**Table S1.** The prediction performance of the classifier model for all diet groups (HFD, HFD + XOS, LFD, LFD + XOS), dietary fat (high, low) and XOS ingestion (true, false). Accuracy and f1 score for each run derived from 5-fold cross validation.

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| --- |
| **Average model accuracy-% and F1 scores from cross-validation. XGBoost classifier** |
| **Only metabolites** |
|  | **Diet group** | **Fat content** | **XOS supplementation** |
| **all biclusters** | 42.5 +/- 12.7, 0.43 | **92.5 +/- 10, 0.92** | **60 +/- 9.4, 0.55** |
| **SCFA bicluster** | 50 +/- 11.2, 0.5 | **92.5 +/- 10, 0.92** | 57.5 +/- 15, 0.58 |
| **Product bicluster** | 32.5 +/- 15, 0.33 | 77.5 +/- 9.4, 0.78 | 35 +/- 14.6, 0.26 |
| **TMA bicluster** | 27.5 +/- 14.6, 0.28 | 60 +/- 14.6, 0.61 | 47.5 +/- 14.6, 0.48 |
| **AA bicluster** | 47.5 +/- 9.4, 0.48 | 75 +/- 7.9, 0.74 | **62.5 +/- 7.9, 0.62** |
| **Isovalerate bicluster** | 37.5 +/- 7.9, 0.38 | **85 +/- 14.6, 0.85** | 52.5 +/- 18.4, 0.49 |
| **Only genera** |
|  | **Diet group** | **Fat content** | **XOS supplementation** |
| **all biclusters** | 50 +/- 17.7, 0.5 | **82.5 +/- 10, 0.83** | 42.5 +/- 12.7, 0.45 |
| **SCFA bicluster** | 45 +/- 21.8, 0.45 | **87.5 +/- 0, 0.87** | 40 +/- 18.4, 0.35 |
| **Product bicluster** | 45 +/- 12.7, 0.45 | **82.5 +/- 10, 0.79** | 40 +/- 9.4, 0.35 |
| **TMA bicluster** | 37.5 +/- 13.7, 0.38 | 60 +/- 16.6, 0.58 | **60 +/- 16.6, 0.57** |
| **AA bicluster** | 30 +/- 17, 0.3 | 75 +/- 13.7, 0.63 | 45 +/- 15, 0.38 |
| **Isovalerate bicluster** | 37.5 +/- 13.7, 0.38 | **92.5 +/- 6.1, 0.9** | 40 +/- 5, 0.39 |