

Supplementary Info – Metabolic Profiling of Murine Radiation-Induced Lung Injury with Raman Spectroscopy and Comparative Machine Learning

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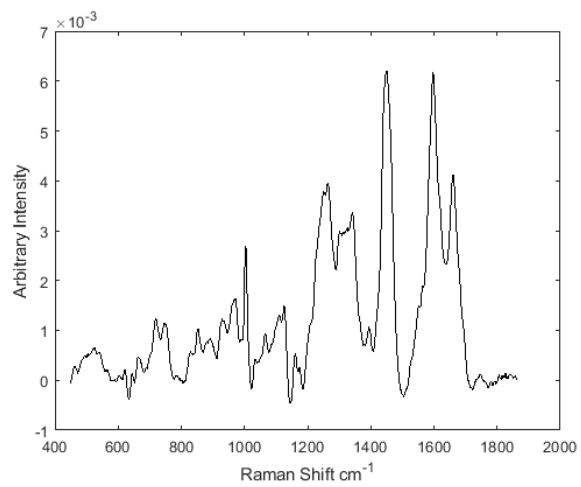
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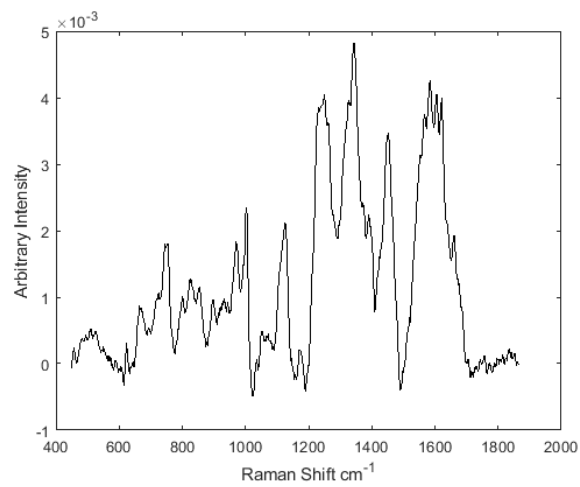
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Table S1. Mouse identifiers and post-radiation date survival times.

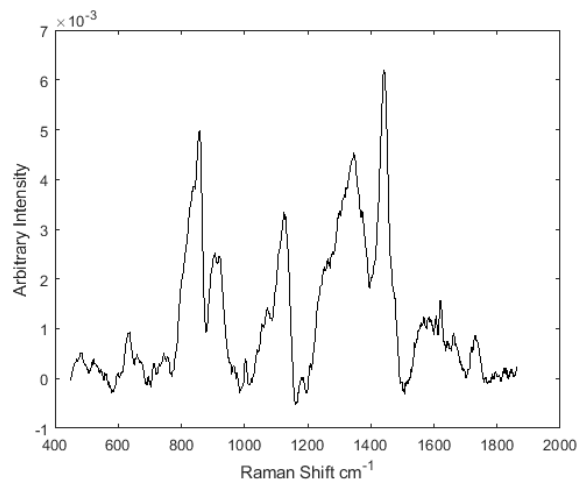
Strain	Mouse Label	Dose	Time from radiation date to euthanasia (days)
C3H/HeJ	Irr 1	16 Gy	88
C3H/HeJ	Irr 2	16 Gy	86
C3H/HeJ	Irr 3	16 Gy	86
C3H/HeJ	Irr 4	16 Gy	88
C3H/HeJ	Irr 5	16 Gy	86
C3H/HeJ	Ctrl 1	0 Gy	86
C3H/HeJ	Ctrl 2	0 Gy	86
C3H/HeJ	Ctrl 3	0 Gy	86
C3H/HeJ	Ctrl 4	0 Gy	91
C3H/HeJ	Ctrl 5	0 Gy	91
C57BL/6	Irr 1	16 Gy	157
C57BL/6	Irr 2	16 Gy	162
C57BL/6	Irr 3	16 Gy	147
C57BL/6	Irr 4	16 Gy	163
C57BL/6	Irr 5	16 Gy	144
C57BL/6	Ctrl 1	0 Gy	157
C57BL/6	Ctrl 2	0 Gy	157
C57BL/6	Ctrl 3	0 Gy	157
C57BL/6	Ctrl 4	0 Gy	164
C57BL/6	Ctrl 5	0 Gy	164



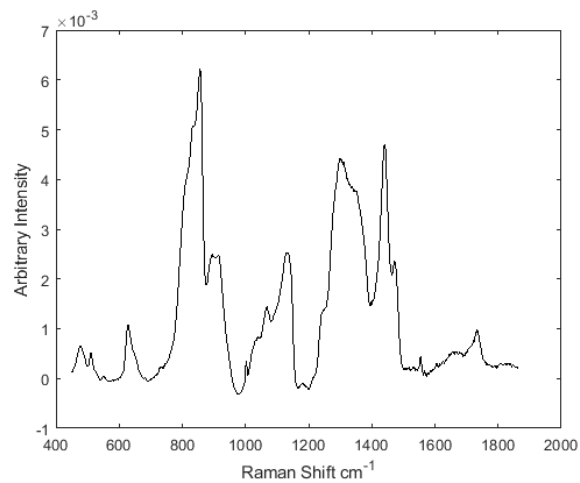
(a)



(b)



(c)



(d)

Figure S1. Examples of variable Raman spectral quality obtained from a C57 mouse lung: (a) high-quality preserved spectrum, (b) low-quality removed spectrum, (c) spectrum removed due to high correlation with OCT-PBS, and (d) a spectrum of pure OCT-PBS for comparison.

Table S2. Raman library for GBR-NMF (group and basis restricted non-negative matrix factorization).

Name	Group
Alanine	Amino acid
Arginine	Amino acid
Asparagine	Amino acid
Aspartic Acid	Amino acid
Cholesterol	Lipid
Citric Acid	TCA cycle
Coenzyme A	TCA cycle
Collagen	Protein
Cysteine	Amino acid
DNA	Nucleic acid
Glucose	Carbohydrate
Glutamic Acid	Amino acid
Glutathione	Antioxidant
Glycerol	Sugar alcohol
Glycogen	Carbohydrate
Histidine	Amino acid
Isoleucine	Amino acid
Lactose	Carbohydrate
Leucine	Amino acid
L-Glutamic Acid	Amino acid
Lysine	Amino acid
Mannose	Carbohydrate
Methionine	Amino acid
OCT-PBS	Stabilizing medium
Oleic Acid	Fatty acid
Palmitic Acid	Fatty acid
Phenylalanine	Amino acid
Phosphatidylcholine	Phospholipid
Phosphatidylserine	Phospholipid
Phosphatidylinositol	Phospholipid
Serine	Amino acid
Stearic Acid	Fatty acid
Threonine	Amino acid
Triglycerides	Lipid
Tryptophan	Amino acid
Tyrosine	Amino acid
Valine	Amino acid

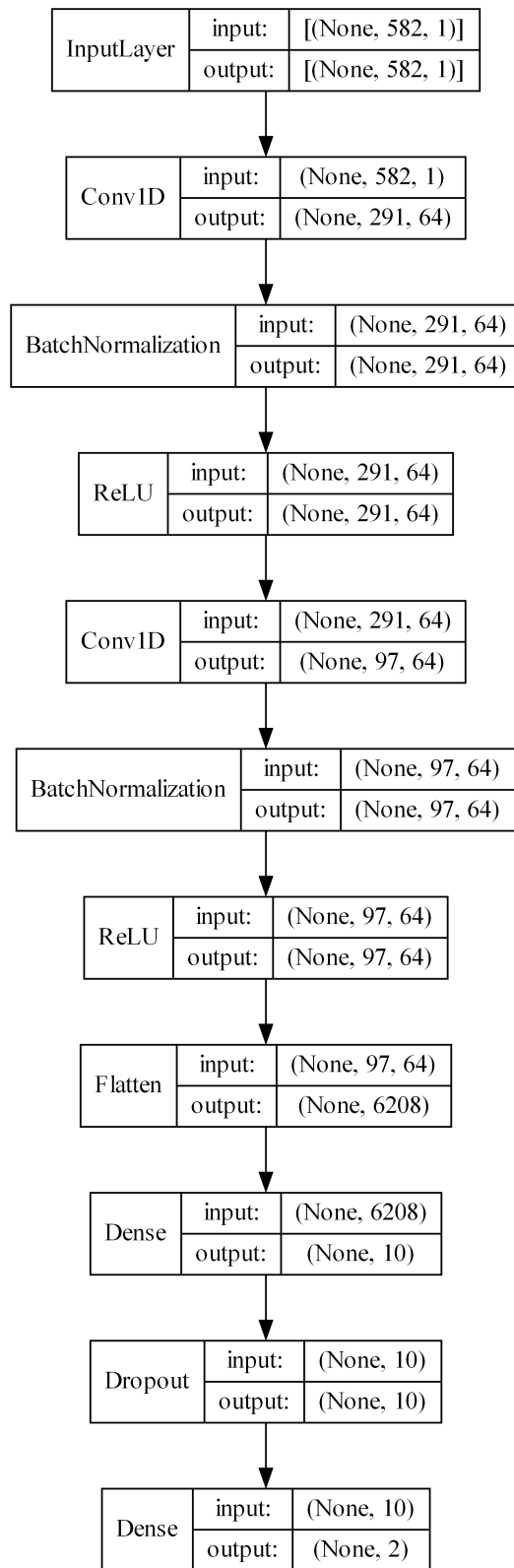
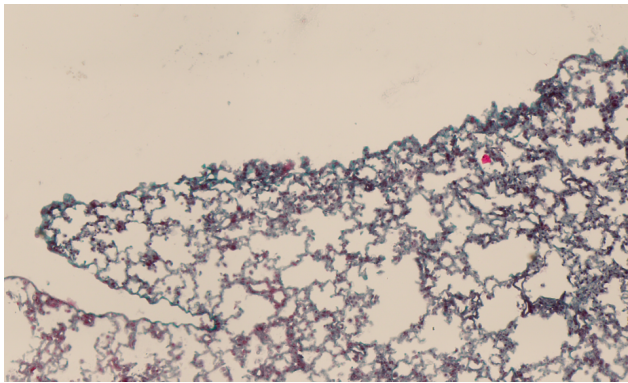
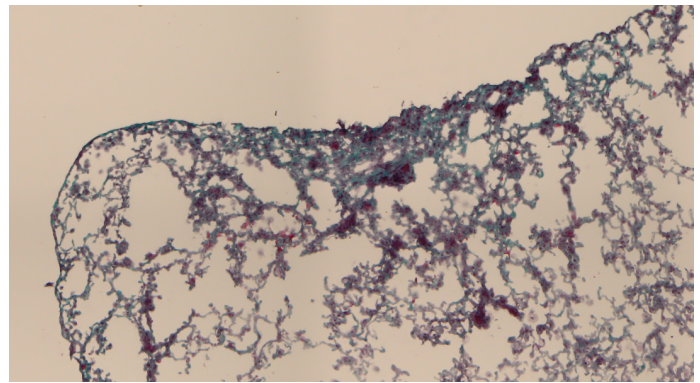


Figure S2. CNN architecture.



(a)



(b)

Figure S3. (a) Collagen presence within a C3H/HeJ mouse lung post-radiation. (b) Collagen presence and alveolar collapse within a C57/BL6J mouse lung post-radiation. Collagen is indicated by cyan regions.