

RF-RDKIT

| Fold | AUC | BACC | Sens | Spec | Kappa |
|----------------|-------------|-------------|-------------|-------------|-------------|
| 0 | 0.86 | 0.64 | 0.30 | 0.98 | 0.36 |
| 1 | 0.87 | 0.67 | 0.36 | 0.99 | 0.45 |
| 2 | 0.88 | 0.65 | 0.31 | 0.98 | 0.39 |
| 3 | 0.86 | 0.66 | 0.35 | 0.98 | 0.41 |
| 4 | 0.88 | 0.67 | 0.36 | 0.98 | 0.43 |
| Average | 0.87 | 0.66 | 0.34 | 0.98 | 0.41 |

RF-MORGAN

| Fold | AUC | BACC | Sens | Spec | Kappa |
|----------------|-------------|-------------|-------------|-------------|-------------|
| 0 | 0.83 | 0.63 | 0.28 | 0.98 | 0.35 |
| 1 | 0.84 | 0.63 | 0.28 | 0.98 | 0.35 |
| 2 | 0.84 | 0.62 | 0.25 | 0.98 | 0.32 |
| 3 | 0.85 | 0.64 | 0.30 | 0.99 | 0.40 |
| 4 | 0.86 | 0.64 | 0.29 | 0.99 | 0.39 |
| Average | 0.84 | 0.63 | 0.28 | 0.98 | 0.36 |

XGB-RDKIT

| Fold | AUC | BACC | Sens | Spec | Kappa |
|----------------|-------------|-------------|-------------|-------------|-------------|
| 0 | 0.87 | 0.65 | 0.32 | 0.97 | 0.37 |
| 1 | 0.87 | 0.68 | 0.39 | 0.97 | 0.45 |
| 2 | 0.88 | 0.67 | 0.37 | 0.97 | 0.43 |
| 3 | 0.87 | 0.69 | 0.40 | 0.97 | 0.46 |
| 4 | 0.88 | 0.68 | 0.39 | 0.98 | 0.45 |
| Average | 0.87 | 0.67 | 0.37 | 0.97 | 0.43 |

XGB-MORGAN

| Fold | AUC | BACC | Sens | Spec | Kappa |
|----------------|-------------|-------------|-------------|-------------|-------------|
| 0 | 0.84 | 0.66 | 0.33 | 0.98 | 0.41 |
| 1 | 0.85 | 0.64 | 0.30 | 0.98 | 0.38 |
| 2 | 0.86 | 0.64 | 0.30 | 0.98 | 0.37 |
| 3 | 0.85 | 0.65 | 0.32 | 0.98 | 0.41 |
| 4 | 0.85 | 0.69 | 0.39 | 0.99 | 0.49 |
| Average | 0.85 | 0.66 | 0.33 | 0.98 | 0.41 |

DNN-RDKIT

| Fold | AUC | BACC | Sens | Spec | Kappa |
|----------------|-------------|-------------|-------------|-------------|-------------|
| 0 | 0.81 | 0.57 | 0.14 | 0.99 | 0.21 |
| 1 | 0.78 | 0.62 | 0.25 | 0.98 | 0.31 |
| 2 | 0.86 | 0.67 | 0.38 | 0.97 | 0.43 |
| 3 | 0.82 | 0.58 | 0.16 | 0.99 | 0.23 |
| 4 | 0.82 | 0.64 | 0.29 | 0.99 | 0.37 |
| Average | 0.82 | 0.62 | 0.24 | 0.98 | 0.31 |

DNN-MORGAN

| Fold | AUC | BACC | Sens | Spec | Kappa |
|------|------|------|------|------|-------|
| 0 | 0.71 | 0.66 | 0.36 | 0.97 | 0.39 |
| 1 | 0.72 | 0.67 | 0.37 | 0.96 | 0.40 |
| 2 | 0.80 | 0.71 | 0.49 | 0.94 | 0.45 |
| 3 | 0.74 | 0.70 | 0.43 | 0.98 | 0.49 |

| | | | | | |
|----------------|------|------|------|------|------|
| 4 | 0.74 | 0.69 | 0.43 | 0.96 | 0.46 |
| Average | 0.74 | 0.69 | 0.42 | 0.96 | 0.44 |

GCNN

| Fold | AUC | BACC | Sens | Spec | Kappa |
|----------------|------------|-------------|-------------|-------------|--------------|
| 0 | 0.85 | 0.69 | 0.42 | 0.96 | 0.44 |
| 1 | 0.81 | 0.59 | 0.20 | 0.99 | 0.27 |
| 2 | 0.88 | 0.63 | 0.28 | 0.97 | 0.33 |
| 3 | 0.86 | 0.65 | 0.32 | 0.98 | 0.36 |
| 4 | 0.87 | 0.69 | 0.41 | 0.97 | 0.46 |
| Average | 0.85 | 0.65 | 0.33 | 0.97 | 0.37 |

| Model | Full Name |
|--------------|--------------------------------------|
| RF | Random Forest |
| XGB | eXtreme Gradient Boosting or XGBoost |
| DNN | Deep Neural Network |
| GCNN | Graph Convolutional Neural Network |

RF-RDKIT

| Fold | AUC | BACC | Sens | Spec | Kappa |
|----------------|------|------|------|------|-------|
| 0 | 0.86 | 0.76 | 0.62 | 0.91 | 0.55 |
| 1 | 0.85 | 0.78 | 0.64 | 0.92 | 0.60 |
| 2 | 0.82 | 0.73 | 0.56 | 0.90 | 0.48 |
| 3 | 0.85 | 0.73 | 0.53 | 0.92 | 0.49 |
| 4 | 0.86 | 0.75 | 0.60 | 0.91 | 0.53 |
| Average | 0.85 | 0.75 | 0.59 | 0.91 | 0.53 |

RF-MORGAN

| Fold | AUC | BACC | Sens | Spec | Kappa |
|----------------|------|------|------|------|-------|
| 0 | 0.83 | 0.77 | 0.63 | 0.91 | 0.56 |
| 1 | 0.82 | 0.75 | 0.61 | 0.90 | 0.53 |
| 2 | 0.76 | 0.69 | 0.52 | 0.87 | 0.41 |
| 3 | 0.81 | 0.73 | 0.54 | 0.91 | 0.48 |
| 4 | 0.81 | 0.71 | 0.56 | 0.87 | 0.44 |
| Average | 0.81 | 0.73 | 0.57 | 0.89 | 0.48 |

XGB-RDKIT

| Fold | AUC | BACC | Sens | Spec | Kappa |
|----------------|------|------|------|------|-------|
| 0 | 0.87 | 0.78 | 0.67 | 0.88 | 0.56 |
| 1 | 0.84 | 0.74 | 0.59 | 0.89 | 0.51 |
| 2 | 0.83 | 0.75 | 0.60 | 0.90 | 0.52 |
| 3 | 0.85 | 0.74 | 0.57 | 0.91 | 0.51 |
| 4 | 0.85 | 0.76 | 0.62 | 0.90 | 0.55 |
| Average | 0.85 | 0.75 | 0.61 | 0.90 | 0.53 |

XGB-MORGAN

| Fold | AUC | BACC | Sens | Spec | Kappa |
|----------------|------|------|------|------|-------|
| 0 | 0.82 | 0.75 | 0.64 | 0.87 | 0.51 |
| 1 | 0.83 | 0.75 | 0.61 | 0.89 | 0.52 |
| 2 | 0.77 | 0.69 | 0.55 | 0.84 | 0.40 |
| 3 | 0.81 | 0.73 | 0.55 | 0.90 | 0.48 |
| 4 | 0.83 | 0.76 | 0.66 | 0.86 | 0.53 |
| Average | 0.81 | 0.74 | 0.60 | 0.87 | 0.49 |

DNN-RDKIT

| Fold | AUC | BACC | Sens | Spec | Kappa |
|----------------|------|------|------|------|-------|
| 0 | 0.86 | 0.8 | 0.83 | 0.76 | 0.54 |
| 1 | 0.81 | 0.71 | 0.45 | 0.96 | 0.46 |
| 2 | 0.82 | 0.74 | 0.64 | 0.83 | 0.47 |
| 3 | 0.81 | 0.74 | 0.63 | 0.85 | 0.5 |
| 4 | 0.84 | 0.77 | 0.75 | 0.79 | 0.52 |
| Average | 0.83 | 0.75 | 0.66 | 0.84 | 0.50 |

DNN-MORGAN

| Fold | AUC | BACC | Sens | Spec | Kappa |
|------|------|------|------|------|-------|
| 0 | 0.78 | 0.76 | 0.7 | 0.82 | 0.51 |
| 1 | 0.77 | 0.72 | 0.62 | 0.83 | 0.46 |
| 2 | 0.71 | 0.68 | 0.54 | 0.82 | 0.37 |
| 3 | 0.74 | 0.71 | 0.63 | 0.79 | 0.42 |

| | | | | | |
|----------------|------|------|------|------|------|
| 4 | 0.78 | 0.74 | 0.63 | 0.84 | 0.47 |
| Average | 0.76 | 0.72 | 0.62 | 0.82 | 0.45 |

GCNN

| Fold | AUC | BACC | Sens | Spec | Kappa |
|----------------|------------|-------------|-------------|-------------|--------------|
| 0 | 0.86 | 0.75 | 0.62 | 0.89 | 0.53 |
| 1 | 0.84 | 0.73 | 0.56 | 0.90 | 0.49 |
| 2 | 0.83 | 0.75 | 0.61 | 0.89 | 0.51 |
| 3 | 0.86 | 0.77 | 0.68 | 0.86 | 0.55 |
| 4 | 0.86 | 0.77 | 0.68 | 0.86 | 0.54 |
| Average | 0.85 | 0.75 | 0.63 | 0.88 | 0.52 |