Supplemental Material

Statistical methodology

Clusterisation using the Kml algorithm.

Kml is a partitioning algorithm, an implementation of k-means designed for longitudinal data, previously used in sociological studies to identify groups of individual developmental trajectories. The aim of the clustering is minimize within-cluster distances and maximize between-cluster distances. Kml uses the Euclidean distance for assignment to clusters. In addition, Kml chooses the optimal number of clusters using the Calinski and Harabasz criterion, by running k-means several times and varying the initial number of seeds (7). Here, all normalized uNGAL concentrations were included in individual trajectories, and the Kml algorithm used to identify clusters of homogeneous trajectories of uNGAL variation.

The *Likelihood Ratio (LR)* summarizes how many times more likely patients with disease are to have a positive result (5), and is considered to provide strong evidence to rule in diagnoses when >10, and to rule out diagnoses when < 0.1.

The *Diagnostic Odds ratio (DOR)* is the ratio of the odds of positivity in patients with disease relative to the odds of positivity in patients without disease, and ranges from zero to infinity (8).

The number needed to screen represents the number of patients required to yield one correct identification (case or non-case) beyond those misidentified, and varies between 1, in the case of the ideal test, and infinity, in the case of a test making random predictions. It is

calculated as the reciprocal of Mitchell's identification index (19), i.e. of the difference between the fraction correctly identified and the fraction misidentified.

The Net Reclassification Improvement (NRI), and the *Integrated Discrimination Improvement (IDI)* are issued from the reclassification methodology, used to quantify the added predictive ability of new biomarkers. NRI determines the proportion of cases correctly reclassified, whereas IDI determines the extent to which the degree of risk is correctly reclassified (23). They are calculated after adding the biomarker as a predictor to a pre-specified model based on clinical variables. Here, the clinical variable was length of bypass.

Accuracy of absolute urine NGAL concentration for the prediction of dialysis and/or in-hospital death.

Absolute urine NGAL concentration (ng/mL)								
Time interval	**Before CPB**	**Within 1 h of CPB**	**1 to 3 h of CPB**	**3 to 6 h of CPB**	**6 to 12 h of CPB**	**12 to 18h of CPB**	**18 to 24 h of CPB**	**24 to 48 h of CPB**
Cutoff	62.4	109.1	138.6	82.4	30.3	7.6	8.8	7.2
Sensitivity and 95%CI*	0.64 [0.45 – 0.87]	0.54 [0.37 – 0.92]	0.55 [0.41 – 1.00]	0.77 [0.54 – 1.00]	0.69 [0.54 – 1.00]	0.94 [0.54 – 1.00]	0.92 [0.50 – 1.00]	0.50 [0.28 -0.94]
Specificity and 95%CI*	0.83 [0.52 – 0.91]	0.85 [0.33 – 0.95]	0.66 [0.27 – 0.95]	0.77 [0.59 – 0.97]	0.84 [0.46 – 0.97]	0.50 [0.40 – 0.96]	0.52 [0.43 -0.96]	0.60 [0.29 – 1.00]
Positive likelihood ratio and 95% CI*	3.88 [1.54 – 7.69]	3.64 [1.42 – 13.11]	1.62 [1.23 – 11.93]	3.39 [2.04 – 21.82]	4.39 [1.79 – 20.38]	1.87 [1.64 – 16.80]	1.92 [1.46 – 27.75]	1.24 [1.19 - ∞]
Negative likelihood ratio and 95% CI*	0.43 [0.11 – 0.74]	0.53 [0.00 – 0.78]	0.68 [0.00 – 0.77]	0.30 [0.00 – 0.57]	0.37 [0.00 – 0.53]	0.12 [0.00 – 0.53]	0.16 [0.00 – 0.67]	0.84 [0.00 – 0.84]
Diagnostic Odds-ratio and 95% CI*	9.08 [3.11 – 55.42]	6.82 [2.54 - ∞]	2.38 [1.77 - ∞]	11.36 [4.44 - ∞]	11.85 [6.86 - ∞]	15.00 [7.91 - ∞]	12.00 [2.27 - ∞]	1.48 [1.50 - ∞]
Net Reclassification Index and 95% CI	0.95 [0.40 – 1.50]	0.79 [0.18 – 1.40]	0.22 [-0.45 – 0.89]	0.98 [0.50 – 1.66]	0.79 [0.27 – 1.30]	0.97 [0.45 – 1.49]	0.88 [0.26 – 1.49]	0.79 [0.21 – 1.36]

P-value	<0.001	0.01	0.52	<0.001	0.003	<0.001	0.005	0.007
Integrated Discrimination	0.13	0.06	0.003	0.10	0.06	0.06	0.09	0.05
Improvement	[0.05 – 0.21]	[-0.01 – 0.13]	[-0.01 – 0.02]	[0.05 – 0.15]	[0.01 – 0.10]	[0.02 – 0.09]	[0.01 – 0.18]	[0.004 – 0.10]
and 95% CI	0.002	0.08	0.72	<0.001	0.008	<0.001	0.02	0.03
P-value								
Number needed to screen	1.50	1.52	3.23	1.83	1.52	12.0	6.23	-6.23
and 95% CI*	[1.26 – 1.86]	[1.29 – 1.91]	[2.17 – 6.28]	[1.44 – 2.76]	[1.32 – 1.82]	[-81.01 – 171.0]	[-40.0 – 79.0]	[-40.0 – 42.0]

*95% Confidence intervals were estimated by boot-strapping with 1000 re-samples.

CPB = cardiopulmonary bypass

Accuracy of the urine NGAL excretion rate for the prediction of dialysis and/or in-hospital death.

	Urine NGAL excretion rate (ng/h)							
Time interval	**Before CPB**	**Within 1 h of CPB**	**1 to 3 h of CPB**	**3 to 6 h of CPB**	**6 to 12 h of CPB**	**12 to 18h of CPB**	**18 to 24 h of CPB**	**24 to 48 h of CPB**
Cutoff	92.7	360.0	1785.6	3165.0	89.2	262.0	55.4	79.3
Sensitivity and 95%CI*	0.50 [0.43 – 0.94]	0.73 [0.54 – 1.00]	0.55 [0.37 – 1.00]	0.46 [0.35 – 0.87]	0.81 [0.39 – 1.00]	0.43 [0.35 – 1.00]	0.92 [0.40 – 1.00]	0.57 [0.23 – 0.87]
Specificity and 95%CI*	0.75 [0.26 – 0.88]	0.70 [0.31 – 0.97]	0.80 [0.36 – 0.99]	0.88 [0.43 – 0.95]	0.49 [0.37 – 0.95]	0.78 [0.20 – 0.90]	0.36 [0.29 – 0.95]	0.64 [0.38 – 1.00]
Positive likelihood ratio and 95% CI*	2.04 [1.23 – 4.40]	2.43 [1.39 – 16.30]	2.79 [1.39 – 33.03]	4.07 [1.28 – 10.21]	1.59 [1.23 – 7.87]	2.01 [1.14 – 4.76]	1.44 [1.22 – 10.5]	1.59 [1.31 - ∞]
Negative likelihood ratio and 95% CI*	0.66 [0.00 – 0.80]	0.39 [0.00 – 0.63]	0.55 [0.00 – 0.72]	0.61 [0.11 – 0.80]	0.39 [0.00 – 0.78]	0.72 [0.00 – 0.85]	0.23 [0.00 – 0.77]	0.67 [0.16 – 0.81]
Diagnostic Odds-ratio and 95% CI*	3.09 [1.77 – 32.46]	6.24 [3.23 - ∞]	5.04 [2.43 - ∞]	6.70 [1.69 – 51.75]	4.13 [2.04 - ∞]	2.80 [1.37 - ∞]	6.25 [1.75 - ∞]	2.39 [1.95 - ∞]
Net Reclassification Index and 95% CI P-value	0.80 [0.25 – 1.35] 0.004	0.87 [0.26 – 1.48] 0.005	0.98 [0.31 – 1.65] 0.004	0.81 [0.23 – 1.39] 0.006	0.95 [0.44 – 1.47] <0.001	1.00 [0.58 – 1.61] <0.001	0.33 [-0.29 – 0.94] 0.30	0.68 [0.10 – 1.26] 0.02
Integrated Discrimination	0.08	0.05	0.01	0.05	0.03	0.04	0.06	0.11

Improvement and 95% CI P-value	[0.02 – 0.14] 0.01	[-0.01 – 0.12] 0.12	[-0.009 – 0.03] 0.28	[0.01 – 0.10] 0.02	[0.007 – 0.04] 0.006	[0.008 – 0.08] 0.01	[0.02 – 0.09] <0.001	[0.02 – 0.19] 0.01
Number needed to screen and 95% CI*	2.15 [1.66 – 3.04]	2.47 [1.82 – 3.80]	1.74 [1.43 – 2.21]	1.49 [1.23 – 1.95]	30.33 [-93.0 - ∞]	2.00 [1.57 – 2.71]	-9.00 [-75 - ∞]	-3.86 [-14.3 - -2.04]

*95% Confidence intervals were estimated by boot-strapping with 1000 re-samples.

CPB = cardiopulmonary bypass