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Integrated NMR and LC-MS based metabolomics approach for biomarker identification for radiation exposure

Ruchi Baghel, Kiran Maan and **Poonam Rana**
Institute of Nuclear Medicine and Allied Sciences-DRDO, India

In the event of an intentional or accidental release of ionizing radiation in a densely populated area, timely assessment and triage of the general population for radiation exposure is critical. Despite decades of research, counter measures still lack. In this study, we describe the potential of integrated NMR and LC-MS approaches in evaluating the radiation biomarkers. Untargeted profiling by means of broad-spectrum, highly sensitive, UPLC-ESI-QTOFMS provides a comprehensive list of metabolites at one go in a single bio fluid. Present study aims to discover new, as well as validate the previously identified metabolic signatures for whole-body irradiation in mice. The study comprised 33 C57BL6 male (8-10 weeks) mice distributed as 5Gy, 7.5Gy and controls having 11 each and irradiated through 60Co gamma source. Urine samples collected post 24 hrs were run in both ESI positive and negative mode. All the data were normalized by sum and were than pareto-scaled followed by multivariate analysis including PCA and PLS-DA. Of the total 1514 (positive) and 1764 (negative) peaks univariate analysis (t-test, $p<0.05$ significant) revealed a total of 658 significant (positive) molecules with creatinine ($p=9.8 \times 10^{-5}$) and L-carnitine ($p=3.6 \times 10^{-8}$) from 5 Gy whereas betaine ($p=2.0 \times 10^{-4}$), 8-hydroxyquinone ($p=9.6 \times 10^{-5}$) and L-carnitine ($p=3.4 \times 10^{-5}$) from 7.5 Gy. Out of 537 significant (negative) molecules taurine (4.7×10^{-4}) and Quinnolinic acid (6.3×10^{-4}) were from 5Gy. Present study thus validates our previously (NMR) reported significant metabolites citric acid, hippuric acid and taurine. The results thus lay foundation for high-throughput triaging by metabolomic biomarkers for effective medical management. Further pathway analysis also revealed results.

ruchi.microbiol24@gmail.com

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