

Appendix I.

Supplementary Table 1. Medication regimen complexity–intensive care unit Scoring Tool

MRC-ICU Scoring Tool	
Parameter	Point Value
High Priority Medications	
Aminoglycosides (amikacin, gentamicin, tobramycin)	3x
Amphotericin B and Liposomal Amphotericin B	1
Antiarrhythmics (amiodarone, dofetilide, sotalol)	1x
Anticoagulants (NOAC's/DOAC's, fondaparinux)	1x
Anticonvulsants (carbamazepine, phenobarbital, phenytoin, valproic acid)	3x
Argatroban	2
Azole antifungals (posaconazole, voriconazole)	2x
Blood Products (Factor products, Antithrombin III)	2x
Chemotherapy (active inpatient)	3x
Clozapine	3
Digoxin	3
Ganciclovir/valganciclovir	1x
Hyperosmolar fluids (hypertonic saline (1.5%, 3%, 23.4%), mannitol)	1x
Immunosuppressants (cyclosporine, sirolimus, tacrolimus)	3x
Lidocaine (continuous infusion)	2
Lithium	3

Prostacyclins (epoprostenol, iloprost, treprostinil)	2x
Theophylline	3
Therapeutic heparins (enoxaparin, heparin infusion)	2x
Vancomycin (IV)	3
Warfarin	3
ICU Medications	
Neuromuscular Blockade	2
Continuous infusions (exclude those listed elsewhere)	1x
Total Parenteral Nutrition	
Managed by non-pharmacist service	1
Managed by clinical specialist pharmacist	3
ICU Prophylaxis and FAST HUGS BID	
Thromboembolic prophylaxis (exclude heparin infusion, therapeutic enoxaparin)	1
Stress ulcer prophylaxis (exclude pantoprazole infusion)	1
Glycemic control (subcutaneous insulin; exclude IV insulin)	1
Bowel regimen	1
Chlorhexidine	1
Analgesia and Sedation	
Opioids and sedatives (scheduled and PRN)	1x
Continuous infusion opioids and sedatives (propofol, fentanyl, dexmedetomidine, ketamine, benzodiazepines)	2x
Antimicrobial Agents	
Antimicrobials (include HIV medications, exclude those listed elsewhere)	1x

Restricted antimicrobials (4 th -5 th generation cephalosporins, carbapenems, linezolid, daptomycin, colistin/polymyxins)	2x
Devices	
Dialysis	2
Extracorporeal membrane oxygenation (ECMO)	2
Intra-aortic balloon pump (IABP)	1
Left ventricular assist device (LVAD)	1
Mechanical ventilation	2

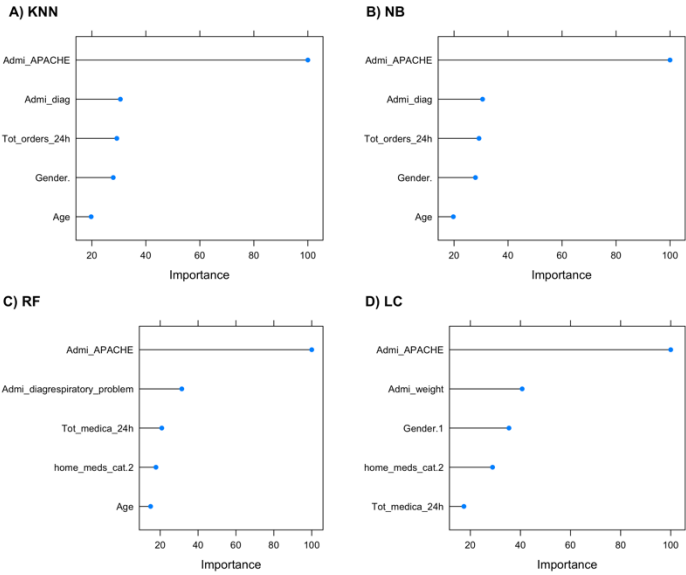
Each individual medication or medication class listed has a weighted score (i.e., 1, 2, or 3 points). This multiplier indicates that for every medication that meets those criteria, the score is multiplied (e.g., if fentanyl and midazolam are prescribed, this total would be 2 points multiplied by each medication for a total of 4 points). The MRC-ICU is then the sum of all the points assigned to the medications.

Supplementary Table 2. Performance of the machine learning algorithms on Sub-model: base model only with medication regimen complexity and MRC-ICU values at 24h

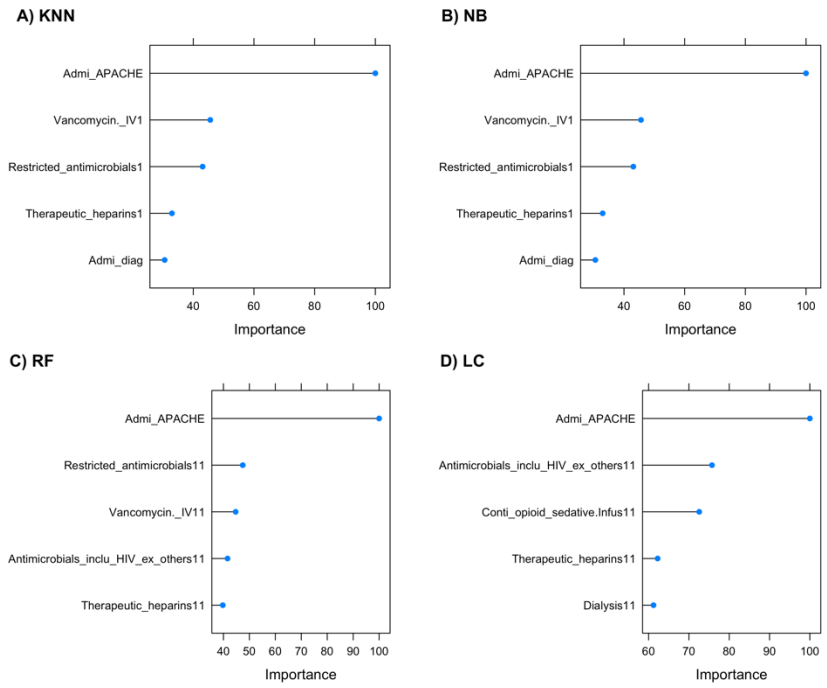
	AUC (95% CI)	Se (95% CI)	Sp (95% CI)	PPV (95% CI)	NPV (95% CI)
KNN	0.81(0.64,0.93)	0.81(0.64,0.93)	0.20(0.10,1.00)	0.91 (0.87,1.00)	0.23(0.12,0.46)
NB	0.78(0.60,0.91)	0.81(0.63,0.93)	0.32(0.11,0.98)	0.96(0.80,1.00)	0.00(0.00,0.46)
RF	0.75(0.57,0.89)	0.82(0.63,0.94)	0.25(0.01,0.81)	0.88(0.70,0.98)	0.17(0.00,0.64)
SVM	0.78(0.60,0.91)	0.85(0.66,0.96)	0.85(0.05,0.85)	0.88(0.70,0.98)	0.33(0.04,0.78)
NN	0.66(0.47,0.81)	0.83(0.61,0.95)	0.22(0.03,0.60)	0.73(0.52,0.88)	0.33(0.04,0.78)
LC	0.75(0.57,0.89)	0.85(0.65,0.96)	0.33(0.04,0.78)	0.85(0.65,0.96)	0.33(0.04,0.78)

Abbreviations: KNN: K-nearest neighbor, NB: naive Bayes, RF: random forest, SVM: support vector machine, NN: neural network, LC: logistic classifier, AUC: Area under the receiver operator characteristics curve, Se: Sensitivity, Sp: Specificity, PPV: positive predictive value, NPV: negative predictive value.

Supplementary Figure 1: Variable importance plot for Model I

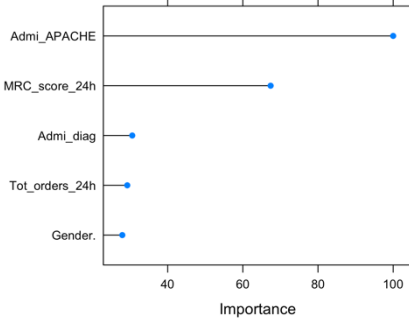


Supplementary Figure 2: Variable importance plot for Model II

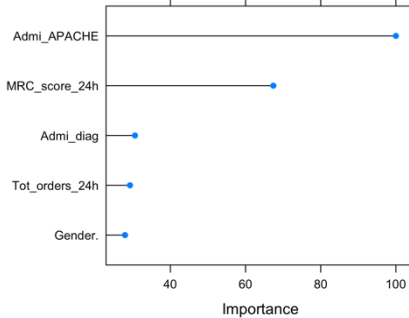


Supplementary Figure 3: Variable importance plot for Model III

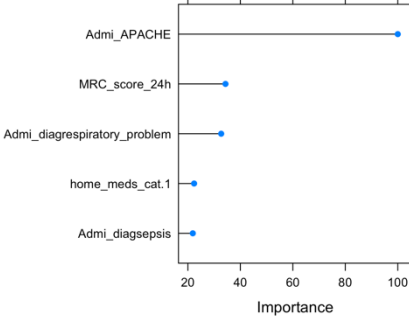
A) KNN



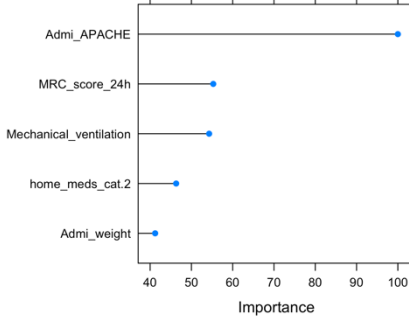
B) NB



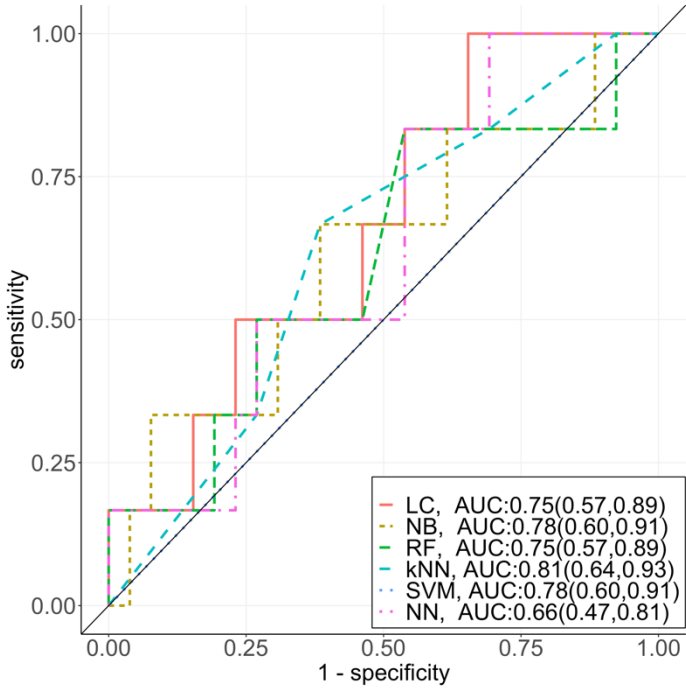
C) RF



D) LC



Supplementary Figure 4: Performance matrix of the machine learning algorithms for predicting mortality among critically ill patients using three different model setups. Sub-model I: Model I with only medication regimen complexity and MRC-ICU values at 24h.



Supplementary Figure 5: Variable importance plot for Sub-model I

