

Additional file 1. Baseline characteristics of patients admitted to the intensive care units.

	Total (n=12377)	Training dataset (n=9901)	Testing dataset (n=2476)	<i>P</i>
(1) Age	70 (57-82)	70 (57-82)	69 (56-82)	0.256
(2) Gender (male)	7966 (64.36)	6345 (64.08)	1621 (65.47)	0.205
(3) Height	162.8 (156-169)	162.5 (156-168.9)	163 (156-169)	0.175
(4) Weight	60.2 (52-70)	60.1 (52-70)	60.25 (52-70)	0.830
(5) Renal function				
Crea	1.43 (0.92-2.74)	1.44 (0.92-2.78)	1.42 (0.92-2.62)	0.405
Cr_0	1.80 (1.04-2.38)	1.80 (1.04-2.41)	1.79 (1.03-2.31)	0.401
Cr_2Max	1.75 (1.05-2.84)	1.75 (1.05-2.87)	1.74 (1.04-2.79)	0.710
BUN	30 (17-51)	30 (17-52)	29 (16.75-50)	0.251
eGFR	40.6 (22-53)	40.60 (22-53)	40.6 (23.75-53)	0.431
(6) Input				
IV Fluid8H	786.8 (300-1699)	792 (304.4-1700)	769 (291.7-1682.1)	0.386
IV Fluid24H	2112.2 (1000-3600)	2120 (1001-3590.7)	2089.75 (1000-3622.65)	0.937
Blood transfusion (ml) 0-8hr	0 (0-240)	0 (0-250)	0 (0-210)	0.322
Blood transfusion (ml) 0-24hr	0 (0-500)	0 (0-510)	0 (0-500)	0.325
(7) Urine output				
UO_8H	400 (90-890)	400 (90-900)	400 (80-850)	0.148
UO_16H	330 (110-650)	340 (120-660)	315 (100-630)	0.036
UO_24H	320 (100-630)	320 (100-640)	330 (100-620)	0.696
Urine (ml)	1280 (550-2190)	1280 (560-2210)	1260 (510-2120)	0.069
(8) I/O balance	1864.43 (542.96-2795.47)	1864.43 (531-2767.8)	1864.43 (586.55-2914.12)	0.192
(9) Vital signs on ICU admission				
Highest BT	37.7 (37.2-38.3)	37.7 (37.2-38.3)	37.7 (37.2-38.3)	0.596
Lowest BT	36 (35.5-36.6)	36 (35.5-36.6)	36 (35.5-36.6)	0.832
Heart rates	110 (96-127)	110 (96-127)	111 (96-128)	0.755
Respiratory rates	25 (22-30)	25 (22-29)	26 (22-30)	<u>0.047</u>
ABPs	91.6 (78-102)	91.6 (78-103)	91.6 (78-102)	0.445
ABPd	48.36 (42-54)	48.36 (42-54)	48.36 (41-53)	0.051
NBP	82 (70-96)	83 (70-97)	81 (70-95)	0.055
NBPd	43 (35-51)	43 (34-51)	43 (35-51)	0.939
(10) Ventilator				
Mechanical ventilation	9210 (74.41)	7392 (74.66)	1818 (73.42)	0.216

Tidal Volume first	546.51 (494-589)	546.51 (493-589)	546.51 (497-588)	0.627
FiO2 first	71.26 (50-100)	71.26 (50-100)	71.26 (50-100)	0.569
Rate first	12 (12-12.48)	12 (12-12.48)	12 (12-12.48)	0.130
PEEP first	5 (5-5.2)	5 (5-5.2)	5 (5-5.2)	0.808
Peak first	24.61 (22-27)	24.61 (22-27)	24.61 (22-26)	0.428
Tidal Volume second	547.09 (507-573)	547.09 (507-574)	547.09 (509-571)	0.581
FiO2 second	41.79 (35-41.79)	41.79 (30-41.79)	41.79 (35-41.79)	0.199
Rate second	11.46 (11.46-12)	11.46 (11.46-12)	11.46 (11.46-12)	<u>0.036</u>
PEEP second	6.23 (5-6.23)	6.23 (5-6.23)	6.23 (5-6.23)	0.604
Peak second	23.64 (22-24)	23.64 (22-24)	23.64 (22-24)	0.372
(11) Oxygenation				
PaO2	133 (86.7-173.8)	133 (87-173.2)	131.95 (85.57-176.07)	0.874
(12) Acidosis and electrolyte				
pH	7.41 (7.38-7.46)	7.41 (7.38-7.46)	7.41 (7.37-7.46)	0.440
PaCO2	31.9 (27.1-35.8)	31.9 (27.1-35.8)	31.9 (27.2-35.9)	0.827
HCO3	21 (18.1-23.2)	21 (18.1-23.3)	21 (18.1-23.2)	0.820
Na	138.78 (138-139)	138.78 (138.78-139)	138.78 (138-139)	0.332
iP	3.62 (2.6-3.8)	3.62 (2.6-3.8)	3.62 (2.6-3.8)	0.325
K	4.05 (3.9-4.05)	4.05 (3.9-4.05)	4.05 (3.9-4.05)	0.327
Ca	7.85 (7.8-8.3)	7.85 (7.8-8.3)	7.85 (7.8-8.3)	0.349
Mg	2.00 (1.77-2.14)	2 (1.78-2.14)	2 (1.75-2.13)	0.316
(13) Hemodynamic status				
CVP_0	10.31 (9-10.31)	10.31 (9-10.31)	10.31 (10-10.31)	0.442
CVP_24	10.39 (10-10.39)	10.39 (10-10.39)	10.39 (10-10.39)	0.546
Usage of norepinephrine	3327 (26.88)	2630 (26.56)	697 (28.15)	0.116
Usage of dopamine	726 (5.87)	586 (5.92)	140 (5.65)	0.665
(14) Liver function				
Total bilirubin	0.95 (0.5-2.06)	0.94 (0.5-2.06)	0.96 (0.52-2.06)	0.386
AST	53 (25-187.95)	52 (25-187.95)	56 (26-187.95)	0.133
ALT	26 (15-68)	26 (15-68)	27 (15-67)	0.158
(15) Inflammatory markers				
WBC	9900 (6500-14200)	9900 (6500-14200)	9900 (6500-14100)	0.815
CRP	10.85 (5.02-13.23)	10.85 (4.93-13.12)	10.85 (5.38-13.57)	0.100
(16) Platelet (K)	164 (100-229)	164 (102-230)	163 (96-226)	0.166
(17) Albumin	2.78 (2.4-3.1)	2.78 (2.4-3.1)	2.78 (2.4-3.1)	0.443
(18) CRP	10.85 (5.02-13.23)	10.85 (4.93-13.12)	10.85 (5.38-13.57)	0.100
(19) CK-MB	37.95 (16-37.95)	37.95 (16-37.95)	37.95 (17-37.95)	0.015
(20) GCS	9 (4-14)	9 (4-14)	9 (4-14)	0.397

(21) RASS				
RASS (high)	0 (0-1)	0 (0-1)	0 (0-1)	0.390
RASS (low)	-2 (-3- -1)	-2 (-3- -1)	-2 (-3- -1)	0.188
(22) Segment (%)	82.4 (72.9-89.1)	82.4 (73-89.2)	82.2 (72.38-89)	0.270
(23) Lymphocyte (%)	8.5 (4.8-15)	8.5 (4.8-15)	8.6 (4.7-14.9)	0.731
(24) Hb	10 (8.6-11.7)	10 (8.6-11.7)	9.9 (8.5-11.7)	0.487
(25) RDW	18.6 (15.1-18.67)	18.5 (15.1-18.67)	18.67 (15.3-18.67)	<u>0.042</u>
(26) PT	14.09 (11.70-14.09)	14.09 (11.70-14.09)	14.09 (11.70-14.09)	0.444
(27) Blood type				
A+	3285 (26.54)	2629 (26.55)	656 (26.49)	0.958
A-	5 (0.04)	3 (0.03)	2 (0.08)	0.263
AB+	708 (5.72)	591 (5.97)	117 (4.73)	0.019
B+	2976 (24.04)	2389 (24.13)	587 (23.71)	0.673
B-	6 (0.05)	3 (0.03)	3 (0.12)	0.099
O+	4797 (38.76)	3808 (38.46)	989 (39.94)	0.181
O-	13 (0.11)	11 (0.11)	2 (0.08)	1.000
(28) Comorbid				
AF	451 (3.64)	363 (3.67)	88 (3.55)	0.853
Asthma	328 (2.65)	250 (2.52)	78 (3.15)	0.091
Autoim	450 (3.64)	361 (3.65)	89 (3.59)	0.948
CAD	2618 (21.15)	2120 (21.41)	498 (20.11)	0.161
CKD	2533 (20.47)	2016 (20.36)	517 (20.88)	0.578
COPD	1277 (10.32)	1026 (10.36)	251 (10.14)	0.766
Cancer	4776 (38.59)	3811 (38.49)	965 (38.97)	0.661
CerebVD	1539 (12.43)	1211 (12.23)	328 (13.25)	0.173
ChronicLiv	1539 (12.43)	1215 (12.27)	324 (13.09)	0.276
Cirrhosis	709 (5.73)	545 (5.5)	164 (6.62)	0.032
DM	3013 (24.34)	2424 (24.48)	589 (23.79)	0.479
DM_Severe	1361 (11)	1113 (11.24)	248 (10.02)	0.086
Dementia	856 (6.92)	692 (6.99)	164 (6.62)	0.534
Dyslipid	1331 (10.75)	1059 (10.7)	272 (10.99)	0.692
GIBleeding	1477 (11.93)	1198 (12.1)	279 (11.27)	0.268
Gout	601 (4.86)	478 (4.83)	123 (4.97)	0.758
HD	2098 (16.95)	1645 (16.61)	453 (18.3)	0.047
HF	1313 (10.61)	1072 (10.83)	241 (9.73)	0.118
HIV	28 (0.23)	24 (0.24)	4 (0.16)	0.636
HStroke	172 (1.39)	137 (1.38)	35 (1.41)	0.931
HTN	3998 (32.3)	3225 (32.57)	773 (31.22)	0.203

IStroke	897 (7.25)	703 (7.1)	194 (7.84)	0.208
KT	174 (1.41)	140 (1.41)	34 (1.37)	0.917
Liverdz	180 (1.45)	135 (1.36)	45 (1.82)	0.089
Liverdz_mi	699 (5.65)	543 (5.48)	156 (6.3)	0.118
MI	440 (3.55)	354 (3.58)	86 (3.47)	0.851
MIHx	35 (0.28)	27 (0.27)	8 (0.32)	0.672
OtherBleed	820 (6.63)	651 (6.58)	169 (6.83)	0.654
PAOD	35 (0.28)	32 (0.32)	3 (0.12)	0.135
PUD	1843 (14.89)	1457 (14.72)	386 (15.59)	0.283
PVD	260 (2.1)	216 (2.18)	44 (1.78)	0.241
Paralysis	60 (0.48)	46 (0.46)	14 (0.57)	0.518
SysEmbol	429 (3.47)	347 (3.5)	82 (3.31)	0.664
TIA	115 (0.93)	93 (0.94)	22 (0.89)	0.898
VHD	389 (3.14)	298 (3.01)	91 (3.68)	0.092
(29) Drug together				
ACEI	1723 (13.92)	1376 (13.90)	347 (14.01)	0.873
AGI	760 (6.14)	605 (6.11)	155 (6.26)	0.782
ARB	3963 (32.02)	3189 (32.21)	774 (31.26)	0.373
ATG	351 (2.84)	287 (2.90)	64 (2.58)	0.455
Adalctone	2285 (18.46)	1825 (18.43)	460 (18.58)	0.864
AlphaBlocker	4173 (33.72)	3355 (33.89)	818 (33.04)	0.433
Antiplatelet	4039 (32.63)	3256 (32.89)	783 (31.62)	0.240
Apixaban	68 (0.55)	56 (0.57)	12 (0.48)	0.751
Aspirin	3538 (28.59)	2864 (28.93)	674 (27.22)	0.096
Basiliximab	116 (0.94)	95 (0.96)	21 (0.85)	0.719
BetaBlocker	5205 (42.05)	4154 (41.96)	1051 (42.45)	0.666
CCB	5696 (46.02)	4584 (46.30)	1112 (44.91)	0.224
CNI	585 (4.73)	479 (4.84)	106 (4.28)	0.267
COX2	2418 (19.54)	1928 (19.47)	490 (19.79)	0.735
Cyclosporine	315 (2.55)	261 (2.64)	54 (2.18)	0.226
DPP4I	1331 (10.75)	1081 (10.92)	250 (10.1)	0.246
Dabigatran	154 (1.24)	131 (1.32)	23 (0.93)	0.132
Diuretics	6590 (53.24)	5250 (53.02)	1340 (54.12)	0.333
Edoxaban	31 (0.25)	25 (0.25)	6 (0.24)	1.000
Entresto	21 (0.17)	19 (0.19)	2 (0.08)	0.287
Everolimus	89 (0.72)	71 (0.72)	18 (0.73)	1.000
GLP1	4 (0.03)	2 (0.02)	2 (0.08)	0.181
Insulin	5130 (41.45)	4126 (41.67)	1004 (40.55)	0.316

MMF	529 (4.27)	421 (4.25)	108 (4.36)	0.828
NSAID	6597 (53.30)	5252 (53.05)	1345 (54.32)	0.260
Nitrate	3877 (31.32)	3133 (31.64)	744 (30.05)	0.127
PPI	6686 (54.02)	5367 (54.21)	1319 (53.27)	0.404
Plavix	2217 (17.91)	1788 (18.06)	429 (17.33)	0.412
Rivaroxaban	174 (1.41)	142 (1.43)	32 (1.29)	0.629
SGLT2	14 (0.11)	11 (0.11)	3 (0.12)	1.000
Statin	2524 (20.39)	2023 (20.43)	501 (20.23)	0.844
Steroid	4229 (34.17)	3425 (34.59)	804 (32.47)	0.047
Sulfonylurea	1535 (12.40)	1237 (12.49)	298 (12.04)	0.561
TZD	369 (2.98)	303 (3.06)	66 (2.67)	0.322
Tacrolimus	335 (2.71)	269 (2.72)	66 (2.67)	0.940
Ticagrelor	116 (0.94)	95 (0.96)	21 (0.85)	0.719
Ticlopidine	451 (3.64)	356 (3.60)	95 (3.84)	0.552
Warfarin	725 (5.86)	575 (5.81)	150 (6.06)	0.635
azathioprine	250 (2.02)	198 (2.00)	52 (2.1)	0.755
glinide	1083 (8.75)	868 (8.77)	215 (8.68)	0.934
mTORi	136 (1.10)	111 (1.12)	25 (1.01)	0.739
metformin	1904 (15.38)	1544 (15.59)	360 (14.54)	0.202
sirolimus	136 (1.10)	111 (1.12)	25 (1.01)	0.739
(30) Ward				
ICUA	4002 (32.33)	3186 (32.18)	816 (32.96)	0.471
ICUB	4017 (32.46)	3253 (32.86)	764 (30.86)	0.058
ICUC	4358 (35.21)	3462 (34.97)	896 (36.19)	0.259
ICU mortality	1993 (16.1)	1594 (16.1)	399 (16.11)	0.977

ACEi, angiotensin-converting enzyme inhibitor; ARB, angiotensin receptor blocker; ICU, intensive care unit; eGFR, estimated glomerular filtration rate; AKI, acute kidney injury.

Additional file 2. The hyperparameters for XGBoost configuration 1.

Hyperparameter	Value
base_score	0.5
colsample_bylevel	1
colsample_bynode	1
colsample_bytree	1
gamma	5
learning_rate	0.300000012
max_delta_step	0
max_depth	2
min_child_weight	1
n_estimators	100
num_parallel_tree	1
random_state	42
reg_alpha	0
reg_lambda	1
scale_pos_weight	2
subsample	1
tree_method	exact
validate_parameters	1

Additional file 3. The hyperparameters for XGBoost configuration 2.

Hyperparameter	Value
base_score	0.5
colsample_bylevel	1
colsample_bynode	1
colsample_bytree	1
gamma	5
learning_rate	0.300000012
max_delta_step	0
max_depth	3
min_child_weight	1
n_estimators	100
num_parallel_tree	1
random_state	42
reg_alpha	0
reg_lambda	1
scale_pos_weight	2
subsample	1
tree_method	exact
validate_parameters	1

Additional file 4. Relative importance of the extreme gradient boosting model (XGBoost, configuration 1) variables for the prediction of mortality in intensive care units (ICUs) among non-ventilated critical patients.

