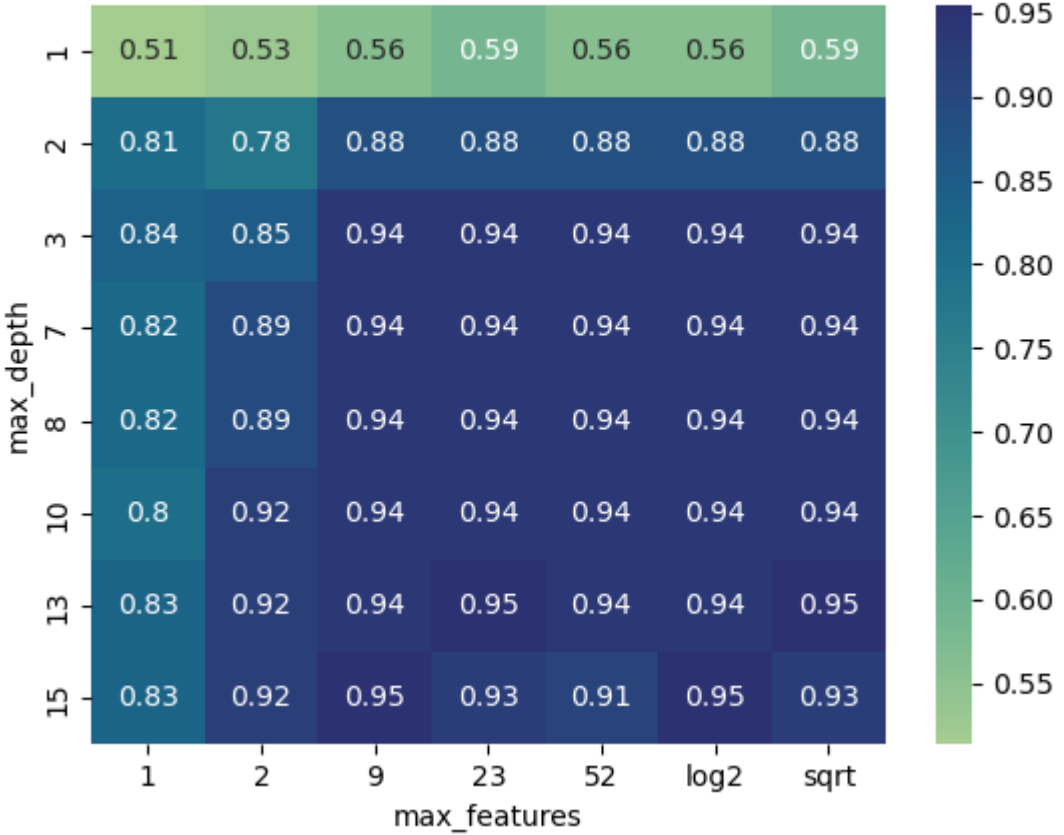
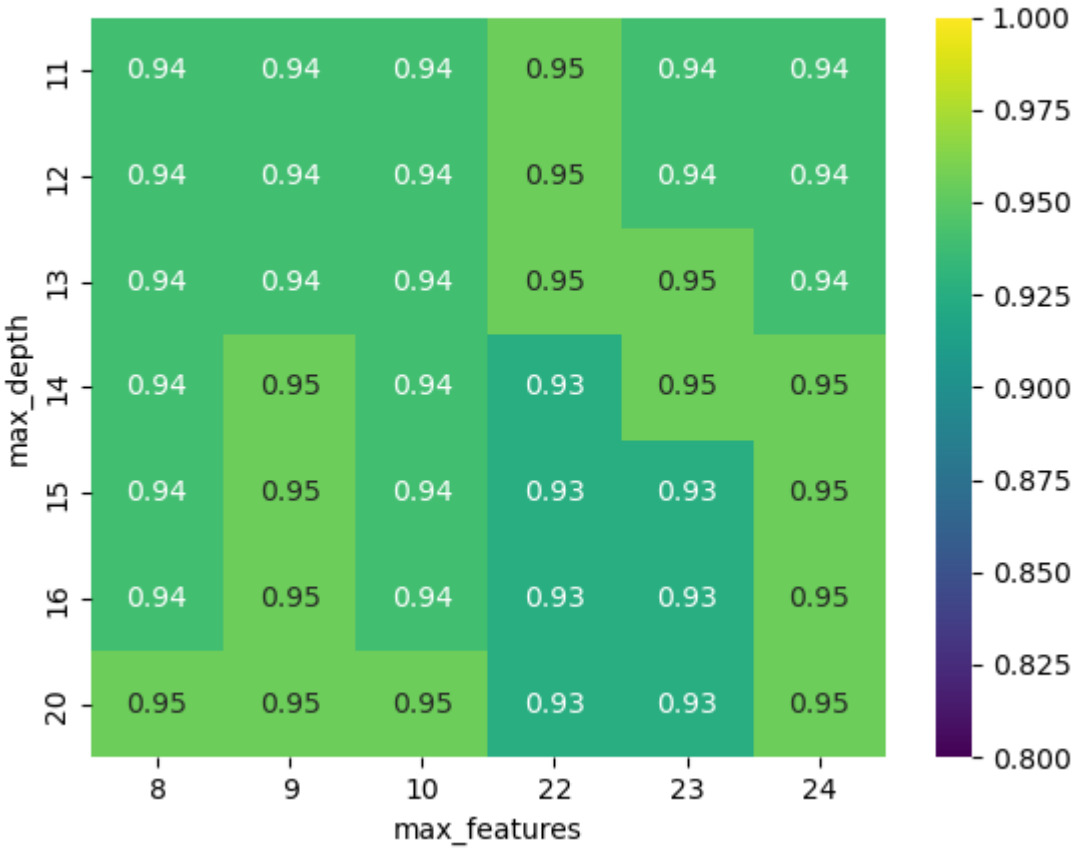
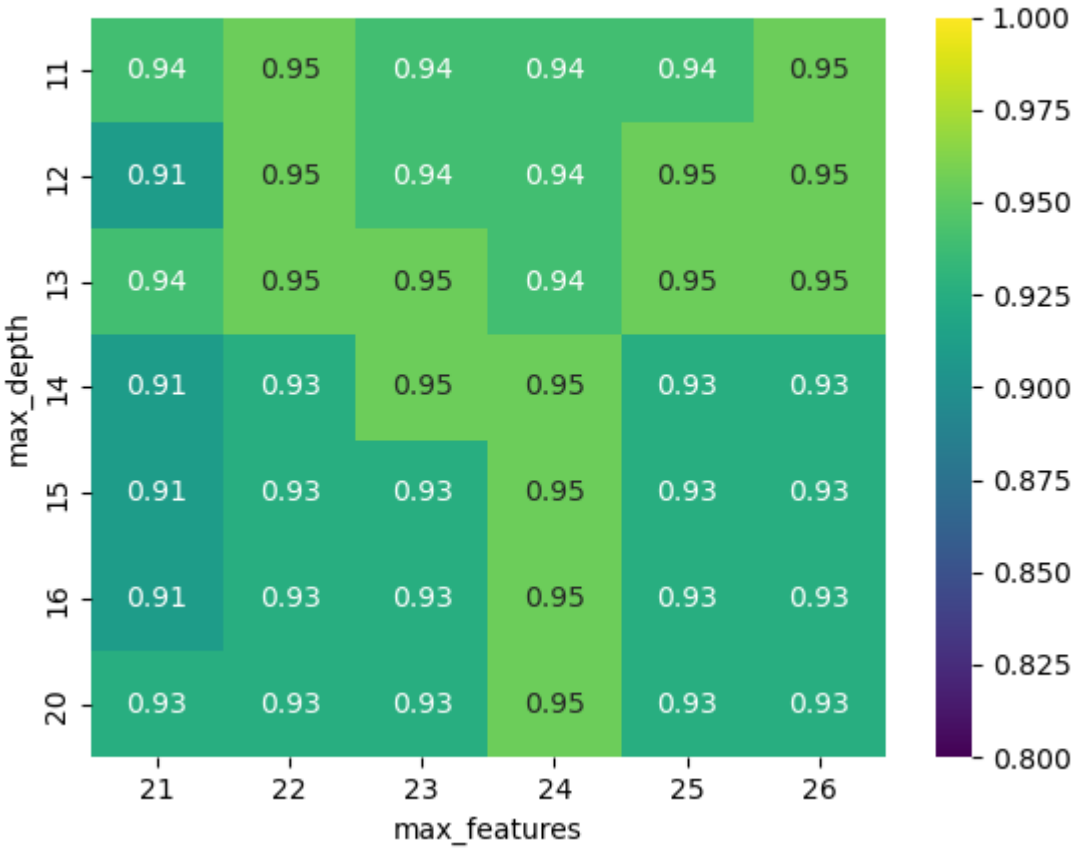
Caspofungin

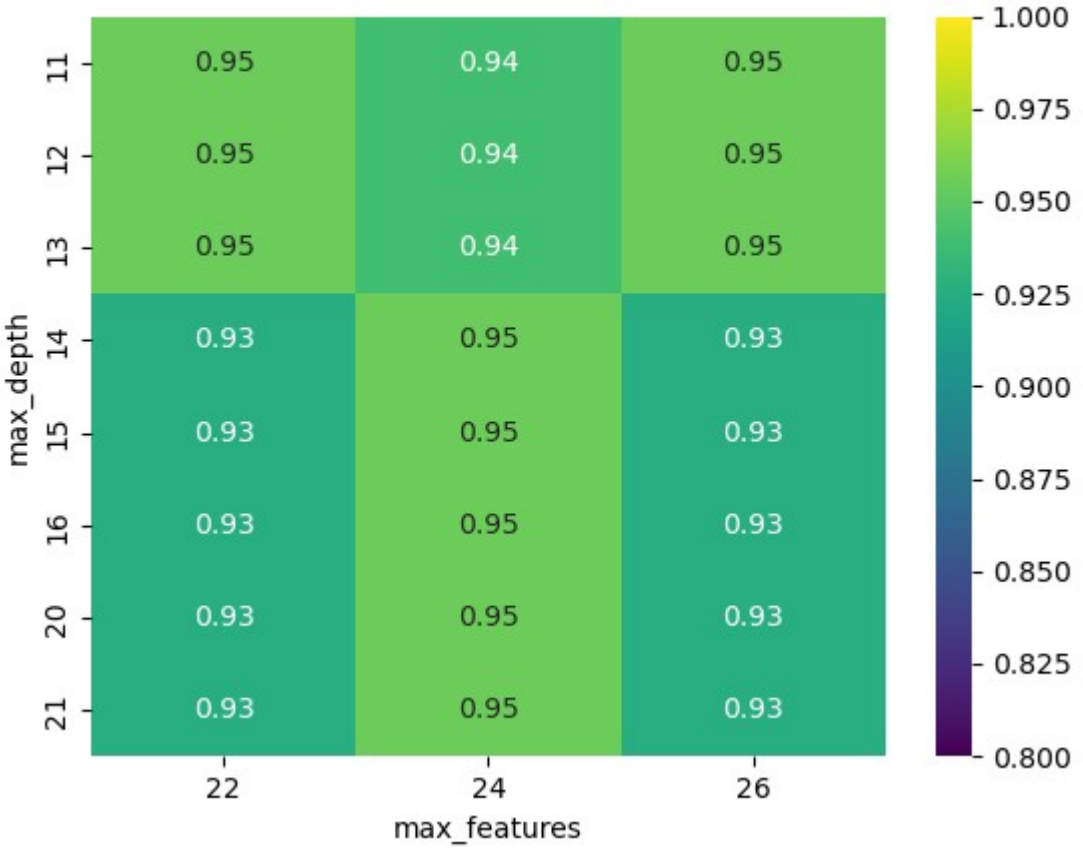
Log2(522) == 9

SQRT(522) == 23

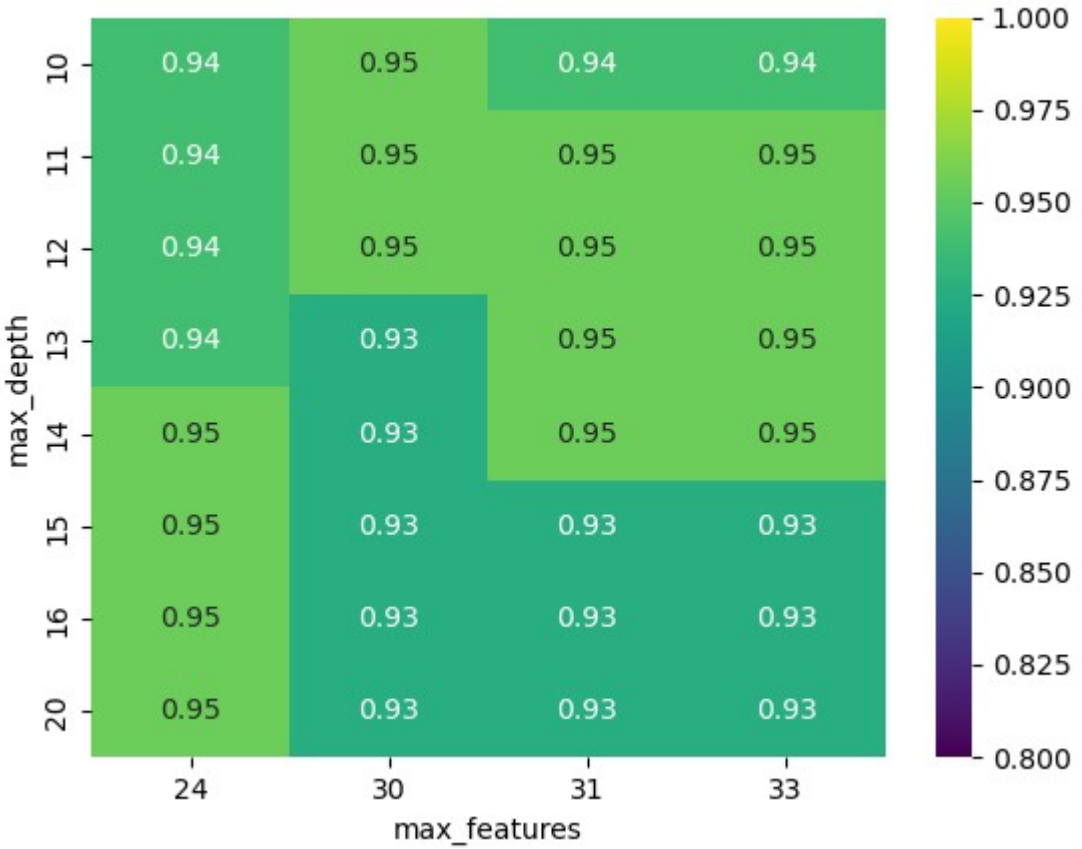



max_depth
11
12
13
14
15
16
20
0.94 0.94 0.94 0.95 0.94 0.94
0.94 0.94 0.94 0.95 0.94 0.94
0.94 0.94 0.94 0.95 0.95 0.94
0.94 0.95 0.94 0.93 0.95 0.95
0.94 0.95 0.94 0.93 0.93 0.95
0.94 0.95 0.94 0.93 0.93 0.95
0.95 0.95 0.95 0.93 0.93 0.95
8
9
10
22
23
24
max_features
1.000
0.975
0.950
0.925
0.900
0.875
0.850
0.825
0.800


max_depth
11
12
13
14
15
16
20
0.94 0.95 0.94 0.94 0.94 0.95
0.91 0.95 0.94 0.94 0.95 0.95
0.94 0.95 0.95 0.94 0.95 0.95
0.91 0.93 0.95 0.95 0.93 0.93
0.91 0.93 0.93 0.95 0.93 0.93
0.91 0.93 0.93 0.95 0.93 0.93
0.93 0.93 0.93 0.95 0.93 0.93
21
22
23
24
25
26
max_features
1.000
0.975
0.950
0.925
0.900
0.875
0.850
0.825
0.800


max_depth
11
12
13
14
15
16
20
21
0.95
0.94
0.95
0.95
0.94
0.95
0.95
0.94
0.95
0.93
0.95
0.93
0.93
0.95
0.93
0.93
0.95
0.93
0.93
0.95
0.93
22
24
26
max_features
1.000
0.975
0.950
0.925
0.900
0.875
0.850
0.825
0.800

Verification



New gridsearch:

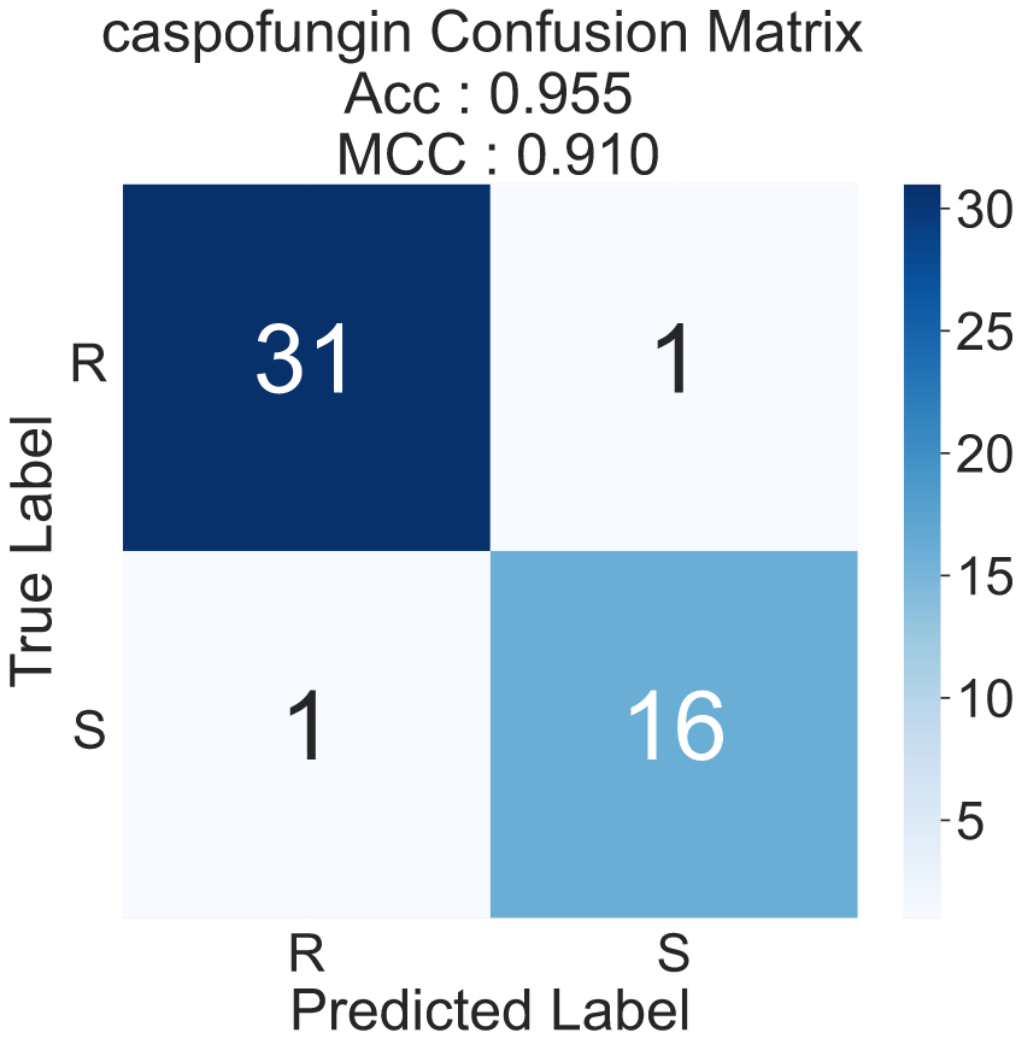
```
grid = {'n_estimators': [100],
        'max_features': [23, 24,25,26,27,28,29,30,31,32,33],
        'max_depth': [10,11,12,13,14,15,16,17,18,19,20],
        'min_samples_split': [2],
        'min_samples_leaf' : [1],
        'random_state': [18]}
```

Best params caspofungin:

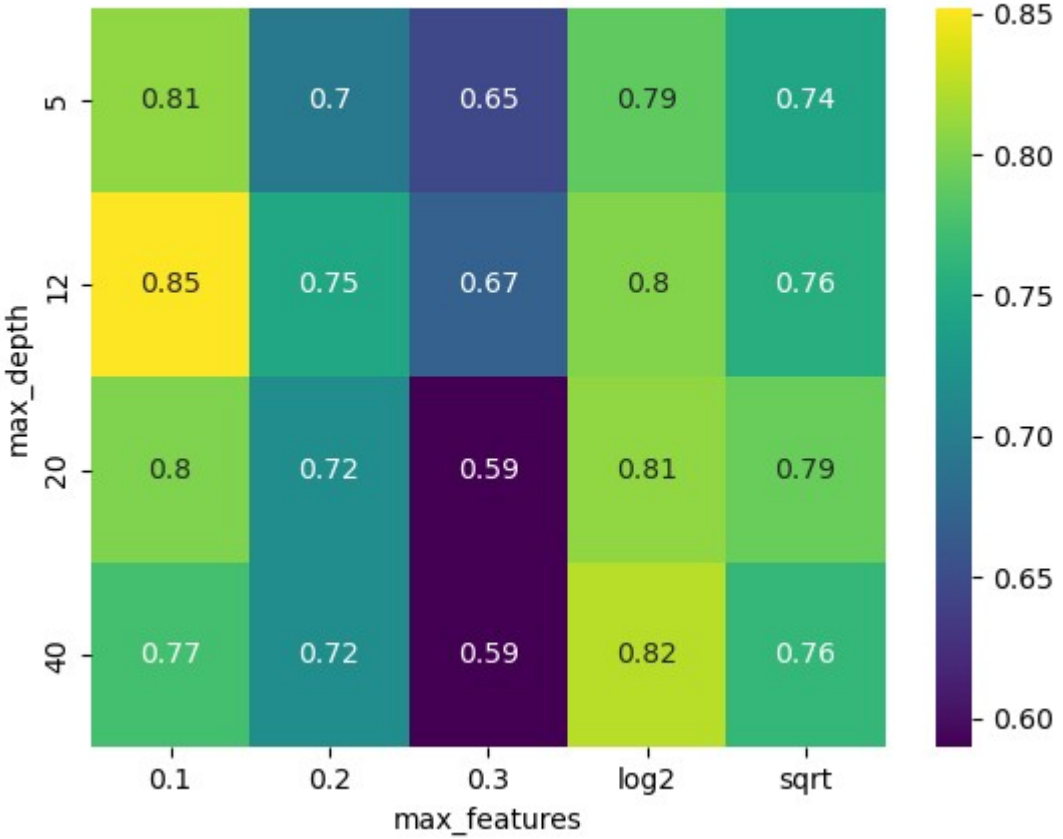
{'max_depth': 12, 'max_features': 30, 'min_samples_leaf': 1, 'min_samples_split': 2, 'n_estimators': 100, 'random_state': 18}

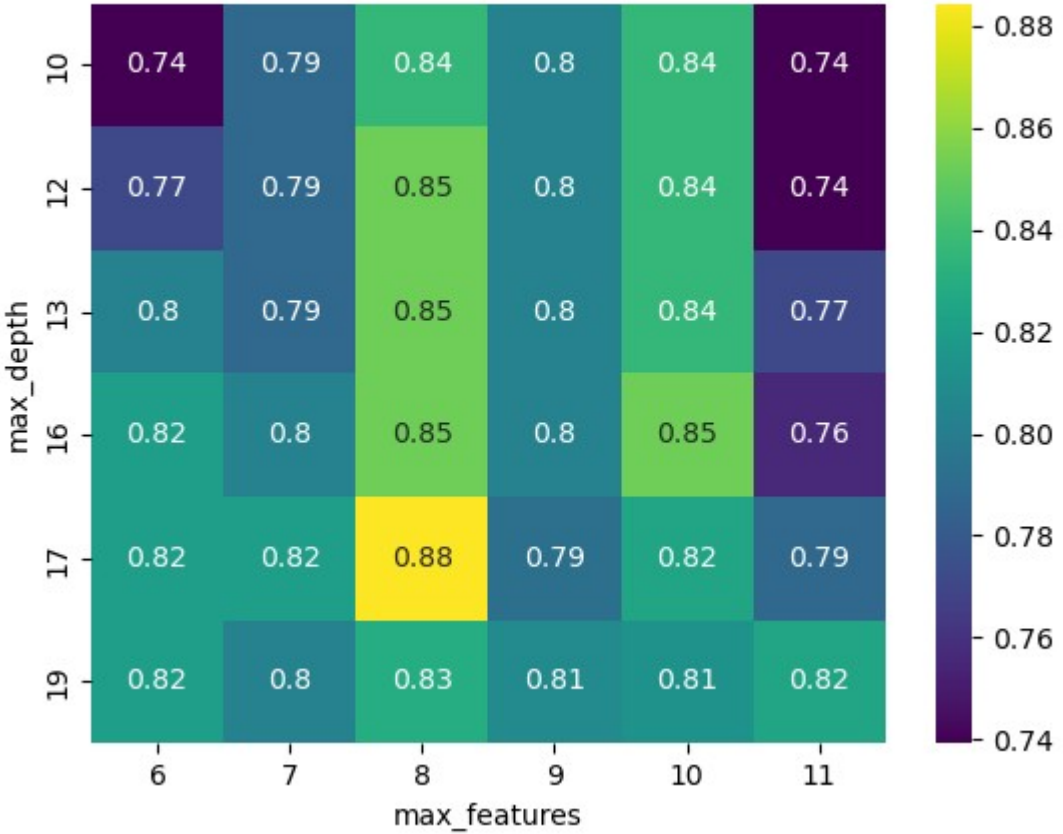
Train Balanced Acc : 0.9898648648648649

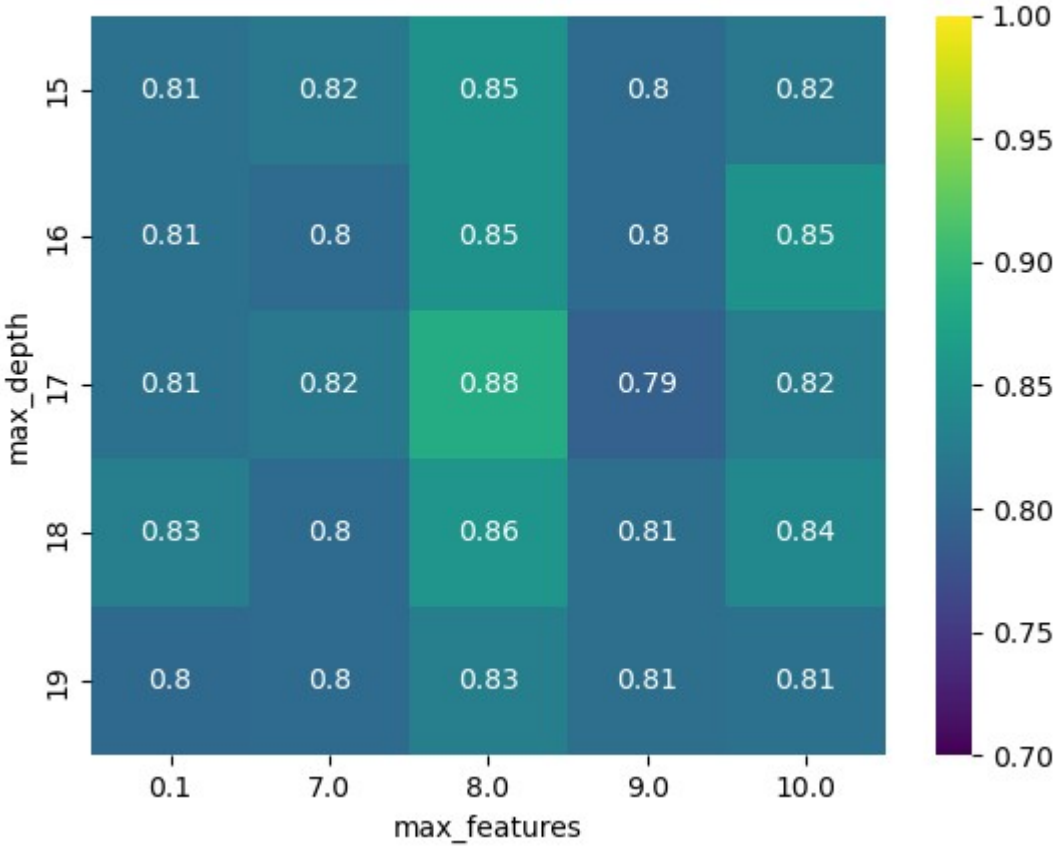
Test Balanced Acc : 0.9549632352941176


caspofungin Confusion Matrix
Acc : 0.955
MCC : 0.910
True Label
R
S
31
1
1
16
30
25
20
15
10
5
R
S
Predicted Label

Anidulafungin

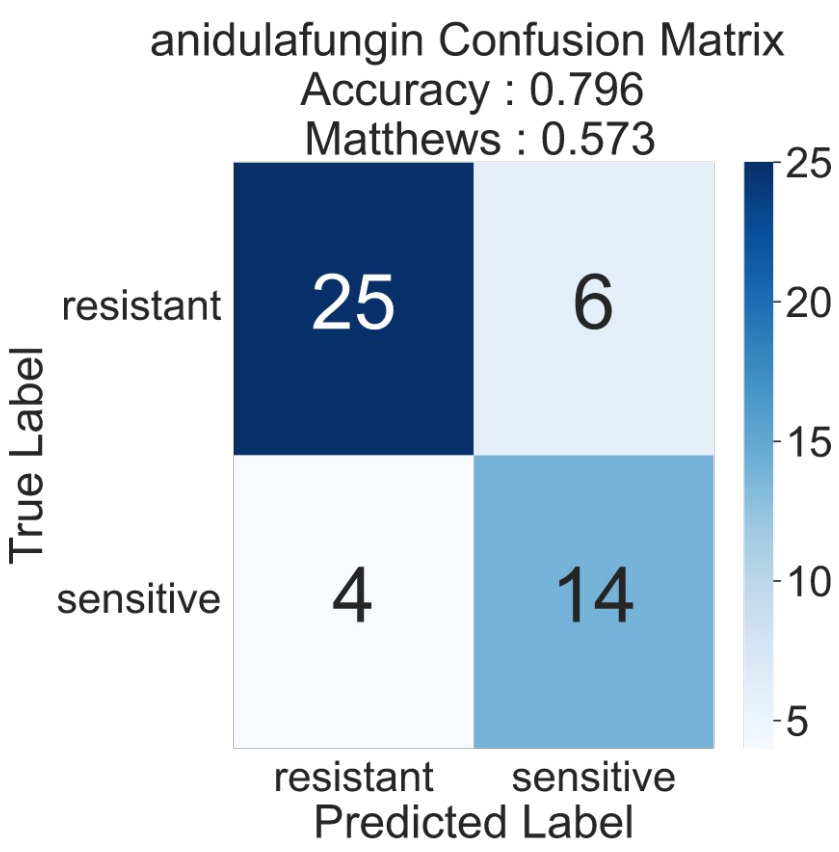

max_depth
5
12
20
40
0.81
0.7
0.65
0.79
0.74
0.85
0.75
0.67
0.8
0.76
0.8
0.72
0.59
0.81
0.79
0.77
0.72
0.59
0.82
0.76
0.1
0.2
0.3
log2
sqrt
max_features
0.85
0.80
0.75
0.70
0.65
0.60

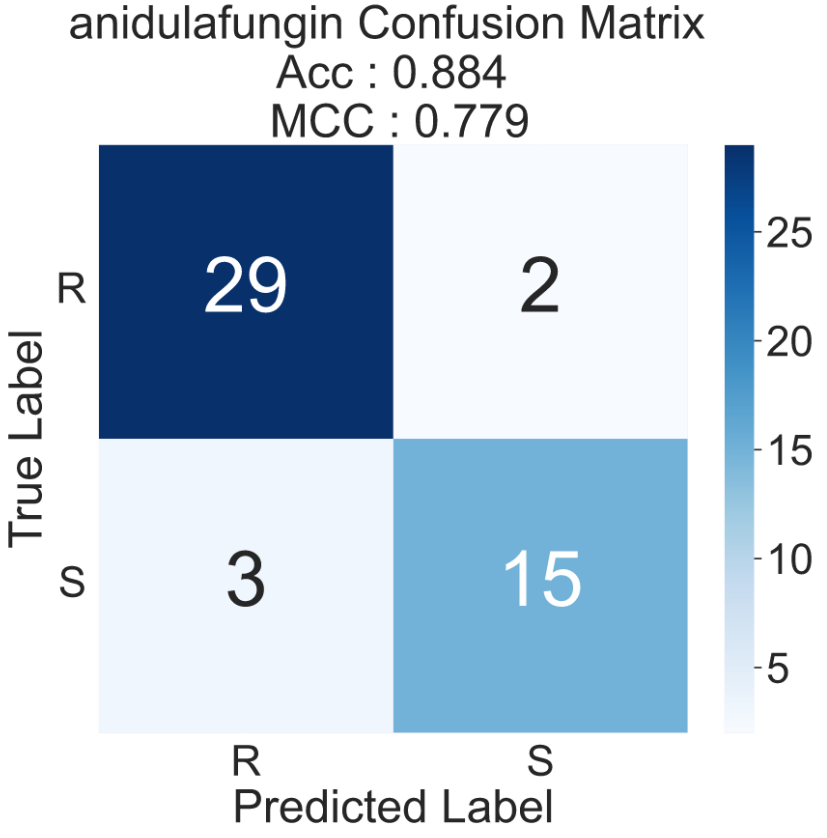

max_depth
10
12
13
16
17
19
0.74 0.79 0.84 0.8 0.84 0.74
0.77 0.79 0.85 0.8 0.84 0.74
0.8 0.79 0.85 0.8 0.84 0.77
0.82 0.8 0.85 0.8 0.85 0.76
0.82 0.82 0.88 0.79 0.82 0.79
0.82 0.8 0.83 0.81 0.81 0.82
6
7
8
9
10
11
max_features
0.88
0.86
0.84
0.82
0.80
0.78
0.76
0.74


max_depth
15
16
17
18
19
0.81 0.82 0.85 0.8 0.82
0.81 0.8 0.85 0.8 0.85
0.81 0.82 0.88 0.79 0.82
0.83 0.8 0.86 0.81 0.84
0.8 0.8 0.83 0.81 0.81
0.1
7.0
8.0
9.0
10.0
max_features
1.00
0.95
0.90
0.85
0.80
0.75
0.70

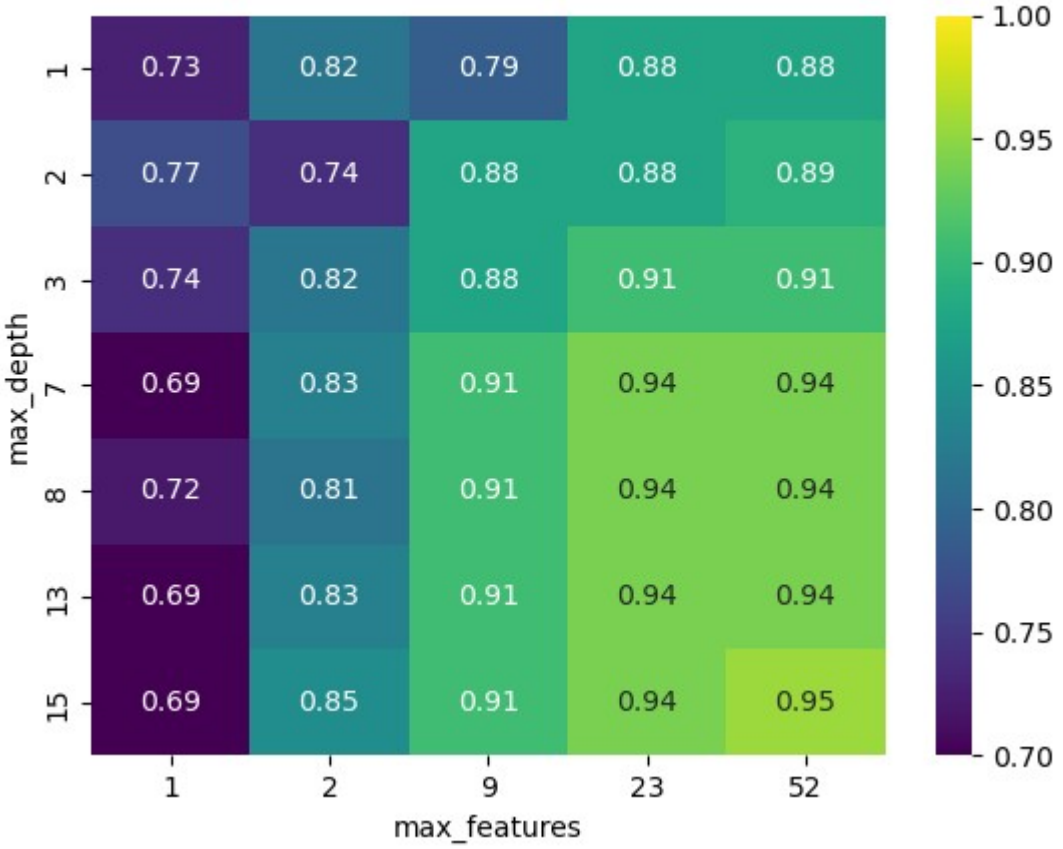
Best params anidulafungin:

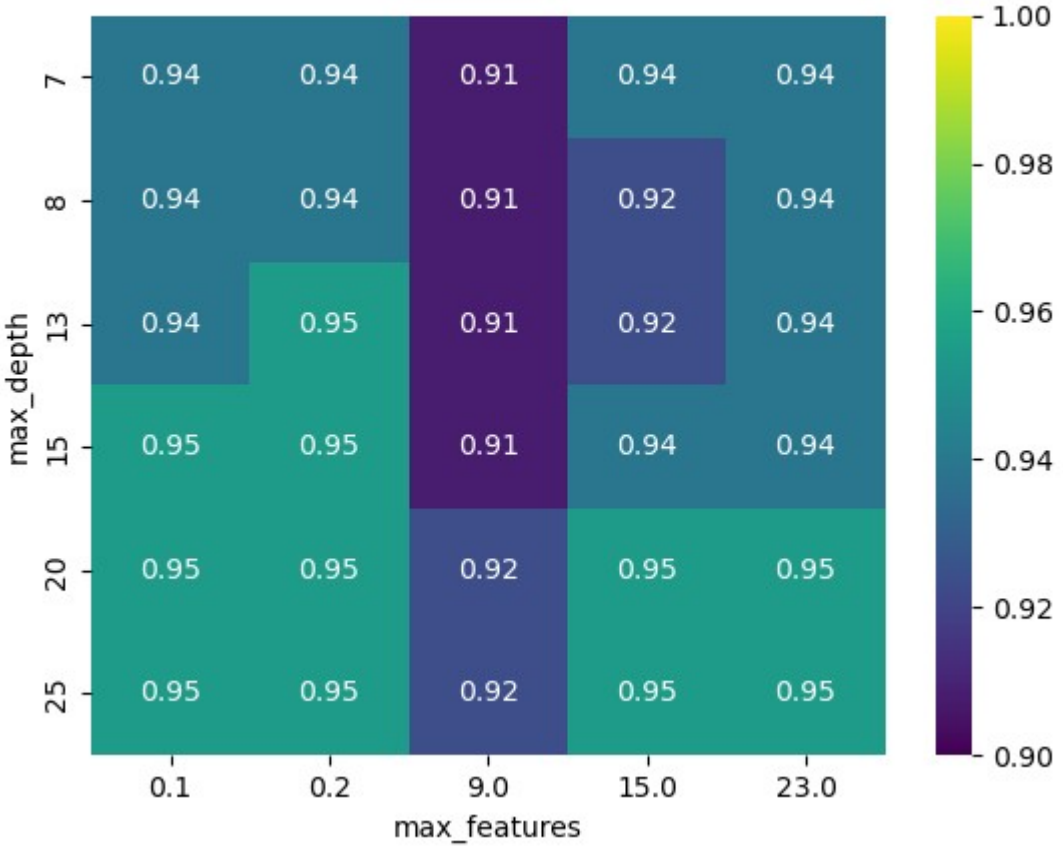
{'max_depth': 17, 'max_features': 8, 'min_samples_leaf': 1, 'min_samples_split': 2, 'n_estimators': 100, 'random_state': 18}

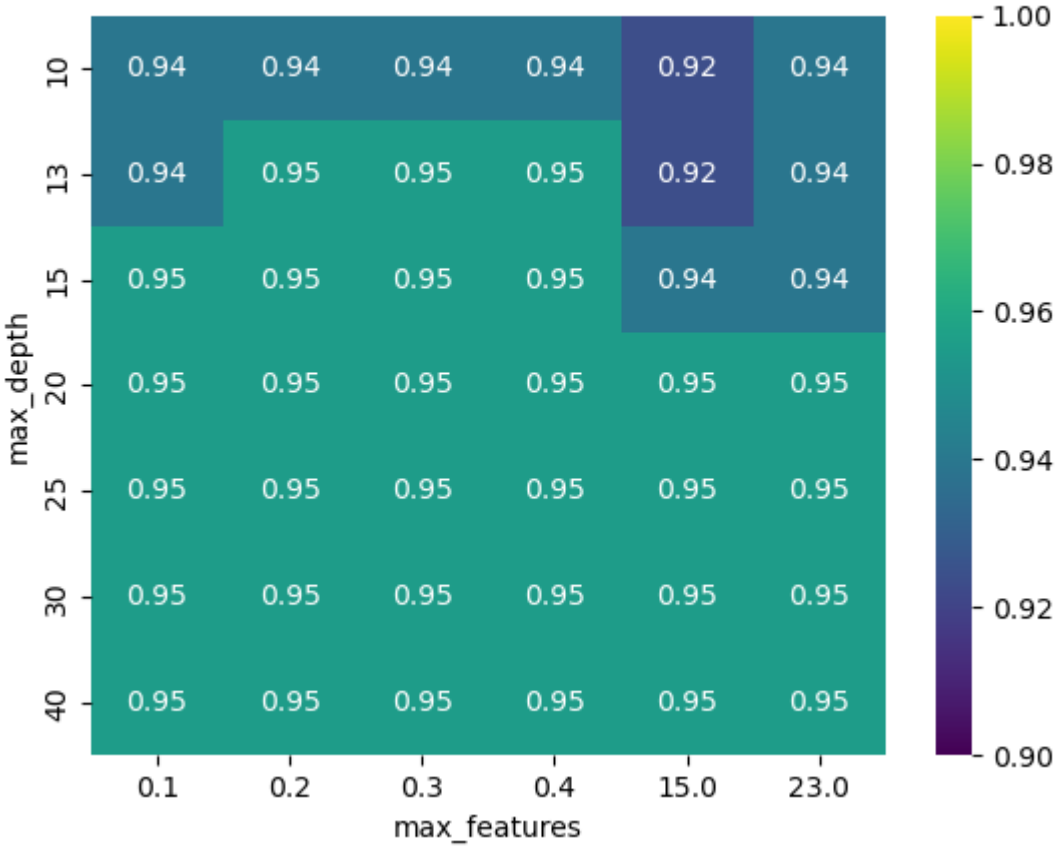

anidulafungin Confusion Matrix
Accuracy : 0.796
Matthews : 0.573
True Label
resistant
sensitive
25
6
4
14
resistant
sensitive
Predicted Label
25
20
15
10
5


anidulafungin Confusion Matrix
Acc : 0.884
MCC : 0.779
True Label
R
S
29
2
3
15
R
S
Predicted Label
25
20
15
10
5

Micafungin

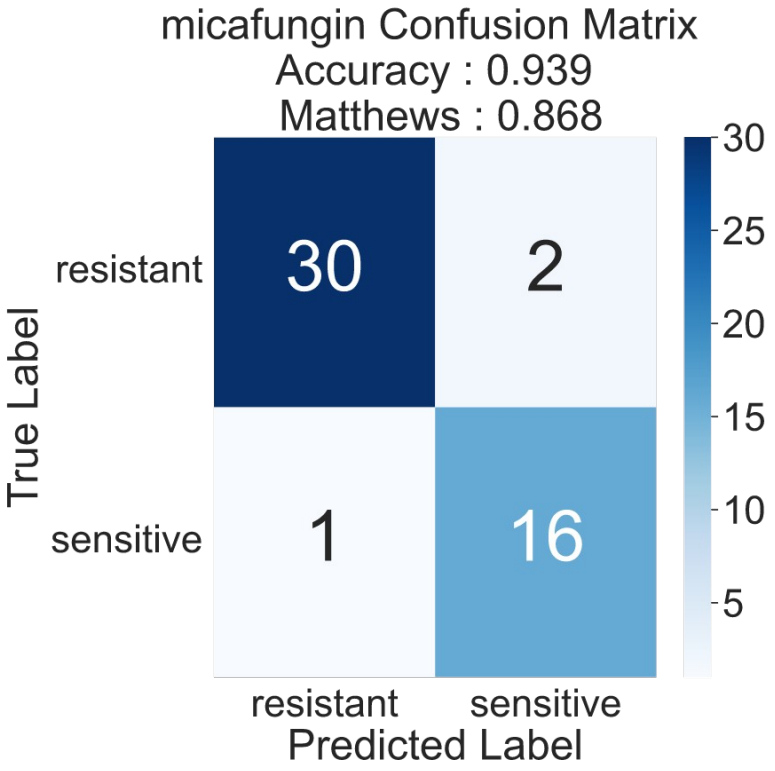

max_depth
1
2
3
7
8
13
15
0.73 0.82 0.79 0.88 0.88
0.77 0.74 0.88 0.88 0.89
0.74 0.82 0.88 0.91 0.91
0.69 0.83 0.91 0.94 0.94
0.72 0.81 0.91 0.94 0.94
0.69 0.83 0.91 0.94 0.94
0.69 0.85 0.91 0.94 0.95
1
2
9
23
52
max_features
1.00
0.95
0.90
0.85
0.80
0.75
0.70

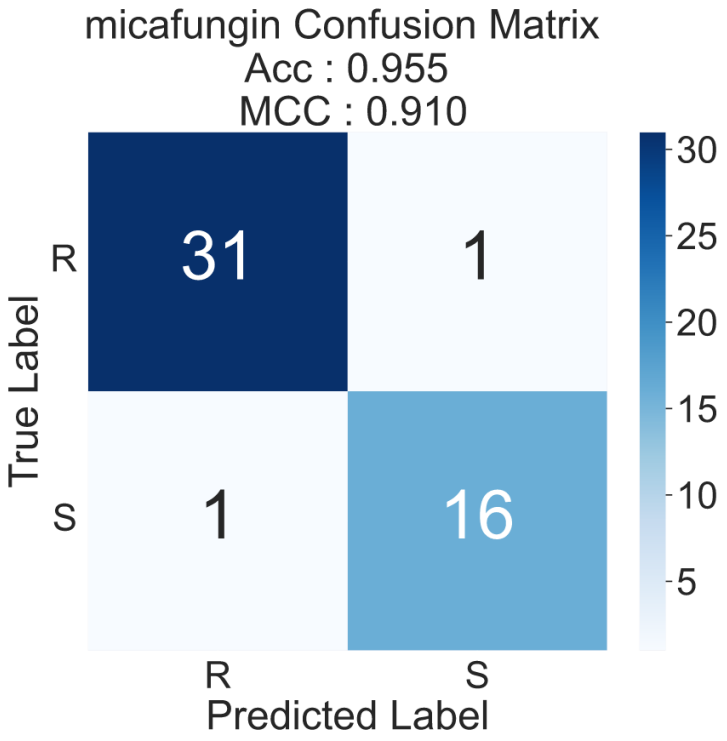

max_depth
7
8
13
15
20
25
0.94 0.94 0.91 0.94 0.94
0.94 0.94 0.91 0.92 0.94
0.94 0.95 0.91 0.92 0.94
0.95 0.95 0.91 0.94 0.94
0.95 0.95 0.92 0.95 0.95
0.95 0.95 0.92 0.95 0.95
0.1
0.2
9.0
15.0
23.0
max_features
1.00
0.98
0.96
0.94
0.92
0.90


max_depth
10
13
15
20
25
30
40
0.94 0.94 0.94 0.94 0.92 0.94
0.94 0.95 0.95 0.95 0.92 0.94
0.95 0.95 0.95 0.95 0.94 0.94
0.95 0.95 0.95 0.95 0.95 0.95
0.95 0.95 0.95 0.95 0.95 0.95
0.95 0.95 0.95 0.95 0.95 0.95
0.95 0.95 0.95 0.95 0.95 0.95
0.1
0.2
0.3
0.4
15.0
23.0
max_features
1.00
0.98
0.96
0.94
0.92
0.90

Best params micafungin:

{'max_depth': 20, 'max_features': 0.4, 'min_samples_leaf': 1, 'min_samples_split': 2, 'n_estimators': 100, 'random_state': 18}


micafungin Confusion Matrix
Accuracy : 0.939
Matthews : 0.868
True Label
resistant
sensitive
30
2
1
16
resistant
sensitive
Predicted Label
30
25
20
15
10
5


micafungin Confusion Matrix
Acc : 0.955
MCC : 0.910
True Label
R
S
31
1
1
16
R
S
Predicted Label
30
25
20
15
10
5