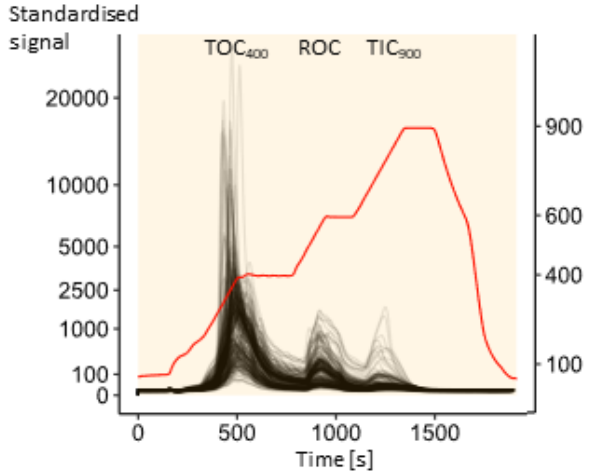
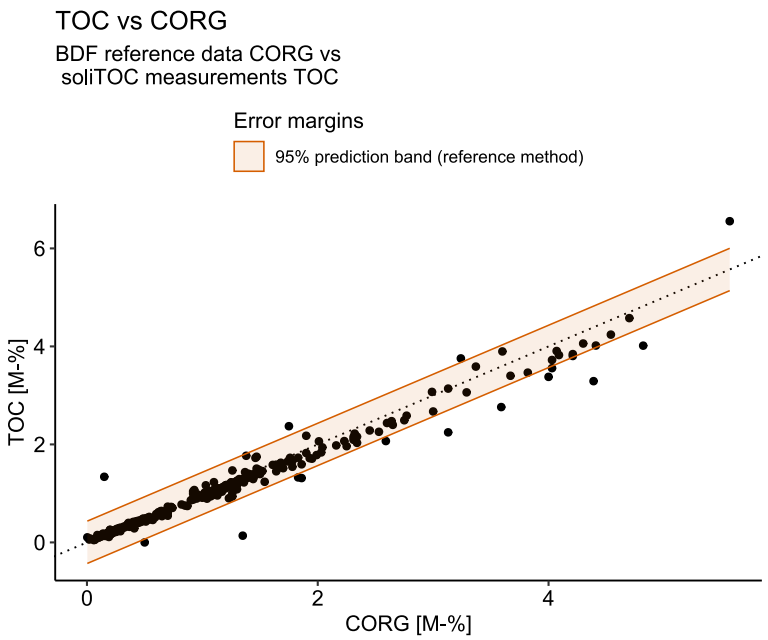
Stepped thermal analysis in accordance with DIN19539

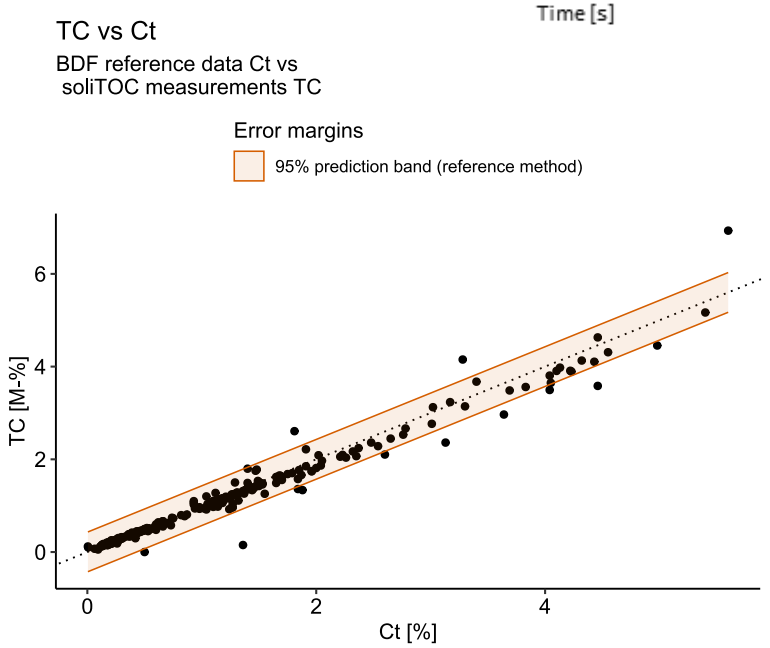
Carbon fractions (DIN19539):
TOC_{400}: labile SOC-Pool
ROC: recalcitrant SOC-Pool
TIC_{900}: inorganic C-Pool

TOC

TC







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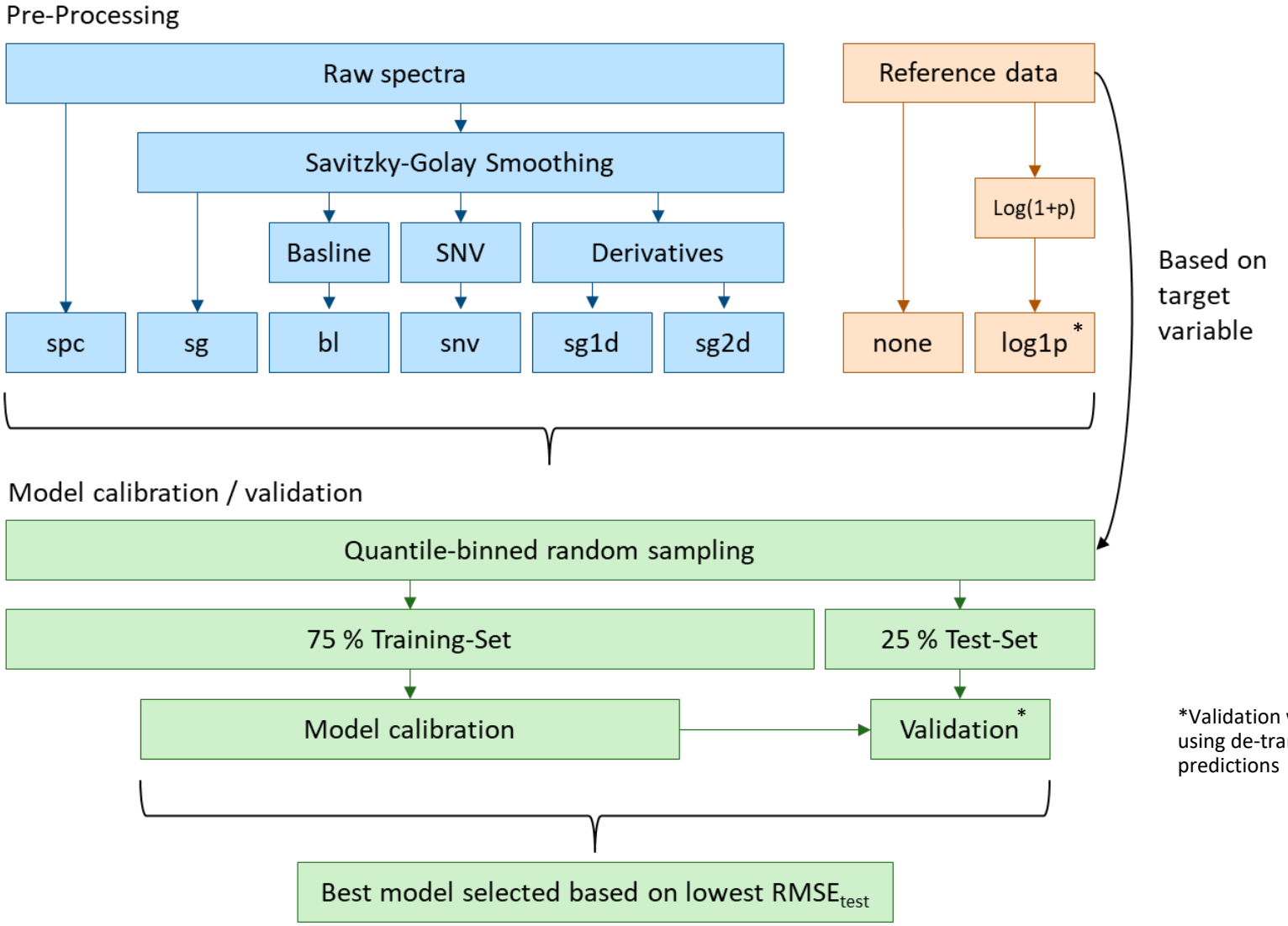
Pre-Processing and model calibration



*Validation was carried out using de-transformed predictions

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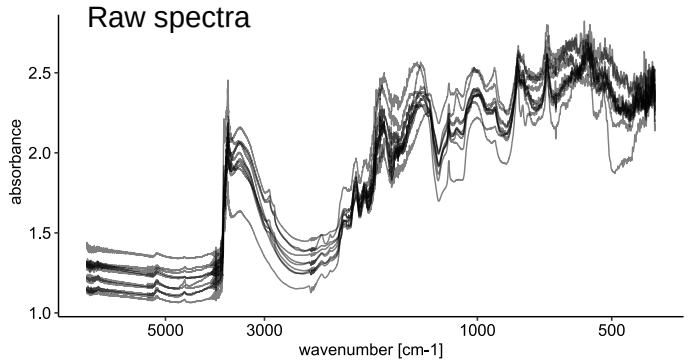
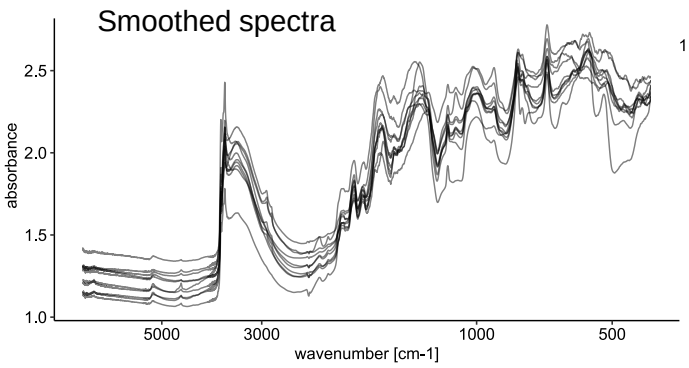
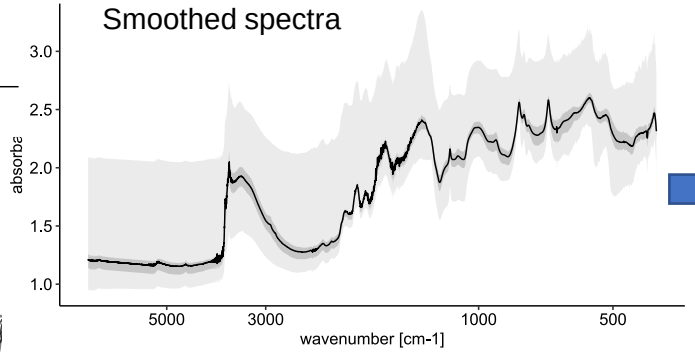
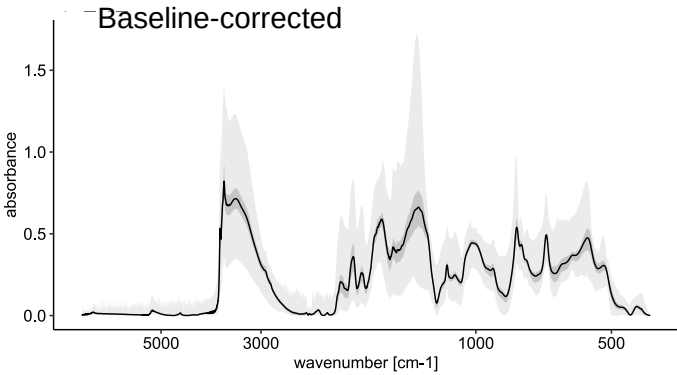
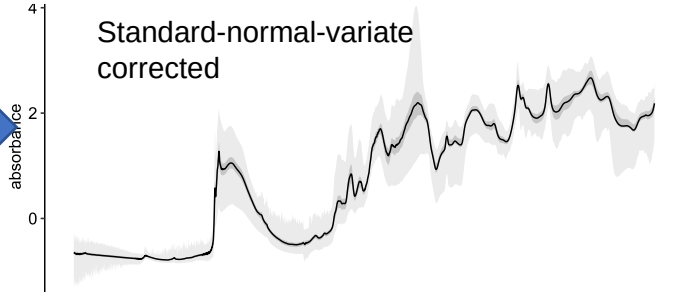
Visualisation of different pre-processing steps

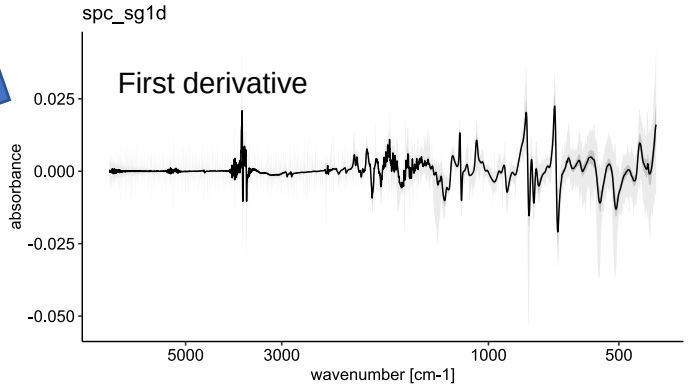












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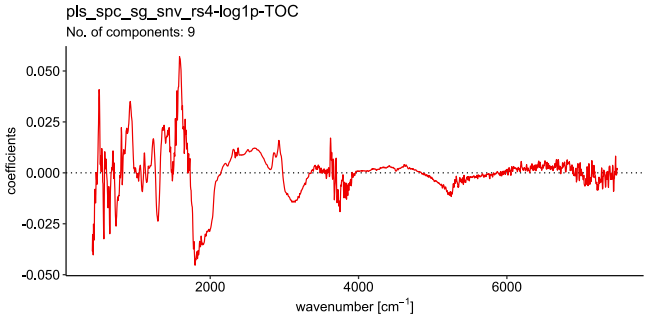
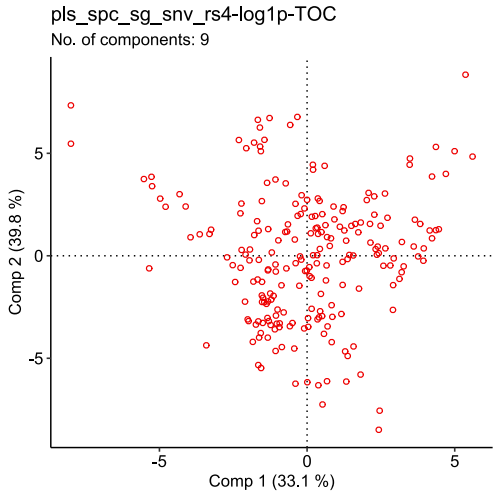
Differnt used model types

PLS

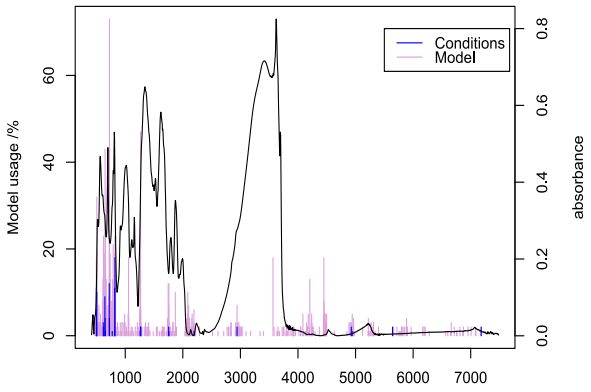
Partial Least Squares Regression using the NIPLS algorithm

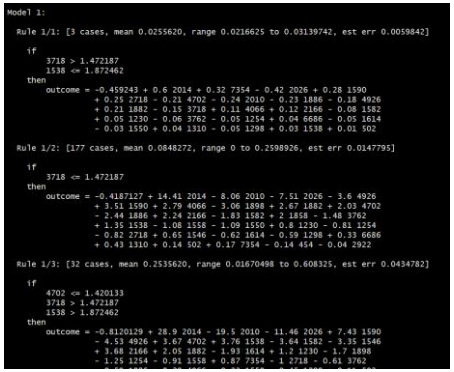




Cubist

Rule-based regression tree
with linear models at terminal nodes





```
Model 1:

 Rule 1/1: [3 cases, mean 0.0255620, range 0.0216625 to 0.03139742, est err 0.0059842]

   if
      3718 > 1.472187
      1538 <= 1.872462
   then
      outcome = -0.459243 + 0.6 2014 + 0.32 7354 - 0.42 2026 + 0.28 1590
                + 0.25 2718 - 0.21 4702 - 0.24 2010 - 0.23 1886 - 0.18 4926
                + 0.21 1882 - 0.15 3718 + 0.11 4066 + 0.12 2166 - 0.08 1582
                + 0.05 1230 - 0.06 3762 - 0.05 1254 + 0.04 6686 - 0.05 1614
                - 0.03 1550 + 0.04 1310 - 0.05 1298 + 0.03 1538 + 0.01 502

 Rule 1/2: [177 cases, mean 0.0848272, range 0 to 0.2598926, est err 0.0147795]

   if
      3718 <= 1.472187
   then
      outcome = -0.4187127 + 14.41 2014 - 8.06 2010 - 7.51 2026 - 3.6 4926
                + 3.51 1590 + 2.79 4066 - 3.06 1898 + 2.67 1882 + 2.03 4702
                - 2.44 1886 + 2.24 2166 - 1.83 1582 + 2 1858 - 1.48 3762
                + 1.35 1538 - 1.08 1558 - 1.09 1550 + 0.8 1230 - 0.81 1254
                - 0.82 2718 + 0.65 1546 - 0.62 1614 - 0.59 1298 + 0.33 6686
                + 0.43 1310 + 0.14 502 + 0.17 7354 - 0.14 454 - 0.04 2922

 Rule 1/3: [32 cases, mean 0.2535620, range 0.01670498 to 0.608325, est err 0.0434782]

   if
      4702 <= 1.420133
      3718 > 1.472187
      1538 > 1.872462
   then
      outcome = -0.8120129 + 28.9 2014 - 19.5 2010 - 11.46 2026 + 7.43 1590
                - 4.53 4926 + 3.67 4702 + 3.76 1538 - 3.64 1582 - 3.35 1546
                + 3.68 2166 + 2.05 1882 - 1.93 1614 + 1.2 1230 - 1.7 1898
                - 1.25 1254 - 0.91 1558 + 0.87 7354 - 1 2718 - 0.61 3762
```

MBL

Memory Based Learner
For each predictor spectra, a set of k most similar spectra are selected based on a similarity metric (Mahalanobis distance). For each predictor spectra an individual weighted averaged pls is created

https://cran.r-project.org/web/packages/resemble/readme/README.html
(modified)

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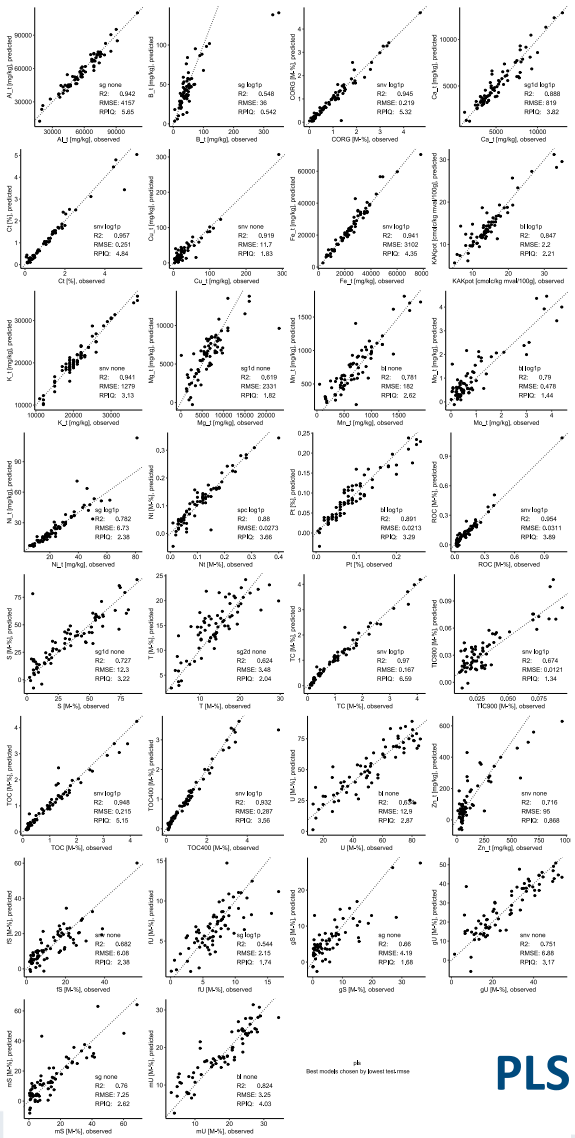
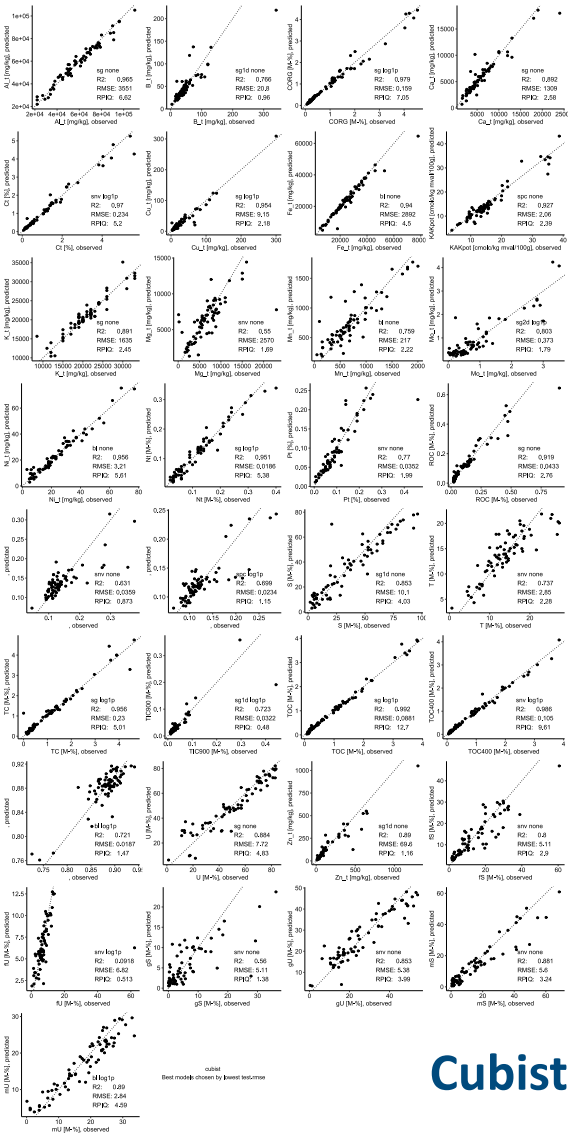
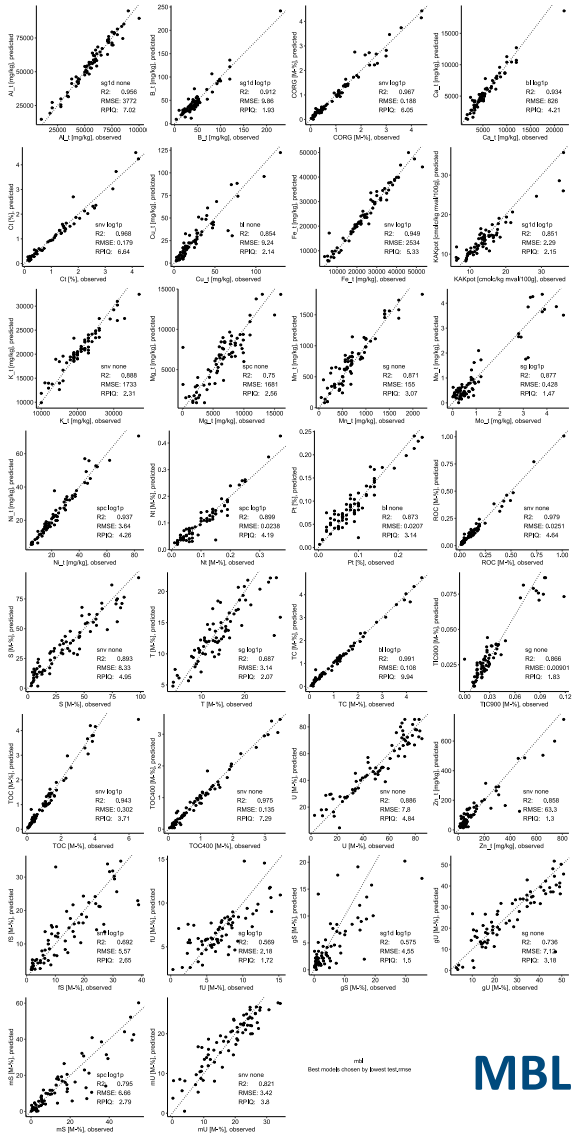
Model Validation



PLS



Cubist



MBL

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Soil properties / target variables

Variable (short)	Variable (long)	Unit	Method
TOC_{400}	Labile organic carbon	wt-%	Stepped themal analysis / DIN19539
ROC	Recalcitrant organic carbon	wt-%	Stepped themal analysis / DIN19539
TIC_{900}	Inorganic carbon	wt-%	Stepped themal analysis / DIN19539
TOC	Total organic carbon (TOC_{400} + ROC)	wt-%	Stepped themal analysis / DIN19539
TC	Total carbon ($TOC+TIC_{900}$)	wt-%	Stepped themal analysis / DIN19539
C_{ORG}	Total organic carbon	wt-%	Determination of total organic carbon
C_t	Total carbon	wt-%	Elemental Analysis (C,H,N,S,O)
N_t	Total nitrogen	wt-%	Elemental Analysis (C,H,N,S,O)
P_t	Total phoaphorous	wt-%	EDRFA
gS	Coarse sand	wt-%	Texture distribution
mS	Medium sand	wt-%	Texture distribution
fS	Fine sand	wt-%	Texture distribution
S	Sand	wt-%	Texture distribution
gU	Coarse silt	wt-%	Texture distribution
mU	Medium silt	wt-%	Texture distribution
fU	Fine silt	wt-%	Texture distribution
U	Silt	wt-%	Texture distribution
T	Clay	wt-%	Texture distribution
KAK_{pot} (CEC_{pot})	Cation exchange capacity	$cmol_c\ kg^{-1}$	$BaCl_2$, exchangeable cations DIN196848
Al_t	Total aluminium	$mg\ kg^{-1}$	HF/HNO_3/HCl microwave digestion, determination of total elemental concentrations
B_t	Total boron	$mg\ kg^{-1}$	HF/HNO_3/HCl microwave digestion, determination of total elemental concentrations
Ca_t	Total calcium	$mg\ kg^{-1}$	HF/HNO_3/HCl microwave digestion, determination of total elemental concentrations
Cu_t	Total copper	$mg\ kg^{-1}$	HF/HNO_3/HCl microwave digestion, determination of total elemental concentrations
Fe_t	Total iron	$mg\ kg^{-1}$	HF/HNO_3/HCl microwave digestion, determination of total elemental concentrations
K_t	Total potassium	$mg\ kg^{-1}$	HF/HNO_3/HCl microwave digestion, determination of total elemental concentrations
Mg_t	Total magnesium	$mg\ kg^{-1}$	HF/HNO_3/HCl microwave digestion, determination of total elemental concentrations
Mn_t	Total manganese	$mg\ kg^{-1}$	HF/HNO_3/HCl microwave digestion, determination of total elemental concentrations
Mo_t	Total molybdenium	$mg\ kg^{-1}$	HF/HNO_3/HCl microwave digestion, determination of total elemental concentrations
Ni_t	Total nickel	$mg\ kg^{-1}$	HF/HNO_3/HCl microwave digestion, determination of total elemental concentrations
Zn_t	Total zinc	$mg\ kg^{-1}$	HF/HNO_3/HCl microwave digestion, determination of total elemental concentrations

Re-analysis using the Elementar soliTOC

Reference values obtained from the BDF database.

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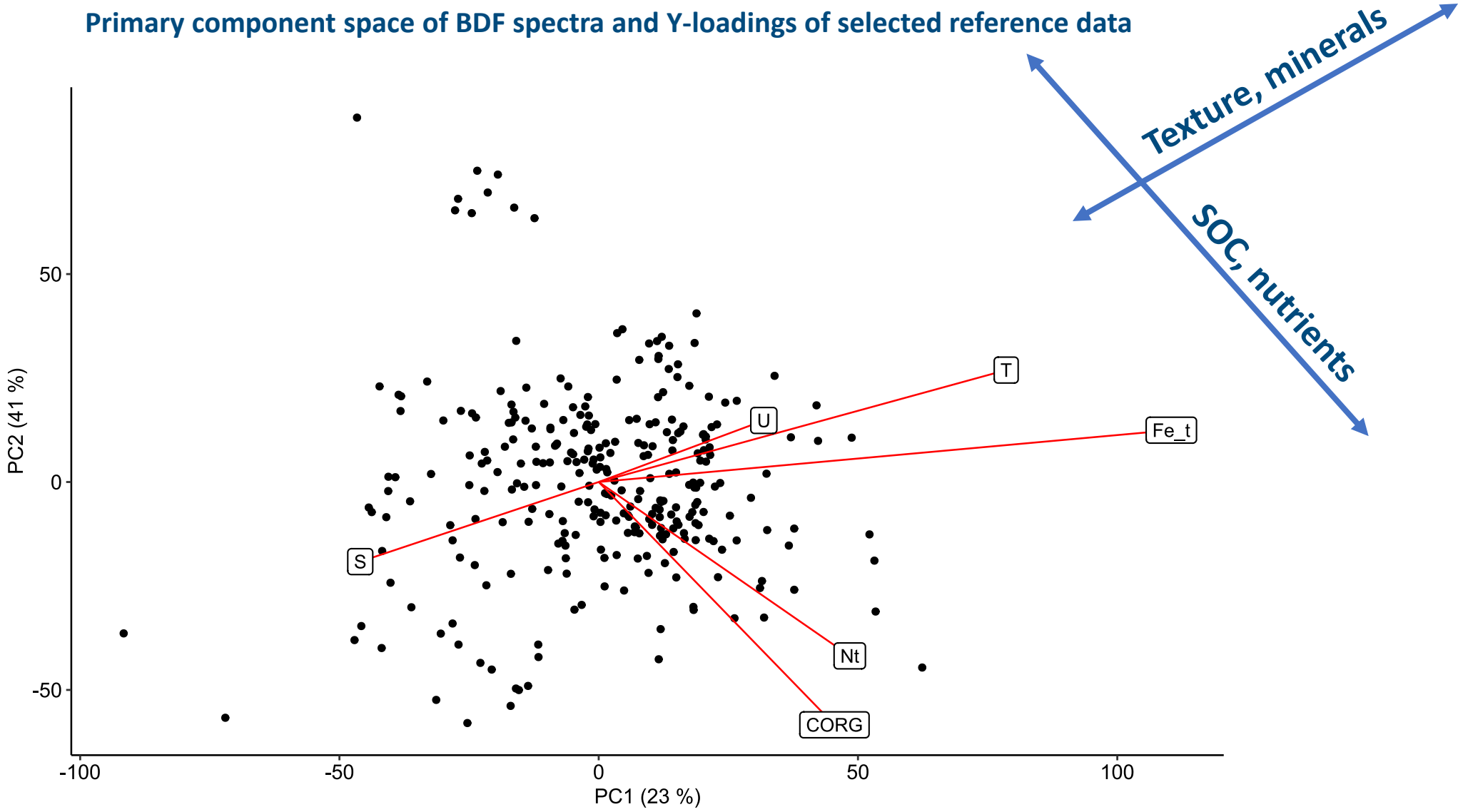
Primary component space of BDF spectra and Y-loadings of selected reference data



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