

Multimedia Appendix 1. Hyperparameter tuning.

The hyperparameters of the ML classifiers obtained through the grid search cross-validation were as follows:

Table 1: Hyperparameter value range and optimal values for all ML methods.

Model	Hyperparameters	Best combination	
		All factors	Oxidative stress factors only
Binary Classification			
LR	C_ values: [0.001, 0.01, 0.1, 1, 10, 100] Penalty: [l1, l2] Solvers: liblinear, lbfgs, newton-cg, sag, saga]	C_ value: 1 Penalty: l2 Solver: liblinear	C_ value: 0.001 Penalty: l2 Solver: liblinear
RF	n_estimators: [50, 100, 150, 200, 300] max_depth: [None, 5, 10, 15, 20, 25, 30] min_samples_split: [2, 5, 10] min_samples_leaf: [1, 2, 4] bootstrap: [True, False] max_features: [auto, sqrt, log2] max_leaf_nodes: [None, 5, 10, 20, 50, 100]	n_estimators: 50 max_depth: 15 min_samples_split: 2 min_samples_leaf: 1 bootstrap: False max_leaf_nodes: None	n_estimators: 50 max_depth: None min_samples_split: 5 min_samples_leaf: 1 bootstrap: False max_leaf_nodes: None
KNN	n_neighbors : [3, 5,7,9,11,13,15] weights: [uniform, distance] metric: [minkowski, euclidean, manhattan]	n_neighbors: 11 weights: distance Metric: manhattan	n_neighbors: 15 weights: distance Metric: manhattan
SVM	C: [0.1, 1, 10, 100] gamma: [1, 0.1, 0.01, 0.001] kernel: [linear, rbf]	C: 1 gamma: 0.1 kernel: rbf	C: 1 gamma: 1 kernel:rbf
NB	Naive Bayes has almost no hyperparameters to tune, so it usually generalizes well		
WLR	solvers = ['newton-cg', 'liblinear'] penalty = ['l1', 'l2'] c_values = [100, 10, 1.0, 0.1, 0.01]	solver: newton-cg penalty: l2 C: 1	solver: liblinear penalty: l2 C: 0.1
WRF	n_estimators: [50, 100, 150, 200, 300] max_depth: [None, 5, 10, 15, 20, 25, 30] min_samples_split: [2, 5, 10] min_samples_leaf: [1, 2, 4] bootstrap: [True, False] max_features: [auto, sqrt, log2] max_leaf_nodes: [None, 5, 10, 20, 50, 100]	n_estimators: 50 max_depth: None min_samples_split: 2 min_samples_leaf: 1 bootstrap: True max_leaf_nodes: None	n_estimators: 100 max_depth: 25 min_samples_split: 2 min_samples_leaf: 1 bootstrap: False max_leaf_nodes: None
Multi-class Classification			

LR	solvers = ['newton-cg', 'lbfgs', 'liblinear'] penalty = ['l1', 'l2'] c_values = [100, 10, 1.0, 0.1, 0.01]	Solver: liblinear Penalty: l2 C: 10	Solver: liblinear Penalty: l2 C: 0.001
RF	n_estimators: [50, 100, 150, 200, 300] max_depth: [None, 5, 10, 15, 20, 25, 30] min_samples_split: [2, 5, 10] min_samples_leaf: [1, 2, 4] bootstrap: [True, False] max_features: [auto, sqrt, log2] max_leaf_nodes: [None, 5, 10, 20, 50, 100]	n_estimators: 100 max_depth: 15 min_samples_split: 2 min_samples_leaf: 1 bootstrap: False max_leaf_nodes: None	n_estimators: 100 max_depth: 15 min_samples_split: 2 min_samples_leaf: 1 bootstrap: False max_leaf_nodes: None
KNN	n_neighbors: [5,7,9,11,13,15] weights: ['uniform','distance'] metric:['minkowski','euclidean', 'manhattan']	n_neighbors: 13 weights: distance Metric: Manhattan	n_neighbors: 15 weights: distance Metric: Manhattan
SVM	C: [1, 10, 100] gamma: [1,0.1,0.01,0.001] kernel: ['rbf']	C: 1 gamma: 0.1 kernel: rbf	C: 100 gamma: 1 kernel: rbf
NB	naive Bayes has almost no hyperparameters to tune, so it usually generalizes well		
WLR	solvers = ['newton-cg', 'liblinear'] penalty = ['l1', 'l2'] c_values = [100, 10, 1.0, 0.1, 0.01]	solver: liblinear penalty: l2 C: 0.001	solver: liblinear penalty: l2 C: 0.1
WRF	n_estimators: [50, 100, 150, 200, 300] max_depth: [None, 5, 10, 15, 20, 25, 30] min_samples_split: [2, 5, 10] min_samples_leaf: [1, 2, 4] bootstrap: [True, False] max_features: [auto, sqrt, log2] max_leaf_nodes: [None, 5, 10, 20, 50, 100]	n_estimators: 50 max_depth: None min_samples_split: 2 min_samples_leaf: 1 bootstrap: True max_leaf_nodes: None	n_estimators: 300 max_depth: 15 min_samples_split: 2 min_samples_leaf: 1 bootstrap: True max_leaf_nodes: None

Multimedia Appendix 2. Confusion Matrices

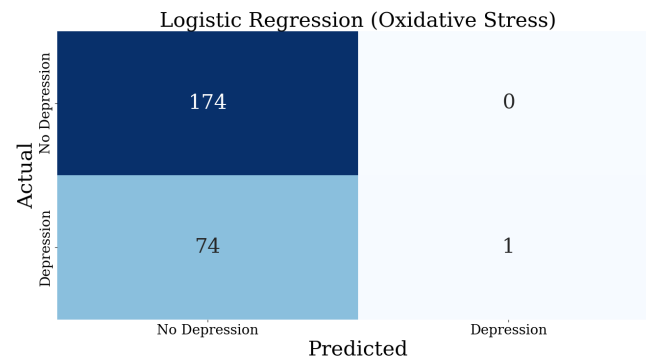


Figure 1: Confusion matrix of LR with oxidative stress biomarkers as the main features.

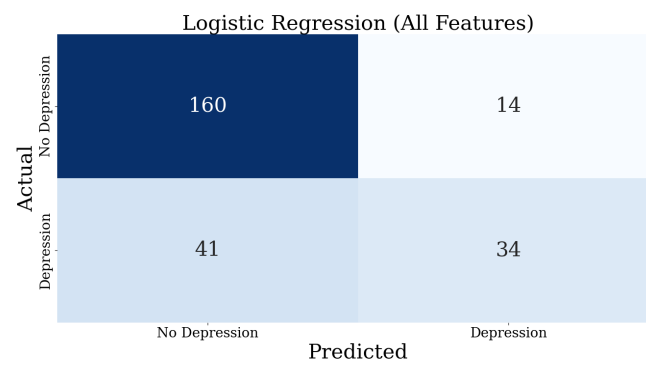


Figure 2: Confusion matrix of LR with all features.

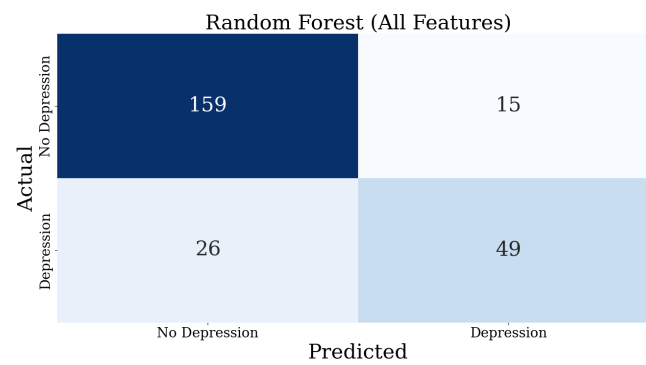


Figure 3: Confusion matrix of RF with all features.

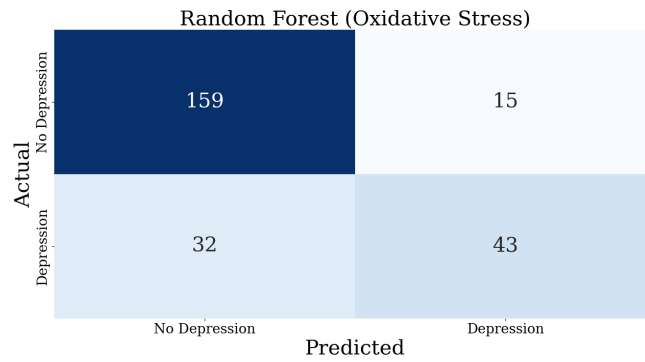


Figure 4: Confusion matrix of RF with oxidative stress biomarkers as the main features.

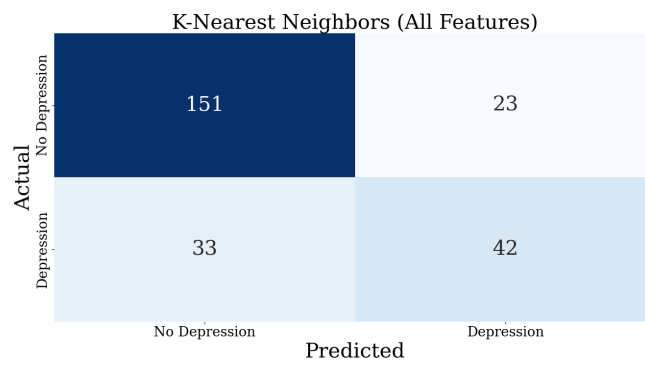


Figure 5: Confusion matrix of KNN with all features.

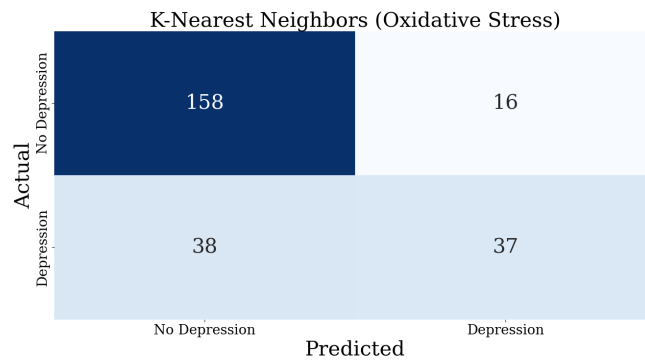


Figure 6: Confusion matrix of KNN with oxidative stress biomarkers as the main features.

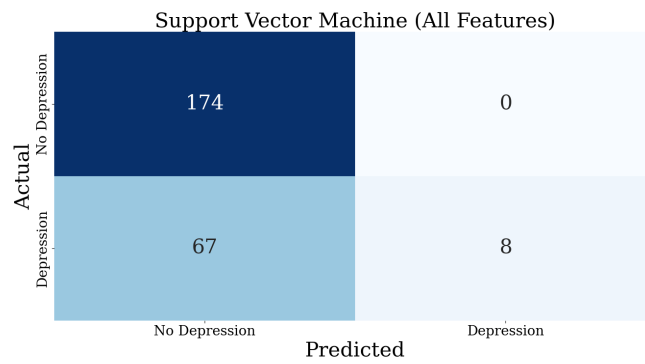


Figure 7: Confusion matrix of SVM with all features.

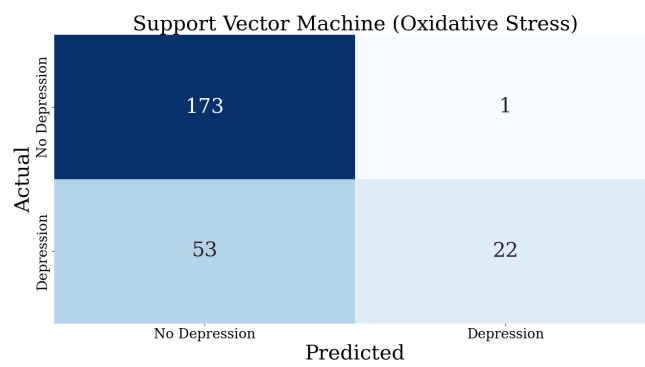


Figure 8: Confusion matrix of SVM with oxidative stress biomarkers as the main features.

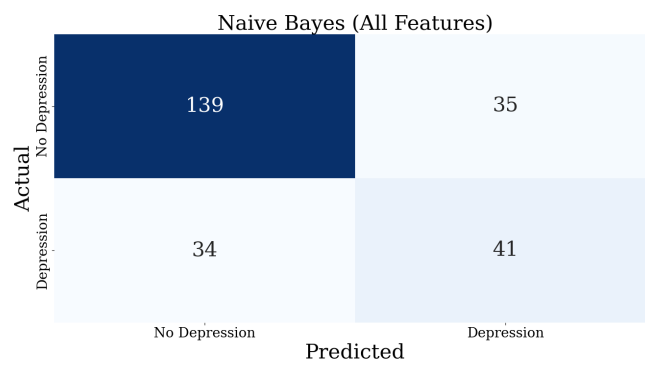


Figure 9: Confusion matrix of NB with all features.

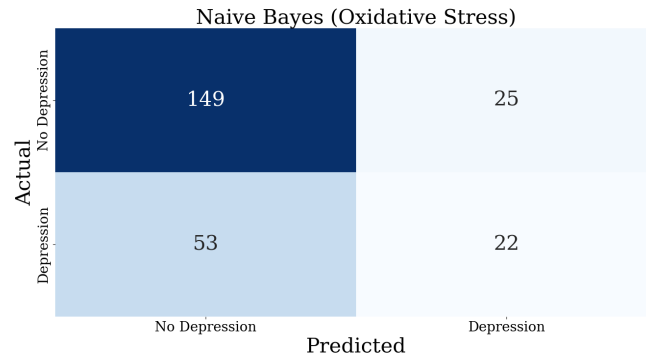


Figure 10: Confusion matrix of NB with oxidative stress biomarkers as the main features.

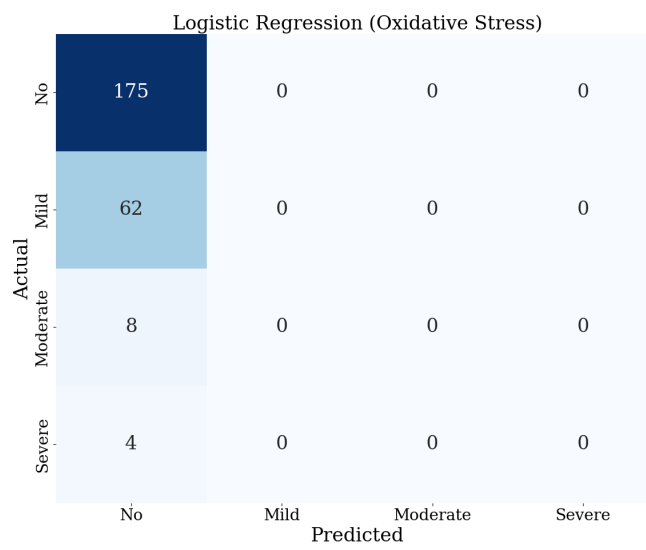


Figure 11: Confusion matrix of LR with oxidative stress biomarkers as the main features.

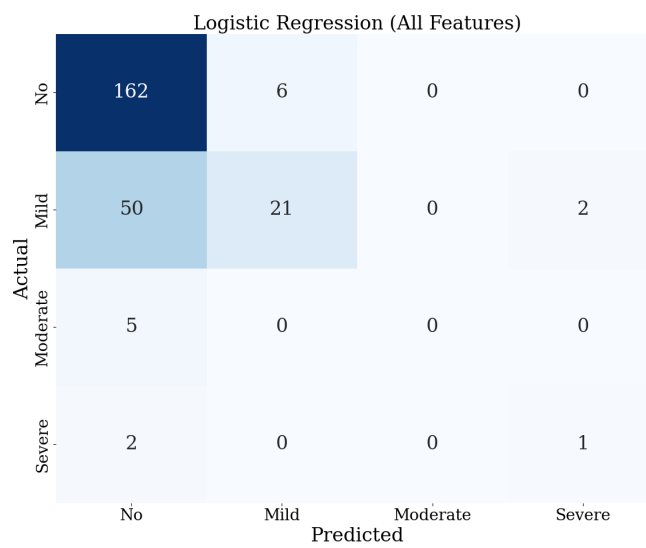


Figure 12: Confusion matrix of LR with all features.

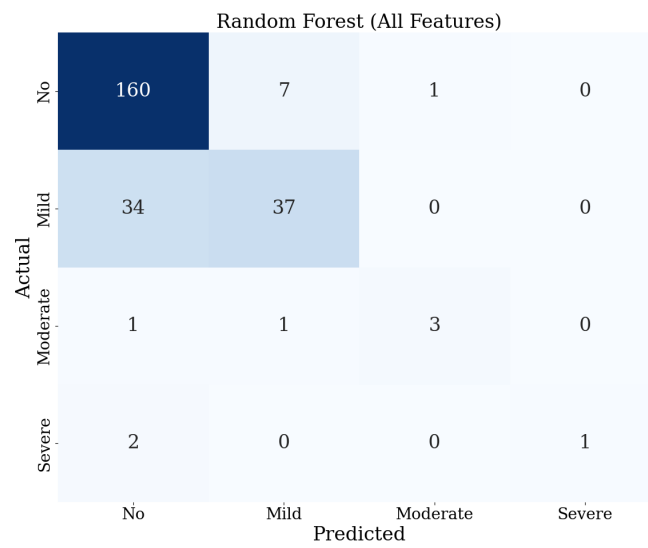


Figure 13: Confusion matrix of RF with all features.

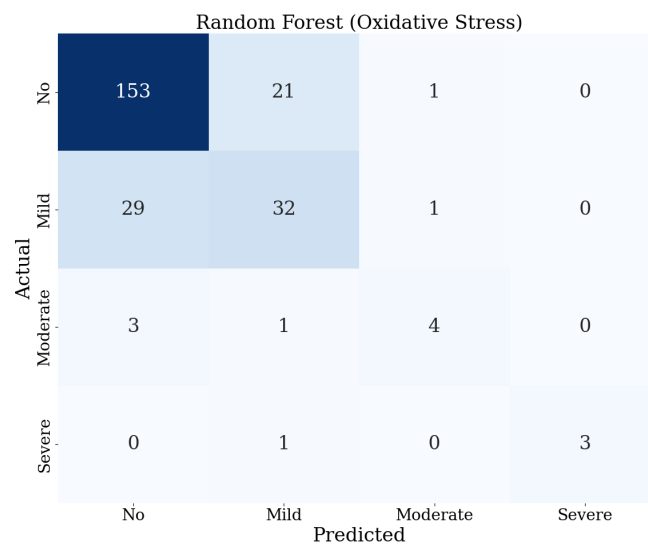


Figure 14: Confusion matrix of RF with oxidative stress biomarkers as the main features.

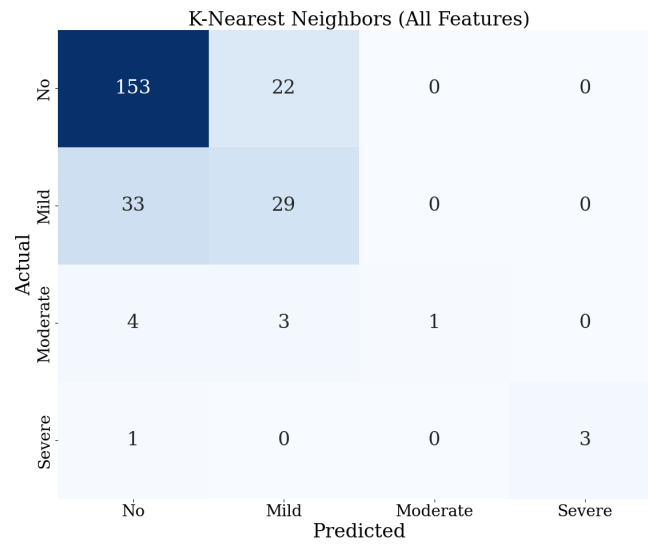


Figure 15: Confusion matrix of KNN with all features.

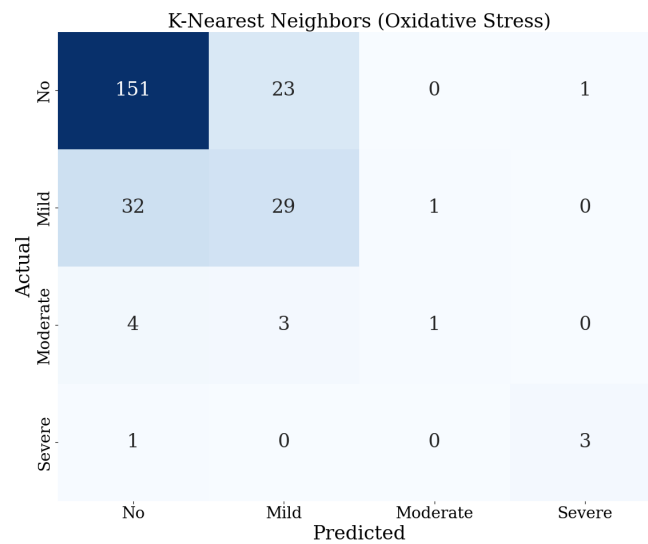


Figure 16: Confusion matrix of KNN with oxidative stress biomarkers as the main features.

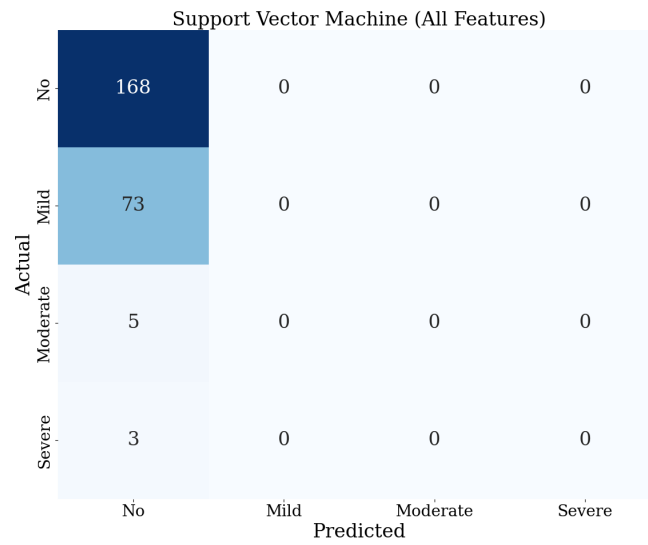


Figure 17: Confusion matrix of SVM with all features.

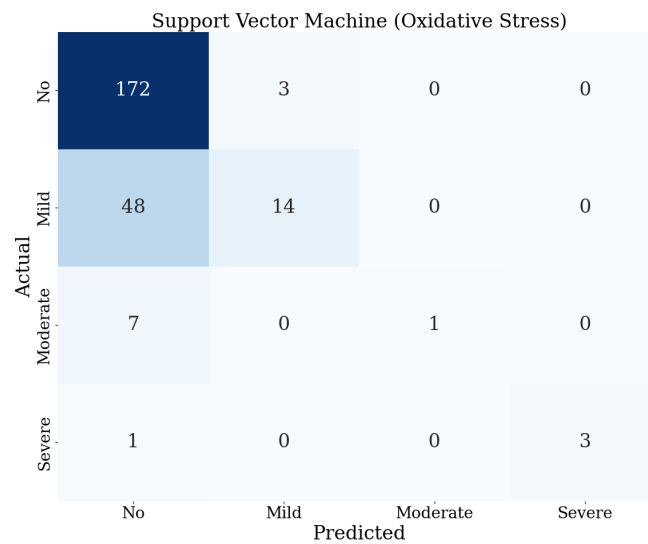


Figure 18: Confusion matrix of SVM with oxidative stress biomarkers as the main features.

Naive Bayes (All Features)

Actual	No	135	26	0	7
	Mild	34	25	0	14
	Moderate	2	2	0	1
	Severe	1	1	0	1
		No	Mild	Moderate	Severe
		Predicted			

Figure 19: Confusion matrix of NB with all features.

Naive Bayes (Oxidative Stress)

Actual	No	146	25	1	3
	Mild	38	19	2	3
	Moderate	6	2	0	0
	Severe	1	0	0	3
		No	Mild	Moderate	Severe
		Predicted			

Figure 20: Confusion matrix of NB with oxidative stress biomarkers as the main features.

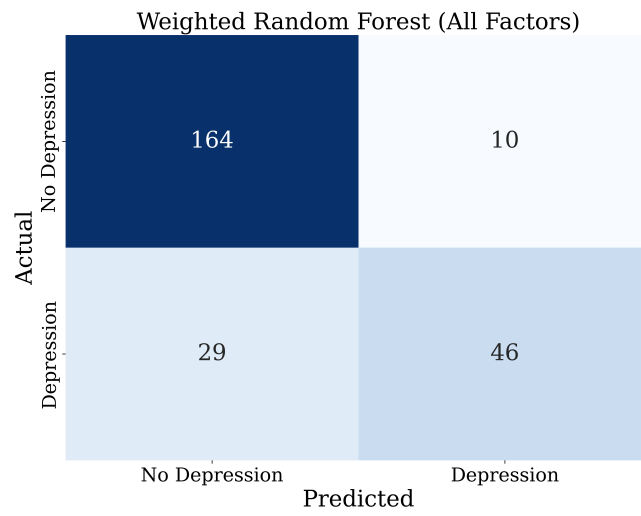


Figure 21: Confusion matrix of weighted RF with all features.

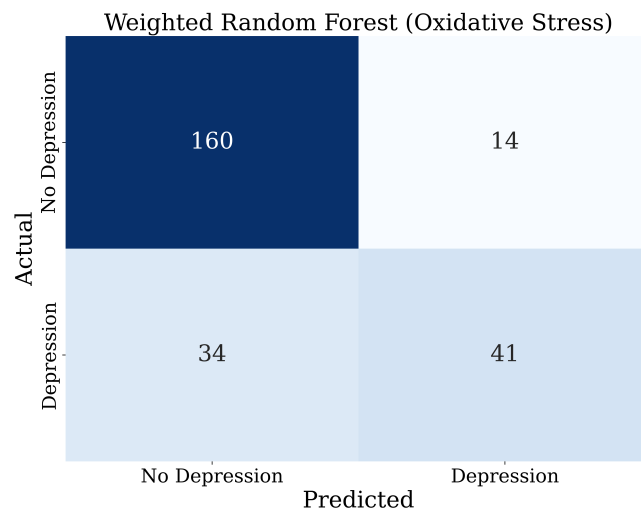


Figure 22: Confusion matrix of weighted RF with oxidative stress biomarkers as the main features.

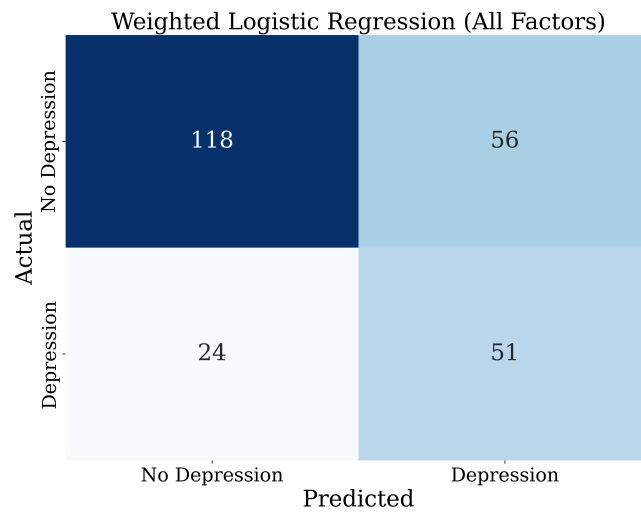


Figure 23: Confusion matrix of weighted LR with all features.

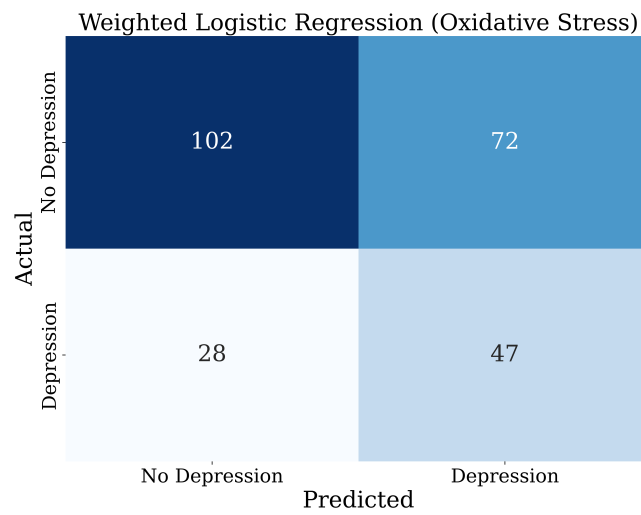


Figure 24: Confusion matrix of weighted LR with oxidative stress biomarkers as the main features.

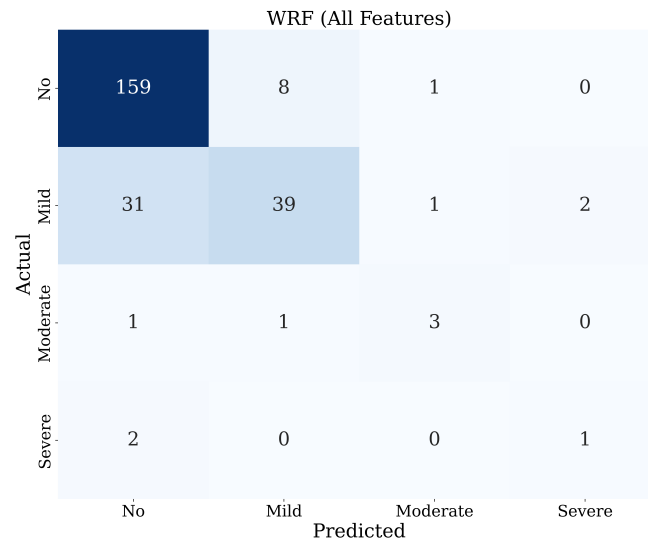


Figure 25: Confusion matrix of weighted RF with all features.

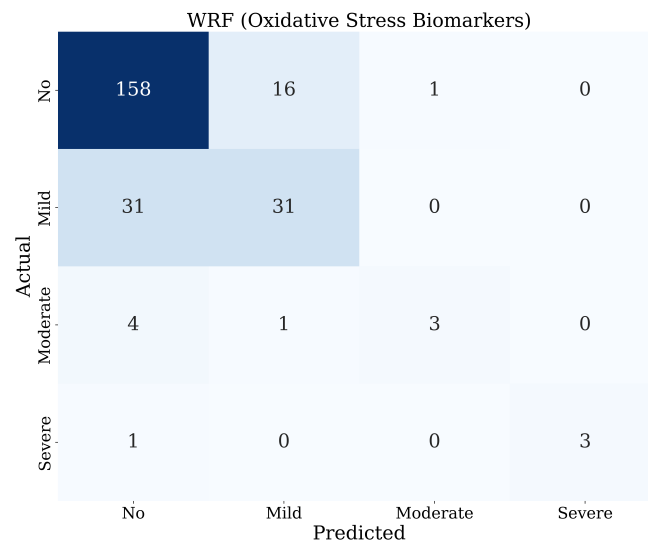


Figure 26: Confusion matrix of weighted RF with oxidative stress biomarkers as the main features.

WLR (All Features)

Actual	No	145	17	5	1
	Mild	30	30	4	9
	Moderate	2	2	0	1
	Severe	1	1	0	1
		No	Mild	Moderate	Severe
		Predicted			

Figure 27: Confusion matrix of weighted LR with all features.

WLR (Oxidative Stress Biomarkers)

Actual	No	162	8	0	5
	Mild	47	10	0	5
	Moderate	8	0	0	0
	Severe	0	1	0	3
		No	Mild	Moderate	Severe
		Predicted			

Figure 28: Confusion matrix of weighted LR with oxidative stress biomarkers as the main features.