

| | Validation set | | | | 8-fold CV | | |
|------------------|----------------|----------|-------------|--------------|-------------|--------------|-------------|
| Model | Train RMSE | Train R2 | Test RMSE | NRM | CVRMSE | NRM | SD SSE |
| PLS | 0.80 | 0.93 | 3.81 | 42.47 | 14.12 | 157.41 | 113.88 |
| Ridge Regression | 1.87 | 0.59 | 2.01 | 22.41 | 5.87 | 65.44 | 20.17 |
| Random Forest | 2.43 | 0.30 | 2.49 | 27.76 | 2.83 | 31.55 | 2.81 |