E. DRN Features

In order to ascertain what features users would want from a DRN, we collated together desired features from three different sources:

- **Survey Results**: We asked users several questions that could elicit desired features, including how technology could make their life easier, what features they would perceive to be the most important for a DRN, and the limitations and barriers they currently face.
- **User Stories**: As demonstrated in Section 2, part of the research for this case study was to produce a large number of storyboards and flows based on user roles and requirements. The features detailed in these were also extracted for the purpose of this exercise.
- **Mural Boards:** During the PSDI partner meetings, several Mural Boards were set up for collaborative use during the meetings for partners and team members to brainstorm about potential functionality and features. These features were also extracted from these different Mural Boards.

The full list of features have been categorised twice, into high level categories and sub categories. Table E. 1 shows the full breakdown of these features and their categories:

Table E. 1: Categorised list of features obtained from engagement activities

High Level Category	Feature Category	Feature
Coding Support	Coding	Code testing
Coding Support	Coding	Code to deal with data
Coding Support	Coding	Collaborative coding
Coding Support	Coding	Document Code
Coding Support	Coding	Record process of developing Code
Coding Support	Coding	Record process of developing model/simulation
Coding Support	Coding	Translation of interactive command-line testing of parameters into a script (including understanding 'delete last thing, it didn't work'), and script documentation generation suitable for users (topic-based, indexed) not just for developers.
Coding Support	Versioning	Establish version of DRN
Coding Support	Versioning	Version control
Collaboration & Management Features	Auditing	Audit Trails
Collaboration & Management Features	Auditing	Lock plans and risk assessments
Collaboration & Management Features	Auditing	Mark as audited
Collaboration & Management Features	Auditing	Moderation: review / approve / reject / rate all data/Code/plans/etc
Collaboration & Management Features	Auditing	Protect Intellectual Property rights
Collaboration & Management Features	Auditing	Reconfigure notebook to share when experiment is marked as complete/approved

Collaboration & Management Features	Auditing	Review and rate experiment
Collaboration & Management Features	Auditing	Review process / data for validity
Collaboration & Management Features	Auditing	See activity logs
Collaboration & Management Features	Auditing	See when notebook was last audited
Collaboration & Management Features	Auditing	Sign off entries
Collaboration & Management Features	Comments	Configurable comment capabilities
Collaboration & Management Features	Notifications	Configurable notifications for all changes
Collaboration & Management Features	Subscribe	Have sign up button for notebook
Collaboration & Management Features	Subscribe	Register interest in projects
Collaboration & Management Features	Subscribe	Subscribe to other researchers/notebooks/projects
Collaboration & Management Features	Team Management	Bulletin board / forum style space
Collaboration & Management Features	Team Management	Create a homepage for notebook
Collaboration & Management Features	Team Management	Message board
Collaboration & Management Features	Team Management	Page statistics
Collaboration & Management Features	Team Management	Plan allocation of capacity
Collaboration & Management Features	Team Management	Recent activity feed
Collaboration & Management Features	Team Management	See overview of research
Collaboration & Management Features	Team Management	Share an update on a notebook
Collaboration & Management Features	Team Management	Task Management
Collaboration & Management Features	Team Management	Team communication
Collaboration & Management Features	Team Management	Team homepage for information in the same place
Collaboration & Management Features	Team Management	Team leaders control data of group
Collaboration & Management Features	Team Management	Team notebooks
Collaboration & Management Features	Team Management	Track meetings and progress
Collaboration & Management Features	Team Management	View collaborators files

Customisation & Extension	Personalisable	Add own plugins
Customisation & Extension	Personalisable	Create user profiles
Customisation & Extension	Personalisable	Personalisable
Customisation & Extension	Personalisable	Tailor system to research domain / researcher
Data Features	API Access	API access to data
Data Features	Data Access	Authentication covers login, data permissions etc.
Data Features	Data Access	Data Access controls with different levels
Data Features	Data Access	See who is accessing data
Data Features	Data Conversion	Conversion tool
Data Features	Data Conversion	Data format converter
Data Features	Data Conversion	Data ingest processes
Data Features	Data Exchange	Data exchange platform
Data Features	Data Integration	Collate together experimental and simulation data
Data Features	Data Integration	Combine data across a team
Data Features	Data Integration	Combine data from multiple sources
Data Features	Data Integration	Easily combining data from multiple sources
Data Features	Data Management	Central database for output data
Data Features	Data Management	Create data management plan
Data Features	Data Management	Curation of existing data resources
Data Features	Data Management	Define data processing pipeline
Data Features	Data Management	Platform for recording and managing data
Data Features	Data Quality	Assurance on quality of data
Data Features	Data Quality	Criteria to categorise resource as trusted
Data Features	Data Quality	Quality check data
Data Features	Data Retention	Perserve data indefinitely
Data Features	Data Retention	Remove obsolete data offline / soft delete
Data Features	Data Retention	Store data for a specified period of time
Data Features	Data Security	Data Security
Data Features	Data Security	Secure storage, backup and archives
Data Features	Data Standards	Data provided in clear and accessible formats
Data Features	Data Standards	Enforce consistent standards.
Data Features	Data Standards	Ensure integrity of data and metadata
Data Features	Data Standards	Have a universal control and data output language
Data Features	Data Standards	Shim layers as a common interface
Data Features	Data Standards	Standardised file formats that work and everyone adheres to.
Data Features	Data Standards	Standardised methods of referring to chemicals
Data Features	Data Standards	Use domain standards

Data Features	Data Storage	Archive at the time of creation
Data Features	Data Storage	Archive Notebook
Data Features	Data Storage	Automatic saves
Data Features	Data Storage	Backup/archive
Data Features	Data Storage	Can handle large datasets
Data Features	Data Storage	Permanent storage options for data. Current limitation of storage providers, i.e. Google, Amazon, Dropbox, etc. is the issue that if you close or lose the account, access to previous uploads is also revoked -- can't refer to them for access to data in articles.
Data Features	Data Storage	Secure storage, backup and archives
Data Features	Data Support	Deal with all different stages of data (raw, cleaned, processed, analysed)
Data Features	Data Support	Download and utlise catalog data
Data Features	Data Support	Drag data from other resources into DRN
Data Features	Data Support	Include data from other software
Data Features	FAIR	Data curation for FAIR
Data Features	FAIR	Publishing FAIR data
Data Features	Identifiers	Link data on chemical identity
Data Features	Identifiers	Link data using standard identifiers
Data Features	Identifiers	Link to third party data through identifiers
Data Features	Identifiers	Link together experiments and samples and data through Unique IDs
Data Features	Identifiers	Researcher identification
Data Features	Identifiers	Unique ID for experiments
Data Features	Identifiers	Unique ID for samples
Data Features	Identifiers	Link data and interpretation
Data Features	Provenance	Display provenance of data
Data Features	Provenance	Provenance of structures
Data Features	Provenance	See algorithm/program used to produce data
Data Features	Provenance	See how datasets are reused
Data Features	Provenance	Tools to capture provenance
Domain Based Features	Chemical/Molecules	Automatic chemical recognition
Domain Based Features	Chemical/Molecules	Global database of chemical values
Domain Based Features	Chemical/Molecules	Handle reagents
Domain Based Features	Chemical/Molecules	Import reaction
Domain Based Features	Chemical/Molecules	Inbuilt understanding of molecules
Domain Based Features	Chemical/Molecules	Include material information
Domain Based Features	Chemical/Molecules	Standard list of instruments and reagents (remove instrument bits)
Domain Based Features	Chemical/Molecules	Table of contents for specific reaction schemes

Domain Features	Based	Default Lists	Create default values
Domain Features	Based	Default Lists	Global database of chemical values
Domain Features	Based	Default Lists	List of data resources
Domain Features	Based	Default Lists	Standard list of instruments and reagents (remove instrument bits)
Domain Features	Based	Equipment Interface	Automatically capture data from instrument and upload to experiment
Domain Features	Based	Equipment Interface	Full availability of all sources, from firmware upwards for all devices and full open hardware
Domain Features	Based	Equipment Interface	Interface with equipment
Domain Features	Based	Equipment Interface	Link to instrument descriptions to view instructions
Domain Features	Based	Equipment Interface	Link to instruments
Domain Features	Based	Equipment Interface	Provide list of available equipment
Domain Features	Based	Equipment Interface	Remote control of instruments
Domain Features	Based	Equipment Interface	Standard list of instruments and reagents (remove reagents bit)
Domain Features	Based	Experiment Planning / Recording	Add dates to experiments
Domain Features	Based	Experiment Planning / Recording	Add titles to experiments
Domain Features	Based	Experiment Planning / Recording	Capture experiment conditions
Domain Features	Based	Experiment Planning / Recording	Copy and modify plan
Domain Features	Based	Experiment Planning / Recording	Create experiment plan
Domain Features	Based	Experiment Planning / Recording	Facilitate different experiments
Domain Features	Based	Experiment Planning / Recording	Keeping track of what environments and simulation parameters I've used for what results
Domain Features	Based	Experiment Planning / Recording	Mark experiments as completed
Domain Features	Based	Experiment Planning / Recording	Protocols

Domain Features	Based	Experiment Planning / Recording	Provide full environment details for data generation
Domain Features	Based	Experiment Planning / Recording	Record experiment at each stage
Domain Features	Based	Experiment Planning / Recording	Record experiment conditions
Domain Features	Based	Experiment Planning / Recording	Record observations
Domain Features	Based	Experiment Planning / Recording	ReCreate experimental conditions for verification
Domain Features	Based	Experiment Planning / Recording	Show experiment status
Domain Features	Based	Health & Safety	Add safety information
Domain Features	Based	Health & Safety	Automatically flag hazardous chemicals
Domain Features	Based	Health & Safety	Automatically populate experiment record with risk assessment info
Domain Features	Based	Health & Safety	Create risk phrase vocabulary
Domain Features	Based	Health & Safety	Flag dangerous chemicals
Domain Features	Based	Health & Safety	Index of COSHH materials
Domain Features	Based	Health & Safety	Link to safety information
Domain Features	Based	Health & Safety	Review safety information
Domain Features	Based	Health & Safety	Risk assessment inclusion
Domain Features	Based	LIMS/ELN	Link to Chemical Inventory Website
Domain Features	Based	LIMS/ELN	Link to ELN
Domain Features	Based	LIMS/ELN	Link to LIMS
Domain Features	Based	LIMS/ELN	Link to materials inventory system
Domain Features	Based	Link to domain-based databases	Link to domain databases
Domain Features	Based	Link to domain-based databases	Automatically link to external chemistry resources
Domain Features	Based	Link to domain-based software	Link to domain software

Domain Based Features	Link to domain-based software	Interface between notebook and domain software
Domain Based Features	Link to domain-based software	Interface with chemspider
Domain Based Features	Link to domain-based software	Link to ChemDraw
Domain Based Features	Link to domain-based software	Link to SciFinder
Generic Features	API Access	API / CMD access
Generic Features	Automation Capabilities	Update links
Generic Features	Automation Capabilities	Automate deletion of files of data that should not be published because of errors (e.g. in input).
Generic Features	Automation Capabilities	Automatic data cleaning/detecting faulty data
Generic Features	Automation Capabilities	Automatic processing and formatting
Generic Features	Automation Capabilities	Automatic updates of DRN
Generic Features	Automation Capabilities	Automation of routine tasks.
Generic Features	Automation Capabilities	Capture exploratory analysis Automatically
Generic Features	Automation Capabilities	Dropbox-esque features (automatic data update)
Generic Features	Automation Capabilities	Extract metadata associated with research data
Generic Features	General	Access planning, notes, data and analysis in one place
Generic Features	General	Easy to use systems that play well with one another
Generic Features	General	Interoperable services
Generic Features	General	Scalable
Generic Features	General	Simple to install
Generic Features	General	Simple to use
Generic Features	General	Simplified login (without multiple passwords)
Generic Features	General	Straightforward and transparent processes
Generic Features	General	User centric design
Generic Features	GUI	GUI access
Generic Features	Localisation	Language support
Generic Features	Localisation	See dates in appropriate timezones
Generic Features	Remote Access	Access from all locations
Generic Features	Remote Access	Access on low bandwidth systems
Generic Features	Remote Access	Remote desktop access to systems
Generic Features	Remote Access	synchronise across multiple devices
Generic Features	Remote Access	Use DRN offline
Generic Features	Synchronisation	Open several things simultaneously
Generic Features	Synchronisation	Upload large numbers of files simultaneously
Generic Features	Synchronisation	View multiple data/notes from different experiments

Metadata, Semantics & AI	AI Tools / Integration	Analyse Data
Metadata, Semantics & AI	AI Tools / Integration	Input search data into AI/ML workflows
Metadata, Semantics & AI	AI Tools / Integration	Provide large datasets for ML use
Metadata, Semantics & AI	AI Tools / Integration	Redirect AI from producing better models to do some of the heavy lifting in data wrangling
Metadata, Semantics & AI	AI Tools / Integration	Smoother integration of ml packages with existing data.
Metadata, Semantics & AI	AI Tools / Integration	Store ML training data
Metadata, Semantics & AI	Metadata	Automated metadata creation & extraction (e.g. instrument settings, Code parameters, timestamps)
Metadata, Semantics & AI	Metadata	Domain and general metadata
Metadata, Semantics & AI	Metadata	Experiment metadata
Metadata, Semantics & AI	Metadata	Extract metadata associated with research data
Metadata, Semantics & AI	Metadata	Hierarchical metadata
Metadata, Semantics & AI	Metadata	Metadata collection at source
Metadata, Semantics & AI	Metadata	Metadata for samples
Metadata, Semantics & AI	Metadata	Metadata in structured form
Metadata, Semantics & AI	Metadata	Metadata knowledge graph
Metadata, Semantics & AI	Metadata	Prepopulate metadata with specific vocabulary or predefined metadata schema
Metadata, Semantics & AI	Metadata	Standard metadata and headers to data
Metadata, Semantics & AI	Metadata	Store metadata
Metadata, Semantics & AI	Metadata	Structure as required metadata (where appropriate)
Metadata, Semantics & AI	Metadata	Support variety of metadata formats
Metadata, Semantics & AI	Metadata	View others metadata in tag cloud
Metadata, Semantics & AI	Semantics	Advanced Semantic Search (Filtered Search)
Metadata, Semantics & AI	Semantics	Automatically link together related experiments
Metadata, Semantics & AI	Semantics	Coherent standardisation of semantisation of materials data and processes to reach interoperability especially across data from electronic atomistic and mesoscopic scales experiments and simulations.

Metadata, Semantics & AI	Semantics	Inferences for similar projects
Metadata, Semantics & AI	Semantics	Inferences for the same molecules of reactions
Metadata, Semantics & AI	Semantics	Link everything together for me
Metadata, Semantics & AI	Semantics	Link files / images / data
Metadata, Semantics & AI	Semantics	Link raw, intermediate and analysed data
Metadata, Semantics & AI	Semantics	Link related notebooks
Metadata, Semantics & AI	Semantics	Link to measurement vocabularies
Metadata, Semantics & AI	Semantics	Link to ontologies
Metadata, Semantics & AI	Semantics	More semantics. An easily searchable keywords lookup tool, that records the semantic meaning of the selected keywords. This would enable joined up research, without requiring researchers to understand ontologies. This should be used when publishing papers in addition to data, so it is easier to identify appropriate papers and data.
Metadata, Semantics & AI	Semantics	Ontology driven workflows
Metadata, Semantics & AI	Semantics	Prepopulate DRN with vocabulary or link to information system so links are Created
Metadata, Semantics & AI	Semantics	Semantic annotations
Metadata, Semantics & AI	Semantics	Tag / classify experiments
Metadata, Semantics & AI	Semantics	Tag / classify notes
Metadata, Semantics & AI	Templates	Create and use templates (public and private)
Metadata, Semantics & AI	Templates	Create flows from a list of standard components
Metadata, Semantics & AI	Templates	Use and Reuse stored models
Notebooking Features	Content support	Annotations and highlights
Notebooking Features	Content support	Audio files
Notebooking Features	Content support	Automatic handwriting recognition
Notebooking Features	Content support	Bar Codes/QR Codes for sample / experiment
Notebooking Features	Content support	Calculations / Formulas / Equations
Notebooking Features	Content support	Checklist with links
Notebooking Features	Content support	Copy sketches into notebook
Notebooking Features	Content support	Data/resources open in correct software
Notebooking Features	Content support	Facilitate sketches and drawing
Notebooking Features	Content support	Facilitate tables
Notebooking Features	Content support	Free text entry

Notebooking Features	Content support	Graph display of data
Notebooking Features	Content support	Handwritten notes
Notebooking Features	Content support	Import literature source
Notebooking Features	Content support	Include reaction scheme
Notebooking Features	Content support	Include structural representations (2D and 3D)
Notebooking Features	Content support	Integrate / store: Excel, Word, PDFs, Pictures,
Notebooking Features	Content support	Numerical entry
Notebooking Features	Content support	Photos / images
Notebooking Features	Content support	Postit notes
Notebooking Features	Content support	Record timings
Notebooking Features	Content support	Support complex images (giga-pixel, z-stacked, hyperspectral imaging)
Notebooking Features	Content support	Support obsolete file formats (future/past proofing)
Notebooking Features	Content support	Text recognition
Notebooking Features	Content support	Thumbnails of documents, graphs etc.
Notebooking Features	Content support	Timelines
Notebooking Features	Content support	TODO Lists
Notebooking Features	Content support	Videos
Notebooking Features	Interaction / Access	As easy to write in as a paper notebook
Notebooking Features	Interaction / Access	Both human and machine access
Notebooking Features	Interaction / Access	Digital pen integration
Notebooking Features	Interaction / Access	Hands free/voice control
Notebooking Features	Interaction / Access	Tablet/Smartphone compliant
Notebooking Features	Interaction / Access	Usable in the lab like a paper notebook
Notebooking Features	Interaction / Access	Voice Capture
Notebooking Features	Interaction / Access	Web based/Platform Independent
Notebooking Features	Link to other files	Link to Code
Notebooking Features	Link to other files	Link to data from other sources
Notebooking Features	Link to other files	Link to external dataset
Notebooking Features	Link to other files	Link to other experiments
Notebooking Features	Organisation / Reconfiguration	Contents Table / Overview Screen
Notebooking Features	Organisation / Reconfiguration	Group together team members and notebooks by topic
Notebooking Features	Organisation / Reconfiguration	Re-orderable list of work
Notebooking Features	Organisation / Reconfiguration	Timeline of experiments / studies by team/project/researcher/topic
Notebooking Features	Organisation / Reconfiguration	View experiments in last edited order

Notebooking Features	Paper Integration	Digitise paper based legacy data
Notebooking Features	Paper Integration	Handwritten notes
Notebooking Features	Paper Integration	Link with paper notebooks
Notebooking Features	Paper Integration	Scan in documents
Notebooking Features	Paper Integration	Transform/migrate digital legacy data
Notebooking Features	Referencing & Literature	Access to reference quality data
Notebooking Features	Referencing & Literature	Add Code citations
Notebooking Features	Referencing & Literature	Add data citations
Notebooking Features	Referencing & Literature	Easy access to published work
Notebooking Features	Referencing & Literature	Export literature references from notebooks for use in formal report
Notebooking Features	Referencing & Literature	Extract data Automatically from legacy literature
Notebooking Features	Referencing & Literature	Import literature source
Notebooking Features	Referencing & Literature	Journal article links
Notebooking Features	Referencing & Literature	Link to reference managers
Notebooking Features	Referencing & Literature	Link to reference managers
Notebooking Features	Referencing & Literature	Share literature resource
Notebooking Features	Referencing & Literature	Store and view literature sources
Notebooking Features	Referencing & Literature	Suggested citations
Notebooking Features	Word Processing	Cut and paste between windows
Notebooking Features	Word Processing	Smart cut and paste (e.g. matching field names)
Notebooking Features	Word Processing	Spell Checker
Notebooking Features	Word Processing	Word processing
Notebooking Features	Word Processing	WYSIWIG Editor for notes
Publishing & Sharing Features	Documentation & Instructions	Create instructions
Publishing & Sharing Features	Documentation & Instructions	Documentation for techniques
Publishing & Sharing Features	Documentation & Instructions	Share instructions
Publishing & Sharing Features	Documentation & Instructions	User documentation
Publishing & Sharing Features	DOIs	DOI generation / permanent links for data

Publishing & Sharing Features	Export	Common data standards for import/export
Publishing & Sharing Features	Export	Downloads/Printing
Publishing & Sharing Features	Export	Export all components of work (e.g. data, Code, graphics)
Publishing & Sharing Features	Export	Export data to chemspider
Publishing & Sharing Features	Export	Export full notebook
Publishing & Sharing Features	Export	Export in multiple formats
Publishing & Sharing Features	Export	Export literature references from notebooks for use in formal report
Publishing & Sharing Features	Export	Export structures in compatible file formats
Publishing & Sharing Features	Export	Migration tools
Publishing & Sharing Features	Export	Export thesis
Publishing & Sharing Features	Licensing	Create Code licenses
Publishing & Sharing Features	Licensing	Create data licenses
Publishing & Sharing Features	Open Access	Default model for making data open once published
Publishing & Sharing Features	Open Access	Free scientific articles
Publishing & Sharing Features	Open Access	Use open source software (where possible)
Publishing & Sharing Features	Open Access	Lower Costs
Publishing & Sharing Features	Publishing	Create package of notes/data/Code
Publishing & Sharing Features	Publishing	Generate report button
Publishing & Sharing Features	Publishing	Methods for publishing data
Publishing & Sharing Features	Publishing	Produce paper publication
Publishing & Sharing Features	Publishing	Thesis generation button
Publishing & Sharing Features	Publishing	View reports
Publishing & Sharing Features	Publishing	Write report
Publishing & Sharing Features	Repositories	Download data from repository
Publishing & Sharing Features	Repositories	Find add and run Code from online repository

Publishing & Sharing Features	Repositories	Upload Code to repository
Publishing & Sharing Features	Repositories	Upload data to repository
Publishing & Sharing Features	Repositories	Upload notebooks to repository
Publishing & Sharing Features	Researcher Attribution	Attribution for combined datasets
Publishing & Sharing Features	Researcher Attribution	Recognition of researcher contribution to data
Publishing & Sharing Features	Sharing	Established data sharing expectations / policies
Publishing & Sharing Features	Sharing	Share data for reuse
Publishing & Sharing Features	Sharing	Share draft data with collaborators
Publishing & Sharing Features	Sharing	Share plan
Publishing & Sharing Features	Sharing	Share with other institutions
Publishing & Sharing Features	Sharing	Share work with collaborators
Publishing & Sharing Features	Sharing	Shareable files
Publishing & Sharing Features	Sharing	Shared electronic notebooks
Publishing & Sharing Features	Sharing	Shared files / notebooks
Publishing & Sharing Features	Sharing	Sharing and accessing large data
Publishing & Sharing Features	Social Media	Integrate with Social Media
Searching	Characteristics Search	Find datasets with specific characteristics
Searching	Domain Search	Making it easier to locate the necessary information and source on studied materials.
Searching	Domain Search	Search by structure
Searching	Domain Search	Search experiment protocols
Searching	Domain Search	Searches include reaction schemes
Searching	Indexing	Indexable
Searching	Indexing	Make things easier to find.
Searching	Indexing	Uniformity of interfaces to data bases and easily accessible search engines for extracting data.
Searching	Keyword/Concept Search via Content Types	Describe datasets to enable searching
Searching	Keyword/Concept Search via Content Types	Find context for the work

Searching	Keyword/Concept Search via Content Types	Keyword Search
Searching	Literature Search	Literature search
Searching	Notebook Search	Search notebook discussion forum
Searching	Notebook Search	Search through previous documents of a project
Searching	Notebook Search	Searchable data across all notebooks
Searching	Similarity Search	Search for similar data
Searching	Similarity Search	See related content upon click
Searching	Visual Search	Search by image
Searching	Visual Search	Search graphs (visual)
Training & User Support	Training	Training
Training & User Support	User Documentation	User Documentation