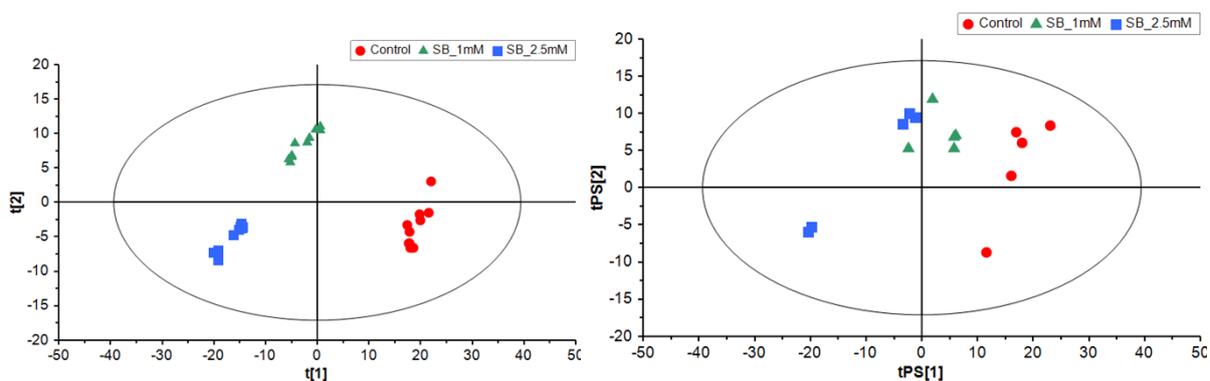
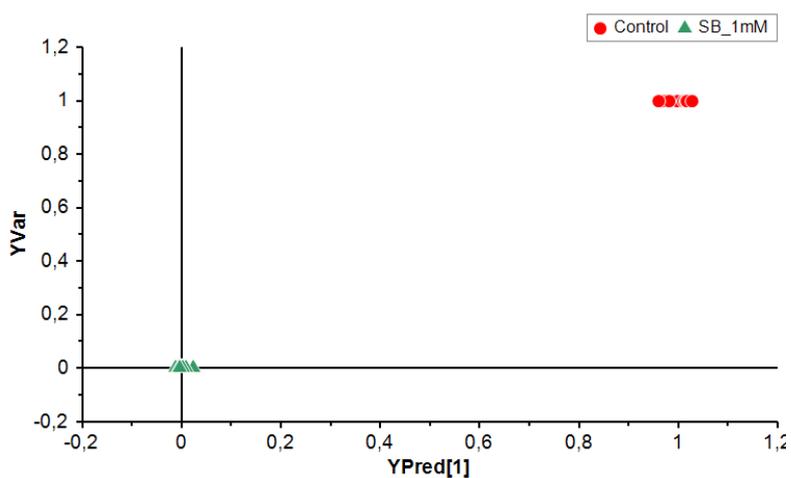


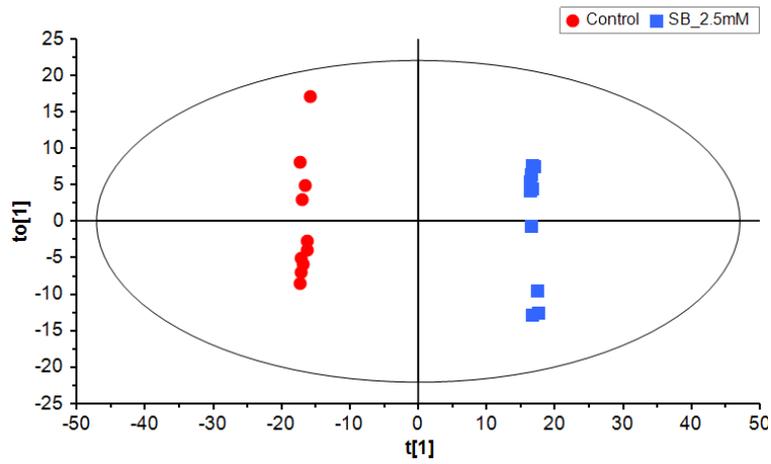
## Supplementary data:



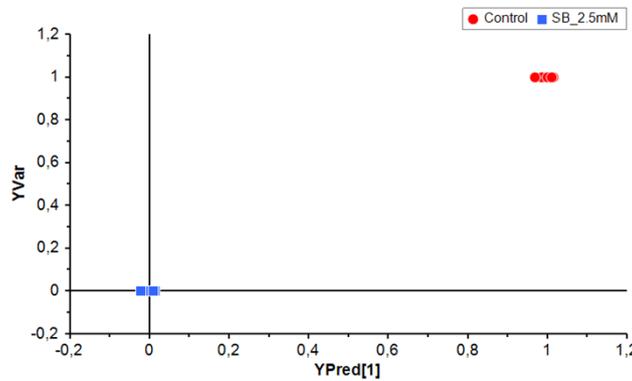
**Fig. S1: Scores plot of the training (left) and the test (right) sets for the three-class PLS-DA model.**



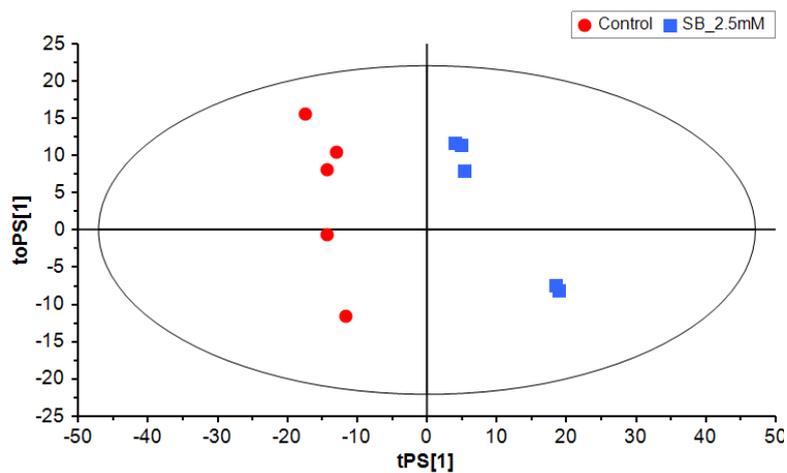
**Fig. S2: Observed versus predicted group values obtained by OPLS-DA of the SB 1 mM training set (n=20).**



**Fig. S3: Classification of control and 2.5 mM SB samples: OPLS-DA scores plot of the training set (n=20).**



**Fig. S4: Observed versus predicted group values obtained by OPLS-DA of the SB 2.5 mM training set (n=20).**



**Fig. S5: Prediction of control and 2.5 mM SB samples: OPLS-DA scores plot of the test set (n=10).**

**Table S1: Contingency table for the three-class PLS-DA model showing that 80% of samples within the test set ( $n=15$ ) were accurately classified. Fisher's exact test was performed on binary classification data to establish classification significance ( $p$ -value  $< 0.05$ ).**

	Members	Correct	Control	SB 1 mM	SB 2.5 mM	No class
Control	5	100%	5	0	0	0
SB 1 mM	5	100%	0	5	0	0
SB 2.5 mM	5	40%	0	3	2	0
No class	0		0	0	0	0
Total	15	80%	5	8	2	0
Fisher's prob.	0.00044					

**Table S2: Contingency table for the two-class OPLS-DA model showing that 100% of control and 1 mM SB samples within the test set ( $n=10$ ) were accurately classified. Fisher's exact test was performed on binary classification data to establish classification significance ( $p$ -value  $< 0.05$ ).**

	Members	Correct	Control	SB 1 mM
Control	5	100%	5	0
SB 1 mM	5	100%	0	5
No class	0		0	0
Total	10	100%	5	5
Fisher's prob.	0.004			

**Table S3: Contingency table for the two-class OPLS-DA model showing that 100% of control and 2.5 mM SB samples within the test set (n=10) were accurately classified. Fisher's exact test was performed on binary classification data to establish classification significance (p-value < 0.05).**

	Members	Correct	Control	SB 2.5 mM
Control	5	100%	5	0
SB 2.5 mM	5	100%	0	5
No class	0		0	0
Total	10	100%	5	5
Fisher's prob.	0.004			