

Arxspan Workflow: Changing the way scientists can work

May 2019

Arxspan- ChemAxon Partnership

Reaction

Upload Reaction

Download Reaction

Overview

Name	Molecular Weight	Molarity/Density	Moles	Mass/Volume	Equivalents	LIMIT
ethyl (3R,4S,5R)-3,4,5-	202.206		2.8 mmol	566 mg		<input type="checkbox"/>
pentan-3-one	86.134		1.4 mmol	120 mg	1	<input checked="" type="checkbox"/>
ethyl (3aR,7R,7aS)-2,2-	270.325				1	

Properties

- Activity
- Activity Class
- Aggregation Pattern
- Alert
- Alerts All Categories
- Alerts All Sources
- Alerts
- Alerts Test
- Alerts Test 2
- Alerts ID Source
- Alerts Image
- Alerts Relationship
- Alerts Source
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Draw a Structure: Substructure Search

Advanced Filters | Make New Chart

Marvin JS
by ChemAxon

Stereochemistry:

Target Therapeutic Area:

Area:

Scientist:

Synonym:

CAS Number:

Request Date:

Project:

Arxspan is now part of Bruker BioSpin



BILLERICA, Mass. - March 14, 2019 - Bruker Corporation (Nasdaq: BRKR) today announced that it has acquired Arxspan LLC, a provider of cloud-based scientific software and workflow solutions, based in Southborough, Massachusetts. Arxspan is known for its line of cloud-based products for the management of research data under the Arxlab® brand. The company has a focus on serving pharmaceutical and biopharma customers. Financial details of the transaction were not disclosed.

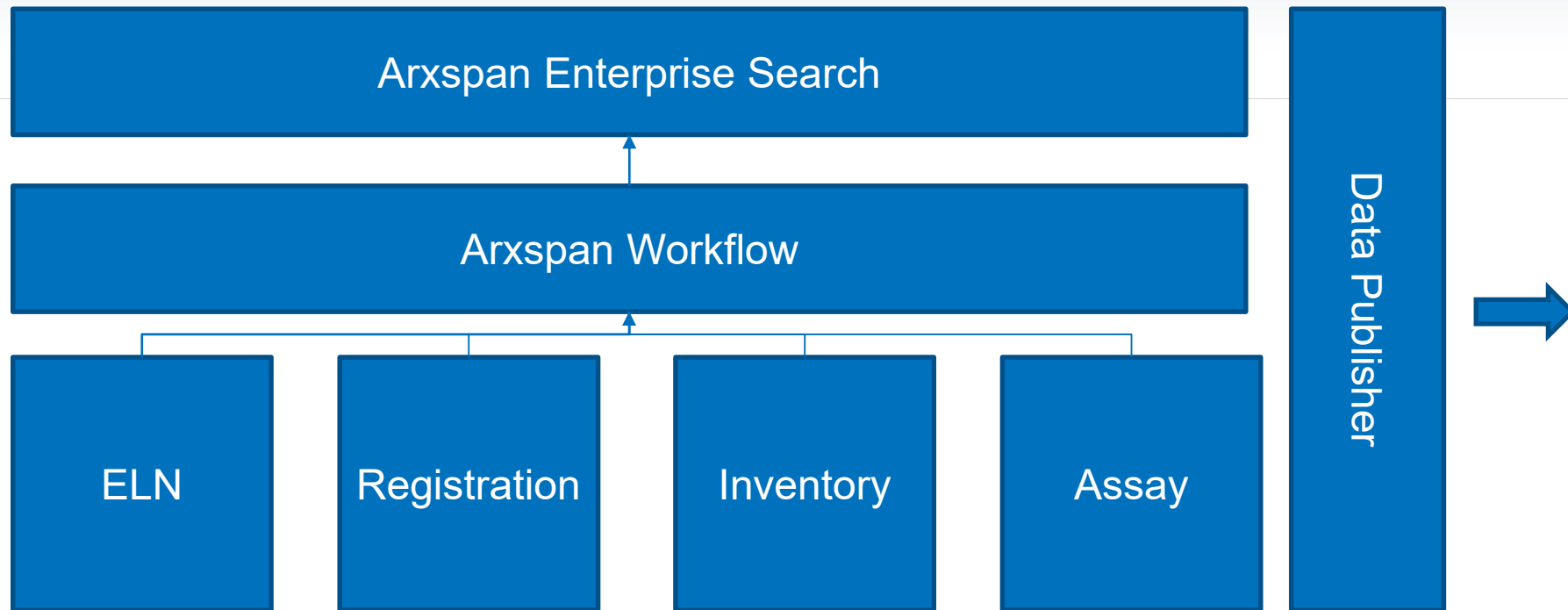
Bruker can now provide a range of software tools for customers in the chemistry, pharmaceutical, biopharma and analytical laboratory markets. Together with the Mestrelab strategic partnership and majority investment, the acquisition of Arxspan will allow Bruker to offer state-of-the-art chemistry and biopharma software tools, supporting discovery and development.

Commenting on the acquisition, Dr. Falko Busse, Group President for Bruker Biospin, stated: "The Arxspan acquisition, coupled with our strategic partnership with Mestrelab, positions Bruker firmly in the field of cloud-based, scientific software for our chemistry and pharma customers. Bruker is committed to providing intuitive end-to-end solutions that make analysis and knowledge extraction in scientific research faster and easier. Our new software solutions enable our biopharma customers to increase their productivity in drug discovery and development

Benefits of Workflow

1. To provide a single solution for the creation of work requests and work execution
2. Allow Users and administrators to configure complete scientific workflows
3. Greatly reduce the number of interfaces researchers are required to navigate daily
4. Simplify working with external collaborators
5. Provide customers a means to completely customize the ELN

Arxspan Enterprise Platform



Workflow Configuration



Dropdown Name
Levels

Dropdown Header Text
Levels

Dropdown Masking

Dropdown Options

+ New Option

Option Name	Disabled	Masking	Group Name	Mask Value
Area 10	<input type="checkbox"/>	<input type="checkbox"/>	Area 10	
Area 9	<input type="checkbox"/>	<input type="checkbox"/>	ChemPartner	
Area 8	<input type="checkbox"/>	<input type="checkbox"/>	External Collaborator	
Area 7	<input type="checkbox"/>	<input type="checkbox"/>	WHSite	
Area 6	<input type="checkbox"/>	<input type="checkbox"/>	WorkflowManagers	
Area 5	<input type="checkbox"/>	<input type="checkbox"/>		
Area 4	<input type="checkbox"/>	<input type="checkbox"/>		
Area 3	<input type="checkbox"/>	<input type="checkbox"/>		
Area 2	<input type="checkbox"/>	<input type="checkbox"/>		
Area 1	<input type="checkbox"/>	<input type="checkbox"/>		

Submit Cancel

Define Data Dictionaries

Number of Frozen Columns in Table
0

Fields

+ Add Field

Default Level
Company Group User

Field	Field Group	Include in Manage Requests	Manage	Sorting
Project Name		<input type="checkbox"/>	Edit	
Project Notebook		<input type="checkbox"/>	Edit	
Partner		<input type="checkbox"/>	Edit	
Status		<input type="checkbox"/>	Edit	
Date Requested		<input type="checkbox"/>	Edit	
Date completed		<input type="checkbox"/>	Edit	
Waybill No		<input type="checkbox"/>	Edit	
Shipping Status		<input type="checkbox"/>	Edit	
Shipping Date		<input type="checkbox"/>	Edit	
Date received		<input type="checkbox"/>	Edit	
Carrier Tracking No		<input type="checkbox"/>	Edit	
Final Report		<input type="checkbox"/>	Edit	
Request Notes		<input type="checkbox"/>	Edit	

Request Item Type(s)

+ Add Request Item Type

Request Item Type	Custom Name	Minimum # of Items	Delete items when editing
Compound UC2	Compound UC2	0	<input type="checkbox"/>

Disabled

Submit Cancel

Add them to forms

Workflow

Name	Date Type	Status	Use Date
Area 10	Area 10	Area 10	Area 10
Area 9	Area 9	Area 9	Area 9
Area 8	Area 8	Area 8	Area 8
Area 7	Area 7	Area 7	Area 7
Area 6	Area 6	Area 6	Area 6
Area 5	Area 5	Area 5	Area 5
Area 4	Area 4	Area 4	Area 4
Area 3	Area 3	Area 3	Area 3
Area 2	Area 2	Area 2	Area 2
Area 1	Area 1	Area 1	Area 1

Configure fields

Workflow Configuration



Allowed Users

	Can Add	Can View	Can Edit	Can Delete
Kate Hardy	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Jeff Carter	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Joe Demo	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Erwin Schrodinger	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Jane Biologist	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Anspan Support	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Bill Russo	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

Allowed Groups

	Can Add	Can View	Can Edit	Can Delete
Apollo	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>
ChemPartner	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
External Collaborator	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
HRPilot	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Workflow Managers	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
WuXi	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

- Restrict Access
- Prioritize After Submission
- Search Registration For Compounds
- Register New Compounds
- Check If Structure Is Requested Before Registering

Default Value

Target Dependencies

Source Value	Target	Target Values	Delete
Syngene	Status	<input checked="" type="checkbox"/> On hold <input checked="" type="checkbox"/> Completed <input type="checkbox"/> Dropped <input type="checkbox"/> Running	Delete
Pharmaron	Status	<input type="checkbox"/> On hold <input type="checkbox"/> Completed <input checked="" type="checkbox"/> Dropped <input checked="" type="checkbox"/> Running	Delete

Allowed Users

- Anspan Support
- Bill Russo
- ChemPartner User
- Chris Forbes
- David Farrell

Allowed Groups

- Apollo
- ChemPartner
- External Collaborator
- HRPilot
- Workflow Managers

Allowed Applications

ELN	Workflow	Assay	Registration	Inventory
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

COMPOUND REQUEST NOTIFICATIONS

Notification Editor

Who	Event Type	Element	Tool Used	Field	Email	Post Notification	Browser
Bill Russo	Update	Request Type (enr-req)	Status		<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
User: UserFunction							

Page 1 of 1

Set Permissions
at the field

Or Form level

Set notifications at create,
edit or completion

Workflow Use cases



Compound Request Template

Complete the Required Fields

Configure the Loading Template

Upload data

Status: Queue

Sourcing date: 05/17/2019

Internal Chem: Partially

Project Notebook

Request Purpose: SAR Build Out

Attachments: Drop files to upload or browse for a file. Choose File Literature Reference.pdf

Project Name

Compound

UPLOAD FILE: compoundRequest.sdf

Show 25 entries

Priority	Structure*	hemistry*	Amount requested (g)*	Number of steps*	Purity requested (%)*	Compound type*	Destination*
1		hemistry	120	4	100	Final Compound	Ship
		hemistry	80	4	100	Intermediate	
		hemistry	100	4	100		

Excel Data:

	B	C	D	E	F	G
1	Body Mass (mg)	MCV	RBC	MCHC	RDW	REGID
2	MD-610829	20.2	42	1106	32	10 APR-000034-01
3	MD-610830	20.6	49	1016	33	10 APR-000035-01
4	MD-610831	21.1	40	1486	30	11 APR-000036-01
5	MD-610832	19.6	42	1134	30	10 APR-000037-01
6	MD-610833	18.2	35	875	28	9 APR-000038-01
7				955	32	11 APR-000034-01
8				1338	29	13 APR-000035-01
9				1345	30	11 APR-000036-01
10				1105	30	13 APR-000037-01
11				811	30	12 APR-000038-01

File Explorer:

Workflow

compoundRequest.sdf (34 KB)

Literature Reference.pdf (803 KB)

Workflow Use cases



Compound Request Template

Status:

Sourcing date:

Internal Chem:

Project Notebook:

FTEs:

Request Purpose:

Attachments: [Literature Reference.pdf](#)

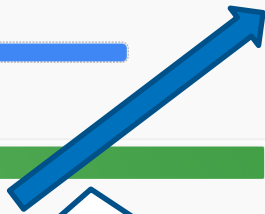
Project Name:

Compound

compoundRequest.pdf

Show 25 entries

Priority	Structure*	chemistry*	Amount requested (g)*	Number of steps*	Purity requested (%)	Compound type*	Destination*	Reg ID	Status
1		chemistry	120	4	100	Final Compound	Ship	AKR-00004	<input type="button" value="AKR-00004"/>
2		chemistry	80	4	100	Intermediate	Ship	AKR-00004	<input type="button" value="AKR-00004"/> <input type="button" value="Queue"/> <input type="button" value="Cancel"/>
3		chemistry	100	4	100	Final Compound	Ship	AKR-00004	<input type="button" value="AKR-00004"/> <input type="button" value="Queue"/> <input type="button" value="Cancel"/>



Request Dashboard

Workflow

Manage Requests

Show 25 entries

Start order	Name	Requestor	Requestor Priority	# of Items	Date Created	Project	Status	# FTEs	Sourcing d
1	External Collabor...	Kate Hardy	3	10	07/11/18 8:40 PM	ATG7	Queued		
2	External Collabor...	Kate Hardy	4	10	07/11/18 9:04 PM	3-GPI	Queued		
3	External Collabor...	Kate Hardy	5	10	07/11/18 9:05 PM	3-GPI	Queued		
4	External Collabor...	Kate Hardy	6	10	07/11/18 9:06 PM	3-GPI	Queued		
5	External Collabor...	Kate Hardy	7	10	07/11/18 9:07 PM	3-GPI	Queued		
6	External Collabor...	Kate Hardy	2	10	07/10/18 11:20 PM	ATG7	Queued		
7	External Collabor...	Jeff Carter	2	10	07/12/18 8:16 AM	AKT	Queued		
8	External Collabor...	Jeff Carter	3	10	07/12/18 9:13 AM	3-GPI	Queued		
9	External Collabor...	Jeff Carter	4	10	07/18/18 9:27 PM	ATG7	Queued	2	
10	External Collabor...	Jeff Carter	5	10	07/19/18 5:19 PM	ADC	Queued		

Collaborators Review, Complete

Project*:

Status*:

Sourcing date:

End date:

Internal Chem*:

Attachments: [Current file: Literature Reference.pdf](#)

Project Notebook:

Workflow Use cases



Hematology
Template

The interface displays a grid of flow cytometry plots for various parameters including CD34, CD34+CD45, CD34+CD45+CD45, CD34+CD45+CD45+CD45, CD34+CD45+CD45+CD45+CD45, CD34+CD45+CD45+CD45+CD45+CD45, CD34+CD45+CD45+CD45+CD45+CD45+CD45, and CD34+CD45+CD45+CD45+CD45+CD45+CD45+CD45. Below the plots is a table with the following data:

Priority	Animal ID	Body Mass (mg)	MCV	RBC	MCHC	RDW
	AB-12350	287.4	92	4.6	35	11
	AB-12351	237.9	86	4.8	37	15
	AB-12352	298.3	86	4.9	36	16
	AB-12353	213.7	91	5.0	32	
	AB-12354	294.5	85	4.9	36	

At the bottom, a message states: "All changes saved to draft - [Click to publish now](#) - (Keyboard shortcut: Ctrl+S)"

The Excel spreadsheet shows the following data:

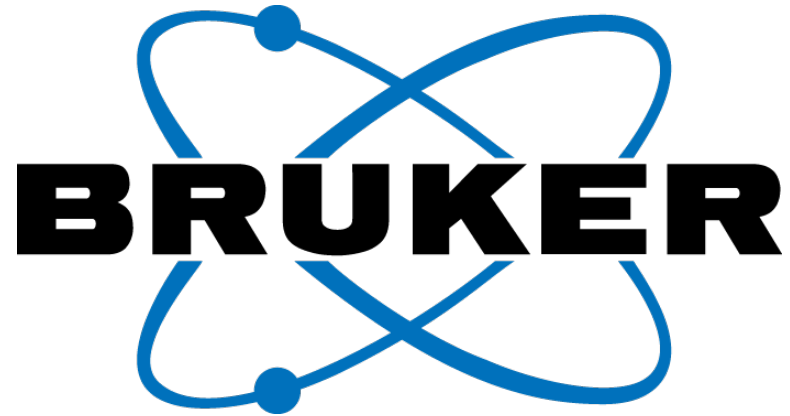
Animal ID	Body Mass (mg)	MCV	RBC	MCHC	RDW	REGID
610829	20.2	42	1106	32	10	APR-000034-01
610830	20.6	49	1016	33	10	APR-000035-01
610831	21.1	40	1486	30	11	APR-000036-01
610832	19.6	42	1134	30	10	APR-000037-01
610833	16.2	35	875	28	9	APR-000038-01
610834	20.0	48	955	32	11	APR-000034-01
610835	48	1338	29	13	13	APR-000035-01
610836	49	1345	30	11	11	APR-000036-01
610837	49	1105	30	13	13	APR-000037-01
610838	39	811	30	12	12	APR-000038-01

Configure the
Loading Template

The file explorer shows a folder named "Custom Experiment" containing a file named "Apolo_Hematology with RegID" with a last modified date of 2019/05/13 21:14.

Upload data

Questions?



Innovation with Integrity