

Supplementary Materials: Modeling of Antioxidant Activity, Polyphenols and Macronutrients Content of Bee Pollen Applying Solid-State ^{13}C NMR Spectra

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Table S1. Spectral regions used for PLS modeling.

Analyzed parameter	Region (ppm)
Reducing sugars	50-200
Protein	10-22 and 53-170
Fat	40-110 and 140-170
Total polyphenols	100-170
Antioxidant activity ABTS	73-158
NHCS	10-200
C	20-200
N	10-22 and 53-170
S	130-160 and 180-200
pH	110-130 and 160-180

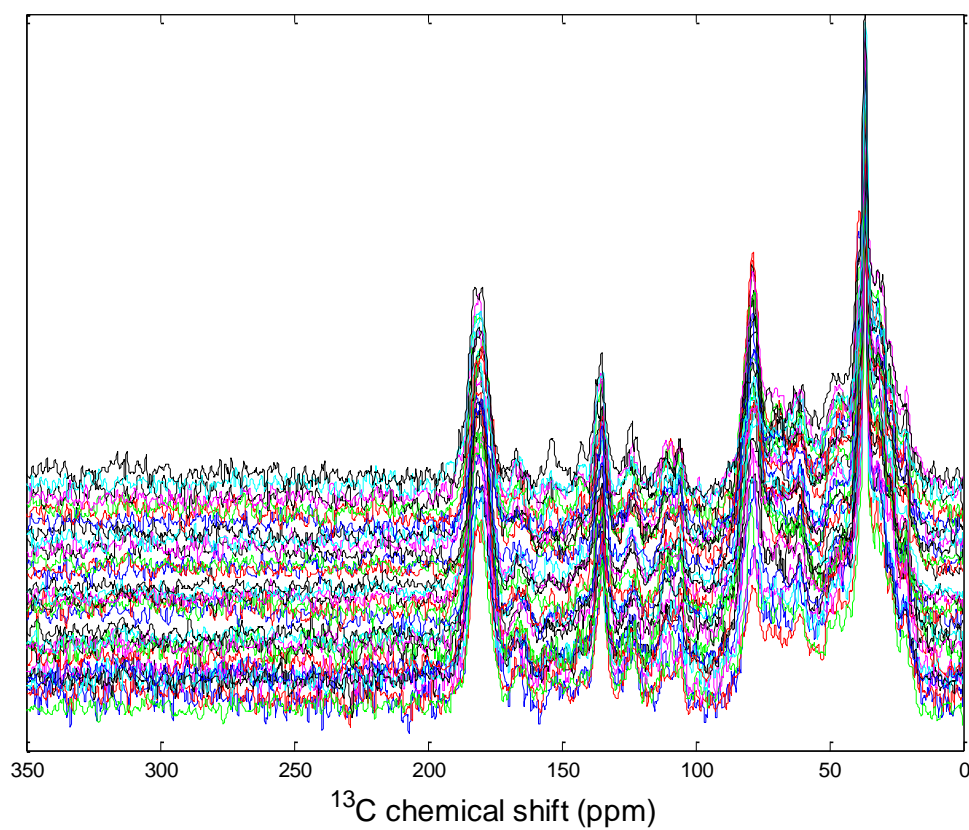
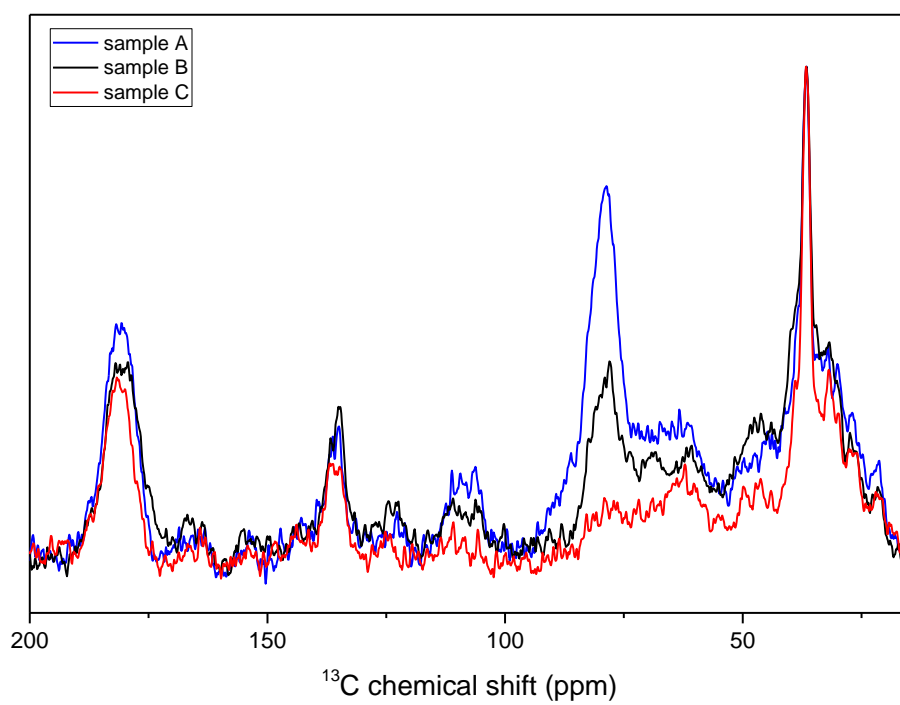


Figure S1. ^{13}C CPMAS NMR spectra of the analyzed bee pollen samples.



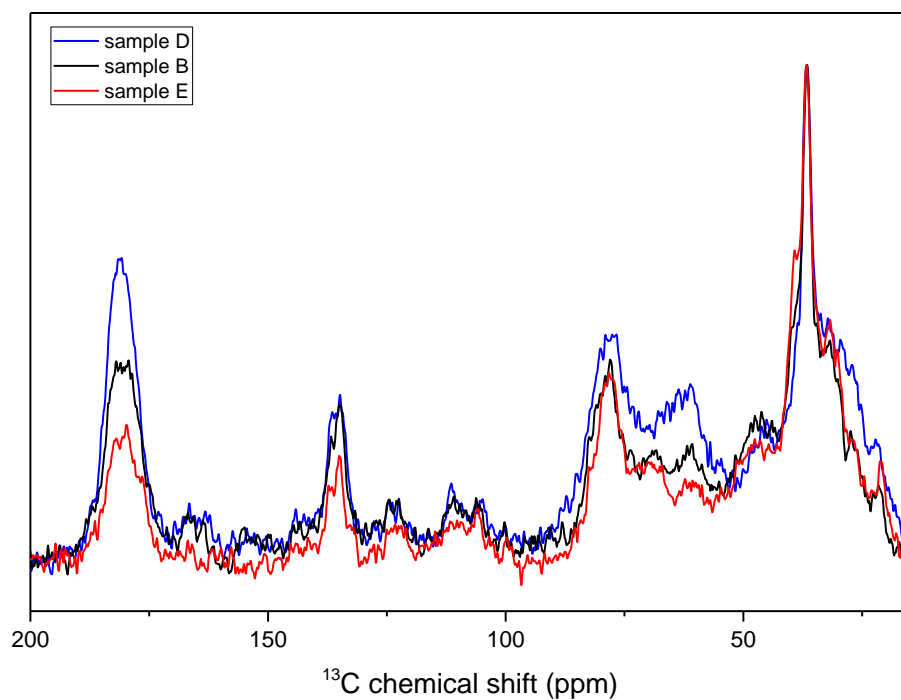


Figure S2. ^{13}C NMR spectra of selected bee pollen samples A-E; labeling as in Fig. 3.

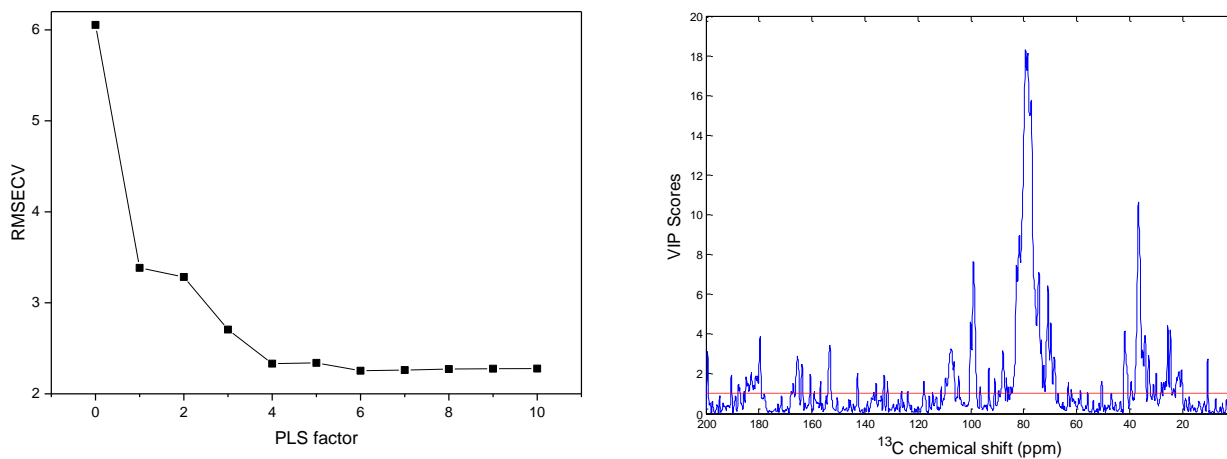


Figure S3. Modeling of reducing sugars content in pollen samples on the basis of ^{13}C NMR spectra; the RMSECV (left) and VIP scores (right) plots.

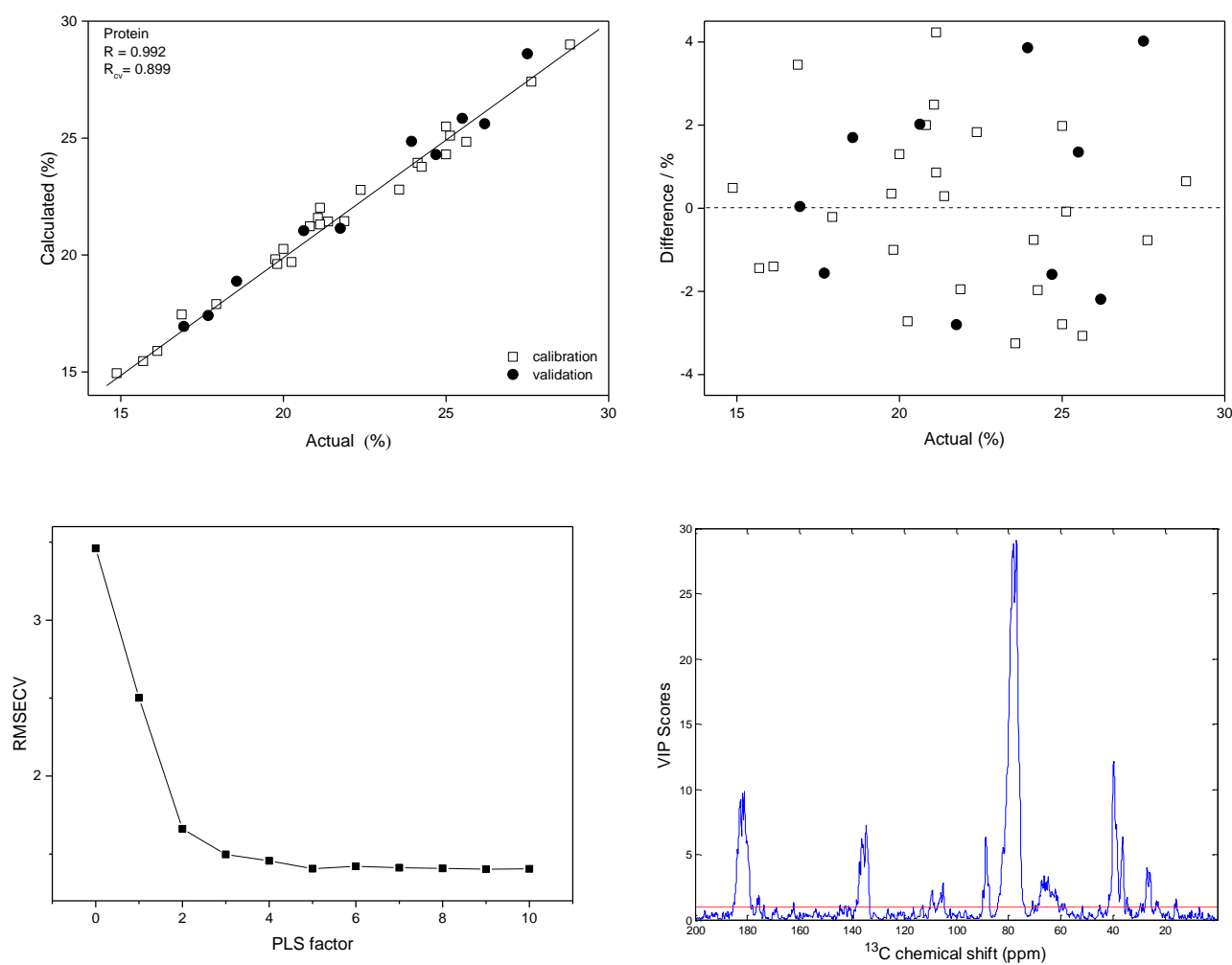


Figure S4. Modeling of protein content in pollen samples on the basis of ^{13}C NMR spectra; top panel: prediction plot (left) and relative errors (right), bottom panel: the RMSECV (left) and VIP scores (right) plots.

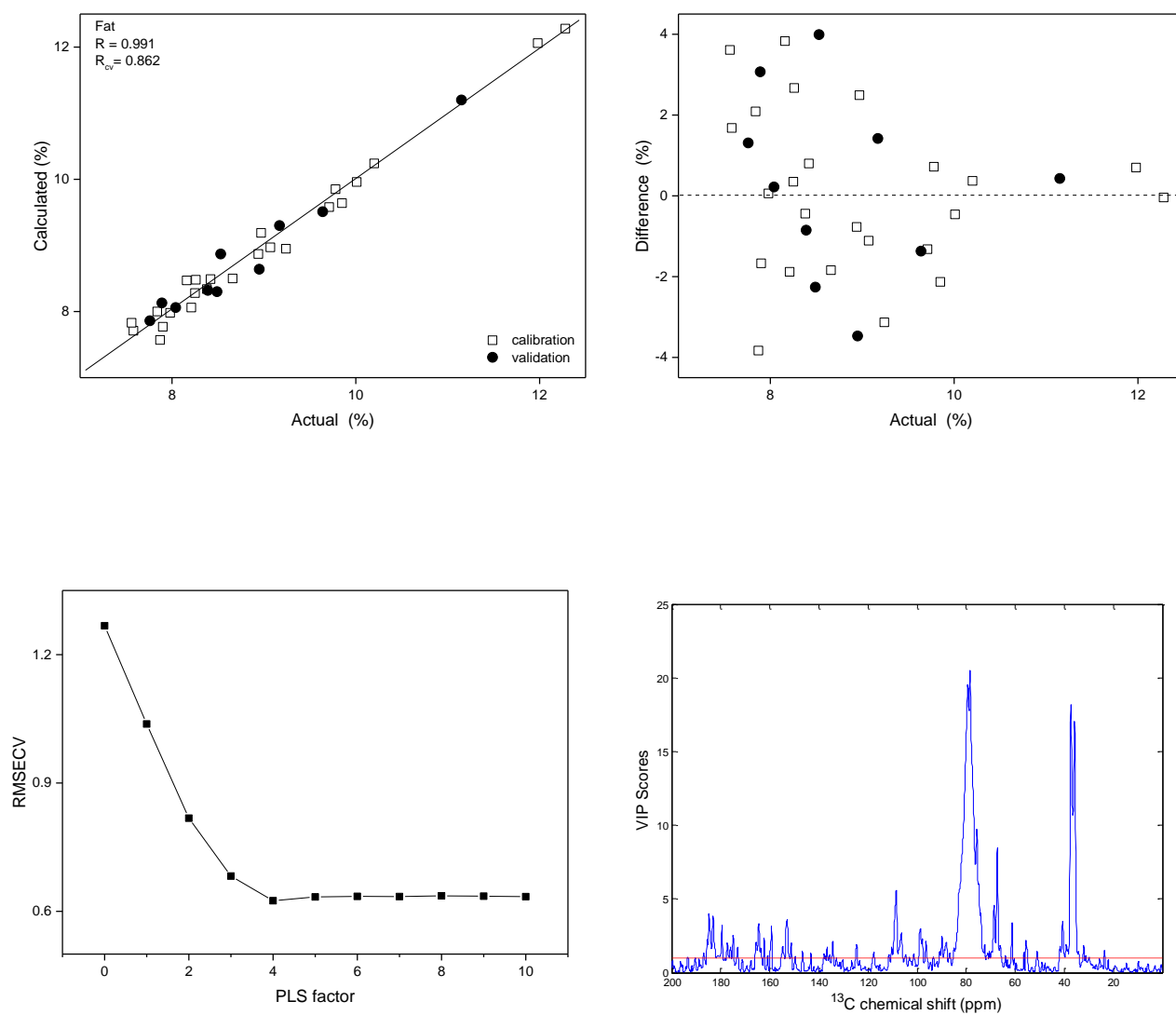


Figure S5 Modeling of fat content in pollen samples on the basis of ^{13}C NMR spectra; top panel: prediction plot (left) and relative errors (right), bottom panel: the RMSECV (left) and VIP scores (right) plots

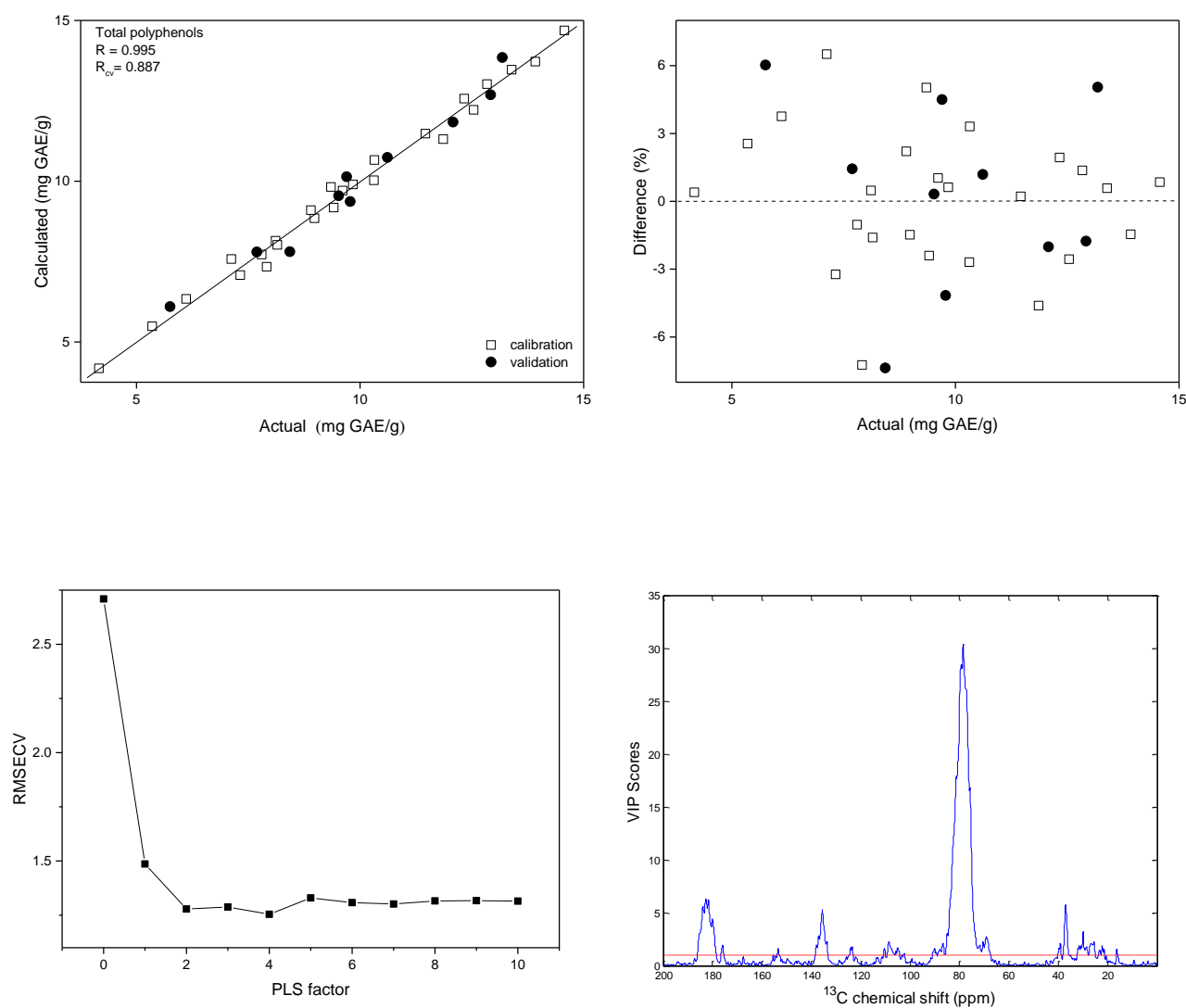


Figure S6 Modeling of total polyphenolic compounds content in pollen samples on the basis of ^{13}C NMR spectra; top panel: prediction plot (left) and relative errors (right), bottom panel: the RMSECV (left) and VIP scores (right) plots

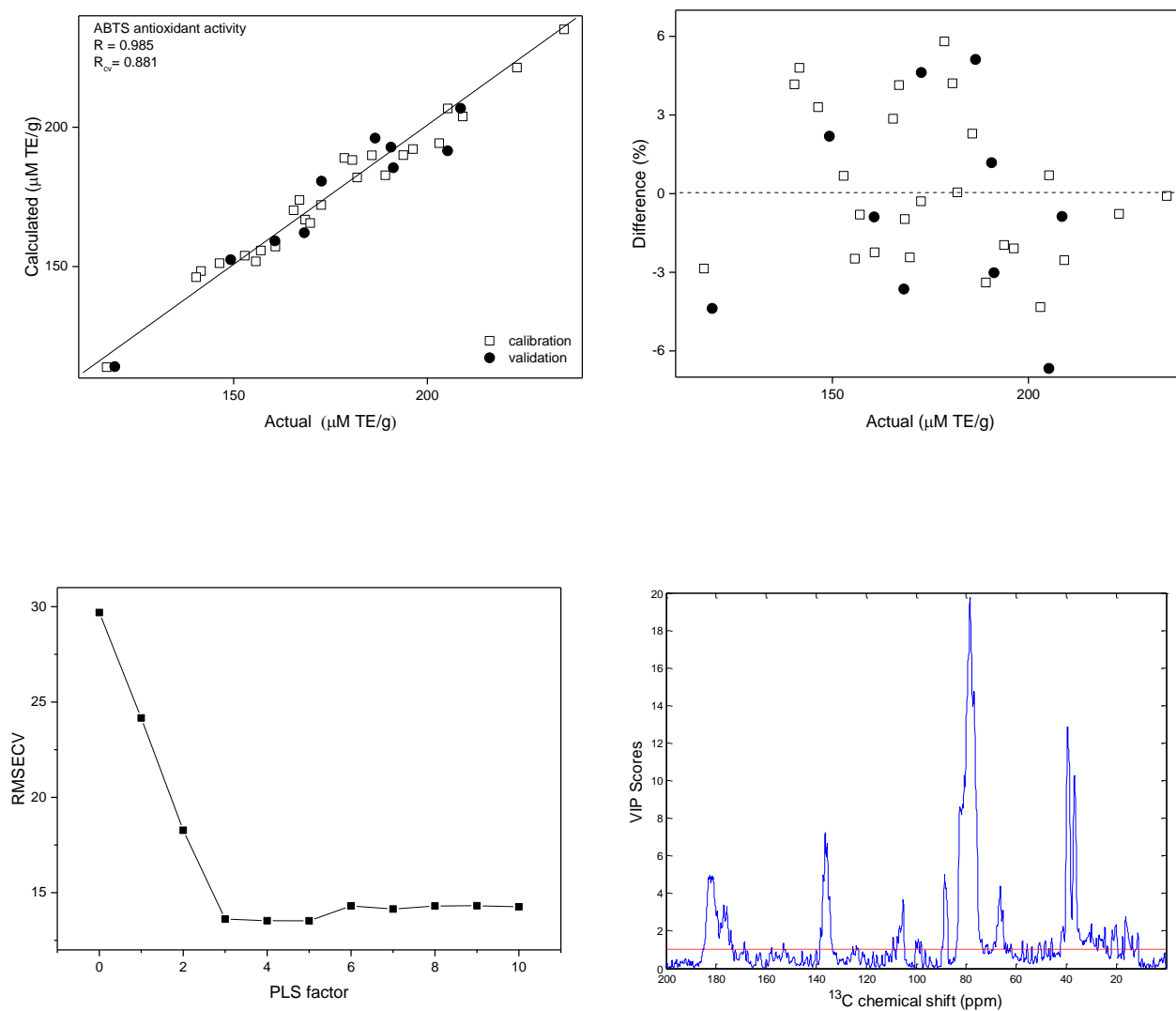


Figure S7 Modeling of ABTS antioxidant activity in pollen samples on the basis of ^{13}C NMR spectra; top panel: prediction plot (left) and relative errors (right), bottom panel: the RMSECV (left) and VIP scores (right) plots

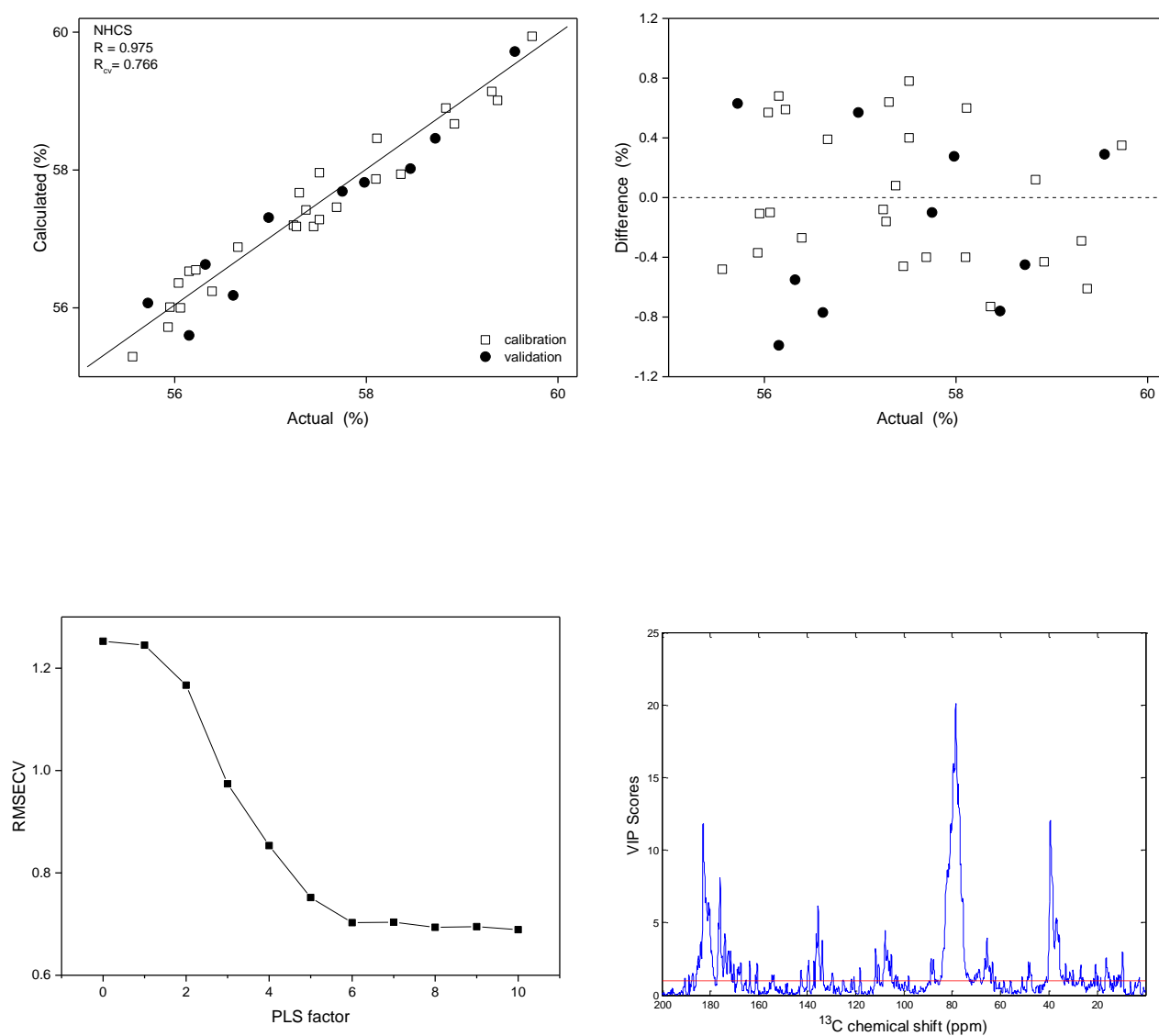


Figure S8 Modeling of NHCS content in pollen samples on the basis of ^{13}C NMR spectra; top panel: prediction plot (left) and relative errors (right), bottom panel: the RMSECV (left) and VIP scores (right) plots

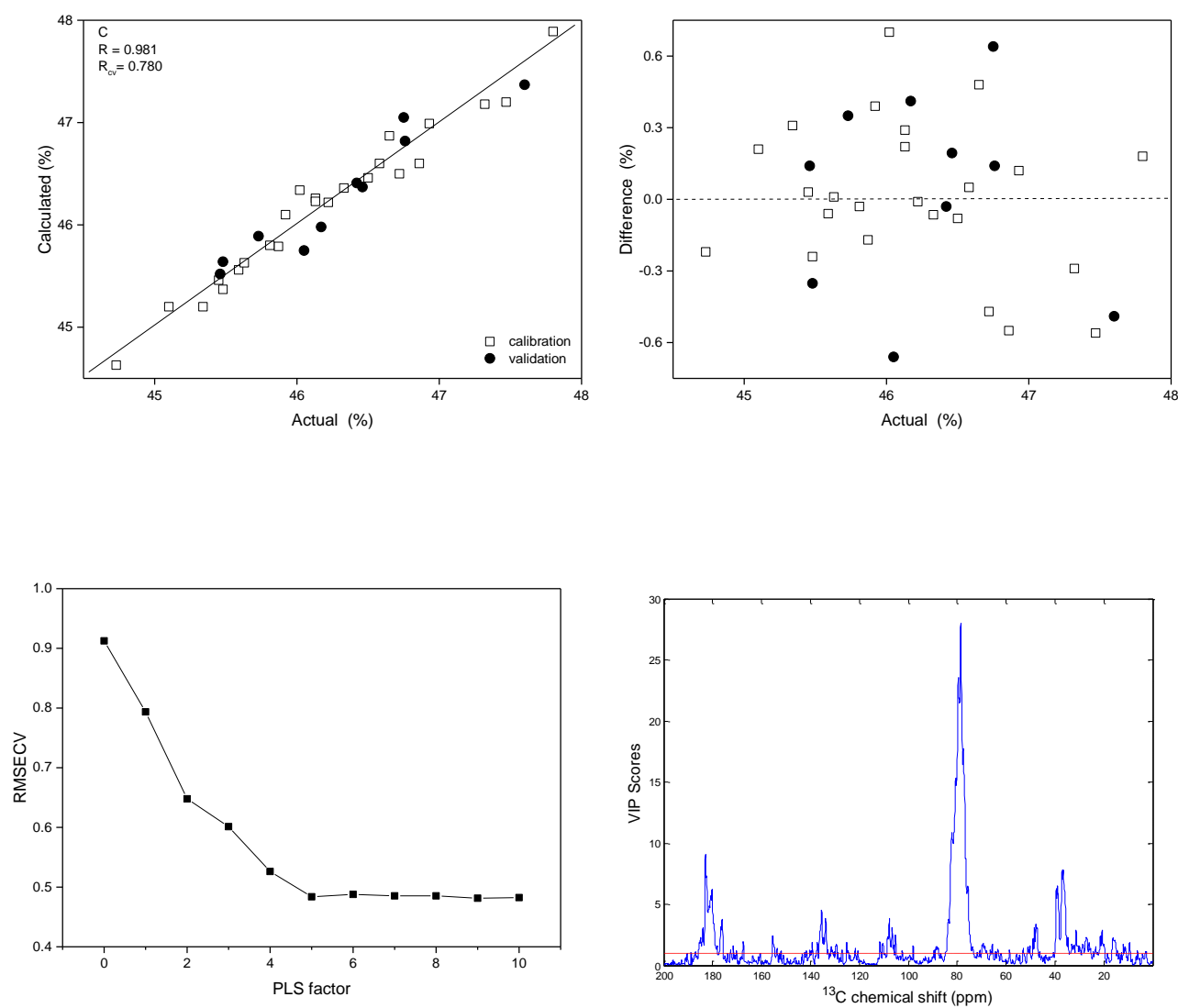


Figure S9 Modeling of C content in pollen samples on the basis of ^{13}C NMR spectra; top panel: prediction plot (left) and relative errors (right), bottom panel: the RMSECV (left) and VIP scores (right) plots

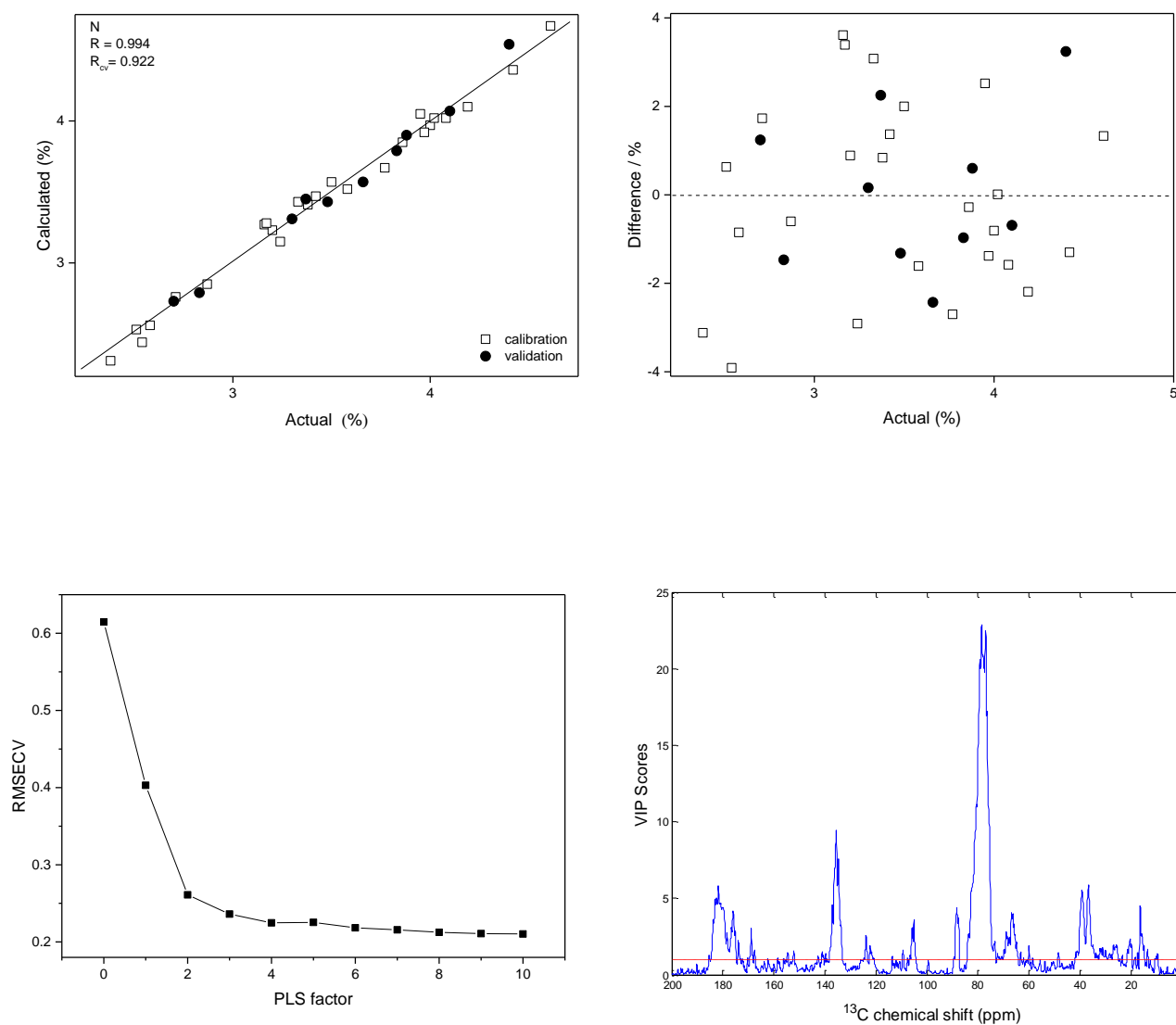


Figure S10 Modeling of N content in pollen samples on the basis of ^{13}C NMR spectra; top panel: prediction plot (left) and relative errors (right), bottom panel: the RMSECV (left) and VIP scores (right) plots

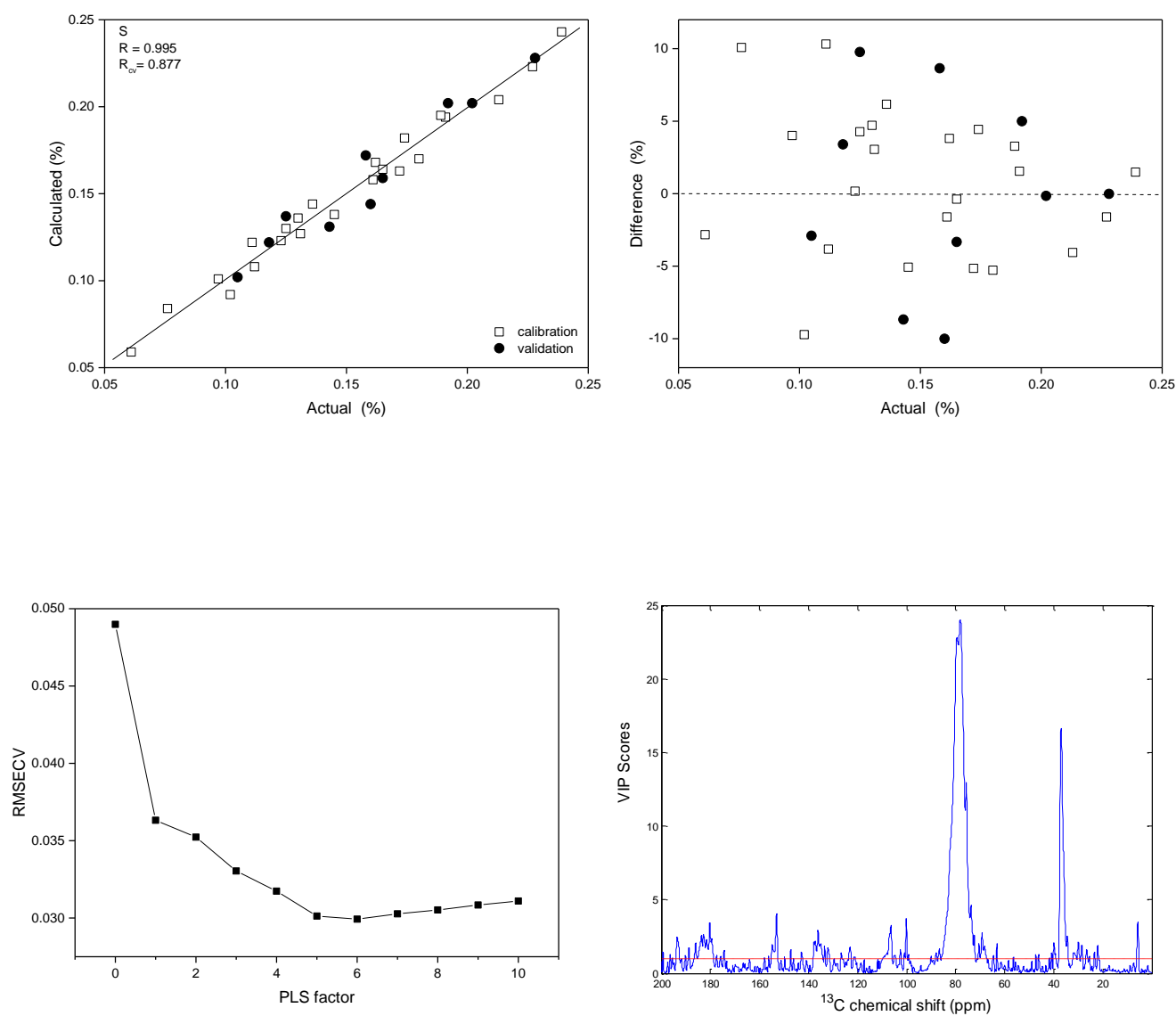


Figure S11 Modeling of S content in pollen samples on the basis of ^{13}C NMR spectra; top panel: prediction plot (left) and relative errors (right), bottom panel: the RMSECV (left) and VIP scores (right) plots

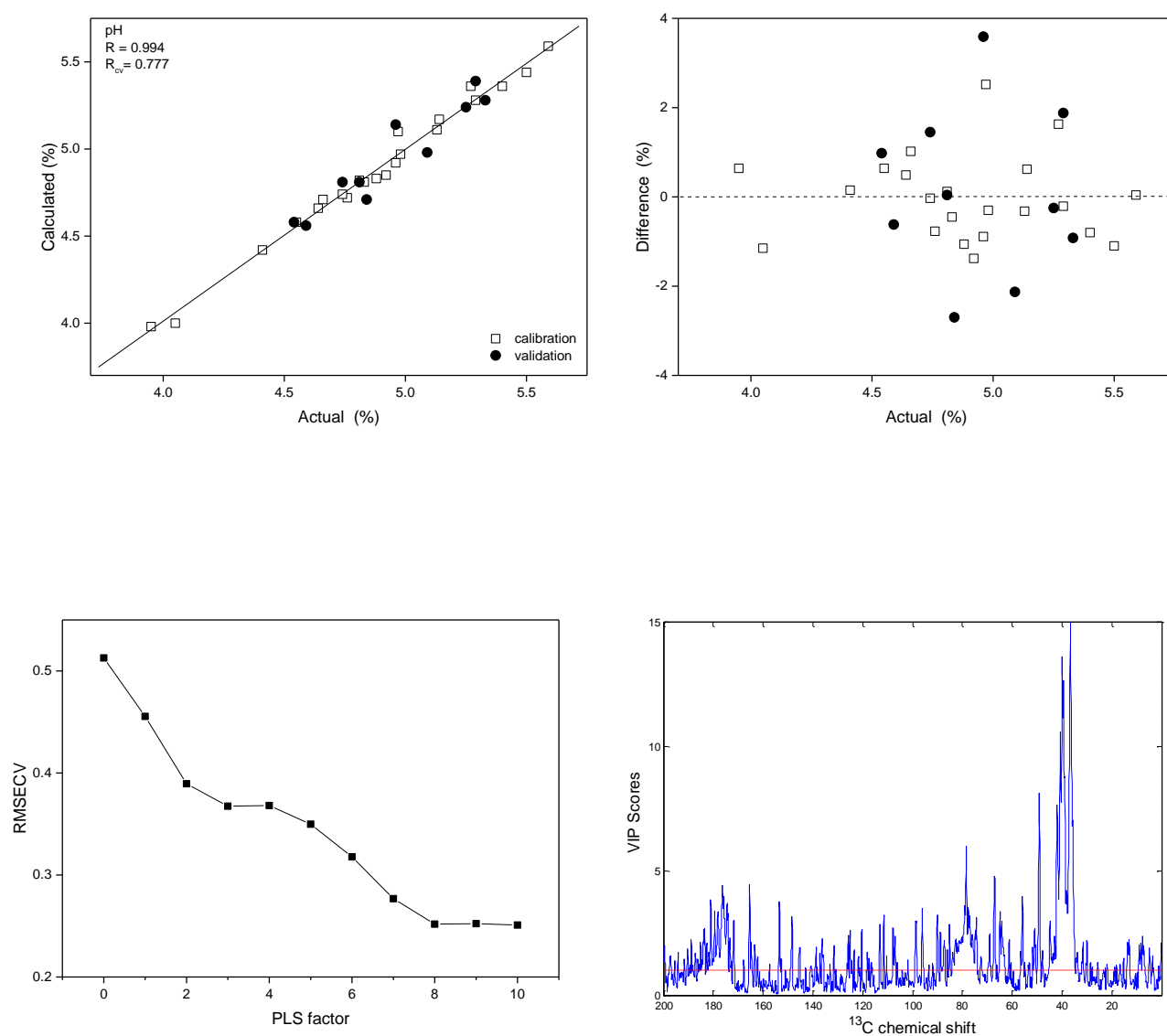


Figure S12 Modeling of pH of pollen samples on the basis of ^{13}C NMR spectra; top panel: prediction plot (left) and relative errors (right), bottom panel: the RMSECV (left) and VIP scores (right) plots