DATA TITLE: Raman spectral data from healthy pregnant patient plasma throughout pregnancy

DATA ABSTRACT:

This dataset aims to share Raman spectral data from healthy pregnant patient plasma samples measured in all three trimesters and is associated with research on predicting earlier onset of preeclampsia. The Raman data shared here is particularly for patients that had normal pregnancy without preeclampsia. The sample collection and Raman measurement details provided below are reproduced from our published paper, listed below, and are represented in .csv file format.

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ASSOCIATED PUBLICATIONS:

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COLLECTION INFORMATION:

Time period(s): May ’23 to July ’23.

Location(s): Nanovaccine Institute, Iowa State University, Ames, IA 50012, USA.

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# ----- FILE DIRECTORY -----

Each Raman data file (\*.csv format) corresponds to one anonymized patient sample, with separate samples taken in each trimester of pregnancy. The first column of each file consists of the wavenumber (cm-1), and each subsequent column corresponds to an individual Raman spectra with intensities at those wavenumbers. There are 100 spectra in total for each sample.

## ----- FILE LIST-----

1. H 1st Tri – folder of spectra taken from samples in the first trimester

1.1 – 1.34: H1.csv … H34.csv – spectra files for samples H1 through H34 for the first trimester timepoint.

2. H 2nd Tri – folder of spectra taken from samples in the second trimester

2.1 – 2.34: H1.csv … H34.csv – spectra files for samples H1 through H34 for the second trimester timepoint.

3. H 3rd Tri – folder of spectra taken from samples in the third trimester.

3.1 – 3.34: H1.csv … H34.csv – spectra files for samples H1 through H34 for the third trimester timepoint.

## ----- CODEBOOK -----

Number Of Columns: 101

Number Of Rows: 1022

Missing Data Codes: N/A

## ----- VARIABLES -----

|  |  |  |
| --- | --- | --- |
| Name *[variable name]* | Description *[what is it?]* | Values *[units, valid data types, etc.]* |
| Wavenumber (column 1) | The shift in incidence light from Raman scattering that composes a Raman spectra. | cm-1 |
| Intensity (column 2-101) | The intensity of scattered light at a given wavenumber, which can be correlated to the abundance of the species that scatters at that wavenumber (e.g., spectral peaks). Each spectra consists of intensity values plotted by wavenumber (X = wavenumber, y= intensity). | Counts (arbitrary unit) |

# ----- METHODS AND MATERIALS -----

## ----- DATA COLLECTION METHODS -----

All patients provided informed consent to have blood collected by the Perinatal Family Tissue Bank from the University of Iowa Hospitals & Clinics Department of Obstetrics and Gynecology (IRB#200910784).

Blood was collected in ACD-A tubes (Becton Dickinson), centrifuged, and plasma was aliquoted, snap-frozen, and stored at −80°C. Patients were not directly recruited for this study. Blood samples and clinical data were obtained from pregnant patients being recruited and enrolled by the Perinatal Family Tissue Bank (PFTB) at the University of Iowa (UI). The PFTB prospectively collects maternal biofluids (blood, urine) throughout gestation as well as at delivery (amniotic fluid, placenta). PFTB continuously recruits and enrolls participants serving as a cross sectional biobank and clinical datamart that provides research substrates for a number of studies both within UI and to other collaborating institutions.

The plasma samples from the patients and associated clinical data were provided to us coded with all of the HIPAA identifiers removed. The reporting of human data aligns with the Helsinki guidelines.

A Renishaw inVia Raman confocal microscope with a 785 nm laser was used to take scans of the dried plasma with WiRE 5.4 software. The spectrophotometer was calibrated daily with a standard silicon wafer at 520.5 nm. After thawing the plasma, 3 μL of sample was aliquoted on a 2 mm CaF2 disk and subsequently dried for 20 min in 37°C. The samples were run under the 50x objective with 100% laser power of 120 mW with 1200 lines per mm grating, 1 accumulation and 10 second exposure time. One hundred points of static scans for all the samples were measured by line maps in the WIRE 5.4 software.

## ----- DATA PROCESSING METHODS -----

Data in this dataset is raw data that has been collated by sample from multiple original output files. No additional processing steps have been applied.

# ------- SOFTWARE -------

Name: WiRE

Version: 5.4

System Requirements: Windows

URL: https://www.renishaw.com/en/raman-software--9450

Developer: Renishaw plc

Additional Notes: Data was generated from WiRE in its native proprietary format (\*.wdf) but was exported to \*.txt files and then collated into \*.csv files.

# ------- EQUIPMENT -------

Manufacturer: Renishaw

Model: InVia

Embedded Software: WiRE

Embedded Software: 5.4

# ------- LICENSING -------

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