Online Resource 3

Quality control and quality assurance reporting checklist

Acute kidney injury is associated with less reversal of urinary metabolomic changes after coronary artery bypass grafting

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Scope of this completed checklist

This is a secondary analysis of two published, processed urine metabolomics matrices. No specimens were collected, no analytical platform was run and no raw mass-spectrometry files were reprocessed for this study. The responses below cover all eight question domains in the mQACC version 1 checklist linked by Metabolomics. They distinguish original sample-acquisition information from checks performed on the reused matrices. An unverified source procedure is not treated as evidence that the original investigators omitted it.

The checklist has been typeset for this secondary analysis; it is not a certification that all original experimental quality-control criteria were met. “Not independently verified” means that no complete, study-specific record was reconstructed for this reanalysis.

Q1. Analytical platform

Response: Secondary reanalysis; no new platform operation.

The urine inputs are processed mass-spectrometry metabolomics features. The independent 55-patient source reports isotope-labeling liquid chromatography–mass spectrometry. The GSE183276 tissue component uses existing cell annotations and is not a metabolomics acquisition. Source matrix provenance is listed in Online Resource 1, Table S5.

Q2. System suitability samples and acceptance criteria

Response: Not applicable to new acquisition; original suitability criteria not independently verified.

No new instrument suitability experiment was performed. This reanalysis does not claim a verified list of suitability compounds, concentration levels, mass/retention-time tolerances or run acceptance thresholds for either original acquisition.

Q3. Internal standards or alternative calibration

Response: No new internal standards; original complete acceptance criteria not independently verified.

The independent urine source describes a pooled isotope-labeled universal metabolite standard and equal-molar sample/reference mixing. This does not by itself verify all internal-standard compositions, concentrations or instrument acceptance criteria in the mQACC sense. No NMR calibration was performed.

Q4. Blank samples and acceptance criteria

Response: No new blanks; original blank-based criteria not independently verified.

No process, extraction or solvent blanks were generated or reprocessed. The submitted analysis does not claim independent verification of blank compositions, blank-to-sample intensity thresholds or blank-based feature exclusions for the original datasets.

Q5. Pooled quality-control samples and criteria

Response: No new pooled QC samples; complete original QC acceptance record not independently verified.

The pooled reference in the independent urine source is documented as an isotope-labeling reference. It is not assumed here to establish an interspersed pooled-QC injection scheme, a QC coefficient-of-variation threshold or batch acceptance criteria. These cannot be inferred from complete feature values alone.

Q6. Collection, storage and thawing

Response: Partially reported; a complete original handling record was not reconstructed.

The longitudinal sampling times were preoperative and approximately 6, 20 and 44 h after CABG. The independent source reports collection within 4 h, centrifugation, filtration and storage at −80 °C. Original study-specific thawing histories and all preanalytical conditions were not independently verified for both cohorts.

Q7. Randomization of sample preparation and acquisition

Response: Not applicable to new acquisition; original preparation/acquisition order not independently verified.

Original laboratory randomization and injection-order records were not reconstructed. Patient-label permutation tests and bootstrap resampling in this reanalysis are statistical procedures, not evidence of randomized laboratory preparation or instrument runs.

Q8. Public availability of QC sample data

Response: QC-specific repository availability not independently verified.

Processed biological-sample matrices are publicly available with the source publications. PXD063754/IPX0009727000 is retained as a source raw-archive identifier, not a claim that this reanalysis inspected or verified deposited QC injections. No new QC-sample dataset was generated.

Checks actually performed in the secondary analysis

Sample identifiers were mapped to patients and scheduled timepoints; complete four-sample series, group counts and the shared feature universe were checked. The longitudinal matrix had 0 non-finite values among 2,517,856 entries; the independent matrix had 0 among 76,120. Transformations, zero handling, scale fallbacks, training-only trajectory preprocessing and patient-level resampling are specified in Online Resource 1 and executable code. These checks assess the usable processed matrices, not instrument performance.

Identification and interpretation

No new authentic-standard confirmation, spectral-library matching or MSI-level assignment was performed. The 4,048 longitudinal measurements are retained as molecular features; no claim is made that they are 4,048 identified compounds. The analyses concern profile distances and directions, not validated metabolite concentrations or compound-specific pathways.

Sources

mQACC Community Engagement Working Group. Minimum reporting standards document—reporting the use of different QC samples in untargeted studies, version 1. Checklist linked in the Metabolomics author instructions: https://media.springer.com/full/springer-instructions-for-authors-assets/pdf/11306_mQACC_minimum_reporting_standard_checklist.pdf

Zhao et al. (2025). Journal of Proteome Research. https://doi.org/10.1021/acs.jproteome.5c00113. Processed Supporting Information Tables S1 and S2 are the longitudinal inputs.

Lee et al. (2026). Metabolomics. https://doi.org/10.1007/s11306-026-02423-7. Source publication section “Experimental procedures” and Supplementary Material 2 document the independent urine input.

GSE183276 source metadata and Lake et al. (2023). Nature. https://doi.org/10.1038/s41586-023-05769-3.