Table S3. Diagnostic parameters of the PLS-DA models discriminating for the C-source (phenanthrene or glucose). The number of components for each model was chosen based on the minimal RMSEP and maximal R^2 values. For the FT-Raman model 4 principal components were used, whereas for the FTIR model 8 principal components were used. RMSC: root mean squared error of calibration, RMSEP: root mean squared error of prediction, R^2_C: coefficient of determination for the calibration, R^2_P: coefficient of determination for predicted values, Sensitivity: ability in discriminating true positives, Specificity: ability in discriminating true negatives.

	FT-Raman spectroscopy	**FTIR spectroscopy**
Sensitivity	0.82	0.92
Specificity	0.75	0.94
RMSEP	0.41	0.28
R^2_p	0.29	0.67
RMSEC	0.35	0.26
R^2_c	0.50	0.71
% variance X	38	87
% variance Y	50	71