**Table L1. Selection of data splitting ratio for ML models at 1 bar.**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  |  | Data Splitting Ratio | | | | |
| 90:10 | 80:20 | 70:30 | 60:40 | 50:50 |
| CH4 Uptake (mol/kg)  N2 Uptake (mol/kg) | R2-Train | 0.99 | 0.99 | 0.99 | 0.98 | 0.99 |
| R2-Test | 0.97 | 0.97 | 0.98 | 0.97 | 0.95 |
| MAE-Train | 1.78×10-2 | 7.91×10-3 | 1.74×10-2 | 2.59×10-2 | 1.19×10-2 |
| MAE-Test | 3.25×10-2 | 3.23×10-2 | 3.04×10-2 | 3.54×10-2 | 3.35×10-2 |
| RMSE-Train | 3.06×10-2 | 1.12×10-2 | 3.50×10-2 | 4.97×10-2 | 1.97×10-2 |
| RMSE-Test | 6.59×10-2 | 6.54×10-2 | 6.02×10-2 | 6.15×10-2 | 8.20×10-2 |
| R2-Train | 0.99 | 0.99 | 0.99 | 0.99 | 0.99 |
| R2-Test | 0.97 | 0.97 | 0.97 | 0.97 | 0.96 |
| MAE-Train | 1.44×10-3 | 1.30×10-3 | 2.42×10-3 | 1.83×10-3 | 3.39×10-3 |
| MAE-Test | 5.44×10-3 | 5.53×10-3 | 5.89×10-3 | 6.08×10-3 | 6.67×10-3 |
| RMSE-Train | 2.15×10-3 | 1.83×10-3 | 3.85×10-3 | 2.78×10-3 | 5.12×10-3 |
| RMSE-Test | 9.69×10-3 | 9.55×10-3 | 1.03×10-2 | 1.11×10-2 | 1.21×10-2 |