**S2 Table. Contingency table results.** a) Pain *vs.* C, b) NP *vs.* C, c) NC *vs*. C, and d) NP *vs*. NC OPLS-DA models

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| 1. Pain *vs.* C
 | Pain | Control | Total |
| OPLS-DA Positive | 32 | 2 | 34 |
| OPLS-DA Negative | 5 | 35 | 40 |
| Total | 37 | 37 | 74 |
| Sensitivity (95% confidence interval): 0.86 (0.71 to 0.95) |
| Specificity (95% confidence interval): 0.85 (0.82 to 0.99) |
| Positive Predictive Value (95% confidence interval): 0.94 (0.80 to 0.99) |
| Negative Predictive Value (95% confidence interval): 0.88 (0.73 to 0.96) |
| P <0.0001 |

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| --- | --- | --- | --- |
| 1. NP *vs.* C
 | Neuropathic Pain | Control | Total |
| OPLS-DA Positive | 23 | 2 | 25 |
| OPLS-DA Negative | 2 | 23 | 25 |
| Total | 25 | 25 | 50 |
| Sensitivity (95% confidence interval): 0.92 (0.74 to 0.99) |
| Specificity (95% confidence interval): 0.92 (0.74 to 0.99) |
| Positive Predictive Value (95% confidence interval): 0.92 (0.74 to 0.99) |
| Negative Predictive Value (95% confidence interval): 0.92 (0.74 to 0.99) |
| P <0.0001 |

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| --- | --- | --- | --- |
| 1. NC *vs.* C
 | Nociceptive Pain | Control | Total |
| OPLS-DA Positive | 8 | 1 | 9 |
| OPLS-DA Negative | 4 | 11 | 15 |
| Total | 12 | 12 | 24 |
| Sensitivity (95% confidence interval): 0.67 (0.35 to 0.90) |
| Specificity (95% confidence interval): 0.92 (0.62 to 1.00) |
| Positive Predictive Value (95% confidence interval): 0.89 (0.52 to 1.00) |
| Negative Predictive Value (95% confidence interval): 0.73 (0.45 to 0.92) |
| P =0.01  |

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| --- | --- | --- | --- |
| 1. NP *vs.* NC
 | Neuropathic Pain | Nociceptive Pain | Total |
| OPLS-DA Positive | 22 | 2 | 24 |
| OPLS-DA Negative | 3 | 10 | 13 |
| Total | 25 | 12 | 37 |
| Sensitivity (95% confidence interval): 0.88 (0.69 to 0.97) |
| Specificity (95% confidence interval): 0.83 (0.52 to 0.98) |
| Positive Predictive Value (95% confidence interval): 0.92 (0.73 to 0.99) |
| Negative Predictive Value (95% confidence interval): 0.77 (0.46 to 0.95) |
| P <0.0001 |