Supplementary Information

Elemental Concentration and Sulfur Chemical Speciation in the Amazonian Plant *Andira surinamensis* Using Synchrotron Radiation Techniques (SR-XRF, XANES), RBS and WD-XRF

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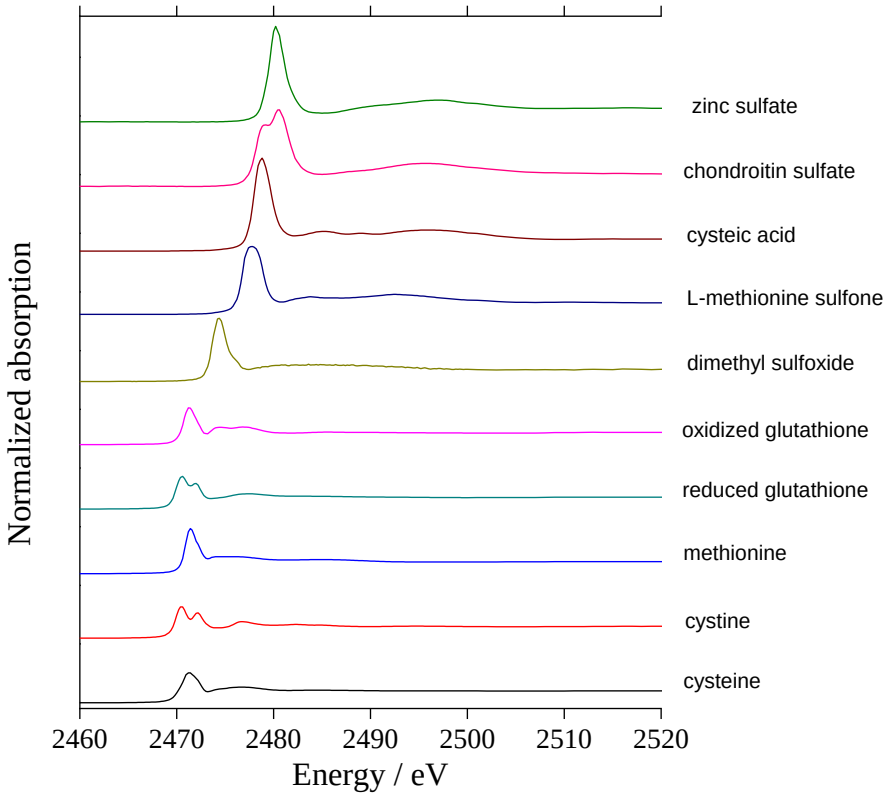

Figure S1. XANES spectra for the set of standards used in the LCF procedure.

Table S1. LLDs and LOQs in WD-XRF

Element	LLD / (μg g^{-1})	LOQ / (μg g^{-1})
Mg	48	160
Al	24	80
Si	16	53
P	10	33
S	7	23
Cl	16	53
K	11	37
Ca	16	53
Mn	9	29
Fe	10	35
Cu	10	33
Zn	10	33
Sr	31	103
Ba	39	129

LLD: lower limit of detection; LOQ: limit of quantification.

Limits of detection were calculated using the spectrometer software. According to the software's manual, the lower limit of detection (LLD) is calculated as:

$$LLD = \frac{3}{m}\sqrt{\frac{I_{Bkg}}{t}} \quad (1)$$

in which m is the sensitivity coefficient; I_{Bkg} the intensity of the background for the wavelength under consideration and t is the counting time on the background. Consequently, a peak can only be detected if it remains above the background fluctuation. LLDs were estimated for the samples or for the standard reference material (SRM) 1570a, whichever contained the element at the lowest concentration.

Limits of quantification (LOQs) were evaluated applying a factor of 10 / 3 to the LLDs.

Table S2. Reference values of SRM 1570a and WD-XRF data

	Reference data / (μg g^{-1})	WD-XRF / (μg g^{-1})	s_{rep} (n = 10) / (μg g^{-1})
Certified value[a]			
Ca	15260 ± 660	15300	600
P	5187 ± 67	5200	270
K	29000 ± 260	30400	1200
Na	18210 ± 230	21400	1200
Al	310 ± 15	270	35
As	0.068 ± 0.012	–	–
B	37.7 ± 1.2	–	–
Cd	2.876 ± 0.058	–	–
Co	0.393 ± 0.030	–	–
Cu	12.22 ± 0.86	–	–
Mn	76.0 ± 1.2	64	9
Hg	0.0297 ± 0.0021	–	–
Ni	2.142 ± 0.058	–	–
Se	0.1152 ± 0.0043	–	–
Sr	55.54 ± 0.50	–	–
Th	0.0480 ± 0.0017	–	–
V	0.568 ± 0.017	–	–
Zn	82.3 ± 3.9	83	6
Reference value[b]			
N	60600 (2000)	–	–
Eu	0.0055 (0.0010)	–	–
Sc	0.0055 (0.0006)	–	–
Rb	12.7 (1.6)	–	–
U	0.155 (0.023)	–	–
Informative value[c]			
S	5000	4800	200
Mg	9000	9300	400
Pb	0.2	–	–
Si		1000	60
Cl	non-informed values[d]	7500	300
Fe		274	14

[a]According to the Certificate of Analysis of the SRM 1570a, certified values are those that "NIST has the highest confidence in its accuracy in that all known or suspected sources of bias have been investigated or taken into account";[1] [b]according to the Certificate of Analysis of the SRM 1570a, reference values are those that "are noncertified values that are the best estimates of the true values based on available data; however, the values do not meet NIST criteria for certification […] and are provided with associated uncertainties that may reflect only measurement reproducibility, may not include all sources of uncertainty, or may reflect a lack of sufficient statistical agreement among multiple analytical methods";[1] [c]according to the Certificate of Analysis of the SRM 1570a, informative values are those that "may be of interest to the SRM user, but insufficient information is available to assess the uncertainty associated with the value, therefore no uncertainty is provided";[1] [d]non-informed values are not included in the SRM certificate but there is information about them in the literature.[2] WD-XRF: wavelength dispersive X-ray fluorescence spectrometry; s_{rep}: standard deviation of the repeatability test.

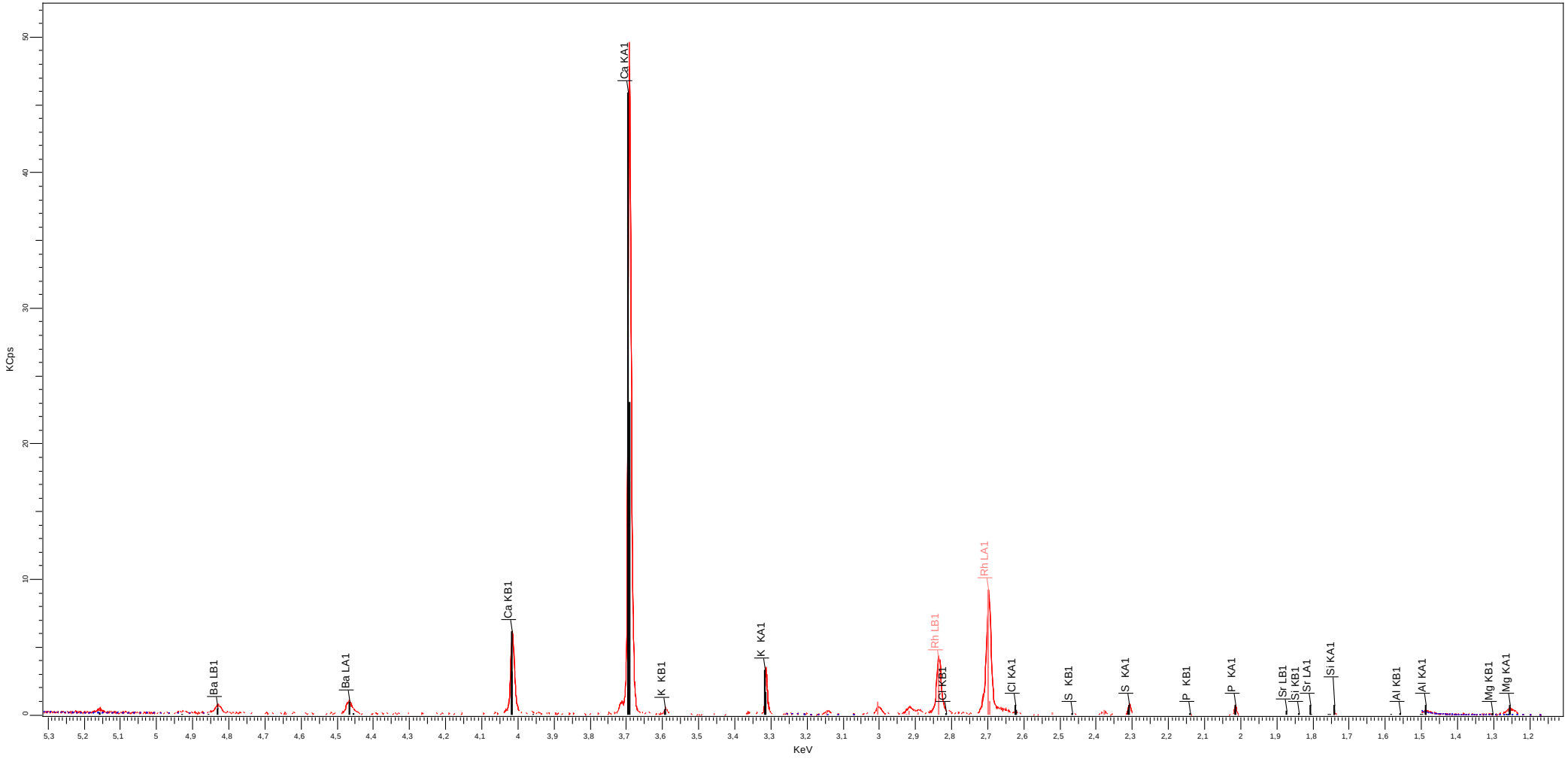

Figure S2. WD-XRF of the bark, part 1 (for a better visualization of lines, zoom in).

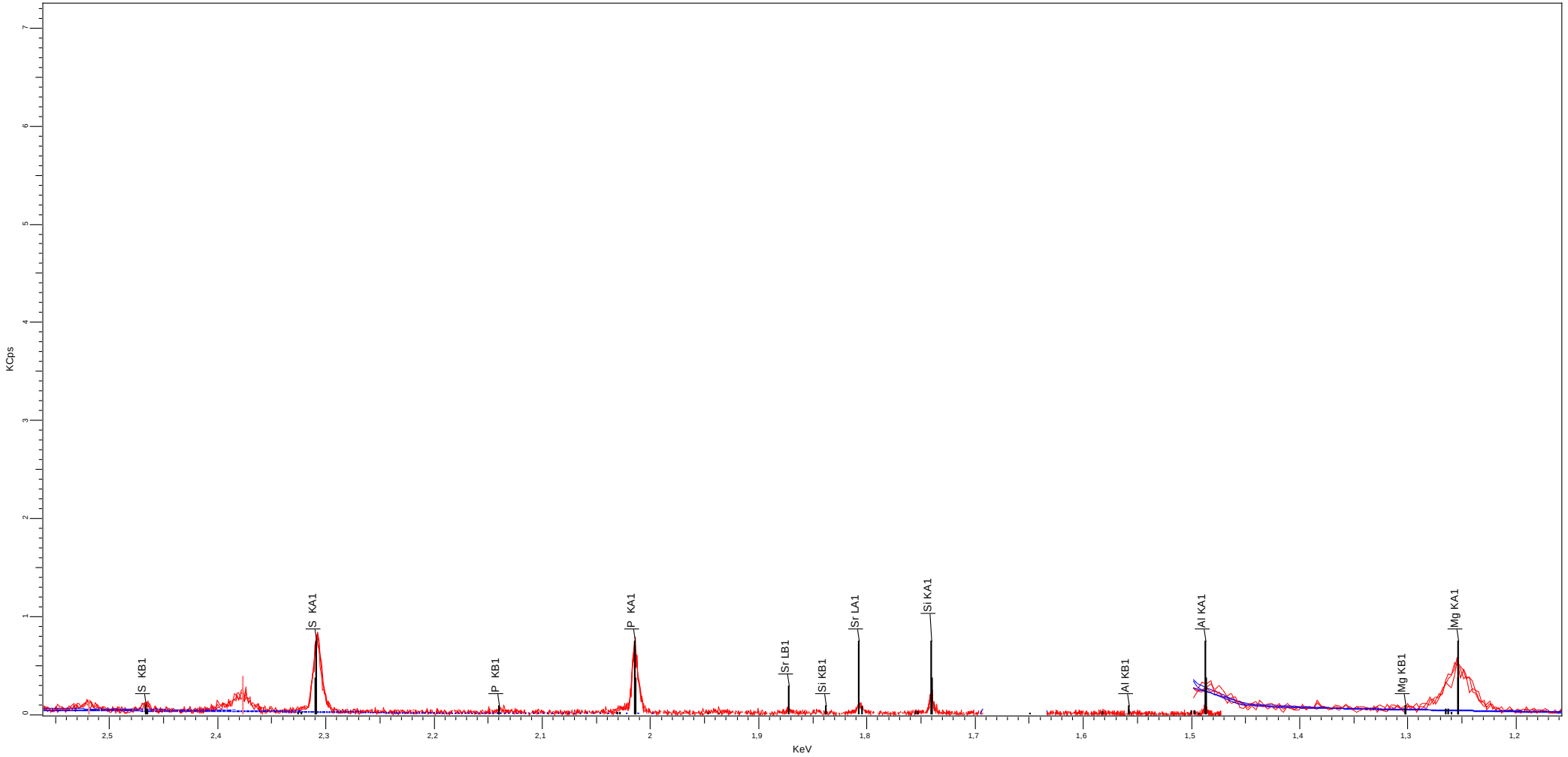

Figure S3. WD-XRF of the bark, part 2 (for a better visualization of lines, zoom in).

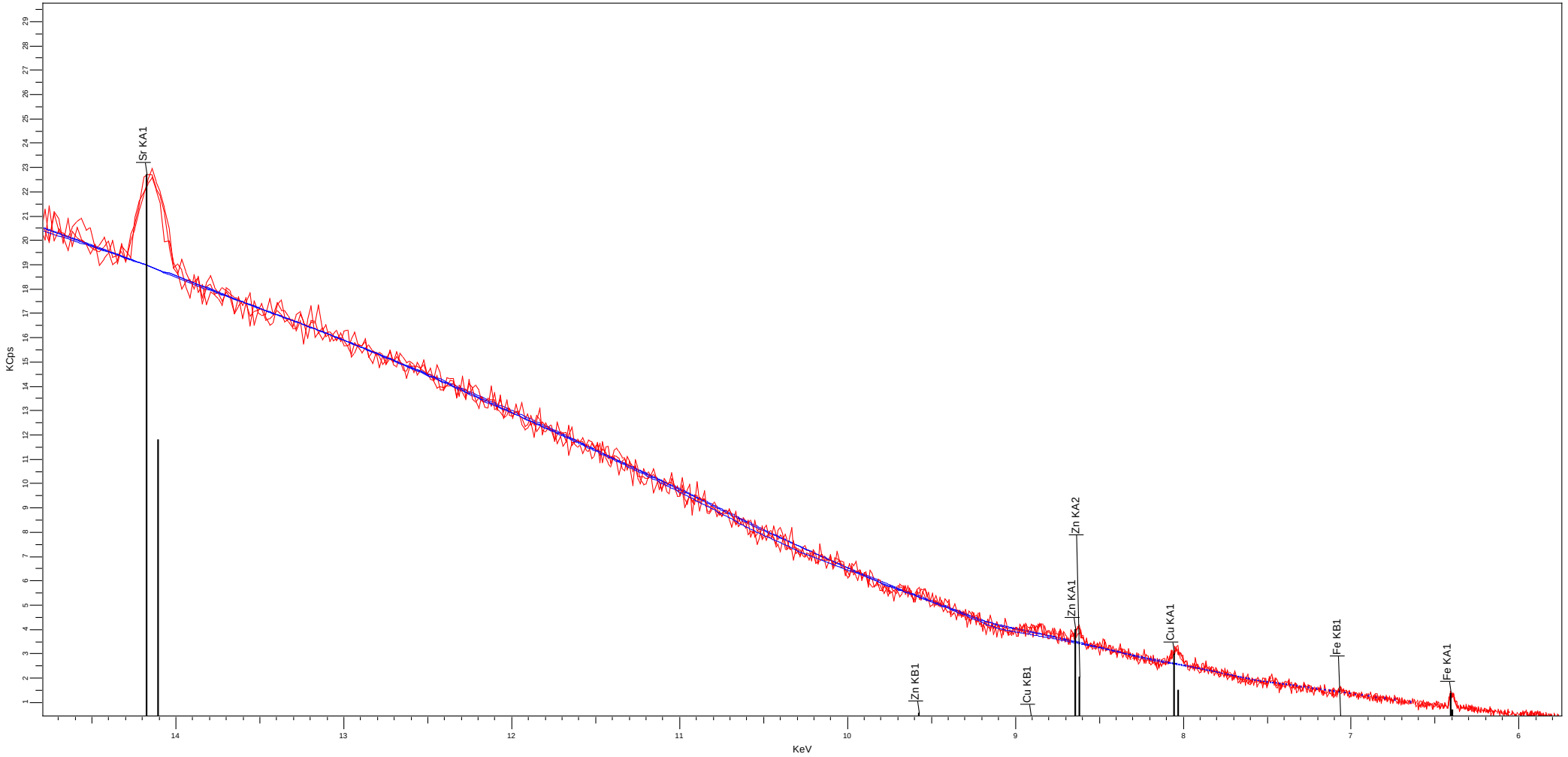

Figure S4. WD-XRF of the bark, part 3 (for a better visualization of lines, zoom in).

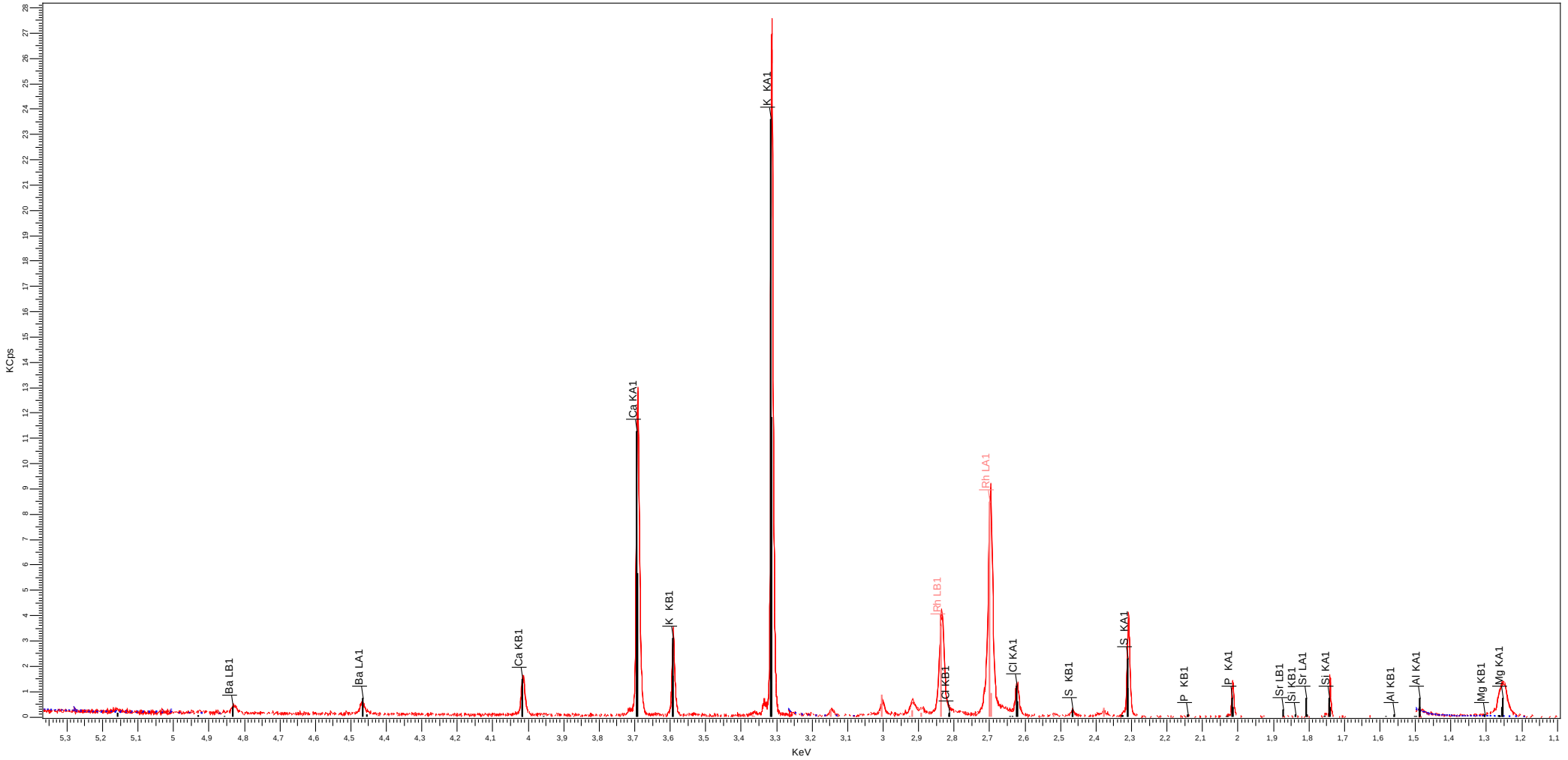

Figure S5. WD-XRF of the leaf, part 1 (for a better visualization of lines, zoom in).

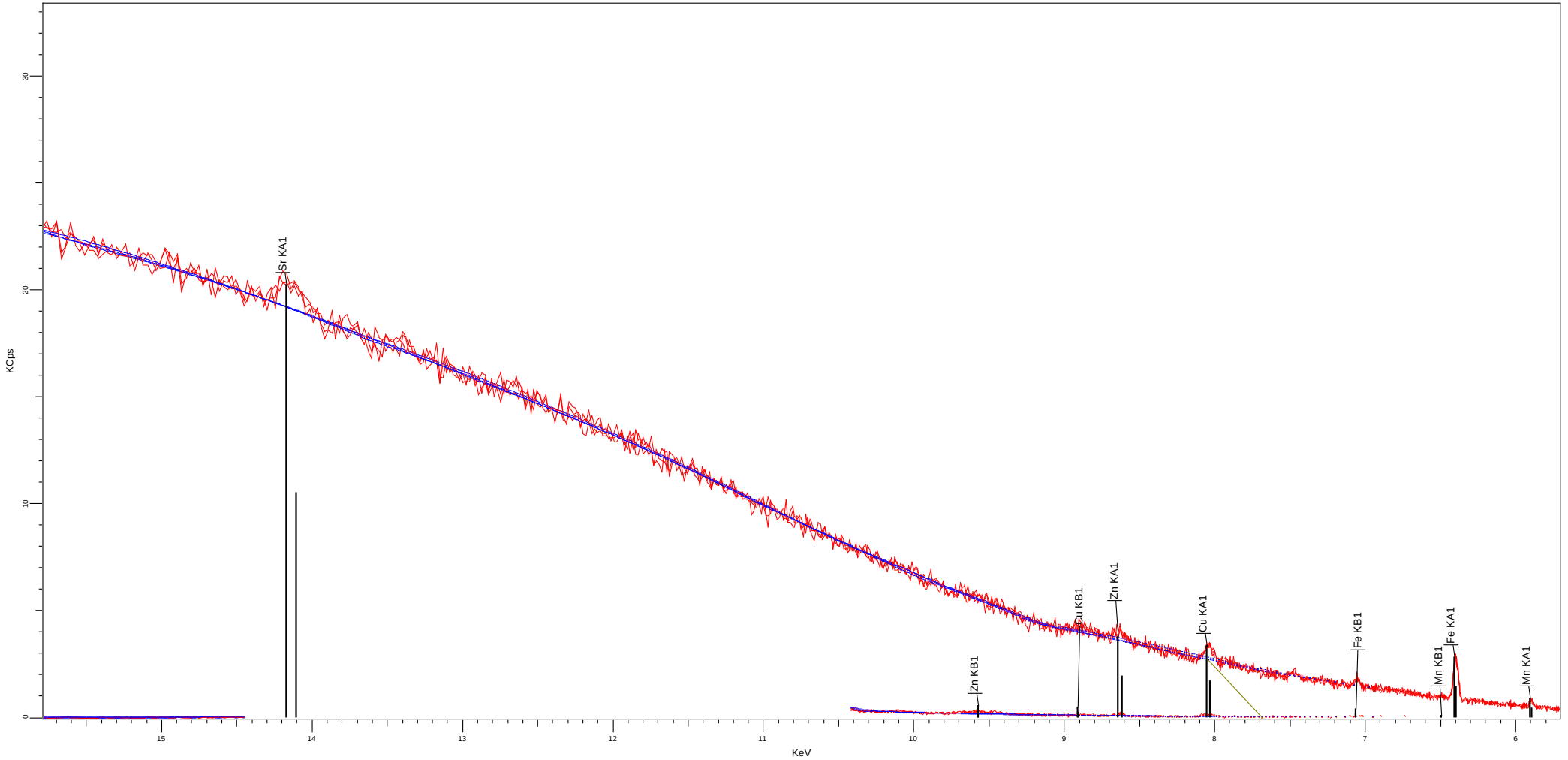

Figure S6. WD-XRF of the leaf, part 2 (for a better visualization of lines, zoom in).

References

1. National Institute of Standards and Technology (NIST); *Standard Reference Material 1570a - Trace Elements in Spinach Leaves*; NIST: Gaithersburg, 2014.

2. Andersen, L. K.; Morgan, T.; Boulamanti, A.; Álvarez, P.; Vassilev, S.; Baxter, D.; *Energy Fuels* **2013**, *27*, 7439.