Table 1: Comparative characteristics of implemented approaches. Test 2 is independent from Train / Test 1 parts. In Part 1 all values presented are medians across 5-times repeated 5-fold cross validation runs. In Part 2 the same partitioning was used but final results were computed as top-N's (see Supplementary S1.2). In Part 3 all values presented are medians across 5-times repeated 4-fold cross validation runs.

Part 1. Results for "winner takes all" strategy. Prediction times are written per one sample.
For classifiers based on features spaces learned with autoencoder additional times for estimation of autoencoder parameters are given in parentheses.

Method	Accuracy, %			F1, %			Time	
	Train	Test 1	Test 2	Train	Test 1	Test 2	Training	Prediction
Logistic regression (autoencoded)	99.8	85.0	72.7	99.8	83.2	79.6	1m 16s (+1h 30m)	0.06ms
Naive Bayes (autoencoded)	90.3	68.4	75.0	90.6	66.7	79.8	8ms (+1h 30m)	0.02ms
Hybrid BN (autoencoded)	92.1	69.2	68.2	92.3	67.5	72.4	50m 47s (+1h 30m)	1.8ms
Large discrete BN	-	78.5	72.7	-	76.5	81.6	3m 14s	9m
Sparse NTD (principal angle)	98.0	77.9	84.1	98.0	76.3	89.8	18h 19m	1.1s
Sparse NMF (principal angle)	99.2	75.4	81.8	99.2	74.4	85.2	28m 46s	1.1s

Part 2. TopN approach. Output is considered to be accurate when correct label is present in TopN results.

Method	Accuracy, %									
	Test 1					Test 2				
	Top1	Top2	Top3	Top4	Top5	Top1	Top2	Top3	Top4	Top5
Logistic regression (autoencoded)	85.0	92.1	94.7	95.6	96.6	72.7	79.5	84.1	86.4	88.6
Naive Bayes (autoencoded)	68.4	77.9	82.1	85.5	87.7	75.0	81.8	84.1	88.6	90.9
Large discrete BN	78.5	85.8	86.9	87.6	87.6	72.7	81.8	86.4	88.6	90.9
Sparse NTD (principal angle)	77.9	82.8	84.2	86.0	86.9	84.1	88.6	90.9	90.9	90.9
Sparse NMF (principal angle)	75.4	79.4	80.7	82.0	82.7	81.8	84.1	86.4	86.4	88.6

Part 3. Plant organ identification.

Method	Accuracy, %			F1, %		
	Train	Test 1	Test 2	Train	Test 1	Test 2
Logistic regression (autoencoded)	87.2	76.9	62.5	87.0	76.2	58.1
Naive Bayes (autoencoded)	77.0	69.4	61.4	76.8	68.3	54.2
Hybrid BN (autoencoded)	75.1	67.0	59.1	74.4	65.7	53.5
Sparse NTD (principal angle)	90.4	80.0	85.2	90.7	80.5	85.8
Sparse NMF (principal angle)	96.3	86.6	84.1	96.4	87.1	84.2