**Table 3** Performances of QSRR models applied to the pesticide dataset

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  |  | Internal set | | | | External set | | | DNN Optimized | | | | | | |
|  |  |  | Training set | | Test set | |  | | |  |  |  |  |
| N° Model | Number of molecular descriptors | Name of the Model | R² | RMSE | R² | RMSE | R² | RMSE | Percentage of error | | Number of neurons per hidden layers | Activation function | | | Solver | Alpha |
| 1 | 16 | *Bade-MLP* | 0.95 | 0.43 | 0.90 | 0.63 | 0.82 | 0.67 | 6% | | 16-16-16-16-16 | ReLu | | | Adam | 10 |
| 2 | 16 | *Lasso-MLP* | 0.60 | 1.19 | 0.50 | 1.27 | 0.49 | 1.36 | 12% | | 16 | tanh | | | SGD | 1 |
| 3 | 16 | *Pearson-MLP* | 0.79 | 0.86 | 0.79 | 0.83 | 0.78 | 0.88 | 8% | | 16-16 | ReLu | | | SGD | 10 |
| 4 | 16 | *RFE-MLP* | 0.69 | 1.04 | 0.60 | 1.15 | 0.63 | 1.16 | 10% | | 16-16-16-16-16 | ReLu | | | SGD | 10 |
| 5 | 16 | *PCA1-MLP* | 0.75 | 0.94 | 0.61 | 1.12 | 0.64 | 1.14 | 10% | | 16 | tanh | | | Adam | 1 |
| 6 | 16 | *PCA2-MLP* | 0.42 | 1.44 | 0.34 | 1.47 | 0.38 | 1.50 | 13% | | 16 | tanh | | | Adam | 1 |
| 7 | 16 | *PCA3-MLP* | 0.61 | 1.18 | 0.53 | 1.24 | 0.56 | 1.26 | 11% | | 16-16-16 | ReLu | | | SGD | 10 |
| 8 | 16 | *PCA4-MLP* | 0.82 | 0.79 | 0.75 | 0.91 | 0.76 | 0.93 | 8% | | 16-16-16-16 | ReLu | | | SGD | 10 |