

Integrating Machine Learning with Metabolic Models for Precision Trauma Care: Personalized Endotype Stratification and Metabolic Target Identification: Supplementary material 4

Marin de Mas I.^{*1,2}, Moura L.³, Antunes F.L.M.³, Guerrero
J.M.^{4,5}, and Johansson P.I.^{1,2}

¹CAG Center for Endotheliomics, Copenhagen University Hospital,
Rigshospitalet, 2100, Copenhagen, Denmark

²Department of Clinical Medicine, Copenhagen University
Hospital, Rigshospitalet, 2100, Copenhagen, Denmark

³Department of Electrical Engineering, Federal University of
Ceará, Fortaleza, 60430-160, Ceará, Brazil

⁴Center for Renewable Energy and Microgrids, Huanjiang
Laboratory, AAU Energy, Zhejiang University, 314423, Zhejiang,
China

⁵Center for Research on Microgrids (AAU CROM), AAU Energy,
Aalborg University, 9220, Aalborg, Denmark

1 Results

This section, results and statistics from the GB model k-fold cross-validation analysis is show. The following tables show the results for the GB model with all the metabolic reactions in the iEC3006 GEM (3006 reactions) (see Table 1), a lighter GB model trained based on the 50 Top Metabolic Reactions (TMR) (see Table 2) based on SHAP analysis [1] and a GB model trained based on the 7 Metabolic "Switch" Reactions (MSR) (See Table 3).

References

- [1] Lloyd S Shapley. "A value for n-person games". In: *Contributions to the Theory of Games* 2.28 (1953), pp. 307–317.

*Corresponding author: Marin de Mas I. Email: igor.bartolome.marin.de.mas@regionh.dk

Table 1: Results and statistics from the GB model trained with the full 3006 reactions from the iEC3006 GEM.

	Precision	Recall	F1-Score	Support
ENDOTYPE A	1.00	1.00	1.00	1809
ENDOTYPE B	1.00	1.00	1.00	1853
ENDOTYPE C	1.00	1.00	1.00	4359
ENDOTYPE D	1.00	1.00	1.00	6229
Accuracy			1.00	14250
Macro avg	1.00	1.00	1.00	14250
Weighted avg	1.00	1.00	1.00	14250

Table 2: Results and statistics from the GB model trained with the 50 TMR.

	Precision	Recall	F1-Score	Support
ENDOTYPE A	1.00	1.00	1.00	1820
ENDOTYPE B	1.00	1.00	1.00	1756
ENDOTYPE C	1.00	1.00	1.00	4265
ENDOTYPE D	1.00	1.00	1.00	6409
Accuracy			1.00	14250
Macro avg	1.00	1.00	1.00	14250
Weighted avg	1.00	1.00	1.00	14250

Table 3: Results and statistics from the GB model trained with the 7 MSR.

	Precision	Recall	F1-Score	Support
ENDOTYPE A	0.82	0.89	0.85	1794
ENDOTYPE B	0.94	0.92	0.93	1824
ENDOTYPE C	0.89	0.88	0.89	4295
ENDOTYPE D	0.95	0.94	0.95	6337
Accuracy			0.91	14250
Macro avg	0.90	0.91	0.90	14250
Weighted avg	0.92	0.91	0.91	14250