Table. F-score in 10-fold cross validation of training dataset

| **Substance** | **Model** | **Mean F-score** | **SE** |
| --- | --- | --- | --- |
| Any Opioids | logistic\_reg | 0.990 | 0.001 |
| Heroin | logistic\_reg | 0.998 | 0.001 |
| Fentanyl | logistic\_reg | 1.000 | 0.000 |
| Prescription.opioids | logistic\_reg | 0.994 | 0.001 |
| Methamphetamine | logistic\_reg | 0.997 | 0.001 |
| Cocaine | logistic\_reg | 0.999 | 0.001 |
| Benzodiazepines | logistic\_reg | 0.903 | 0.007 |
| Alcohol | logistic\_reg | 0.845 | 0.008 |
| Others | logistic\_reg | 0.963 | 0.002 |

Table. Best performing models in 10-fold cross validation of training dataset

| **Substance** | **Model** | **Mean F-score** | **SE** |
| --- | --- | --- | --- |
| Any Opioids | logistic\_reg | 0.990 | 0.001 |
| Heroin | logistic\_reg | 0.998 | 0.001 |
| Fentanyl | logistic\_reg | 1.000 | 0.000 |
| Prescription.opioids | logistic\_reg | 0.994 | 0.001 |
| Methamphetamine | logistic\_reg | 0.997 | 0.001 |
| Cocaine | logistic\_reg | 0.999 | 0.001 |
| Benzodiazepines | logistic\_reg | 0.903 | 0.007 |
| Alcohol | logistic\_reg | 0.845 | 0.008 |
| Others | logistic\_reg | 0.963 | 0.002 |

Table. Diagnostic metrics of best performing models in test dataset

| **Substance** | **F-score** | **Accuracy** | **Kappa** | **Sensitivity (Recall)** | **Specificity** | **Positive predictive value (Precision)** | **Negative predictive value** | **AUROC** |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Any Opioids | 0.990 | 0.997 | 0.988 | 0.984 | 0.999 | 0.996 | 0.997 | 0.998 |
| Heroin | 0.997 | 1.000 | 0.997 | 0.994 | 1.000 | 1.000 | 1.000 | 1.000 |
| Fentanyl | 0.998 | 1.000 | 0.998 | 0.999 | 1.000 | 0.998 | 1.000 | 1.000 |
| Prescription.opioids | 0.994 | 1.000 | 0.993 | 0.996 | 1.000 | 0.992 | 1.000 | 0.996 |
| Methamphetamine | 0.999 | 1.000 | 0.999 | 1.000 | 1.000 | 0.997 | 1.000 | 1.000 |
| Cocaine | 0.998 | 1.000 | 0.998 | 0.996 | 1.000 | 1.000 | 1.000 | 1.000 |
| Benzodiazepines | 0.905 | 0.995 | 0.902 | 0.834 | 1.000 | 0.988 | 0.995 | 0.977 |
| Alcohol | 0.868 | 0.981 | 0.858 | 0.767 | 1.000 | 1.000 | 0.980 | 0.915 |
| Others | 0.969 | 0.995 | 0.966 | 0.946 | 0.999 | 0.993 | 0.995 | 0.995 |

Table. Bootstrapped diagnostic metrics and 95% confidence intervals of best performing models in test dataset

| **Substance** | **F-score** | **Lower** | **Upper** | **Accuracy** | **aLower** | **aUpper** | **Kappa** | **kLower** | **kUpper** | **Sensitivity (Recall)** | **sLower** | **sUpper** | **Specificity** | **spLower** | **spUpper** | **Positive predictive value (Precision)** | **ppLower** | **ppUpper** | **Negative predictive value** | **npLower** | **npUpper** | **AUROC** | **auLower** | **auUpper** |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Any Opioids | 0.987 | 0.980 | 0.994 | 0.996 | 0.994 | 0.998 | 0.985 | 0.977 | 0.992 | 0.981 | 0.969 | 0.991 | 0.999 | 0.997 | 1 | 0.994 | 0.983 | 1 | 0.996 | 0.994 | 0.998 | 0.996 | 0.990 | 1.000 |
| Heroin | 0.995 | 0.983 | 1.000 | 1.000 | 0.998 | 1.000 | 0.995 | 0.983 | 1.000 | 0.995 | 0.976 | 1.000 | 1.000 | 0.999 | 1 | 0.995 | 0.975 | 1 | 1.000 | 0.999 | 1.000 | 1.000 | 0.999 | 1.000 |
| Fentanyl | 0.999 | 0.996 | 1.000 | 1.000 | 0.999 | 1.000 | 0.999 | 0.995 | 1.000 | 0.999 | 0.997 | 1.000 | 1.000 | 0.999 | 1 | 0.999 | 0.994 | 1 | 1.000 | 1.000 | 1.000 | 1.000 | 0.997 | 1.000 |
| Prescription.opioids | 0.979 | 0.952 | 1.000 | 0.999 | 0.997 | 1.000 | 0.979 | 0.951 | 1.000 | 0.971 | 0.929 | 1.000 | 1.000 | 0.998 | 1 | 0.987 | 0.950 | 1 | 0.999 | 0.998 | 1.000 | 0.990 | 0.969 | 1.000 |
| Methamphetamine | 0.996 | 0.985 | 1.000 | 1.000 | 0.998 | 1.000 | 0.996 | 0.984 | 1.000 | 0.995 | 0.972 | 1.000 | 1.000 | 0.999 | 1 | 0.996 | 0.985 | 1 | 1.000 | 0.998 | 1.000 | 0.999 | 0.986 | 1.000 |
| Cocaine | 0.998 | 0.991 | 1.000 | 1.000 | 0.999 | 1.000 | 0.998 | 0.990 | 1.000 | 0.998 | 0.989 | 1.000 | 1.000 | 0.999 | 1 | 0.998 | 0.987 | 1 | 1.000 | 0.999 | 1.000 | 1.000 | 1.000 | 1.000 |
| Benzodiazepines | 0.882 | 0.829 | 0.926 | 0.994 | 0.991 | 0.996 | 0.879 | 0.824 | 0.924 | 0.814 | 0.731 | 0.887 | 0.999 | 0.997 | 1 | 0.963 | 0.900 | 1 | 0.995 | 0.992 | 0.997 | 0.962 | 0.925 | 0.992 |
| Alcohol | 0.867 | 0.837 | 0.894 | 0.981 | 0.977 | 0.985 | 0.857 | 0.826 | 0.886 | 0.780 | 0.726 | 0.835 | 0.998 | 0.995 | 1 | 0.978 | 0.939 | 1 | 0.981 | 0.976 | 0.986 | 0.915 | 0.896 | 0.934 |
| Others | 0.951 | 0.929 | 0.968 | 0.992 | 0.989 | 0.995 | 0.947 | 0.923 | 0.965 | 0.919 | 0.885 | 0.950 | 0.999 | 0.997 | 1 | 0.985 | 0.962 | 1 | 0.993 | 0.990 | 0.996 | 0.988 | 0.974 | 0.997 |







































































