### Deal with messy AMR data the clever way

Escape disconnected workflows with a novel digital laboratory infrastructure.

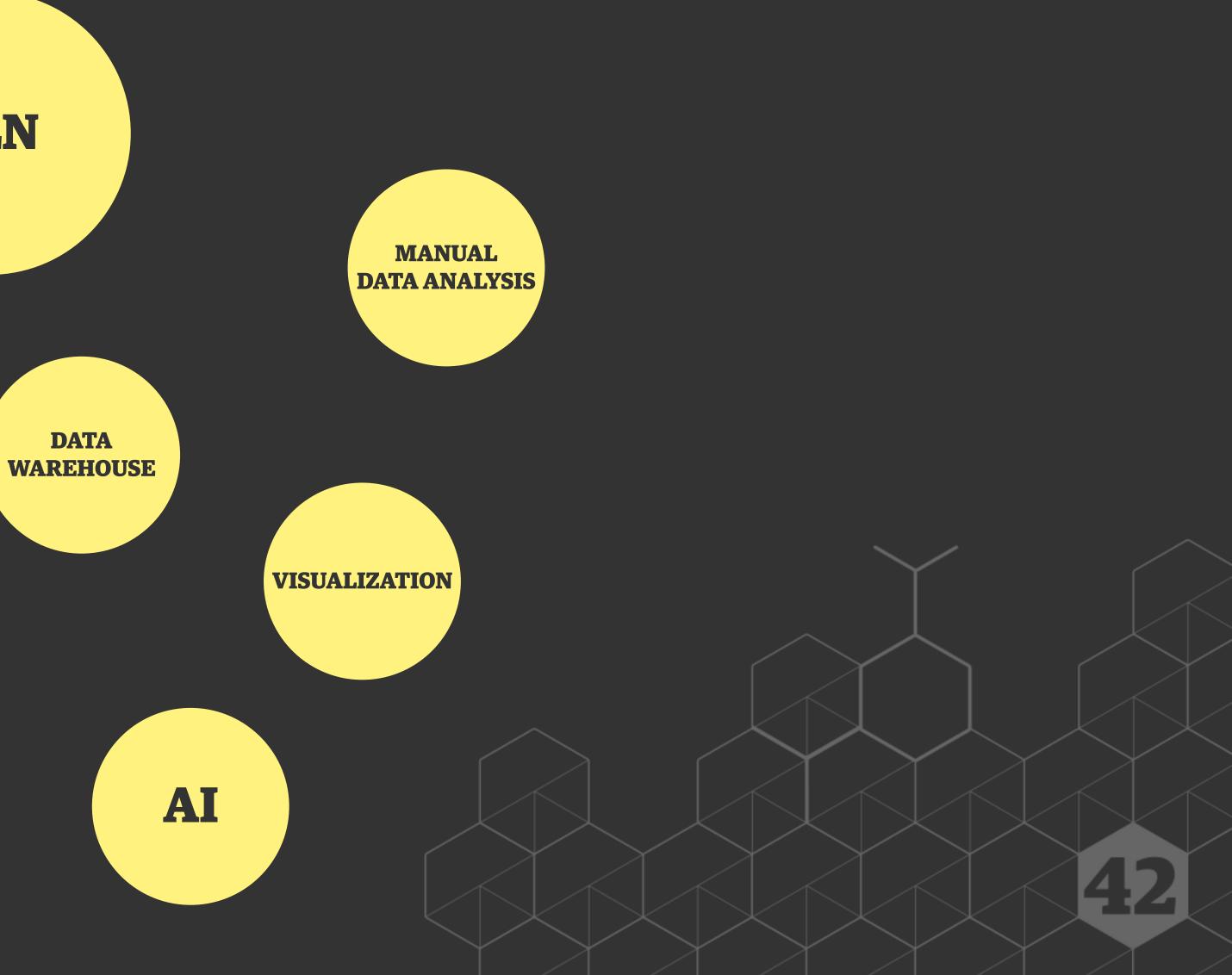
Copenhagen



### The research and lab software landscape

**ELN** 





"For Big-Data Scientists, spending upwards of 80% of their time doing 'janitor work' is the key hurdle to insights."

"76% of data scientists view data preparation as the least enjoyable part of their work."

- New York Times

"79% of data scientists said they spent most of their time collecting, cleaning, and organizing data sets."

- Forbes

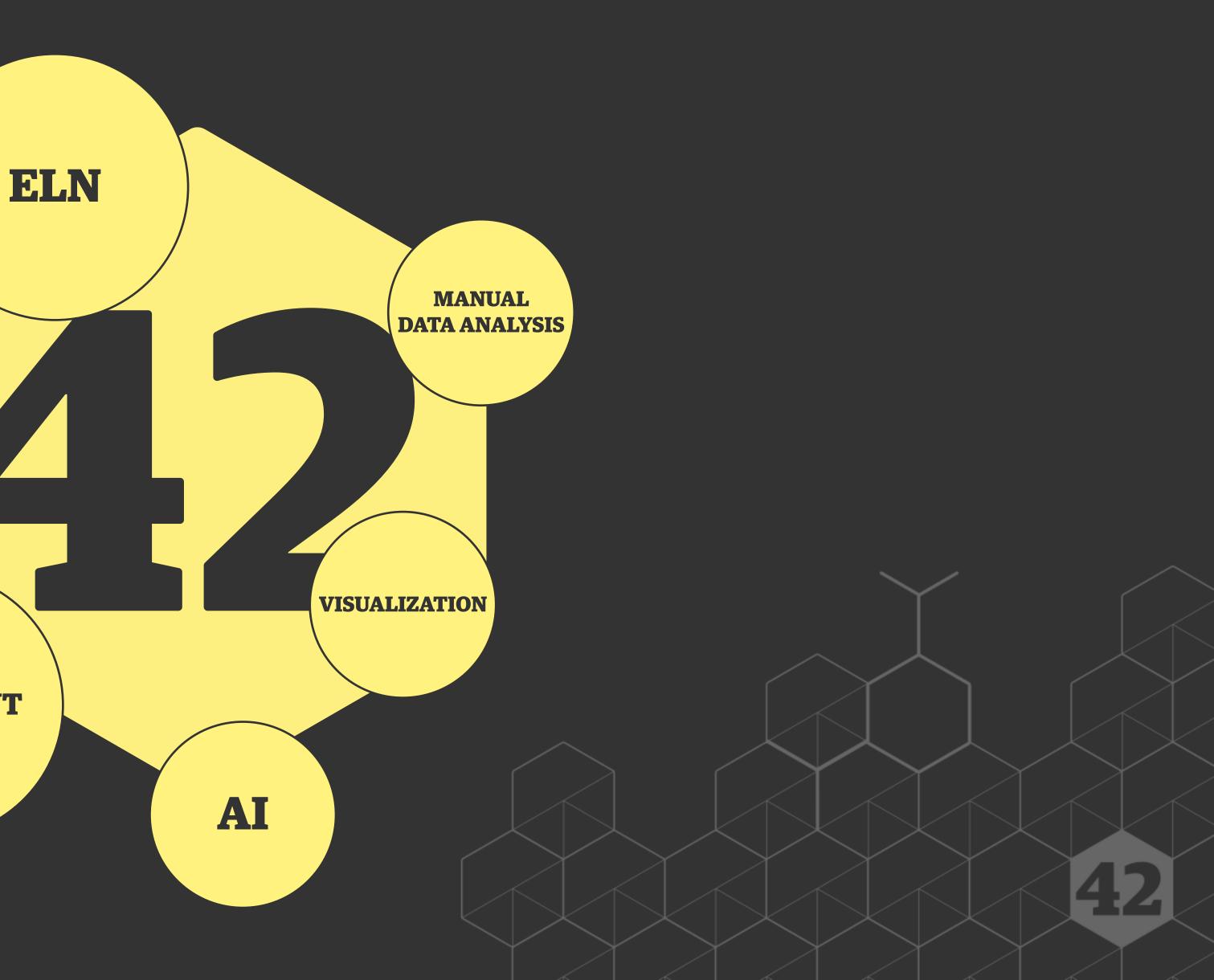
- Figure Eight





### Our take on research and lab informatics

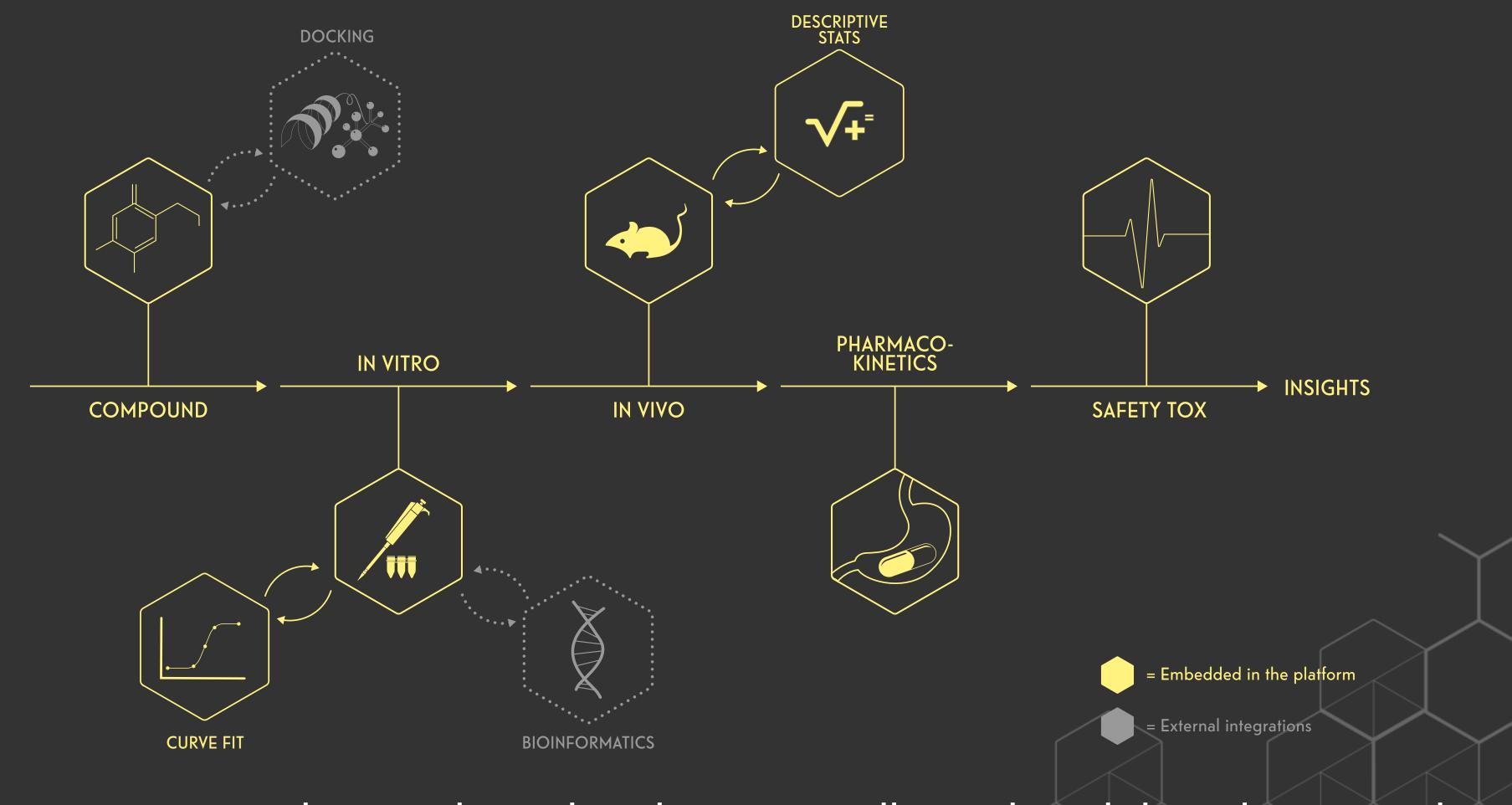
LAB EQUIPMENT DATA



### All types of data is captured close to the source, tagged, and stored on the platform



## The grit42 platform



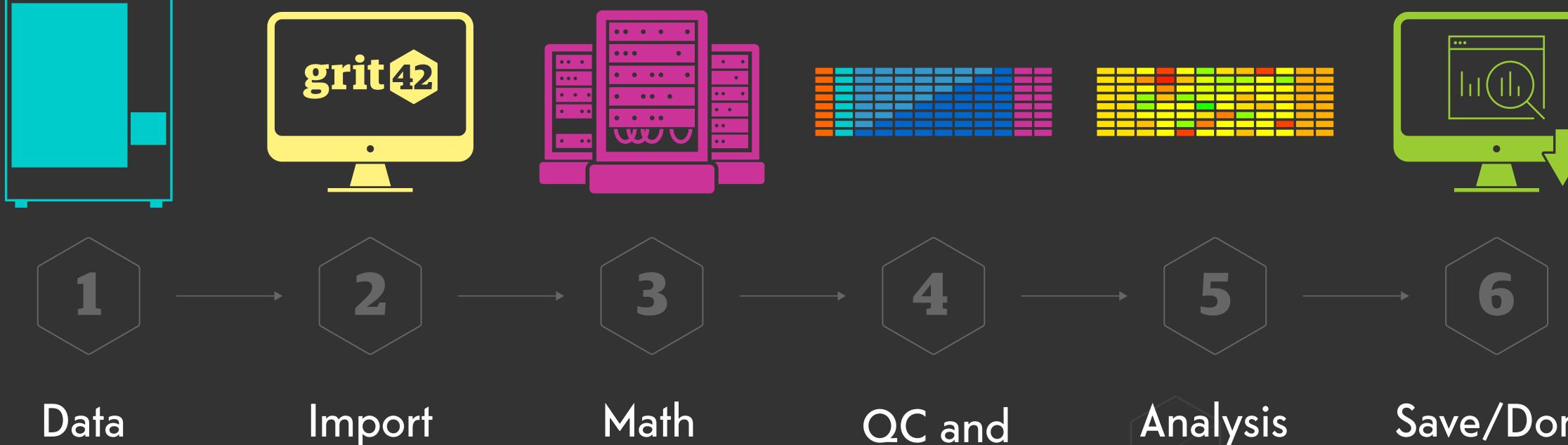
Capture, manage, analyse, and visualise data across all pre-clinical drug discovery phases



### I wish I could spend my day copying and pasting ...said no one ever



### A workflow example



#### QC and visualisation

Analysis

#### Save/Done



E COM	POUNDS SAR TAB	LES SETUP	S EXPERI	MENTS	LISTS ANIN	IALS BRO	WSE				<b>()</b>	zbb	v	grit 🔁
_001, P	M_002								Setup:	Phen	otype Microar	rayStatus:	Publis	hed for review
Data	Growth curves	Parameter	rs Detai	ls						Import	Export	Com	Ipare	Publish
		PM01 (Carbon	Sources) AU	ic	~ 🖌	Show Heatma	ap 📕 Subtract	Negative Con	trol					
Plate 个		01	02	03	04	05	06	07	08	09	10	11	12	
PM01 (Carb	on Sources) 🛛 🔒 A	1423.60	1651.55	3456.76	1003.35	4753.98	977.79	3227.16	4059.93	2627.35	1944.62	1690.85	2196.77	
PM01 (Carb	on Sources) B	1708.26	1227.41	3581.76	923.76	913.93	4666.13	1180.17	1475.94	4143.25	2309.23	3307.47	4485.94	
PMO2 (Carb	on Sources) C	1057.94	815.72	4728.86	1208.02	4227.92	834.99	2904.87	4015.34	4429.55	914.90	1051.03	1651.64	
PM02 (Carb	on Sources)	4575.75	786.97	735.10	1471.76	4523.65	4534.06	1822.88	667.66	1014.61	941.13	961.71	2089.86	
PMO3 (Nitro	gen Sources) E	4594.32	661.39	704.96	850.30	4265.86	681.02	1476.73	655.52	775.52	975.43	1059.31	2608.28	
PM03 (Nitro	gen Sources) F	1083.40	4773.65	463.66	570.90	4657.95	3861.08	3387.41	653.33	667.27	658.58	793.60	3734.81	
M04 (Phos	phorus and Su G	1108.64	494.98	1293.84	1142.71	2995.59	751.59	1180.72	755.00	2449.05	3292.46	978.04	5196.29	
MO4 (Phos	phorus and Su H	3948.88	3521.69	589.26	2967.22	657.51	831.71	680.92	3089.14	826.43	714.29	1023.85	3410.07	
M01 (Carb	on Sources) Baktus vs	s Karius												≡ **
hemical		01 02	03 04	05 06	07 08	09 10	11 12	01 (	02 03	04 05	06 07	08 09	10 11	12
Anennear	A	-25.98 -13.96 -	16.73 - 29.10 -	1.39 -14.55	-17.39 -14.20 -2	3.67 -14.57 -1	11.21 -10.76	^						
↑ (	В	-38.41 -31.40 -	10.72 - 19.82 -	18.25 -5.93 -	-23.85 0.16 -	8.46 -15.62 -1	12.18 -8.86	в						
% NaCl	c			-+-+	-31.25 -8.08 -	-+-+		د						
% Sodium F	D		-+-+	-+-+	-23.68 -24.83 -1	-+-+		•						
	-		-+-+	-++	-38.58 - 29.37 - 2	-+-+		E						
% Sodium L	· · · · · · · · · · · · · · · · · · ·	-+-+	-+-+	-+-+	-7.00 -28.85 -1	-+ +		F						
2-Propaneo		-++	-+-+		57.21 - 14.30 3	-+-+		G						
Thio-b-D-G	ilucose H	8.20 -7.76 -	9.01 -4.05 -	1.46 6.02	11.91 -20.16 -	7.07 -12.96	6.27 -12.17							

### We're combining data capture, scientific analyses, visualisations, and logistics



## Workflow example

grit42 platform	General data management,	SAR table
Compounds	In vitro	
Chemists	Plate readers	Lab
Drawing Meta data	Text files	Manı sr
	Curve fit	M (
Phys / chem parameters	Plate views	Anim
Structures	Curve plots	
	Submit values	Sub
SAR tables	Compounds / results / curves	Dose
	<b>Experiment app</b>	In vitro,
<b>Logistics</b> app	Sample and compound mana	gement.

les, and ordering.

#### In vivo

b observations

ually generated preadsheets

Maths / stats Group stats

nal / group data

Box plots

omit conclusion

es / compounds

DMPK

HPLC

Spreadsheets Instrument data export

Maths

Numeric values

Plots

Submit hypothesis

ds Earlier batches / compounds

, in vivo, and ex vivo + ADME analyses.

Animal handling app Animal management.

#### Discipline

Data production Raw data Algorithms Results Visualisation Conclude exp.

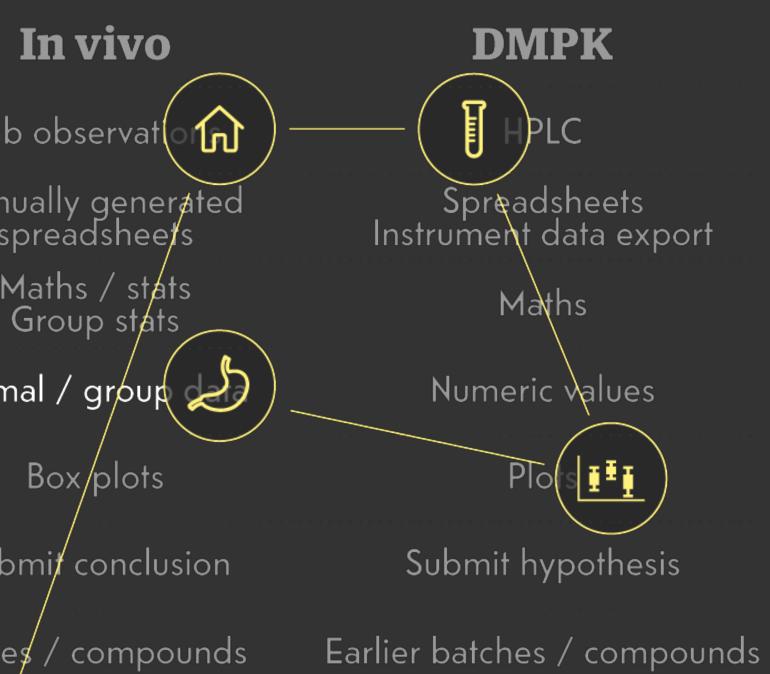
Compare to



### Workflow example

grit42 platform	General data management,	SAR tabl
Compounds	In vitro	
Chemists	Plate readers	Lab
Drawing Meta data	Text files	Manı sp
	Curve fit	M (
Phys / chem parameters	Plate views	Anim
Structura	Curve plots	
	Submit values	Sub
SAR tables	Compounds / results / curves	Dose /
	<b>Experiment app</b>	In vitrø,
		_
Logistics app	and compound mana	gement.

les, and ordering.



in vivo, and ex vivo + ADME analyses.

Animal handling app Animal management.

#### Discipline

Data production Raw data Algorithms Results Visualisation Conclude exp. Compare to









### The built-in advantage of defining roles and parameters for each assay

Copenhagen

SAS



### The roles of parameters

### Hypothesis roles

### Definition of roles

of - CFU's (dependent)

#### • Bacteria (subject) - gives - infection (predicate) - in - mouse (object)

#### Mouse (controlled) - infected with - bacteria (independent) - get's this level



# The intelligent way of searching using parameters

Copenhagen



### Filter - Text

Sele

Com

ium

	HOME	COMPOUNDS	SETUPS	EXPERIMENTS	LISTS	BROWSE		
Bı	rowse				© <sup>1</sup>	Filtor + New		
Sh	ow filter					Filter <b>Filter</b>		
S	Setup like Ir	עו⊗				Facets of yo	ur Searc	ch
	name							
	nVitro mu	ultipoint Bindin	g IFN (Exp	eriment)		Name:		C
		type 3a LS90876				Select filter		
		// type 3a LS78881				Animal (16)		(
		type 3b LS90876				Comment (16)		
	1163 HCV	type 1 LS90876				Compound (2	4)	t
	8963 HCV	type 6 LS90221				Donor (8)		
	1163 HCV	type 2 LS10001				Dose (24)		
	8963 HCV	type 3a LS90876 re	etest			Effect (16) IC50 (24)		
	2283 HCV	type 4 LS38546				Response (8)		
	nvivo For	ced Swimming	Test (Expe	riment)		catalyst (8)		
	N29200-9	6 Ec IR5 q3				compoundCV (1	.6)	
	N73788-9	6 Ec 5649 q3				textConst (8)		
	N31434-5	3 Kp VA384 q3						
	N73891-5	6 Pa 1484185 q3						
	N83764-6	8 Ec ALL q3						
	N92751-7	6 Ec ALL q3						
	N92751-7	6 Ec ALL q3 repeat						
	N815621-	71 Ec ATCC25922 c	16					
	N93456-4	4 Ec 5649 q1						

- .....

			admin	~	grit 42
					Clear A
e:	Hypotesis:	Experimenal:		Value:	
ïlter	Select filter	Select filter		Select filt	ier 🗸 🗸
ound (24) ric (24)	Object (24) Object variable (24)	CV (24) DV (24)			
(4)	Predicate (24)	IV (24)			
	Subject (24) Subject variable (24)	const (24)			



### Filter - Structure

	HOME	COMPOUNDS	SETUPS	EXPERIMENTS	LIS	TS	BROWSE		
B	rowse				$\bigcirc$	Filt	ers		
Sh	ıow filter					Fil	ter		
	Setup like Ir	עו⊗				Мо	lecule		) Exa
	name								) Sut
	nVitro mı	ultipoint Bindin	g IFN (Expe	eriment)					
	8963 HCV	type 3a LS90876				F	acets of y	our Se	arch
	8963 HCV	type 3a LS78881					,		
	8963 HCV	type 3b LS90876							
	1163 HCV	type 1 LS90876				Na	ame:		D
	8963 HCV	type 6 LS90221				s	elect filter		
	1163 HCV	type 2 LS10001							
	8963 HCV	type 3a LS90876 re	etest				nimal (16)	<b>`</b>	C
	2283 HCV	type 4 LS38546					omment (16) ompound (		г +
	nvivo For	ced Swimming	Test (Expe	riment)			nor (8)	(24)	U
	N29200-9	6 Ec IR5 q3					ose (24)		
	N73788-9	6 Ec 5649 q3					fect (16)		
	N31434-5	3 Kp VA384 q3				IC	50 (24)		
	N73891-5	6 Pa 1484185 q3				Re	sponse (8)		
	N83764-6	8 Ec ALL q3					talyst (8)		
	N92751-7	6 Ec ALL q3						(16)	
	N92751-7	6 Ec ALL q3 repeat				tex	(tConst (8)		
	N815621-	71 Ec ATCC25922 c	16						
	N93456-4	4 Ec 5649 q1							



admin 🗸 🗸



act	Apply	
ubstructure		

					Clear All
Data Type:	Hypotesis:	E	Experimenal:	Value:	
Select filter	Select filter		Select filter	Select filter	
Compound (24) numeric (24) text (24)	Object (24) Object variable (24) Predicate (24) Subject (24) Subject variable (24)	[ 	CV (24) DV (24) V (24) const (24)		



### Filter - Facet/Numeric

HOME COMPOUNDS SETUPS EXPERIMENTS LI	STS BROWSE						admin	~	grit4	2
Browse	Filters									
Show filter	Filter + New									
Setup like Inv 🛞	Facets of yo	ur Searc	h							
Smiles like c1ccccc1 🛞									Cle	ear All
	Name:		Data Type:		Hypotesis:	Experimenal:		Value:		
name	Select filter		Select filter		Select filter	Select filter		Selec	t filter	
InVitro multipoint Binding IFN (Experiment)	Dose (5)		numeric (5)		Predicate (5)	DV (5)				
8963 HCV type 3a LS90876	IC50 (5)				Subject variable (5)	IV (5)				
8963 HCV type 3b LS90876	Response (5)									
1163 HCV type 1 LS90876										
8963 HCV type 6 LS90221										
2283 HCV type 4 LS38546										
	> Greater than	Enter Numl	ber	٢						
	< Less than	Enter Numl		\$						



	HOME	COMPOUNDS	SETUPS	EXPERIMENTS	LIST	rs Bi	ROWSE		
B	rowse				$\bigotimes$	Filters			
Sł	now filter					Filter	+ New		
	Setup like In	ıv ⊗				Face	ets of yo	ur Sea	arch
	Smiles like o	clcccccl 🛞							
						Name:			
	name					Select	t filter		
	InVitro mu	ultipoint Bindir	ng IFN (Expe	eriment)		IC50 (3)			
	8963 HCV	type 3a LS90876							
	8963 HCV	type 3b LS90876							
	1163 HCV	type 1 LS90876							
						> Gr	eater than	75	
						< Le	ss than	102	

### Filter - Values

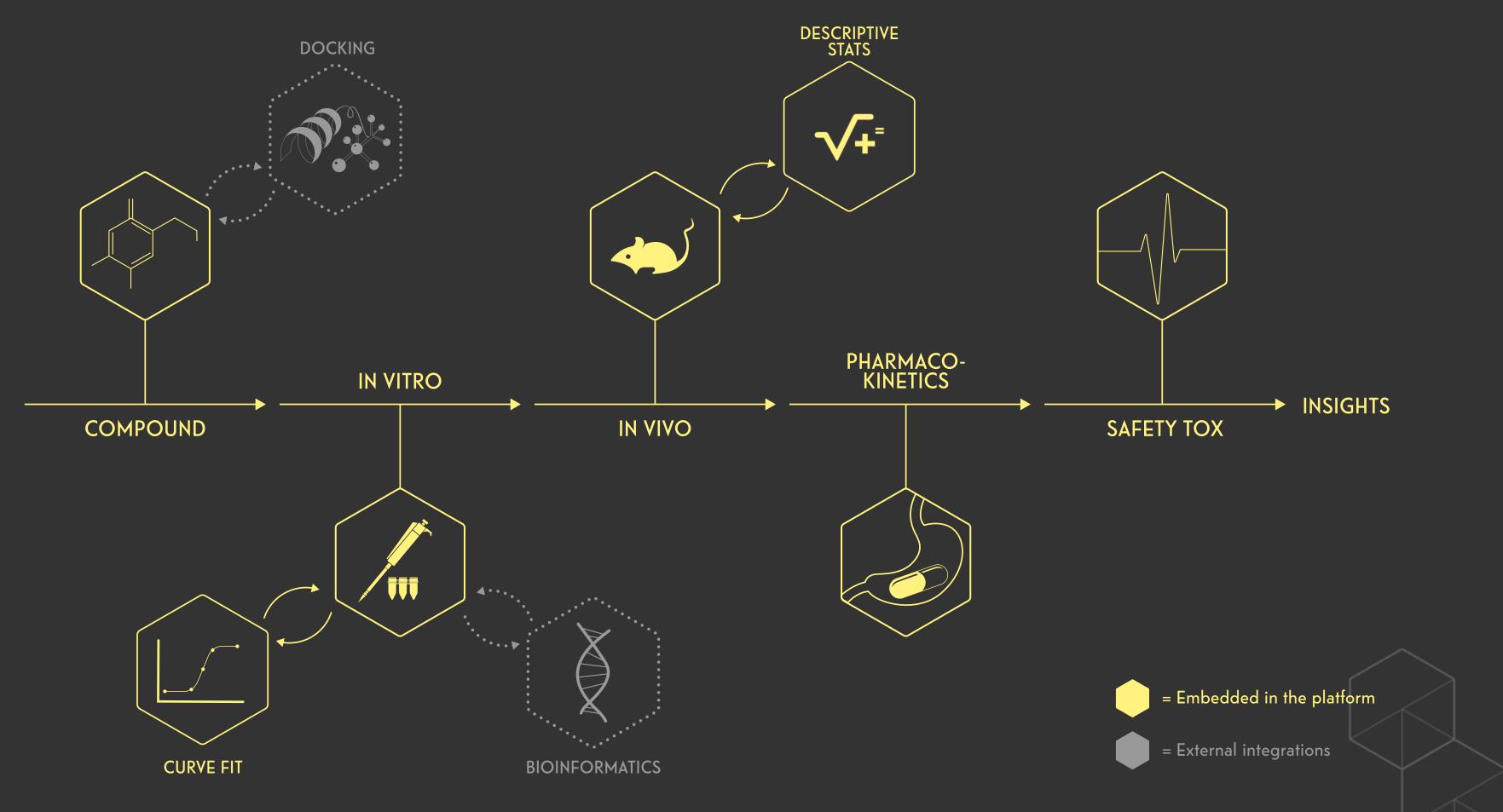
				admin	~ <b>g</b>	rit 42
						Clear All
ype:		Hypotesis:	Experimenal:		Value:	
t filter		Select filter	Select filter		Select filter	
		Predicate (3)	DV (3)			
	\$ \$					
	$\Diamond$					







### A dynamic platform that supports your digital lab infrastructure



It's all here. It's all integrated. And always ready for realtime analyses.



### The six major advantages of grit42

- 1. Data capture, scientific analyses, visualisations, and logistics the grit42 platform supports all your day-to-day workflows
- 2. Compare results across new and old datasets
- 3. Streamlined and replicable experiments across domains and departments
- 4. Perform advanced queries and faceted searches on your data
- 5. Perfect data structure to run advanced analyses, ie. artificial intelligence
- 6. All the data is inherently ready for RDF, graph analysis, FAIR, etc.



### Some of our customers









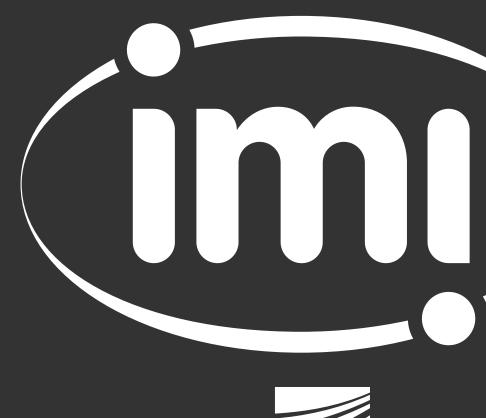


#### **DK**•**JPENSCREEN**

HELMHOLTZ ZENTRUM FÜR INFEKTIONSFORSCHUNG



# AMR-related collaborations ND4BB TRANSLOCATION





**Innovative Initiative** 

Fraunhofer

SANOFI

Johnson Johnson



# DONT PANIC

We offer a viable solution if you're tired of wasting your time on disconnected workflows and messy data

Copenhagen

