***Concentrations of 7-aminoclonazepam measured by UPLC-MS/MS* *in human urine after frozen storage***

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**Abstract**

7-aminoclonazepam is a metabolite of the benzodiazepine clonazepam, and is frequently tested in toxicology and pain management settings. Characterizing the stability of analytes in clinical testing is essential to ensure accurate and precise results. This data article contains the processed data for 7-aminoclonazepam concentrations in human urine. The aim of the study is to characterize the stability of 7-aminoclonazepam in human urine under frozen storage conditions for use in clinical drug monitoring. Analyzing this data set can provide insights into 7-aminoclonazepam stability and provide a template for similar analyses with other analytes.

**Specifications Table**

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| Subject area | *Medicine* |
| More specific subject area | *Therapeutic drug monitoring* |
| Type of data | *GraphPad Prism file; Data tables (Excel)* |
| How data was acquired | *UPLC-MS/MS (Waters system)* |
| Data format | *Analyzed*  |
| Experimental factors | *Drug-free urine spiked with 7-aminoclonazepam calibrator* |
| Experimental features | *Concentrations of 7-aminoclonazepam in human urine from (1) samples prepared from calibrators frozen or refrigerated then compared with reference laboratory method, and (2) samples spiked with refrigerated calibrators prepared freshly or frozen for three months* |
| Data source location | *Boston, MA, USA* |
| Data accessibility | *All data are included herein* |
| Related research article | *Dahlin, JL, Petrides, AK. Instability of 7-aminoclonazepam in frozen storage conditions. Clinical Mass Spectrometry (in press)* |

**Value of the Data**

* The data provide insight the stability of 7-aminoclonazepam when stored in frozen conditions.
* The data is useful in the following areas: clinical chemistry, therapeutic drug monitoring, assay development and validation.
* The formatted data can be applied to other analytes.

**Data**

Concentrations of 7-aminoclonazepam in human urine matrix are provided as part of two experiments: (1) samples prepared from calibrators frozen or refrigerated then compared with reference laboratory method, and (2) samples spiked with refrigerated calibrators prepared freshly or frozen for three months.

Two files are provided: GraphPad Prism 7 file (.pzfx) containing the 7-aminoclonzepam concentrations from both experiments along with accompanying statistical analyses and figure plots; Microsoft Excel file (.xls) containing the same data and statistical reports in spreadsheet format, minus figure plots.

**Experimental Design, Materials, and Methods**

7-aminoclonazepam concentrations in human urine were measured using a recently reported dilute-and-shoot UPLC-MS/MS assay to quantify benzodiazepines and related metabolites in human urine for use in clinical pain management (1). Urine samples are diluted with water and deuterated internal standard, separated by UPLC, then measured by ESI tandem MS. The assay was validated according to FDA bioanalytical guidelines, including for accuracy, precision, analytical range, stability, matrix effects, specificity, and carryover.

For the first experiment, 7-aminoclonazepam calibrators (Cerilliant) were either stored in 4 °C refrigerator according to manufacturer specifications, or stored in -20 °C for approximately one month. Drug-free human urine (Bio-Rad) was spiked with varying concentrations of 7-aminoclonazepam (0 to 1000 ng/mL) from either of the aforementioned calibrators in otherwise identical fashion. The concentration of 7-aminoclonazepam was measured by a validated in-house UPLC-MS/MS assay and compared with the same sample tested by a reference laboratory LC-MS/MS method (ARUP Laboratories). Concentrations obtained from the two methods for each sample are plotted and analyzed by Deming regression.

For the second experiment, 7-aminoclonazepam calibrators (Cerilliant) were either stored in 4 °C refrigerator according to manufacturer specifications. Drug-free human urine (Bio-Rad) was spiked with specified concentrations of 7-aminoclonazepam (5 to 2000 ng/mL). Samples were either prepared fresh or stored in -20 °C for three months, but in otherwise identical fashion. The concentration of 7-aminoclonazepam was measured for each set of spiked samples by the in-house UPLC-MS/MS assay in the same experimental run. Concentrations obtained from the two sets samples for each sample are plotted and analyzed by Deming regression.

**References**

1. Dahlin, JL, Palte, MJ, LaMacchia, J, Petrides, AK. A rapid dilute-and-shoot UPLC-MS/MS assay to simultaneously quantify 37 opioid, benzodiazepine, drugs of abuse, and related metabolites in human urine for use in clinical pain management. (in review)