	1	33
ag13-22-u2-f1_gnd_pwd_A@290610_074525	63	280	4	1	0	259	3	29

Ka



The End