Title: Rapid urine-based diagnostics using ATR-FTIR Spectroscopy

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Abstract

Attenuated total reflectance-Fourier transform infrared (ATR-FTIR) spectroscopy is a non-destructive and cost-effective analytical technique with significant potential for urine analysis. Recent studies demonstrates to apply in clinical diagnostics and forensic investigations.

In clinical applications, Rachawanmuang and colleagues used ATR-FTIR spectroscopy to discriminate urinary spectral biomarkers associated with chronic kidney disease (CKD). A total of 145 urine samples (45 healthy individuals and 100 CKD were analyzed and spectral data were further examined using multivariate analysis and machine learning approaches. Principal Component Analysis (PCA) plots demonstrated clear discrimination between healthy individuals and CKD patients, particularly in the C–H (3000-2800 cm^{-1}) and phosphate region (1400-1000 cm^{-1}). Six machine-learning models were developed to classify healthy and early-stage CKD samples. The neutral network (NN) model showed the best predictive performance on an independent test dataset (85% sensitivity, 73% specificity, and 77% accuracy). Similarly, in forensic applications, Yu and colleagues applied ATR-FTIR spectroscopy to detect common drug metabolites in urine, including heroin (6-acetylmorphine; 6-AM), cocaine (benzoylecgonine; BE), and ecstasy (3,4-methylenedioxyamphetamine; MDA), achieving limits of detection as low as 0.02 mg/mL. Multivariate analyses (PCA, Partial Least Squares-Discriminant Analysis; PLS-DA) and Orthogonal Partial Least Squares-Discriminant Analysis; OPLS-DA) showed clear discrimination between blank and drug-spiked samples, with OPLS-DA providing the best separation. However, as the analysis was performed using spiked samples, further validation with real samples is required.

Overall, these findings highlight the potential of ATR-FTIR spectroscopy as a rapid and promising tool for both forensic investigations and urine-based clinical screening.

Reference

Rachawangmuang, P., Chatchawal, P., Tippayawat, P., Jusakul, A., Kraiklang, R., Lert-itthiporn, W., Najermploy, A., & Wongwattanakul, M. (2026). Discrimination of urine infrared spectral biomarkers for early-stage chronic kidney disease patients using attenuated total reflectance fourier transform infrared spectrometry. *Clinica Chimica Acta*, *579*. https://doi.org/10.1016/j.cca.2025.120665

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