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Project acronym:
HeCaTos

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Modelling toxic response in case studies for predictive human safety assessment

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Deliverable Report D5.3:
Report on meta data of samples delivered to Workpackage 9

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Work package 5

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PP	Restricted to other programme participants (including the Commission Services)	
RE	Restricted to a group specified by the consortium (including the Commission Services)	
CO	Confidential, only for members of the consortium (including the Commission Services)	

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PUBLISHABLE SUMMARY

A system of sample numbering and information presentation and curation was established and provided for all assays to identify and inform on each 3D *in vitro* sample.

OBJECTIVES

Establish a robust, reproducible numbering procedure along with exhaustive information on each sample set to present and transmit to WP09 for accessibility to all partners.

INTRODUCTION

WP05 produces a substantial amount of *in vitro* samples (over 1000 as of September 2017), which are supplied to *in vitro* labs, analytical labs and data analysis labs. It is therefore critical that all information of possible interest to analytical labs and data analysts concerning samples is available in an efficient and presentable manner.

RESULTS

Metadata for all assays is presented in an Excel file which is updated regularly each time a new assay is terminated and wrapped up. The new metadata file is sent to WP09 who will update the version on the EBI's BioStudies server available to all partners.

NB: In addition similar files are sent directly to sample analysis consortium partners via email containing additional information on nucleic acid yields in the case where samples have been processed before shipment.

The file is composed as such:

- Each *in vitro* assay is named by the compound (or control) used in the assay and has its own tab within the file;
- The tabs of assays in the file are in chronological order.

Each assay is sorted by sample numbers in the assay, which contain the following information for each samples:

- **Sample#:** samples are organised in a chronological, consecutive ordering system comprised of a number and series of letters (DNA: epigenomics analysis, RNA: transcriptomics analyses, P: proteomics analysis, M: metabolomics analysis). The numbering system is common and non-specific to heart or liver tissue;
- **Sampling date:** date that the sample was generated i.e. removed from the assay plate and stored at -80°C;
- **Compound:** compound used in the assay, when no compound or a vehicle is used it is specified;
- **Time range:** start time and end time in the assay (counting the first treatment at 0 hours) during which the microtissues were incubated with a certain concentration;
- **Incubation time with respective conc. [µM]:** duration (in hours) of incubation with a specific concentration of compound that the microtissues received;

- **Sampling time point:** time at which the sample was generated i.e. removed from the assay plate and stored at -80°C. Ex. The timepoint T0 indicates the time when microtissues received their first dose, T72 indicated the microtissues received their first dose 72 hours ago;
- **Dose:** dose category the samples were treated with, either toxic or therapeutic. In the case of controls the column is crossed out.

Example of datasheet sent for one assay: Sample #0752DNA was sampled 24hours after the assay began, underwent 3 concentration adjustments and was analysed for epigenomics markers

Phenytoin: RNA samples						
sample#	sampling date	compound	time range	incubation time with	sampling time point	dose
#0 742 RNA	17/01/2017	Phenytoin	0 h	0 h	T0	
#0 743 RNA	17/01/2017	Phenytoin	0 h	0 h	T0	
#0 744 RNA	17/01/2017	Phenytoin	0 h	0 h	T0	
#0 745 RNA	17/01/2017	Phenytoin	0 - 2 h	2 h 1.238167059	T2	Therapeutic
#0 746 RNA	17/01/2017	Phenytoin	0 - 2 h	2 h 1.238167059	T2	Therapeutic
#0 747 RNA	17/01/2017	Phenytoin	0 - 2 h	2 h 1.238167059	T2	Therapeutic
#0 748 RNA	17/01/2017	Phenytoin	0 - 2 h 2 - 8 h	2 h 1.238167059 6 h 1.67623637	T8	Therapeutic
#0 749 RNA	17/01/2017	Phenytoin	0 - 2 h 2 - 8 h	2 h 1.238167059 6 h 1.67623637	T8	Therapeutic
#0 750 RNA	17/01/2017	Phenytoin	0 - 2 h 2 - 8 h	2 h 1.238167059 6 h 1.67623637	T8	Therapeutic
#0 751 RNA	18/01/2017	Phenytoin	0 - 2 h 2 - 8 h 8 - 24 h	2 h 1.238167059 6 h 1.67623637 16 h 1.151052013	T24	Therapeutic
#0 752 RNA	18/01/2017	Phenytoin	0 - 2 h 2 - 8 h 8 - 24 h	2 h 1.238167059 6 h 1.67623637 16 h 1.151052013	T24	Therapeutic
#0 753 RNA	18/01/2017	Phenytoin	0 - 2 h 2 - 8 h 8 - 24 h	2 h 1.238167059 6 h 1.67623637 16 h 1.151052013	T24	Therapeutic
#0 754 RNA	20/01/2017	Phenytoin	0 - 2 h 2 - 8 h 8 - 24 h 24 - 26 h 26 - 32 h 32 - 48 h 48 - 50 h 50 - 56 h 56 - 72 h	2 h 1.238167059 6 h 1.67623637 16 h 1.151052013 2 h 2.057054131 6 h 2.406778373 16 h 1.651177487 2 h 2.407800877 6 h 2.713146763 16 h 1.859978849	T72	Therapeutic

This datasheet has been completed with all assays since establishment of the 3D *in vitro* assay protocol in June 2015 up to the most recent assay performed. It contains the following assays with the information previously mentioned including sampling number and date, concentrations, etc:

Start date	End date	Compound	Start sample#	End sample#	Experimentor	Tissue
02/06/2015	16/06/2015	Idarubicin	211	252	RN	Heart
14/07/2015	28/07/2015	Cardiac control	253	273	RN	Heart
21/07/2015	04/08/2015	Doxorubicin	274	315	RN	Heart
13/10/2015	27/10/2015	Epirubicin	316	357	RN	Heart
01/12/2015	15/12/2015	Idarubicin proteomics repeat	358	399	OC	Heart
19/01/2016	02/02/2016	Cardiac untreated control	400	420	OC	Heart
16/02/2016	01/03/2016	Hepatic untreated control	421	444	OC	Liver
16/02/2016	01/03/2016	Hepatic 0.1% DMSO control	445	465	OC	Liver
08/03/2016	22/03/2016	Azathioprine	466	507	OC	Liver
12/04/2016	26/04/2016	Acetaminophen	508	549	OC	Liver
14/06/2016	28/06/2016	Daunorubicin I	550	591	OC	Heart
05/07/2016	19/07/2016	Cardiac Fluctuating DMSO control	592	615	OC	Heart
11/10/2016	25/10/2016	Daunorubicin II	616	657	OC	Heart
08/11/2016	22/11/2016	Cardiac 5-Fluoruracil	658	699	OC	Heart
06/12/2016	20/12/2016	Hepatic 5-Fluoruracil	700	741	OC	Liver
17/01/2017	31/01/2017	Phenytoin	742	783	OC	Liver
07/02/2017	21/02/2017	Cyclosporin A THE	784	807	OC	Liver
07/03/2017	21/03/2017	Mitoxantrone <T72	808	849	OC	Heart
14/03/2017	28/03/2017	Amiodarone The	850	873	OC	Heart
14/03/2017	28/03/2017	Docetaxel The	874	894	OC	Heart
28/03/2017	11/04/2017	Isoniazid THE	895	918	OC	Liver
28/03/2017	11/04/2017	Valproic Acid THE	919	939	OC	Liver
28/03/2017	11/04/2017	Cyclosporin A TOX	940	957	OC	Liver
13/06/2017	27/06/2017	Fluctuating DMSO II	958	981	OC	Heart
13/06/2017	23/06/2017	Isoniazid TOX	982	1002	OC	Liver
13/06/2017	23/06/2017	Valproic Acid TOX	1003	1020	OC	Liver
27/06/2017	07/07/2017	Amiodarone TOX	1021	1041	OC	Heart
27/06/2017	07/07/2017	Docetaxel TOX	1042	1059	OC	Heart
27/06/2017	11/07/2017	Mitoxantrone >T72	808	849	OC	Heart
11/07/2017	25/07/2017	Paclitaxel	1060	1101	OC	Heart
08/08/2017	22/08/2017	Celecoxib	1102	1143	OC	Heart

In short, a simple manner of manually recording comprehensive assay metadata has been established and has proved functional over the last 2 years with the accumulation of over 30 assays and 1000 samples.

DIFFICULTIES

n/a