

SUPPLEMENTARY MATERIALS

Metabolomic Response of Human Skin Tissue to Low Dose Ionizing Radiation

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I.

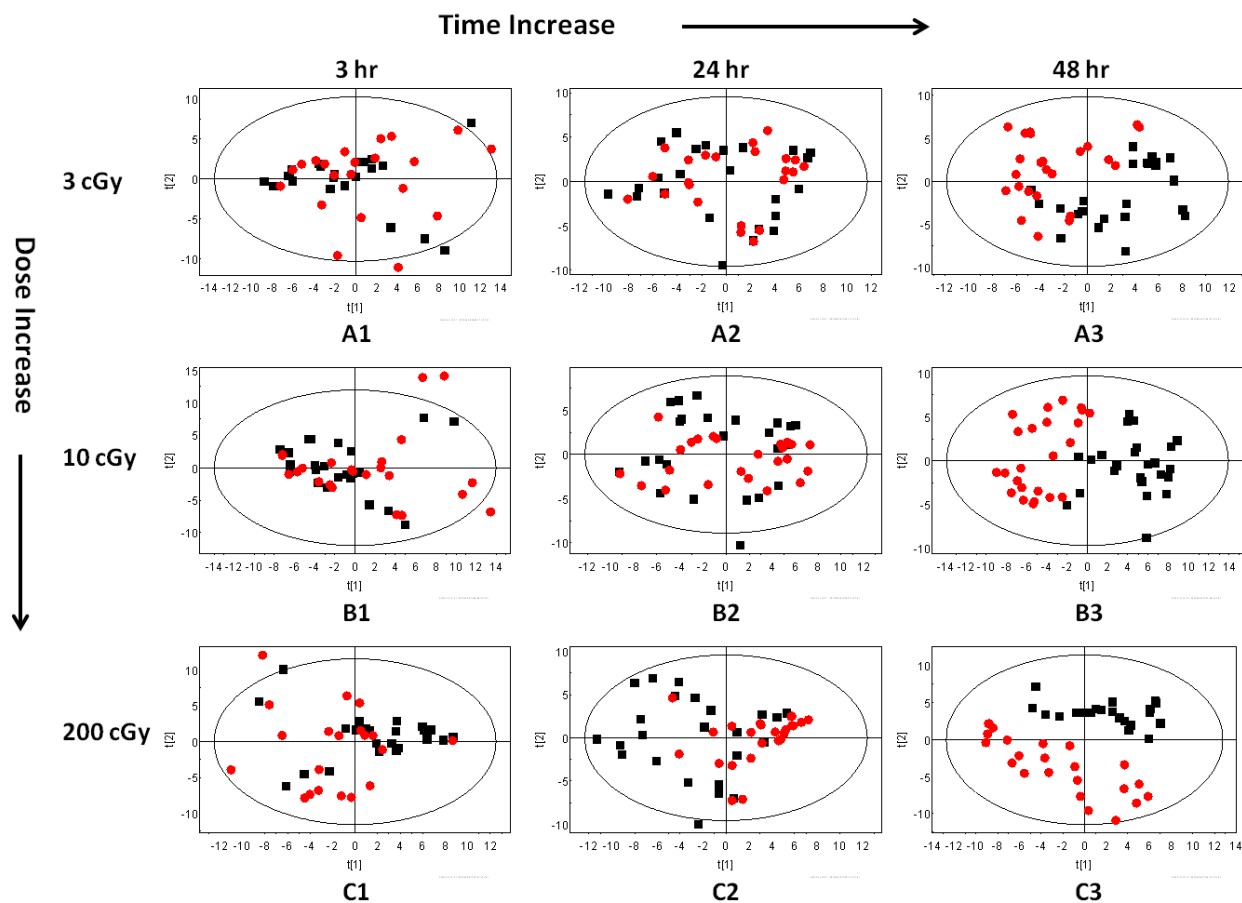


Figure 1. PCA scores plots for water-soluble metabolite samples extracted from sham and X-ray irradiated human skin tissues. Each panel shows a different irradiation dose (3, 10 and 200 cGy) at different time point post-irradiation (3, 24 and 48 hr). Each biological sample ($n = 12$ for each group) was analyzed by GC-MS in duplicate. Outlier samples were removed prior to PCA analysis. The IR-associated metabolic perturbations in human skin manifested at dose- (vertically) and time- (horizontally) dependent manner. Red dot: sham; Black square: irradiated. **A1**, scores plot from sham vs 3 cGy datasets, 3 hr post irradiation (6 components, $R^2X = 0.69$, $Q^2Y = 0.409$); **B1**, scores plot from sham vs 10 cGy datasets, 3 hr post irradiation (6 components, $R^2X = 0.719$, $Q^2Y = 0.428$); **C1**, scores plot from sham vs 200 cGy datasets, 3 hr post irradiation (7 components, $R^2X = 0.745$, $Q^2Y = 0.393$); **A2**, scores plot from sham vs 3 cGy datasets, 24 hr post irradiation (8 components, $R^2X = 0.566$, $Q^2Y = 0.0558$); **B2**, scores plot from sham vs 10 cGy datasets, 24 hr post irradiation (4 components, $R^2X = 0.378$, $Q^2Y = 0.103$); **C2**, scores plot from sham vs 200 cGy datasets, 24 hr post irradiation (7 components, $R^2X = 0.55$, $Q^2Y = 0.114$); **A3**, scores plot from sham vs 3 cGy datasets, 48 hr post irradiation (9 components, $R^2X = 0.68$, $Q^2Y = 0.226$); **B3**, scores plot from sham vs 10 cGy datasets, 48 hr post irradiation (8 components, $R^2X = 0.689$, $Q^2Y = 0.311$); **C3**, scores plot from sham vs 200 cGy datasets, 48 hr post irradiation (8 components, $R^2X = 0.679$, $Q^2Y = 0.289$).

II.

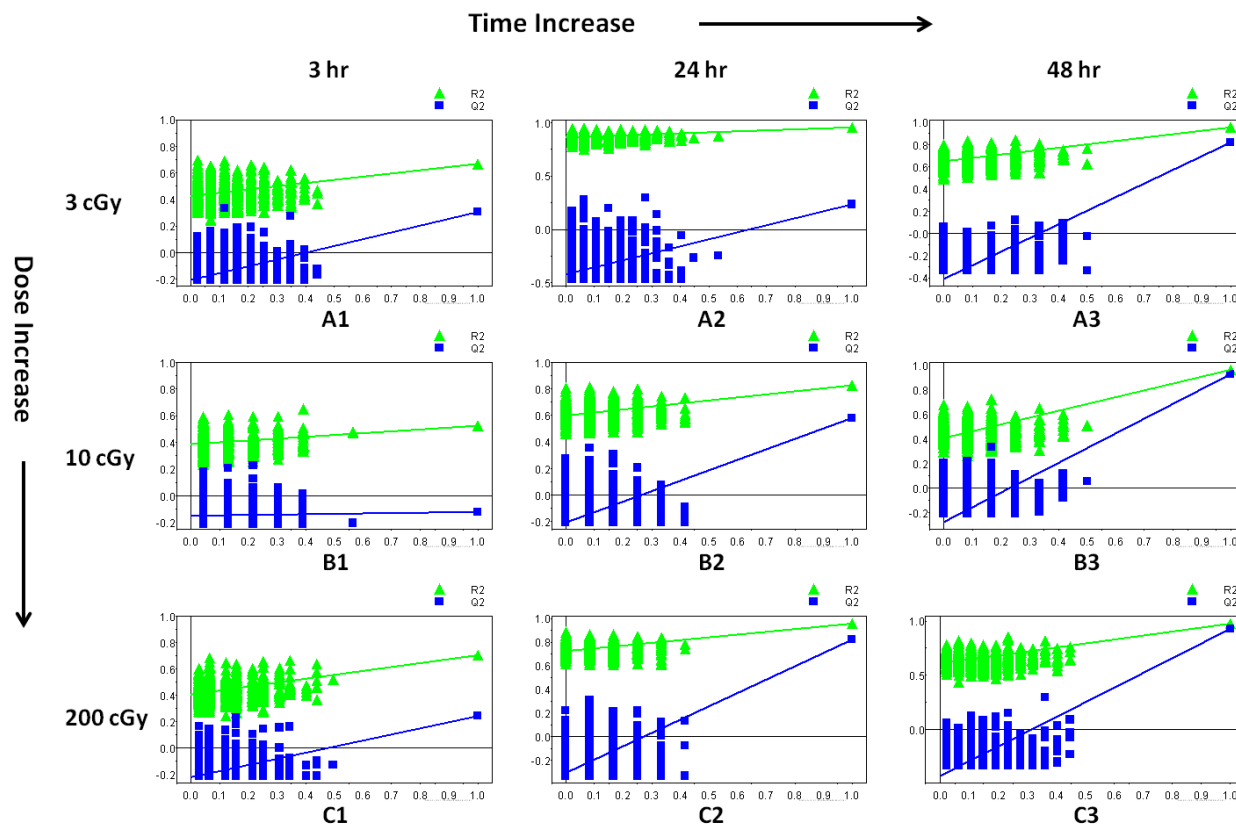


Figure 2. Validation results by performing a 999 random permutation test for the PLS-DA models generated from sham and irradiated human skin tissues. Each panel shows a different irradiation dose (3, 10 and 200 cGy) at different time point post-irradiation (3, 24 and 48 hr). Each biological sample ($n = 12$ for each group) was analyzed by GC-MS in duplicate. Outlier samples were removed prior to PLS-DA analysis. **A1**, permutation test for the PLS-DA model of 3 hr, sham vs 3 cGy datasets, Y-axis intercepts: $R^2 = (0, 0.425)$, $Q^2 = (0, -0.206)$; **B1**, permutation test for the PLS-DA model of 3 hr, sham vs 10 cGy datasets, Y-axis intercepts: $R^2 = (0, 0.386)$, $Q^2 = (0, -0.148)$; **C1**, permutation test for the PLS-DA model of 3 hr, sham vs 200 cGy datasets, Y-axis intercepts: $R^2 = (0, 0.404)$, $Q^2 = (0, -0.226)$; **A2**, permutation test for the PLS-DA model of 24 hr, sham vs 3 cGy datasets, Y-axis intercepts: $R^2 = (0, 0.864)$, $Q^2 = (0, -0.41)$; **B2**, permutation test for the PLS-DA model of 24 hr, sham vs 10 cGy datasets, Y-axis intercepts: $R^2 = (0, 0.603)$, $Q^2 = (0, -0.211)$; **C2**, permutation test for the PLS-DA model of 24 hr, sham vs 200 cGy datasets, Y-axis intercepts: $R^2 = (0, 0.722)$, $Q^2 = (0, -0.309)$; **A3**, permutation test for the PLS-DA model of 48 hr, sham vs 3 cGy datasets, Y-axis intercepts: $R^2 = (0, 0.644)$, $Q^2 = (0, -0.413)$; **B3**, permutation test for the PLS-DA model of 48 hr, sham vs 10 cGy datasets, Y-axis intercepts: $R^2 = (0, 0.407)$, $Q^2 = (0, -0.28)$; **C3**, permutation test for the PLS-DA model of 48 hr, sham vs 200 cGy datasets, Y-axis intercepts: $R^2 = (0, 0.612)$, $Q^2 = (0, -0.422)$.