

Figure S1. (A) Box-and-whisker plot showing the BBB scores, which confirm the successful establishment of the model. In SCI rats, the scores were 0, 0, 1, 0, 1 and 0, while all sham rats maintained a score of 21, indicating no neurological impairment. (B) Contiguous spinal cord sections with intact spinal cord morphology were selected for mass spectrometry imaging analysis. (C) Correlation analysis of the spatially shrunken centroid clustering results indicates the degree of the correlation between different clusters. The Pearson correlation coefficient followed by Bonferroni correction was used to measure the degree of linear correlation between two clusters. Red indicates a positive correlation, and blue indicates a negative correlation. The dot size represents the absolute value of the correlation coefficient. SCI, spinal cord injury; BBB, Basso, Beattie and Bresnahan scale. * $P < 0.05$, ** $P < 0.01$ and *** $P < 0.001$ vs. sham or the correlated cluster.

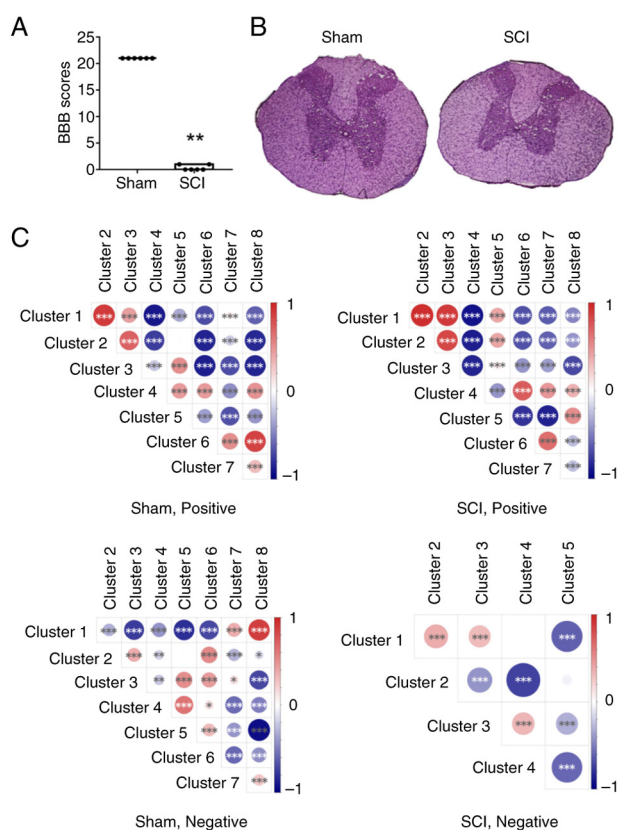


Figure S2. Validation plot of the OPLS-DA model for the gray and white matter. Seven-fold cross-validation and 200 response permutation testing were used to examine the quality of the OPLS-DA. The model parameters for each group were as follows: Gray matter, positive: $R^2Y=0.98$, $Q^2Y=0.97$, $R^2=(0.00, 0.50)$ and $Q^2=(0.00, -0.53)$; gray matter, negative: $R^2Y=0.85$, $Q^2Y=0.81$, $R^2=(0.00, 0.05)$ and $Q^2=(0.00, -0.17)$; white matter, positive: $R^2Y=0.99$, $Q^2Y=0.97$, $R^2=(0.00, 0.55)$ and $Q^2=(0.00, -0.64)$; white matter, negative: $R^2Y=0.89$, $Q^2Y=0.84$, $R^2=(0.00, 0.21)$ and $Q^2=(0.00, -0.34)$. R^2Y represents the proportion of variation in the response variable (Y) that the model can explain, serving as a measure of the model's goodness-of-fit. Q^2Y indicates the model's predictive accuracy, determined through cross-validation. R^2 refers to the overall proportion of variance explained by the model. Q^2 similarly represents the cross-validated predictive power of the model. High R^2Y and Q^2Y values (with Q^2Y ideally >0.5) suggest a robust and reliable model. Additionally, in permutation tests, a negative Q^2 intercept is a good indicator that the model is not overfitted. OPLS-DA, orthogonal partial least squares-discriminant analysis.

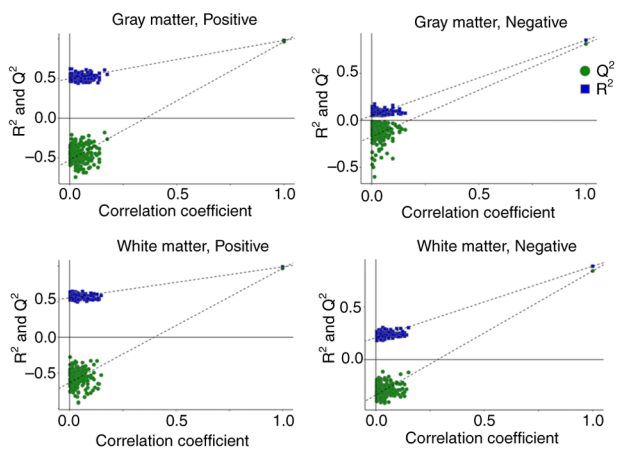


Figure S3. Validation plot of the OPLS-DA model for the ventral and dorsal horns. Seven-fold cross-validation and 200 response permutation testing were used to examine the validity of OPLS-DA. The model parameters for each group were as follows: Ventral horn, positive: $R^2Y=0.99$, $Q^2Y=0.97$, $R^2=(0.00, 0.51)$ and $Q^2=(0.00, -0.54)$; ventral horn, negative: $R^2Y=0.97$, $Q^2Y=0.95$, $R^2=(0.00, 0.33)$ and $Q^2=(0.00, -0.53)$; dorsal horn, positive: $R^2Y=1.00$, $Q^2Y=0.99$, $R^2=(0.00, 0.55)$ and $Q^2=(0.00, -0.68)$; dorsal horn, negative: $R^2Y=0.85$, $Q^2Y=0.55$, $R^2=(0.00, 0.10)$ and $Q^2=(0.0, -0.30)$. R^2Y represents the proportion of variation in the response variable (Y) that the model can explain, serving as a measure of the model's goodness-of-fit. Q^2Y indicates the model's predictive accuracy, determined through cross-validation. R^2 refers to the overall proportion of variance explained by the model. Q^2 similarly represents the cross-validated predictive power of the model. OPLS-DA, orthogonal partial least squares-discriminant analysis; SCI, spinal cord injury.

