

S170900 Organotypic Bronchial- Submitted Data

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1. Purpose

The purpose of this file is to describe the submitted raw data files of the Philip Morris International Reduced Risks Products System Toxicology study S170900 Organotypic Bronchial.

2. File Types

The file extensions used are the following:

- *.txt and *.csv: can be opened with a text editor.
- *.xlsx: can be opened with Microsoft Excel.
- *.pdf: can be opened with Adobe Acrobat Reader.
- *.tif: format used for histology pictures, can be opened with any image viewer.

3. Study Phase Description

A Study comprised of

- Dose Range Assessment (DRA), also referred to as Dose Range Finding (DRF)
- Main Phase (abbreviated as MP, also referred to as "Study Phase" (SP) or as "Experimental Repetition")
 - MP2 (also referred to Experimental Repetition 1 in the Final Report)
 - MP3 (also referred to Experimental Repetition 2 in the Final Report)
 - MP4 (also referred to Experimental Repetition 3 in the Final Report)
 - MP6 (also referred to Experimental Repetition 4 in the Final Report)
 - MP7 (also referred to Experimental Repetition 5 in the Final Report)
 - MP8 (also referred to Experimental Repetition 6 in the Final Report)

4. Folders organization

The folders organization is presented below.

Information on the data contained in the folder is given using parentheses.

S170900

❖ AK

- S170900-AK-RawData.xlsx (containing list of the measured values for the adenylate kinase assay for the phases reported in the final report)
- S170900-AK-MetaData.xlsx (full metadata in Isa-Tab format, including the following tabs:
 - i_Organism, describing the overall study and methods used
 - s_Organism, listing the samples included in the study with the protocols (exposure, measurements) that were applied to them
 - s_DP_AK, listing the samples from which AK was measured
 - a_DP_AK, listing the samples on which AK parameters have been determined and gives the links to the Raw Data file)

❖ CARBONYLS

- S170900-Carbonyls-RawData.csv (measured values of carbonyls deposited in the exposure system, as a quality control measure)

❖ CYP1A11B1

- S170900-CYP-RawData.xlsx (containing list of the measured values for the Cytochrome P450 1A1/1B1 activity assay for the phases reported in the final report)
- S170900-CYP-MetaData.xlsx (full metadata in Isa-Tab format, including the following tabs:
 - i_Organism, describing the overall study and methods used
 - s_Organism, listing the samples included in the study with the protocols (exposure, measurements) that were applied to them
 - s_DP_CYP, listing the samples from which CYP1A11B1 was measured

- a_DP_CYP, listing the samples on which CYP1A11B1 parameters have been determined and gives the links to the RawData file

❖ DOCUMENTS

- S170900-*-ExposurePlan.xlsx (Exposure Plan, where * signifies the study phase as described in [section 3](#), containing the following tabs:
 - Inserts & Endpoints, listing the total number of culture inserts needed and allocation of samples
 - Exposure Plan, illustrating the exposure plan layout)

❖ HE

- S170900-*-HistoLog.xlsx (where * signifies the study phase as described in [section 3](#), listing all the hematoxylin and eosin (HE)-stained sections, including the sample annotation corresponding to the each image ID)
- S170900-*-HE-imageID.tif (where * signifies the study phase as described in [section 3](#): individual images of tissue stained with HE)

❖ IHC

- S170900-IHC-RawData.xlsx (containing list of the measured values of the immunohistochemistry (IHC) analysis)
- S170900-IHC-MetaData.xlsx (containing annotation of the Raw Data file, containing the following tabs:
 - i_Organism, describing the overall study and methods used
 - s_Organism, listing the samples included in the study with the protocols (exposure, measurements) that were applied to them
 - s_DP_IHC, listing the samples from which IHC was conducted
 - a_DP_IHC, listing the samples on which IHC parameters have been determined and gives the links to the Raw Data file)
- S170900-MP*-FOXJ1-XX.tif (where * refers to study phase, as described in [section 3](#) and XX refers to image ID: FOXJ1-stained sections)
- S170900-MP*- Ki67-XX.tif (where * refers to study phase, as described in [section 3](#) and XX refers to image ID: Ki67-stained sections)
- S170900-MP*- P63-XX.tif (where * refers to study phase, as described in [section 3](#) and XX refers to image ID: P63-stained sections)

❖ MAP

- S170900-MAP-RawData.xlsx (containing list of the measured values for multianalyte profiling, for the phases reported in the final report)

- S170900-MAP-MetaData.xlsx (containing annotation of the Raw Data file, containing the following tabs:
 - i_Organism, describing the overall study and methods used
 - s_Organism, listing the samples included in the study with the protocols (exposure, measurements) that were applied to them
 - s_DP_MAP, listing the samples from which MAP was measured
 - a_DP_MAP, listing the samples on which MAP parameters have been determined and gives the links to the Raw Data file)

❖ **MIRNAMA**

- S170900_MP_BR_MIRNA_PROCESSED.csv (referring to processed miRNA expression data. Each row is designating a gene symbol, while each column is a sample. The numbers are log2-expression values.)
- S170900_MP_BR_MIRNA_Metadata.xlsx (referring to the sample meta-data, including the study design and the meta-data collected during the laboratory process (from sample to Affymetrix CEL file). The column “Array.Name” describes the original CEL file name and is matching the headers of the PROCESSED file described above; while the column “Array.Name.TXT” is matching the text export of the original CEL file (File extension .txt))
- S170900_MP_BR_MIRNA_S-*.txt (Individual raw data CEL files converted to text files. The star represents the sample id for each sample)

❖ **MRNAMA**

- S170900_MP_BR_MRNA_PROCESSED.csv (referring to processed gene expression data. Each row is designating a gene symbol, while each column is a sample. The numbers are log2-expression values.)
- S170900_MP_BR_MRNA_Metadata.xlsx (referring to the sample meta-data, including the study design and the meta-data collected during the laboratory process (from sample to Affymetrix CEL file). The column “Array.Name” describes the original CEL file name and is matching the headers of the PROCESSED file described above; while the column “Array.Name.TXT” is matching the text export of the original CEL file (File extension .txt))
- S170900_MP_BR_MRNA_S-*.txt (Individual raw data CEL files converted to text files. The star represents the sample id for each sample)

❖ **NICOTINE**

- S170900-NicEXtrelut-RawData.xlsx (referring to the measured values in the smoke/aerosol trapped in EXtrelut columns)

5. File Naming Convention

[Study Number]-[MPX]-[Endpoint]-[Description]

Where:

- [Study Number] is "S" followed by 6 digits number
- [MPX]: optional, refers to study phase as explained in [section 3](#)
- [Endpoint] refers to a biological endpoint measurement
- [Description] can be any of the following:
 - RawData, containing list of the measured values for the phases reported in the final report
 - Metadata, containing annotation of the RawData file
 - ExposurePlan, containing the following tabs:
 - Inserts & Endpoints, listing the total number of culture inserts needed and allocation of samples
 - Exposure Plan, illustrating the exposure plan layout
 - FOXJ1-imageID, referring to FOXJ1-stained sections, followed by the imageID (e.g., A1, A2, B1, B2, etc.)
 - Ki67-imageID, referring to Ki67-stained sections, followed by the imageID (e.g., A1, A2, B1, B2, etc.)
 - P63-imageID, referring to P63-stained sections, followed by the imageID (e.g., A1, A2, B1, B2, etc.)
 - HE-imageID, referring to the HE-stained sections, followed by the imageID (e.g., A1, A2, B1, B2, etc.)

6. Abbreviations

AK:	adenylate kinase
BR:	bronchial organotypic tissue
CYP:	cytochrome P450
DRA:	dose range assessment
DRF:	dose range finding
HE:	hematoxylin and eosin
IHC:	immunohistochemistry
MAP:	multi analytes profiling
MIRNAMA:	microRNA microarray
MP:	main phase
MRNAMA:	messenger RNA microarray
Nic:	nicotine
SP:	study phase
THS2.2:	Tobacco Heating System (version 2.2), also referred to as ZRH or P1