Fig. S1 Compounds of importance when predicting TAC_{Mch} of *P. atlantica* extracts shown on a (a) an overlay chromatogram, as evaluated using (b) regression coefficients of PLS after column centering, (c) regression coefficients of PLS after normalization and column centering, and (d) regression coefficients of PLS after standard normal variate and column centering.

Fig. S2 Compounds of importance when predicting TAC_{ROO} of *P. atlantica* extracts shown on a (a) an overlay chromatogram, as evaluated using (b) regression coefficients of PLS after column centering, (c) regression coefficients of PLS after normalization and column centering, and (d) regression coefficients of PLS after standard normal variate and column centering.

Fig. S3 Compounds of importance when predicting TAC_{OH} of *P. atlantica* extracts shown on a (a) an overlay chromatogram, as evaluated using (b) regression coefficients of PLS after column centering, (c) regression coefficients of PLS after normalization and column centering, and (d) regression coefficients of PLS after standard normal variate and column centering.

Fig. S4 Compounds of importance when predicting TAC_{NO} of *P. atlantica* extracts shown on a (a) an overlay chromatogram, as evaluated using (b) regression coefficients of PLS after column centering, (c) regression coefficients of PLS after normalization and column centering, and (d) regression coefficients of PLS after standard normal variate and column centering.

Fig. S5 Compounds of importance when predicting $TACO_2^{-\bullet}$ of *P. atlantica* extracts shown on a (a) an overlay chromatogram, as evaluated using (b) regression coefficients of PLS after column centering, (c) regression coefficients of PLS after normalization and column centering, and (d) regression coefficients of PLS after standard normal variate and column centering.