Electronic Supplementary Material (ESI) for Lab on a Chip. This journal is © The Royal Society of Chemistry 2020

1	Models & Devices +										
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			View	Edit	Model Name	Center	0	Base Model	Organ *	Device	Disease
			View	Edit	2D Mono-layer Hepatocytes	University of Pittsburgh Drug Discovery Institute			Liver	96 Well Flat Clear Bottom Black Polystyrene TC-Treated	None
			Ciew	Edit	Hepatocyte Suspension	University of Pittsburgh Drug Discovery Institute			Liver	Eppendorf Tube 1.5 mL	None
			0 View	Edit	Mimetas liver	University of Pittsburgh Drug Discovery Institute		Liver (Mimetas)	Liver	Mimetas OrganoPlate	None
			View	Edit	Mimetas Liver 2.0	University of Pittsburgh Drug Discovery Institute		Liver (Mimetas)	Liver	Mimetas Organoplate 400	None
			View	Edit	LAMPS	University of Pittsburgh Drug Discovery Institute		Liver (UPDDI)	Liver	Nortis Single Chamber	None
			View	Edit	SQL-SAL 1.0	University of Pittsburgh Drug Discovery Institute		Liver (UPDDI)	Liver	Nortis Single chamber (v0.9)	None
			View	Edit	SQL-SAL 1.0 CS Rhomb 24uL	University of Pittsburgh Drug Discovery Institute		Liver (UPDDI)	Liver	Rhombic Chamber Chip 24uL	None
			View	Edit	SQL-SAL 1.5	University of Pittsburgh Drug Discovery Institute		Liver (UPDDI)	Liver	Nortis Single Chamber	None

**Supplemental Figure S1: Selecting the appropriate MPS experimental model.** The MPS database contains detailed bench ready protocols the user can print to assemble and test compounds in various liver models. In this example, the traditional 2D monolayer culture for toxicity and metabolism testing, the gold standard hepatocyte suspension culture for metabolism, a 4 cell organoid type 3D microfluidic liver system in a 96 well Mimetas® plate suitable for high throughput screening, the a 4 cell supervised/self assembly 3D microfluidic Liver Acinus MicroPhysiology (LAMPS) and the earlier version of the LAMPS called the Sequentially Layered, Self Assembly Liver (SQL-SAL) models, and the Vascularized Liver Acinus MicroPhysiology (vLAMPS) model are choices available to meet user needs. The models vary by cell number, types, organization and complexity for the user to select one appropriate to answer the experimental hypothesis.

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	Compounds -			Adver	rse Events	S			
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	View Drug Trials View Adverse Events	Search: liver View	Compound	Event 0	Number of Reports 😧 🍷	Normalized # of Reports	Estimated Usage 😧	Show Organ 🖕	50 • entries Black Box Warning
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ery Institute Microph	Requires Permission	View	TOLCAPONE	BLOOD BILIRUBIN INCREASED	4	3.92	10,195	Liver	0
nces Tissue Chips	Add Compound	View	TOLCAPONE	LIVER FUNCTION TEST ABNORMAL	4	3.92	10,195	Liver	0
		View	ENTACAPONE	ASPARTATE AMINOTRANSFERASE INCREASED	40	2.29	174,449	Liver	
		View	ENTACAPONE	ALANINE AMINOTRANSFERASE INCREASED	34	1.95	174,449	Liver	
		View	ENTACAPONE	HEPATIC FUNCTION ABNORMAL	25	1.43	174,449	Liver	
		View	ENTACAPONE	GAMMA- GLUTAMYLTRANSFERASE INCREASED	20	1.15	174,449	Liver	
		View	ENTACAPONE	LIVER DISORDER	17	0.97	174,449	Liver	

**Supplemental Figure S2: Selecting the appropriate compounds for testing.** Clinical adverse events reporting records are contained within the database. In this example, filters are used to identify compounds with black box warning (!) for liver toxicity, increased incidents of liver enzyme elevations and suitable compounds without liver effects from all reported adverse events found in the FDA Adverse Events Reporting System (FAERS) to test in the LAMPS model. The incidents of adverse events found in the FAERS database are 'normalized' to estimated drug use from the CDC database.



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	View	Drug Trial 🔺 ID	Treatment	Species ¢	Trial Type	Finding	♦ +/- ♦ Frequency ♦	Value 🛊	Value Units
	View	187	ACETAMINOPHEN	Human	Clinical	Blood :: PK :: Cmax	Pos	21.0	µg/mL
	View	174	ENTACAPONE	Human	Clinical	Blood :: PK :: Cmax	Pos	1.22	µg/mL
	View	184	NIMESULIDE	Human	Clinical	Blood :: PK :: Cmax	Pos	6.5	µg/mL
	View	178	TOLCAPONE	Human	Clinical	Blood :: PK :: Cmax	Pos	7.2	µg/mL
	View	172	TROGLITAZONE	Human	Clinical	Blood :: PK :: Cmax	Pos	2.82	µg/mL
	5 View	178	TOLCAPONE	Human	Clinical	Blood :: PK :: Cmax	Pos	7.2	µg/mL
	View	172	TROGLITAZONE	Human	Clinical	Blood :: PK :: Cmax	Pos	2.82	µg/mL
pplemental Figure S4: Selecting the a	the National Cen and in part by the	ter for Adva Vanderbilt		nces Tissue C for Organoty	Chip Testing C pic Models for	enters Program, Predictive Toxicology	ound Cmax		Bute on Gith



**Supplemental Figure S5.** Albumin data from 14 compounds. Data are measured as ng/ml and normalized to percent of the control response in efflux media collected on Days 5, 11 and 17. The MPS experimental models in duplicate or triplicate devices were treated 18 consecutive days by continuous perfusion flow to entacapone (40  $\mu$ M); tolcapone (88  $\mu$ M), tolcapone (220  $\mu$ M); caffeine (600  $\mu$ M); Valproic Acid (1500  $\mu$ M); Warfarin (90  $\mu$ M); Buspirone ( 0.5  $\mu$ M); Methotrexate (0.03  $\mu$ M); Rifampicin (12  $\mu$ M); Erythromycin (54  $\mu$ M); Famotidine (0.5  $\mu$ M); Levofloxacin (600  $\mu$ M); Rosiglitazone (30  $\mu$ M) or Trovafloxacin (200  $\mu$ M).



**Supplemental Figure S6. BUN data from 14 compounds.** Data are measured as ng/ml and normalized to percent of the control response in efflux media collected on Days 5, 11 and 17. The MPS experimental models in duplicate or triplicate devices were treated 18 consecutive days by continuous perfusion flow to entacapone (40  $\mu$ M); tolcapone (88  $\mu$ M), tolcapone (220  $\mu$ M); caffeine (600  $\mu$ M); Valproic Acid (1500  $\mu$ M); Warfarin (90  $\mu$ M); Buspirone ( 0.5  $\mu$ M); Methotrexate (0.03  $\mu$ M); Rifampicin (12  $\mu$ M); Erythromycin (54  $\mu$ M); Famotidine (0.5  $\mu$ M); Levofloxacin (600  $\mu$ M); Rosiglitazone (30  $\mu$ M) or Trovafloxacin (200  $\mu$ M).



**Supplemental Figure S7. LDH data from 14 compounds.** Data are measured as ng/ml and normalized to percent of the control response in efflux media collected on Days 1 - 18. The MPS experimental models in duplicate or triplicate devices were treated 18 consecutive days by continuous perfusion flow to entacapone (40  $\mu$ M); tolcapone (88  $\mu$ M), tolcapone (220  $\mu$ M); caffeine (600  $\mu$ M); Valproic Acid (1500  $\mu$ M); Warfarin (90  $\mu$ M); Buspirone ( 0.5  $\mu$ M); Methotrexate (0.03  $\mu$ M); Rifampicin (12  $\mu$ M); Erythromycin (54  $\mu$ M); Famotidine (0.5  $\mu$ M); Levofloxacin (600  $\mu$ M); Rosiglitazone (30  $\mu$ M) or Trovafloxacin (200  $\mu$ M).



**Supplemental Figure S8. Cytochrome C data from 14 compounds.** A High Content Analysis instrument was used to measure fluorescent intensity on Days 5 and 18 of the mitochondria located Cytochrome C GFP biosensor. The data was normalized to control levels. The MPS experimental models in duplicate or triplicate devices were treated 18 consecutive days by continuous perfusion flow to entacapone (40  $\mu$ M); tolcapone (88  $\mu$ M), tolcapone (220  $\mu$ M); caffeine (600  $\mu$ M); Valproic Acid (1500  $\mu$ M); Warfarin (90  $\mu$ M); Buspirone ( 0.5  $\mu$ M); Methotrexate (0.03  $\mu$ M); Rifampicin (12  $\mu$ M); Erythromycin (54  $\mu$ M); Famotidine (0.5  $\mu$ M); Levofloxacin (600  $\mu$ M); Rosiglitazone (30  $\mu$ M) or Trovafloxacin (200  $\mu$ M).



**Supplemental Figure S9.** Increasing Incidents of Adverse Responses in LAMPS and Tracked FAERS Data by Clinical Hepatotoxicity in the MPS-Db. Pink designates hepatotoxic compounds, yellow designates DILI compounds and green designate non liver toxic compounds. Although the absolute order varies slightly between the in vitro and clinical assessments of liver toxicity, the overall concordance can be accurately categorized.



**Supplemental Figure S10: Detailed analysis of inter-study reproducibility assessment.** The detailed analysis shows the data used to calculated the inter-study reproducibility with links to the individual items (with same treatment) and the studies being compared. The intra-study reproducibility status is given for the samples in each of the studies being compared. The graphs show the individual data points for each of the samples (Items), the average value of the samples and a trimmed version of the average graph showing only the time points that overlapped between the studies. A) Albumin study to study reproducibility; and B) Cytochrome C study to study reproducibility.



Supplemental Figure S11. Additional information generated to assess the human MPS experimental model by Power Analysis. In this example, the effect of warfarin on albumin secretion is being compared with the no compound control. The user selects the treatments to be analyzed (A) and a graph of the experimental data is generated (B). The user then selects the desired method of calculating the effect size (C, see Methods and Materials), the desired significance level (D), and runs the analysis. The p-values and the power values for the difference between the samples is plotted for each point on the data curve (E and F, respectively). Finally, a power curve is generated showing the required sample size to achieve different statistical power values for the given dataset (G). See Figure 6 for selecting the Target/Analyte to analyze, power estimates for different sample sizes and estimates for different sample sizes.

	Disease Overview Disease Biology	Clinical Data Disease M	odels & Studies
letastatic Brea	st Cancer Disease Biology		
the mammary gland. idermal growth factor btype), hormone reco- promore receptor posi- thways, and stimulat- totein have been confi ly three genes (TPS3 sference: KEGG Bree		e presence or absence of hormon 12 negative (luminal A subtype), hr receptor negative and HER2 nega y. In HER2 positive breast tumour in TNBC, the deregulation of varior reditary, a phenomenon linked to <u>c</u>	e receptors (estrogen and progesterone subtypes) and hum rmone receptor positive and HER2 positive (luminal B tive (basal-like or triple-negative breast cancers (TNBCs)). s, HER2 activates the PI3K/AKT and the RAS/RAF/MAPK us signalling pathways (Notch and Wnt/beta-catenin), EGFR
Genomic Databa	es Cancer Genomic Resources		KEGG: Metastatic Breast Cancer Diseas
ochonne bulubu			Entry
Name	Description		
Gene Expression Omnibus	The Gene Expression Omnibus (GEO) is a public repository the distributes comprehensive sets of microarray, next-generation forms of high-throughput functional genomic data submitted be The disease biology portal delivers a prequeried link to the mo-	n sequencing, and other by the scientific community.	
OMIM Gene- Phenotype Relationship	OMIM is a comprehensive, authoritative compendium of huma phenotypes with full-text, referenced overviews of all known M disease biology portal delievers a curated query of the most re	Mendelian disorders. The	
DISEASES.org	DISEASES is a weekly updated web resource that integrates associations from automatic text mining, manually curated lite data, and genome-wide association studies. The disease biolo that displays disease relevant search results.	erature, cancer mutation	Click to view an interactive pathway map for Metastation Breast Cancer.
roteomics, Me	tabolomics, and Pharmacogenomic Resour	rces	
ProteomicsDB	by SAP	Metabolomicswor	kbench
ProteomicsDB by SA and chromosomes of	P is a proteomic database that allows you to browse proteins f interest.	Metabolomicsworkbench metabolomics data.	serves as a national and international repository for
PharmaGKB		DrugBank	
			informatics and chemoinformatics database that combines

**Supplemental Figure S12. Disease Biology portal.** The <u>Disease Biology</u> portal allows the user to link to various genomic, proteomics, metabolomics, and pharmacogenomic databases. The links on this page are automatically pre-queried for the disease of interest.

Copy C Search:	CSV Print C	olumn visibility							Show 50	<ul> <li>entries</li> </ul>
View	Drug Trial ID	Compound	Species 🛊	Trial Type ♦	Finding	Descriptor	\$ <b>+/</b> - \$	Frequency \$	Value 🝦	Value Units
View	225	EVEROLIMUS 10.0 mg   Exemestane 25.0 mg	Human	Clinical	All :: Other :: No Toxicity	Progression Free Survival	Pos			
View	225	Exemestane 25.0 mg	Human	Clinical	All :: Other :: No Toxicity	Progression Free Survival	Pos			
View	227	Fulvestrant 500.0 mg	Human	Clinical	All :: Other :: No Toxicity	Progression Free Survival	Pos			
View	226	LETROZOLE 2.5 mg	Human	Clinical	All :: Other :: No Toxicity	Progression Free Survival	Pos			
View	226	LETROZOLE 2.5 mg	Human	Clinical	All :: Other :: No Toxicity	Progression Free Survival	Pos			
View	227	Palbociclib 125.0   Fulvestrant 500.0 mg	Human	Clinical	All :: Other :: No Toxicity	Progression Free Survival	Pos			
howing 1 to	o 6 of 6 entries		Review	Comple	eted Drug Tri	ials		Previ	ous 1	Next
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**Supplemental Figure S14. Disease Models & Studies portal.** The <u>Disease Models & Studies</u> portal provides a list of all in vitro experimental models and studies in the MPS-Db for the disease of interest. All of the information for the experimental models and studies is easily accessible through the View and View/Edit links.

Chip D       No1         Chip D       No1         Asay Pide D       noe         Asay Weil D       Noe         Three       D9 H0M         Mitch Kith       Peden Fluerescene (mCherry)         Target Analysis       Tumor Cells (mCherry, red)         Target Analysis       Tumor Cells (manor Cells (more)         Target Analysis       Tumor Cells (manore)         Target Analysis       Tumor Cells (manore)			Tumor Cells (mCherry   RED)
Asay Plate IDoneAsay Well IDoneTimeD9 H0 M0Method/KitProtein Fluorescence (mCherry)Target-Stain PairingsTumor Cells (mCherry, red)Target/AnalyteTumor CellsSample LocationChamberNotesThis is one in a time series of images showing cell proliferation.Image Field20Image Field1.0xImage Resolution1.0xImage Resolution2.1 µmImage Resolution2.1 µmImage Resolution8.7610Image Color Mappingred	and with the owned with		Note: This image may have been altered to assist with viewing. To perform analysis, please download the unaltered image.
Asay Well ID       one         Time       D9 H0 M0         Method/Kit       Protein Fluorescence (mCherry)         Target-Stain Pairings       Tumor Cells (mCherry, red)         Target/Analyte       Tumor Cells         Sample Location       Chamber         Notes       This is one in a time series of Images showing cell proliferation.         Image File Name       \$737 + E2 D9 B.tf         Image File Pield       1.0x         Image Resolution       1.0x         Image Resolution       2.2 µm         Image Sample Label       mcherry         Image Wavelength Lex/em       \$77610         Image Color Mapping       red		Chip ID	N0341
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Method/Kit       Protein Fluorescence (mCherry)         Target-Stain Pairings       Tumor Cells (mCherry, red)         Target/Analyte       Tumor Cells         Sample Location       Chamber         Notes       This is one in a time series of images showing cell proliferation.         Image File Name       Y537's +E2 D9 B.tif         Image File Mame       2.0         Image Resolution       1.0x         Image Resolution       2.2 µm         Image Sample Label       mCherry         Image Wavelength (ex/em m)       567/610         Image Color Mapping       red	and the set where is there in	Assay Well ID	none
Target-Stain Pairings       Tumor Cells (mCherry, red)         Target/Analyte       Tumor Cells         Sample Location       Chamber         Notes       This is one in a time series of images showing cell proliferation.         Image File Name       Y537's +E2 D9 B.tif         Image File Name       2 • • • • • • • • • • • • • • • • • • •		Time	D9 H0 M0
Target/Analyte       Tumor Cells         Sample Location       Chamber         Notes       This is one in a time series of images showing cell proliferation.         Image File Name       Y537S +E2 D9 B.tif         Image Field       2         Image Magnification       1.0x         Image Resolution       2 μm         Image Sample Label       mCherry         Image Wavelength (ex/em m)       587/610         Image Color Mapping       red		Method/Kit	Protein Fluorescence (mCherry)
Sample Location       Chamber         Notes       This is one in a time series of images showing cell proliferation.         Image File Name       Y537S +E2 D9 B.tif         Image Field       2         Image Magnification       1.0x         Image Resolution       2 µm         Image Sample Label       mCherry         Image Wavelength (ex/em m)       587/610         Image Color Mapping       red	and the second	Target-Stain Pairings	Tumor Cells (mCherry, red)
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Image File Name     Y537S +E2 D9 B.tf       Image Field     2 Φ       Image Magnification     1.0x       Image Resolution     2 μm       Image Sample Label     mCherry       Image Wavelength (ex/em m)     587/610       Image Color Mapping     red	and the second s	Sample Location	Chamber
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**Supplemental Figure 15: Images and video data are also supported in the MPS-Db.** Day 9 growth of mCherry containing MCF7 Y537S cells in the MPS device. The metadata contains the information on device number, day of exposure, magnification and fluorescent wavelengths. Images can also be downloaded as tif files for additional analysis.

**Supplemental Table S1.** List of methods used to generate data for a variety of targets in different MPS organ models, which have been uploaded into the MPS-Db.

						Or	gan I	Mod	els i	n MPS-	Db		
Assay Category	Target	Method/Kit	Adipose	Bone	Brain	Heart	Intestine	Kidney	Liver	Skeletal Muscle	Skin	Vasculature	Liver Metastasis
	Beat Interval	Microscopy Video Quantification (MotionGUI)				х							
	Beat Rate	EarlyTox Cardiotoxicity Kit, Microscopy Video Quantification (Manual, MotionGUI)				х					1		
	Bile Efflux	Bile Efflux, Image Algorithm (UPDDI)							х				
	Collagen	Picrosirius Red Stain Kit (Polysciences: 24901-250)	х										
	Contractile Force	Force Transducer (Thorlabs)								х			
	Contraction Velocity	Microscopy Video Quantification (MotionGUI)				х							
	CYP3A4	P450-Glo CYP3A4 Assays (Promega: V9001)							х				
	Decay/Rise Ratio	EarlyTox Cardiotoxicity Kit (Molecular Devices: R8211)				х							
	Dextran-FITC (10kDa)	Fluorescence (490/525) (Sigma-Aldrich: FD10S)			х		х						
	E-Cadherin	anti-E-Cadherin							х				
Cell morphology/function	Fatty Acid	BODIPY 500/510 C1, C12 (ThermoFisher: D3823)	х										
centilor photogy/function	Glucose Uptake	Flow-through Biosensor B.LV5							х				
	Image	ICC/IFC (DAPI, FITC, Cy5), Live imaging, Phase Contrast							х				
	Lipid Droplets, Lipid to Nuclei Ratio	Lonza AdipoRed Assay Reagent (Lonza: PT-7009), Hoechst 33342	х										
	Maximum Elongation	Stimulation and Microscopy Video Quantification (1, 5, 10, or 20 Hz)								х			
	Neutral lipids	BODIPY 493/503 (ThermoFisher: D3922)	х										
	Relaxation Velocity	Microscopy Video Quantification (MotionGUI)				х							
	Steatosis (macro and micro)	HCS LipidTOX Red Neutral Lipid Stain (Thermo: H34476)							х				
	Transepithelial Electrical Resistance	EVOM2 Volt/Ohm Meter (WPI: 300523)					х						
	Tumor Area, Intensity	Protein Fluorescence (DAPI, Texas Red) with Quantification (ImageJ, AngioTool)										х	
	Tumor Integrated Intensity	mCherry 587/610											х
	Vessel Area, Length, Junctions	Protein Fluorescence (DAPI, Texas Red) with Quantification (ImageJ, AngioTool)										х	
	Cell Viability (Quantitative)	CellTiter-Glo Luminescent Cell Viability Assay (Promega: G7573)					х		х			х	
	Cellular Metabolism	MTT Assay Kits							х		х		
	Lactate Dehydrogenase	Multiple commercial kits	х	х	х			х	х		х		
Cell viability/proliferaton/toxicity	Live Cells / Dead Cells	LIVE/DEAD Cell Imaging Kits	х					х	х				
cen viability/promeratori/toxicity	Mitochondria	Fluorescence (490/525)							х				
	PrestoBlue	PrestoBlue Cell Viability (ThermoFisher: A13261, A13262)	х	х	х			х	х		х		
	Tumor Growth	Cell Proliferation Kit II (XTT) (Sigma: 11465015001)										х	
	WST-1	WST-1 Assay Reagent - Cell Proliferation (ready to use) (ab155902)											х
Compound Level	User define compound(s) of interest	RapidFire-MS, HPLC-MS, LC-MS/MS, ICP-MS, IM/MS		х	х	х	х	х	х		х		
Device Characterization	Flowrate	Flowrate (by setting, volume, or weight)						х	х				
Gene Expression	User defined gene(s) of interest	RT-PCR (Applied Biosystems: StepOnePlus and SYBR Green Reaction Mix)		x									
	Cytochrome C	CytC Biosensor, Image Algorithm	_	×					х				
Intracellular Biosensor	GCaMP6	Live Imaging Algorithm (FITC)	-						x	x			
	Luciferase Expression	ONE-Glo Luciferase Assay System (Promega: E6110, E6120, E6130)		x						^			
Protoin Dinding	· · · · · · · · · · · · · · · · · · ·												
Protein Binding	User defined compound of interest	Single-Use RED Plate with Inserts (Thermo Scientific: 2034.6) and ICP-MS		х				х	х				
	Alpha-fetoprotein	Human alpha-Fetoprotein DuoSet (R&D Systems: DY1369)		<u> </u>					х		-		
	Ammonium	Ammonia Assay Kit (abcam: ab83360)		<u> </u>				х			-		
	Blood Urea Nitrogen	BUN Liquid Reagent (Stanbio Laboratory: SB-0580-250)		<u> </u>					х				
Secreted Protein/Compound	Glucose	Amplex Red Glucose/Glucose Oxidase Assay Kit, Flow-through Biosensor B.LV5		<u> </u>					х		-		
Secreted Protein/Compound	Insulin Secretion	Insulin ELISA		<u> </u>					х		-		
	L-lactate User define protein(s) of interest	Flow-through Biosensor B.LV5 Human ELISA Kits from various vendors	x	x	×		x	x	x x				