Table 1. Summary of results.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Outcome | Quality measure | PPCpred | Design 1 | Design 2 | … | The best design |
| material production failed | Sensitivity | 78.2 |  |  |  |  |
| Specificity | 67.6 |  |  |  |  |
| PredictiveACC | 74.5 |  |  |  |  |
| **MCC** | **0.449** |  |  |  |  |
| purification failed | Sensitivity | 90.1 |  |  |  |  |
| Specificity | 26.8 |  |  |  |  |
| PredictiveACC | 77.5 |  |  |  |  |
| **MCC** | **0.199** |  |  |  |  |
| crystallization failed | Sensitivity | 86.2 |  |  |  |  |
| Specificity | 46.6 |  |  |  |  |
| PredictiveACC | 81.5 |  |  |  |  |
| **MCC** | **0.277** |  |  |  |  |
| crystallizable | Sensitivity | 61.0 |  |  |  |  |
| Specificity | 83.6 |  |  |  |  |
| PredictiveACC | 76.1 |  |  |  |  |
| **MCC** | **0.455** |  |  |  |  |
| **averageMCC** | | **0.345** |  |  |  |  |
| *accuracy* | | 54.8 |  |  |  |  |