- Supplementary Data - Introducing an R package for luminescence dating analysis Ancient TL

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June 8, 2012

Contents

List of Figures

List of Tables

1 Example: Fitting loop

This **R** script uses the *Luminescence* package and selects all ramped signal data from a BIN-file. It is assumed that every 2nd curve is a background curve. A 3-component fit is tried for every curve after background subtraction. For every fit a plot is produced. The output is written in the previously defined output folder. The numerical values of the parameter output are written in a CSV-file. Additional values are appended.

```
##fit loop for LM-OSL curve data

##INSERT INPUT AND OUTPUT PATH HERE
input<-"~/Desktop/LM_CurveMeasurement.BIN"
output.path<-"~/Desktop/"
n.components<-3


##load library
library(Luminescence)

##==============================================================================##
## READ AND PREPARE DATA
##==============================================================================##

##read BIN file
temp<-readBIN2R(input)

##grep IDs for signal and background curves
values.ID<-temp@METADATA[temp@METADATA[,"LTYPE"]=="RBR","ID"]
values.HIGH<-temp@METADATA[temp@METADATA[,"LTYPE"]=="RBR","HIGH"]

 ##set IDs for curves
 values.signal.ID<-values.ID[seq(1,length(values.ID),2)]
 values.BG.ID<-values.ID[seq(2,length(values.ID),2)]

 #set stimulation time for curves
 values.signal.HIGH<-values.HIGH[seq(1,length(values.HIGH),2)]
 values.BG.HIGH<-values.HIGH[seq(2,length(values.HIGH),2)]

##==============================================================================##
## FIT LOOP
##==============================================================================##

for(i in 1:(length(values.ID)/2)){

     ##set individual data.frame for signal and BG

       ##assuming that signal and bg have the same resolution and stimulation time
       x<-seq(values.signal.HIGH[i]/length(unlist(temp@DATA[values.signal.ID[i]])),
              values.signal.HIGH[i],
              values.signal.HIGH[i]/length(unlist(temp@DATA[values.signal.ID[i]])))

       ##set data.frame
       values.signal<-data.frame(x=x,y=unlist(temp@DATA[values.signal.ID[i]]))
       values.BG<-data.frame(x=x,y=unlist(temp@DATA[values.BG.ID[i]]))

    ##--------------------------------------------------------------------------##
    ##START FITTING WITH JPEG OUTPUT
    jpeg(file=paste(output.path,"FittedCurves_",i,".jpg",sep=""), quality=100,
           height=3000, width=3000,res=300)

    fit_LMCurve(values.signal, values.BG,
                log_scale="x",
                n.components=n.components,
                fit.advanced=TRUE,
```

```
                    output.path=output.path,
                    main=paste("sample␣",i,sep=""))
    dev.off()
  ##——————————————————————————————————————————————————##

}#EOF
```

2 Fitting comparison

To provide a comparison of different approaches to fit models to luminescence curves the routine of the *Luminescence* package is compared with those of the programs Fitbin9 (Bailey, 2008) and Hybfit (Grzegorz Adamiec, principle described in Bluszcz and Adamiec (2006)) (Tab. 1). Without applying any background subtraction the curves almost coincide (indistinguishable curve shapes). The results as a sum curve for a 2-,3- and 4-component function are shown in Fig. 1. In addition, for 7-components the result for sample Rom16 is shown in Fig. 3 using **R** and the program Hybfit. In Fig. 2 the outcome seems to be affected by the way the background is subtracted (linear or polynomial fit) and therefore differences between the programs can be noticed. However, as far as the BG is fitted in the course of one of the slow components, the outcomes of the three programs appear to be very comparable. The detailed results (n- and b-values) are listed in Tab. 2. All fits were produced using the automatic start parameter estimation functions of the programs. Note: Not all possible combinations of components, samples and programs were applied.

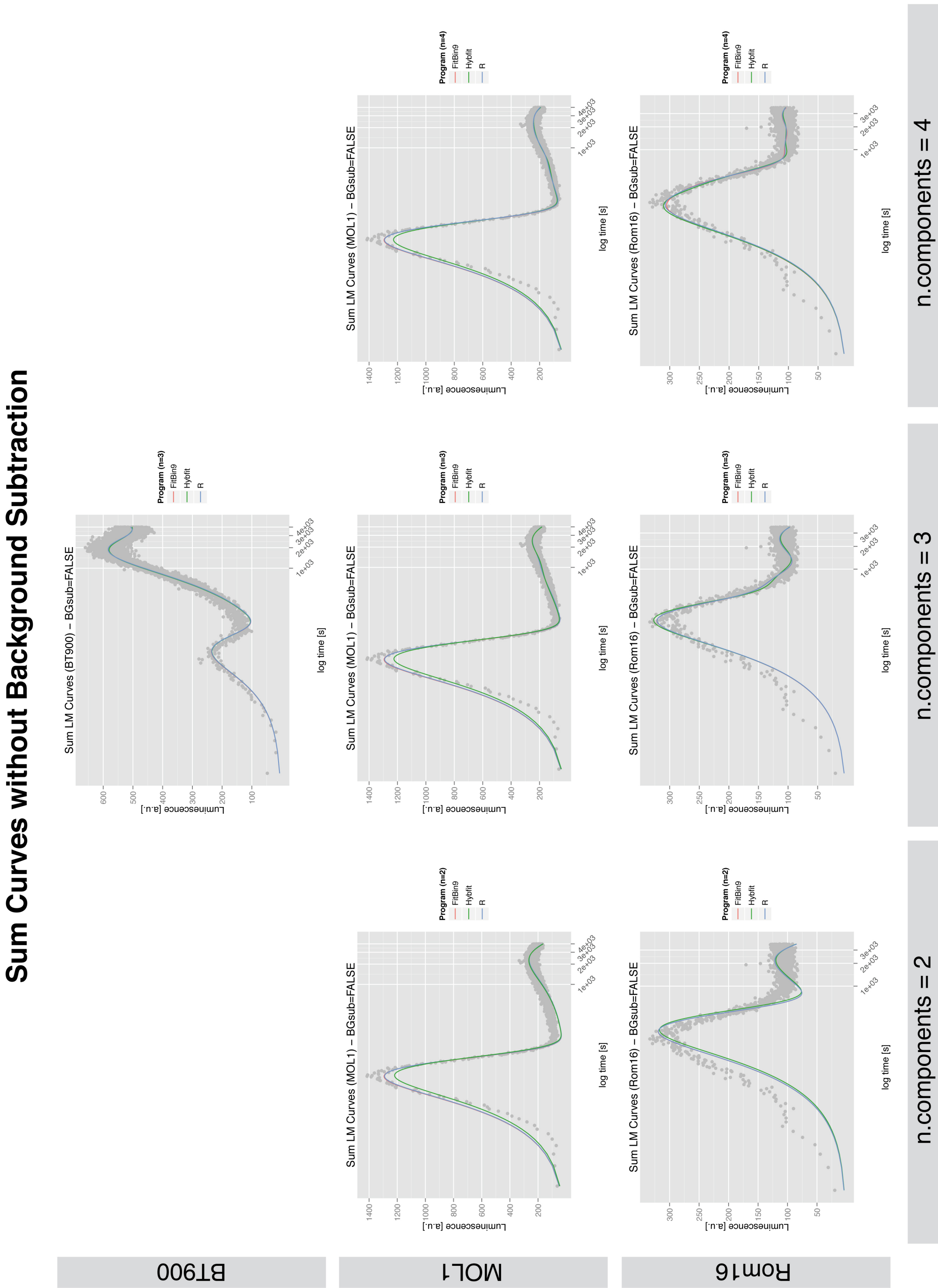

Figure 1: LM-OSL fitting results as sum curves using three different programs for three different samples without background subtraction.

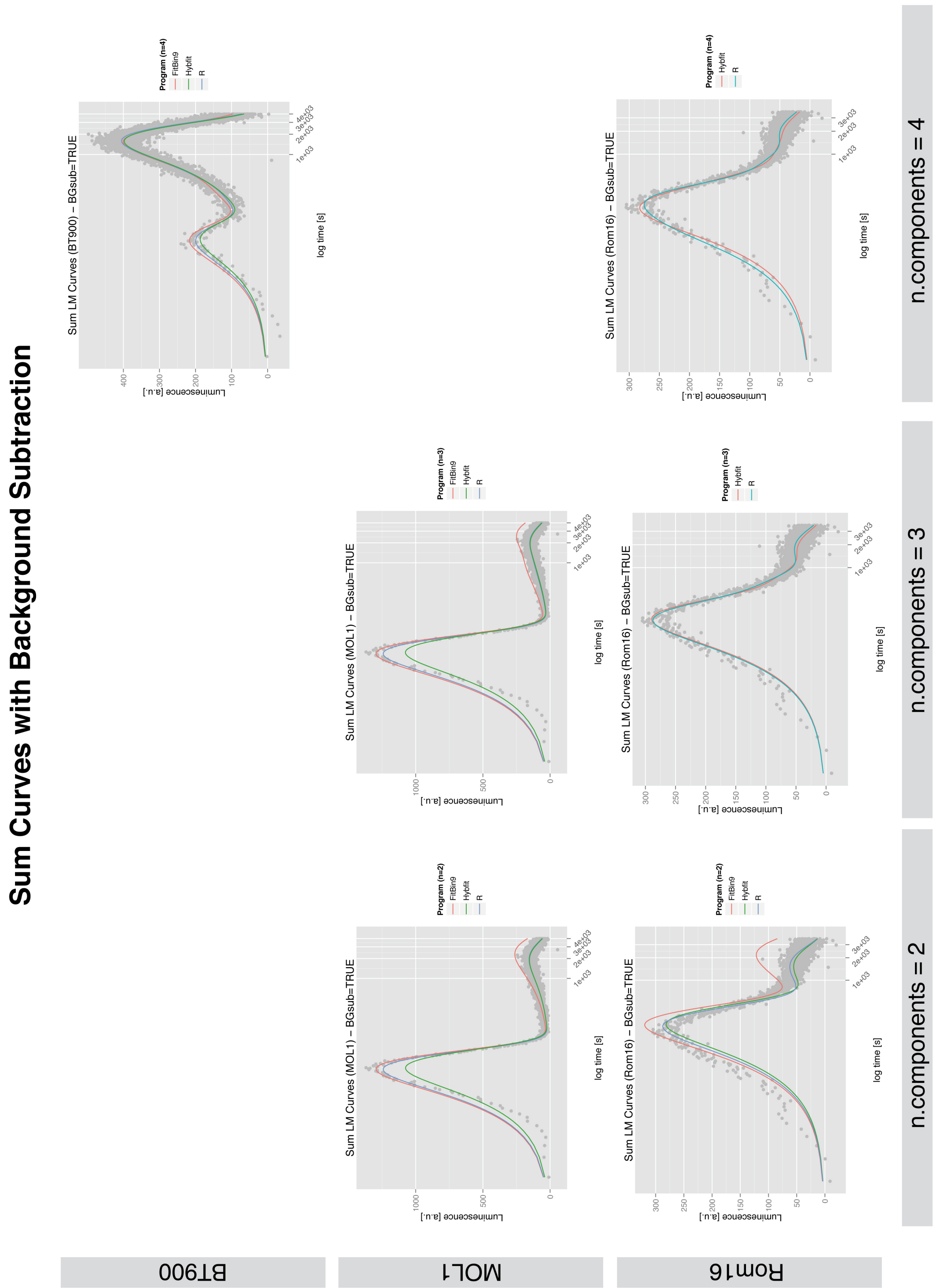

Figure 2: LM-OSL fitting results as sum curves using three different programs for three different samples with background subtraction. Not for all combinations a fit was applied.

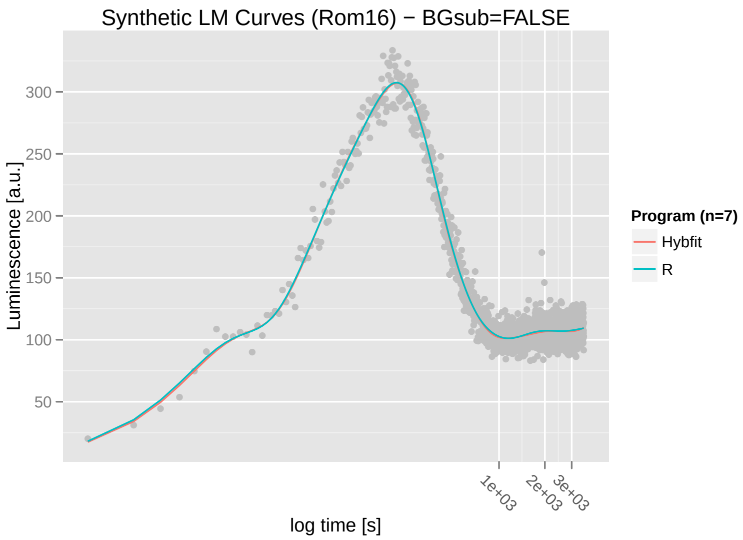

Figure 3: LM-OSL fitting result comparing R and the program Hybfit for sample Rom16 using a 7-component function.

Table 1: Samples used for the fitting test

sample id	description	grain size	laboratory	reference
BT900	beach deposit Norway (quartz)	90 - 250 μm	Bayreuth	Fuchs et al. (2011)
MOL1	Mol sand Belgium (quartz)	90 - 200 μm	Bayreuth	Gullentops and Vandenberghe (1995)
Rom16	archaeological artefact Romania (chalcedony)	100 - 200 μm	Cologne	Schmidt et al. (prep)

Table 2: Results fitting

#	program	sample	BG[1]	n[2]	n1	b1	n2	b2	n3	b3	n4	b4	n5	b5	n6	b6	n7	b7
1	FitBin9	BT900	F	3	1.88E+04	1.28E+00	8.76E+05	1.91E-03	8.19E+06	6.55E-05	NV	NV	NV	NV	NV	NV	NV	NV
2	Hybfit	BT900	F	3	1.86E+04	1.28E+00	7.70E+05	2.09E-03	4.52E+06	1.40E-04	NV	NV	NV	NV	NV	NV	NV	NV
3	R	BT900	F	3	1.88E+04	1.27E+00	8.78E+05	1.90E-03	8.30E+06	6.44E-05	NV	NV	NV	NV	NV	NV	NV	NV
4	FitBin9	BT900	T	4	1.44E+04	1.72E+00	1.05E+04	1.09E-01	9.54E+05	1.75E-03	1.49E+09	3.09E-08	NV	NV	NV	NV	NV	NV
5	R	BT900	T	4	1.27E+04	1.78E+00	4.26E+03	2.59E-01	5.54E+03	4.43E-02	1.06E+06	1.58E-03	NV	NV	NV	NV	NV	NV
6	FitBin9	MOL1	F	2	9.05E+04	2.19E+00	1.00E+06	7.46E-04	NV	NV	NV	NV	NV	NV	NV	NV	NV	NV
7	FitBin9	MOL1	T	2	9.05E+04	2.19E+00	1.00E+06	7.46E-04	NV	NV	NV	NV	NV	NV	NV	NV	NV	NV
8	R	MOL1	F	2	9.07E+04	2.17E+00	1.00E+06	7.46E-04	NV	NV	NV	NV	NV	NV	NV	NV	NV	NV
9	R	MOL1	T	2	8.63E+04	2.23E+00	4.94E+05	1.08E-03	NV	NV	NV	NV	NV	NV	NV	NV	NV	NV
10	FitBin9	MOL1	F	3	8.95E+04	2.23E+00	5.60E+04	1.12E-02	1.03E+06	6.33E-04	NV	NV	NV	NV	NV	NV	NV	NV
11	FitBin9	MOL1	T	3	8.95E+04	2.23E+00	5.60E+04	1.12E-02	1.03E+06	6.33E-04	NV	NV	NV	NV	NV	NV	NV	NV
12	R	MOL1	F	3	8.97E+04	2.20E+00	5.60E+04	1.12E-02	1.03E+06	6.33E-04	NV	NV	NV	NV	NV	NV	NV	NV
13	R	MOL1	T	3	8.60E+04	2.24E+00	1.55E+04	1.46E-02	4.92E+05	1.02E-03	NV	NV	NV	NV	NV	NV	NV	NV
14	FitBin9	MOL1	F	4	8.87E+04	2.25E+00	1.99E+04	4.37E-02	9.48E+04	3.62E-03	1.06E+06	5.24E-04	NV	NV	NV	NV	NV	NV
15	Hybfit	MOL1	F	4	8.52E+04	2.18E+00	1.54E+04	6.40E-02	7.78E+04	4.76E-03	1.05E+06	5.56E-04	NV	NV	NV	NV	NV	NV
16	R	MOL1	F	4	8.89E+04	2.23E+00	2.02E+04	4.23E-02	9.66E+04	3.54E-03	1.06E+06	5.21E-04	NV	NV	NV	NV	NV	NV
17	FitBin9	Rom16	F	2	1.18E+05	6.14E-02	4.36E+05	7.59E-04	NV	NV	NV	NV	NV	NV	NV	NV	NV	NV
18	FitBin9	Rom16	T	2	1.18E+05	6.14E-02	4.36E+05	7.59E-04	NV	NV	NV	NV	NV	NV	NV	NV	NV	NV
19	Hybfit	Rom16	F	2	1.23E+05	5.60E-02	4.36E+05	7.38E-04	NV	NV	NV	NV	NV	NV	NV	NV	NV	NV
20	Hybfit	Rom16	T	2	8.06E+04	1.00E-01	7.20E+04	1.48E-02	NV	NV	NV	NV	NV	NV	NV	NV	NV	NV
21	R	Rom16	F	2	1.19E+05	6.12E-02	4.36E+05	7.59E-04	NV	NV	NV	NV	NV	NV	NV	NV	NV	NV
22	R	Rom16	T	2	1.04E+05	6.61E-02	1.54E+05	1.59E-03	NV	NV	NV	NV	NV	NV	NV	NV	NV	NV
23	FitBin9	Rom16	F	3	7.25E+04	1.08E-01	7.66E+04	1.74E-02	4.74E+05	5.69E-04	NV	NV	NV	NV	NV	NV	NV	NV
24	Hybfit	Rom16	F	3	8.06E+04	1.00E-01	7.20E+04	1.48E-02	4.76E+05	5.49E-04	NV	NV	NV	NV	NV	NV	NV	NV
25	R	Rom16	F	3	7.29E+04	1.07E-01	7.64E+04	1.72E-02	4.74E+05	5.68E-04	NV	NV	NV	NV	NV	NV	NV	NV
26	R	Rom16	T	3	5.89E+04	1.15E-01	6.55E+04	2.48E-02	1.49E+05	1.21E-03	NV	NV	NV	NV	NV	NV	NV	NV
27	FitBin9	Rom16	F	4	1.92E+04	2.84E-01	8.78E+04	5.78E-02	6.25E+04	7.26E-03	5.18E+05	4.43E-04	NV	NV	NV	NV	NV	NV
28	Hybfit	Rom16	F	4	2.83E+04	2.27E-01	8.59E+04	4.82E-02	6.26E+04	5.69E-03	5.37E+05	4.01E-04	NV	NV	NV	NV	NV	NV
29	R	Rom16	F	4	2.25E+04	2.49E-01	8.70E+04	5.42E-02	6.25E+04	6.67E-03	5.25E+05	4.29E-04	NV	NV	NV	NV	NV	NV
30	R	Rom16	T	4	5.07E+03	6.48E-01	7.16E+04	8.66E-02	5.25E+04	1.79E-02	1.48E+05	1.13E-03	NV	NV	NV	NV	NV	NV
31	R	Rom16	F	5	3.74E+03	1.68E+00	5.50E+04	1.17E-01	6.74E+04	3.11E-02	7.22E+04	3.61E-03	6.14E+05	3.02E-04	NV	NV	NV	NV
32	R	Rom16	T	5	2.89E+03	1.15E+00	5.47E+04	1.09E-01	5.82E+04	3.04E-02	5.07E+04	3.48E-03	1.33E+05	6.55E-04	NV	NV	NV	NV
33	R	Rom16	F	6	9.60E+02	2.06E+01	4.55E+03	9.04E-01	5.96E+04	1.06E-01	6.33E+04	2.83E-02	7.54E+04	3.32E-03	6.38E+05	2.80E-04	NV	NV
34	R	Rom16	T	6	5.20E+02	1.96E+01	3.34E+03	7.82E-01	5.67E+04	1.04E-01	5.62E+04	2.90E-02	5.35E+04	3.27E-03	1.32E+05	6.18E-04	NV	NV
35	Hybfit	Rom16	F	7	9.35E+02	2.02E+01	4.20E+03	9.59E-01	5.23E+04	1.14E-01	5.80E+04	3.62E-02	2.82E+04	1.02E-02	1.24E+05	1.77E-03	1.77E+06	6.37E-05
36	R	Rom16	F	7	9.13E+02	2.18E+01	3.60E+03	1.12E+00	3.39E+04	1.40E-01	5.17E+04	5.82E-02	4.39E+04	1.96E-02	8.80E+04	2.62E-03	7.44E+05	2.10E-04
37	R	Rom16	T	7	5.01E+02	2.02E+01	2.74E+03	9.15E-01	4.28E+04	1.20E-01	4.45E+04	4.71E-02	3.10E+04	1.85E-02	7.63E+04	2.31E-03	1.39E+05	3.29E-04

Note

[1] background subtraction T (TRUE) or F (FALSE)

[2] number of components used for fitting

—

n is the number of initial trapped electrons

b is the detrapping probability

NV = No Value

References

Bailey, D. J. E. (2008). *Development of LM OSL Analysis Techniques for Applications to Optical Dating*. PhD thesis, Research Laboratory for Archæology and the History of Art Keble College. unpublished.

Bluszcz, A. and Adamiec, G. (2006). Application of differential evolution to fitting OSL decay curves. *Radiation Measurements*, 41(7-8):886–891.

Fuchs, M., Kreutzer, S., Fischer, M., Sauer, D., and Sørensen, R. (2011). OSL and IRSL dating of raised beach sand deposits along the southeastern coast of Norway. *Quaternary Geochronology*, 10.1016/j.quageo.2011.11.009.

Gullentops, F. and Vandenberghe, N. (1995). Toelichtingen Bij De Geologische Kaart Van Belgie Vlaams Gewest: Kaartblad 17 Mol. Belgische Geologische Dienst.

Schmidt, C., Sitlivy, V., Anghelinu, M., Chabai, V., Kels, H., Uthmeier, T., Hauck, T., Băltean, I., Hilgers, A., Richter, J., and Radtke, U. (in prep.). Unexpectedly old: thermoluminescence dating of heated artefacts from the Aurignacian open-air site of Româneşti-Dumbrăviţa I, Romania. *in preparation*.