CRIPT OPERATION MANUAL

Community Resource for Innovation in Polymer Technology

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Introduction

INTRODUCTION

The Community Resource for Innovation in Polymer Technology (CRIPT) provides a platform for researchers working in polymer science and engineering to capture and share data. CRIPT is hosted by a team at the Massachusetts Institute of Technology (MIT) along with collaborators in academia, industry, and government, with support from the Convergence Accelerator Program of the National Science Foundation (NSF).



PREREQUISITES

Before attempting to access the CRIPT platform, users must verify their identity. Verification consists of obtaining a unique identification number from two third-party organizations. This ensures the user's identity while protecting their work.

The two organizations are: Open Researcher and Contributor ID (ORCID) and Globus ID.

ORCID

Open Researcher and Contributor ID (ORCID) is a global, not-for-profit organization. ORCID provides a persistent digital identifier (ORCID iD) that distinguishes one user from all other researchers.

To obtain an ORCID iD, visit the official ORCID website at **www.orcid.org**.

GLOBUS

Globus is a group at the University of Chicago that develops and operates a non-profit service for use by the research community.

Globus products and services are developed and operated by the University of Chicago and Argonne National Laboratory to assist researchers in sharing their work with universities, laboratories, and companies around the world.

A Globus ID allows users the ability to share research without providing private organizational or personal contact information or credentials.

To obtain a Globus ID, visit the Globus ID website at **www.globusid.org**. If the user does not have a Globus ID, they may create one as part of the CRIPT account creation process.

EDUCATIONAL/GOVERNMENTAL ORGANIZATIONS

Some unique identification credentials provided by universities and governmental agencies can be used to access the CRIPT platform. These must be obtained from the user's institution.

CONTACT TECHNICAL SUPPORT

This manual was created to instruct users on the proper usage of the CRIPT platform. Additional support may also be found using the following resources:

- The CRIPT blog can be found on the CRIPT platform home page at **blog.criptapp.org**. It contains helpful usage tips.
- "Share a Thought" links are featured on many CRIPT platform pages. Clicking on these links allow users to comment and voice their concerns regarding CRIPT platform usage.
- Email requests for help can be sent to **CRIPT@mit.edu**.

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Chapter 1

{ **CRIPT** }

INITIAL SETUP REGISTRATION WITH CRIPT

Before registering with CRIPT, the user will require an ORCID identification number (ID). For more information, see "Prerequisites" on page i-i in the Introduction.

- 1. Navigate to the CRIPT website, https://criptapp.org.
- 2. Select Login/Register (1) on top right corner of page.

Synthesize. Network. Transform 귀 Login / Register
(1)
What is CRIPT? Mission & vision Repetits of CRIPT Team Dors & more
The Community Resource for Innovation in Polymer Technology (CRIPT) provides a platform for people working in polymer science and engineering to capture and share data. CRIPT is led by a team at the Massachusetts Institute of
Technology (MIT) along with collaborators in Academia, Industry, and Government, with support from the Convergence
Accelerator Program of the National Science Foundation (NSF). Learn more

Figure 1-1

- 3. Use drop-down (2) to select institution. If institution is not listed, the consent form can be downloaded from the link (3). The link to the form can be downloaded from the hyperlink, **Institutional consent form.**
- 4. Complete the form and email back to cript@mit.edu.

¢ RIPT		a Back to Home
	Account verification I wil use CRIPT on behalf of My institution is not listed here The Terms of Use must be agreed and signed by an authorized representative of your institution. Please download and complete the institutional consent and signature form below and email it to cript@mit.edu. Pownload the institutional consent form 3	CEI002
		CRIU084

Figure 1-2

INITIAL SETUP

- 5. CRIPT will automatically launch Globus, which will offer several ways to enter the user's unique ID.
- 6. Select Sign in with ORCID iD (4) to launch the ORCID sign-in page.

🕑 globus		
	Log in to use CRIPT	
	Use your existing organizational login e.g., university, national lab, facility, project	
	Look-up your organization	•
	By selecting Continue, you agree to Globus terms of service and privacy policy.	
	G Sign in with Google Sign in with ORCID iD	
	Figure 1-3	CRI0003

- 7. Enter the users Email or 16-digit ORCID iD (5) and Password (6), and select SIGN IN (7).
- 8. If lacking an ORCID iD, select Register now (8).

ORCID Connecting research and researchers	English 🗸 Search
ABOUT FOR RESEARCHERS MEMBERSHIP DOCUMENTATION RESOURCES NEW	/S & EVENTS
5 5 5 5 5 5 5 5 5 5 5 5 5 5	CRI0004

Figure 1-4

INITIAL SETUP

9. Enter user information and select NEXT (9).

Personal data	Security and notifications	Visibility ar	nd terms
	Create your ORCID This is step 1 of 3	iD	
Per ORCID's for yourself.	s terms of use , you may only regi Already have an ORCID iD? Sign	ster for an ORCID iD In	
First name – Sample			0
Last name (O	ptional) ————————————————————————————————————		
Primary emai	il		
anyuser@	esample.com		
Confirm prim	ary email Sample.com		
Additional en anyuser@	nail (Optional) Sample.com		0
+ Add and	other email	9	
GO BACK	(NEXT	

Figure 1-5

10. Verify that there is not an ORCID iD associated with user name by using the scroll bar (10) to scan through names.

11. Once confirmed, select NONE OF THESE ARE ME, CONTINUE WITH REGISTRATION (11).

	<i>с. 1</i>	0.0000 10	
Could this be	you?		
We found some accounts with yo account, please confirm that non	, ur name, which means you may have a e of these records belong to you. Not s	lready created an ORCID iD using a different email address ure if any of these are you? Contact us.	s. Before creating an
First Name	Last Name	Affiliations	View Record
Sample	User	Newcastle University, University of Aberdeen, University of Birmingham, University of California Davis, University of California San Francisco, University of Glasgow, University of Leeds Faculty of Biological Sciences, University of Surrey	View Record
Test	User	Auckland District Health Board, New Zealand Institute of Medical Radiation Technology	View Record
• • •			
I ALREAD	Y HAVE AN ID, GO BACK TO SIGN	IN NONE OF THESE ARE ME, CONTINUE WIT	H REGISTRATION
	your primary email addr	ess.	
	After you've registered, you at any time in the account se	can change your notification settings ettings section of your ORCID record.	
	GO BACK	NEYT	

Figure 1-6

INITIAL SETUP

- 12. Create ORCID iD by entering a Password (12), Confirm password (13) by entering it again.
- 13. An optional check box (14) can be selected for quarterly notifications.
- 14. Select NEXT (15) to continue.

Personal data Security and notifications Visibility and terms Create your ORCID iD This is step 2 of 3 Pessoord So or more characters S 1 letter or symbol 1 1 Confirm password C			3
<section-header> Create your ORCID DD This is step 2 of 3 Image: Serverd Serverd Image: Serverd Intervery Serverd Image: Servery Serverg Intervery Serverg Image: Serverg Image: Serverg Image: Serverg Image: Serverg Image: Serverg Image: Serverg<th>Personal d</th><th>ata Security and notifications Visibility</th><th>and terms</th></section-header>	Personal d	ata Security and notifications Visibility	and terms
This is step 2 of 3 Pessword		Create your ORCID iD	
Password So more characters A letter or symbol I letter or symbol I number Orfirm password Orfirm password Orfirm password Orfirm password Orfirm password Ordification settings OkclD sends email notifications about items related to your account, and changes made to your record by those organizations. Okcount, security, and privacy, including requests from ORCID member organizations for permission to update your record, and changes made to your record by those organizations. Ok can also choose to receive emails from us about new features and tips for making the most of your ORCID record. Please send me quarterly emails about new ORCID features and tips. To receive these emails, you will also need to verify your primary email address. After you've registered, you can change your notification settings at any time in the account settings section of your ORCID record. GUBACK		This is step 2 of 3	
So a more characters A letter or symbol I and the confirm password Confirm p	(12)	- Password	0
 S or more characters 1 letter or symbol 1 number 1 number Confirm password Motification settings ORCID sends email notifications about items related to your account, security, and privacy, including requests from ORCID member organizations for permission to update your record, and changes made to your record by those organizations. You can also choose to receive emails from us about new features and tips for making the most of your ORCID record. Please send me quarterly emails about new ORCID features and tips. To receive these emails, you will also need to verify your primary email address. After you've registered, you can change your notification settings at any time in the account settings section of your ORCID record. 			
 1 letter or symbol 1 number 1 number Confirm password Motification settings ORCID sends email notifications about items related to your account, security, and privacy, including requests from ORCID member organizations for permission to update your record, and changes made to your record by those organizations. You can also choose to receive emails from us about new features and tips for making the most of your ORCID record. Please send me quarterly emails about new ORCID features and tips. <i>To receive these emails, you will also need to verify your primary email address.</i> After you've registered, you can change your notification settings at any time in the account settings section of your ORCID record. 		8 or more characters	
 Confirm password Confirm password Notification settings ORCID sends email notifications about items related to your account, security, and privacy, including requests from ORCID member organizations for permission to update your record, and changes made to your record by those organizations. You can also choose to receive emails from us about new features and tips for making the most of your ORCID record. Please send me quarterly emails about new ORCID features and tips. <i>To receive these emails, you will also need to verify your primary email address.</i> After you've registered, you can change your notification settings at any time in the account settings section of your ORCID record. 		 1 letter or symbol 1 number 	
Motification settings ORCID sends email notifications about items related to your account, security, and privacy, including requests from ORCID member organizations for permission to update your record, and changes made to your record by those organizations. You can also choose to receive emails from us about new features and tips for making the most of your ORCID record. Please send me quarterly emails about new ORCID features and tips. <i>To receive these emails, you will also need to verify your primary email address.</i> After you've registered, you can change your notification settings at any time in the account settings section of your ORCID record. GO BACK	(13)		
Notification settings ORCID sends email notifications about items related to your account, security, and privacy, including requests from ORCID member organizations for permission to update your record, and changes made to your record by those organizations. To u can also choose to receive emails from us about new features and tips for making the most of your ORCID record. Please send me quarterly emails about new ORCID features and tips. To receive these emails, you will also need to verify your primary email address. After you've registered, you can change your notification settings at any time in the account settings section of your ORCID record.		· ·····	
ORCID sends email notifications about items related to your account, security, and privacy, including requests from ORCID member organizations for permission to update your record, and changes made to your record by those organizations. You can also choose to receive emails from us about new features and tips for making the most of your ORCID record. Please send me quarterly emails about new ORCID features and tips. <i>To receive these emails, you will also need to verify your primary email address.</i> After you've registered, you can change your notification settings at any time in the account settings section of your ORCID record.		Notification settings	
account, security, and privacy, including requests from ORCID member organizations for permission to update your record, and changes made to your record by those organizations. You can also choose to receive emails from us about new features and tips for making the most of your ORCID record. Please send me quarterly emails about new ORCID features and tips. <i>To receive these emails, you will also need to verify</i> <i>your primary email address.</i> After you've registered, you can change your notification settings at any time in the account settings section of your ORCID record.		ORCID sends email notifications about items related to your	
 You can also choose to receive emails from us about new features and tips for making the most of your ORCID record. Please send me quarterly emails about new ORCID features and tips. <i>To receive these emails, you will also need to verify your primary email address.</i> After you've registered, you can change your notification settings at any time in the account settings section of your ORCID record. 		account, security, and privacy, including requests from ORCID member organizations for permission to update your record, and	
You can also choose to receive emails from us about new features and tips for making the most of your ORCID record. Please send me quarterly emails about new ORCID features and tips. <i>To receive these emails, you will also need to verify</i> <i>your primary email address.</i> After you've registered, you can change your notification settings at any time in the account settings section of your ORCID record.		changes made to your record by those organizations.	
 Please send me quarterly emails about new ORCID features and tips. To receive these emails, you will also need to verify your primary email address. After you've registered, you can change your notification settings at any time in the account settings section of your ORCID record. GO BACK 	(14)	You can also choose to receive emails from us about new features and tips for making the most of your ORCID record.	
and tips. <i>To receive these emails, you will also need to verify your primary email address.</i> After you've registered, you can change your notification settings at any time in the account settings section of your ORCID record.		Please send me quarterly emails about new ORCID features	
your primary email address. After you've registered, you can change your notification settings at any time in the account settings section of your ORCID record.		and tips. <i>To receive these emails, you will also need to verify</i>	
After you've registered, you can change your notification settings at any time in the account settings section of your ORCID record.		your primary email address.	
GO BACK NEXT		After you've registered, you can change your notification settings at any time in the account settings section of your ORCID record.	(15)
		GO BACK	

Figure 1-7

- 15. Set visibility settings (16) and Terms of Use (17).
- 16. Select the reCAPTCHA box (18) and then select REGISTER (19).

<section-header><section-header></section-header></section-header>	Personal c	lata Security and noti	fications	3 Visibility and terms
Create your ORCID iD This is step 3 of 3 Visibility settings Your ORCID iD connects with your ORCID record that can contain linkinons, awards, other versions of your name, and more. You control this content and who can see it. By default, what visibility should be given to new items added to your ORCID Record? Image:				
This is step 3 of 3 Visibility settings Vour ORCID Die connects with your ORCID record that can contain figure to your research activities, affiliations, awards, other versions of your name, and more. You control this content and who can see it. By default, what visibility should be given to new items added to your ORCID Record? If I be Everyone (87% of users choose this) If I consent of users choose this Dease choose a default visibility settings Terms of Use I consent to the privacy policy and terms of use and agree to my data being publicly accessible where marked as "Visible to zeryone". I consent to my data being processed in the United States. More information on how ORCID process your data. To continue creating your ORCID ID you must accept the terms of use and consent to your data being processed in the United States. The information on Noroe CID process your data. To continue creating your ORCID ID you must accept the terms of use and consent to your data being processed in the United States. The information on the VICID ID you must accept the terms of use and consent to your data being processed in the United States. The information on how ORCID process your data. The information on the VICID ID you must accept the terms of use and consent to your data being processed in the United States. The information on how ORCID process your data. The information on how ORCID process your data. The information on boor ORCID ID you must accept the terms of use and consent to your data being processed in the United States. The information an boor VICID ID you must accept the terms of use and consent to your data being processed in the United States. The information on boor ORCID ID you must accept the terms of use and consent to your data being processed in the United States. The or the terms of use the terms of use the terms of use the terms of use the terms		Create you	r ORCID iD	
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Vour ORCID iD connects with your ORCID record that can contain links to your research activities, affiliations, awards, other versions of your name, and more. You control this content and who can see it. By default, what visibility should be given to new items added to your ORCID Record? Image: the transmission of transmission of transmission of the transmission of the transmission of transmission of the transmission of the transmission of transmission of transmission of transmission of transmission of the transmission of transmission of transmission of the transmission of the transmission of transmission of the tra		Visibility settings		
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 C* Trusted Organizations (5% of users choose this) Doly me (8% of users choose this) Please choose a default visibility setting. More information on visibility settings Terms of Use I consent to the privacy policy and terms of use and agree to my data being publicly accessible where marked as "Visible to Everyone". I consent to my data being processed in the United States. More information on how ORCID process your data. To continue creating your ORCID iD you must accept the terms of use and consent to your data being processed in the United States. To continue creating your ORCID iD you must accept the terms of use and consent to your data being processed in the United States. I'm not a robot Please check the recaptcha box GO BACK 		O 4 Everyone (87% of users c	hoose this)	
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(18) I'm not a robot PrecaPTCHA Pricey 'Tama GO BACK REGISTER		To continue creating your ORCID use and consent to your data beir States.	iD you must accept t ng processed in the l	he terms of Jnited
Please check the recaptcha box GO BACK REGISTER	(18)	i'm not a robot	reCAPTCHA Privacy * Terms	
GO BACK REGISTER		Please check the recaptcha box		
		GO BACK		REGISTER

Figure 1-8

CRI0039



17. The globus site will launch. Select Continue (20).

🕒 globus		
	Welcome – You've Successfully Logged In	
	This is the first time you are accessing Globus with your ORCID login.	
20	If you have previously used Globus with another login you can link it to your ORCID login. When linked, both logins will be able to access the same Globus account permissions and history.	
	Continue Link to an existing account Why should I link accounts?	
© 2010-2022 University of Ch	icano Arconne National Jaboratory Leoal Privacy	
		CRI0040

Figure 1-9

- 18. Enter Email address (21) and Organization (22).
- 19. Select which purpose the account will be used for (23).
- 20. Select Terms of Service (24) to accept Privacy Policy and then select Continue (25).

🔊 globus		
Complete Your Sign I	Jp For 0000-0000-0000-0000@orcid.org	
Name	Sample User	(21)
Email		
(23) Organization		
Account will be used for	 non-profit research or educational purposes 	
	 commercial purposes 	
(25)	☐ I have read and agree to the Globus Terms of Service [2] and Privacy Policy [2].	
	Continue	
	* This field is specified by the identity provider, and cannot be modified by Globus. If you change it with your identity provider, it will propagate to Globus the next time you log in.	
@ 2010. 2022 Linkswitz of Chicago. Avenue: Netland Linkswitz, 1	al. Drivery	
© 2010-2022 University of Chicago, Argonne National Laboratory Le	au rivacy	CRI004
	Figuro 1-10	011001

Figure 1-10

21. The ORCID Authorize access page will open, displaying the user's ORCID credentials. Selecting Authorize access (26) will launch the CRIPT home page.

	ORCID Authorize access
	You are currently signed in as:
	User https://orcid.org/0000-0000-000X Sign out
	Globus Auth ?
26	Get your ORCID iD
	Authorize access
	Deny access
	If authorized, this organization will have access to your ORCID record, as outlined above and described in further detail in ORCID's privacy policy.
	You can manage access permissions for this and other Trusted Organizations in your account settings .

Figure 1-11

LOGIN TO CRIPT

The CRIPT home page allows the user to create new projects, search for existing projects, and find helpful tips on the CRIPT platform.

CRIPT HOME PAGE

¢ RIPT	iame v Search materials	@~ Q
My CRIPT	Hello, user! • 0000-0000-0000-0000	From the CRIPT blog
III Browse -	Quick Tips for Getting Started	Love ChemDraw? Hate ChemDraw? Either way, CRIPT will work for you!
Q Advanced Search Featured Help	With the brand new user interface of CRIPT, you can: Set display name + visibility in the CRIPT user directory in	Destruct Transmit Statu Lia MT BREAD Statut Constrained with your chemistrations the CERT structure editor and how it can integrate with your chemistrate workflows:
	How You Can Help · · · · · · · · · · · · · · · · · · ·	Haley Beech (Olsen Lab, MIT) Why a reluctant experimentalist was convinced that learning BigSMILES and using CRIPT are worthwhile endeavors.
	A Note to Our Early Adopter Community	Collaboration at MONET, an NSF Center
	In the Pipeline Y	Staphen Crass MCNRT: Due (University) How a highly collective polymer research center can benefit from sharing data through a platform such as CRIPT. Visit the blog \Rightarrow
		CR10006



CREATE A PROJECT

The first step in working with user data in CRIPT is to create a project. A project is an organizational tool that will contain a collection of thematically related work that is typically a collaboration between a number of individuals and can lead to a series of scientific publications. The project will hold a set of collections, which are publishable groupings of research (i.e. papers) as well as a set of materials that are used between research performed within the project. By default, the user project will be non-public when first created. Therefore, it can only be viewed and modified by collaborators that are added to the project.

1. Select Browse drop-down (1) and select Projects (2).

¢ RIPT	Name v Search materials	Q~ Q 🚯 About 😁 -
My CRIPT	Hello, user! • consecutive and the second and the s	From the CRIPT blog
Browse 👻	Quick Tips for Getting Started	Love ChemDraw? Hate ChemDraw? Either way, CRIPT will work for you!
Projects Collections Collections Collections Attended At	-2 With the brand new user interface of CRIPT, you can: • Set display name + visibility in the CRIPT user directory in ⊕ Account Settings. • Create and manage & Access Groups with your colleagues and collaborators. • Use the idebact to browge Collections, 2 Experiments, and more • Tell us what you think using the built-in feedback channels. To upload you own data, you can use our Excel template + parser or Python SDK. Please visit the	And the approximation of the a
Q Advanced Search	How You Can Help 🗸	CRIPT are worthwhile endeavors.
ET. Contrard	A Note to Our Early Adopter Community	
Help	In the Pipeline	Stephen Craig (MONET, Duke University) How a highly collaborative polymer research center can benefit from sharing data threads have a fastere much ar CPIOT
	© 2022 MTT All Rights Reserved	
₩ Share a thought		
	E'	CRI0

Figure 1-13

2. Select New project (3).

¢ RIPT	Name 🗸 Se	earch materials.				
My CRIPT Browse - Advanced Search Featured		Projects My recent projects Sample Protect Sample Projects 3				
🗎 Help		Showing	g 1-15 of 2	2 Projects		■ Ⅲ Ⅱ 2
				Name 1	E Collections 1	t⊜ Files 1
			٩	Sample		
			٩	SDK test project	 Tutorial Examples 	esc.bd, nmr.bd
			٩	Test Project Almon	Almon Collection	
			\$	DMREF-Redox		
			٩	CRIPT Examples	1 Tutorial	
			٢	Expo2022	① Expo2022	example_template_v0·
			٩	CRIPT_1	1 CRIPT test	
			٩	waldow_lab	1 test_synthesis1	
			٩	Weak bond network toug	RAFT networks toughe	
			٩	Strong-weak	1 Strong-weak test colle	
			٩	OlsenLab_rubberrecycling	 Polyethylene Grafting 	
			٩	Alexis private project test	Olyethylene Grafting	1 LLDPEmysample.tri
			٩	olsenlab	3 SANS	F127_merged.txt
			٩	AFRL-VaiaProject	1 Binary Polymer Solutio	
. Share a thought			٩	CRIPT_Test		
						CRI0008

Figure 1-14

- 3. Enter a valid project Name (4).
- 4. Enter a Description (5) for the project.
- 5. Select Create (6).
- **NOTE:** New projects are private by default and can only be viewed and modified by collaborators that are associated with the project.

CRIPT Editor	ack to CRIPT			Cancel Create :
(4) (5)	New project Name Description		Create	
	Collections () 👗 Materials ()	Files () Description	Contents	↔ New Collection
- Chara a thought				
N ; Share a thought		Editor v0.4.15 © 20	22 MIT All Rights Reserved	CRI007

Figure 1-15



ADD COLLABORATORS TO A PROJECT

Once a project is created, specify which users can contribute to that project. Add all collaborators, including principal investigators. If a collaborator is not added, they will not be able to view any data in the project until it is public, and will not be able to modify any data.

- 1. Select Browse drop-down (1) and select Users (2).
- 2. Check box (3) allows user to add or remove name from the CRIPT directory.
- 3. Locate the user name (4) for collaboration and copy their ORCID iD (5).

CRIPT Name	e 🗸 Search materials		3_	@~~ Q. 1 About 😁 -
My CRIPT	(1) User directory		0 -	Remove me from the CRIPT directory
Browse -	Showing 1-5 of 5 Members		0	
Projects	± Display name ™ (4)	ORCID 1	(5)	
Collections	sheld	0000-0003-4	4419-249x	
Inventories	0000-0002-5937-7721	0000-0002-	5937-7721	
Materials	Monthly Meeting Staff	0000-0002-8	8098-1026	
References	2 havidh	0000-0001-5	5015-5279	
22 Users	ardiana	0000-0002-	5532-0285	
Q Advanced Search				
* Featured				
🖹 Help				
		© 2022 MIT All Rights Reserved		

Figure 1-16

4. Select Browse drop-down (6), select Projects (7), and select project name (8).

¢RIPT Name ~	Search materials			Q~ Q	About 😁 -
My CRIPT 6 6 Frojects Collections & Deperiments Materials	Project: My recent project My recent project My Refine No fine O collections	s ts 8			New project
 Data References 	Showing 1-15 of	22 Projects			1 2
22t Users		Name %	Collections %	€ Files 1	
Q Advanced Search	□	Sample			
Featured	\$	SDK test project	1 Tutorial Examples	esc.txt, nmr.txt	
Help	٩	Test Project Almon	Almon Collection		
	٩	DMREF-Redox			
	٩	CRIPT Examples	 Tutorial 		
	\$	Expo2022	Expo2022	example_template_v0·	
	٩	CRIPT_1	 CRIPT test 		
	\$	waldow_lab	1 test_synthesis1		
	\$	Weak bond network toug	 RAFT networks toughe 		
	S	Strong-weak	 Strong-weak test colle 		
	\$	OlsenLab_rubberrecycling	 Polyethylene Grafting 		
	\$	Alexis private project test	 Polyethylene Grafting 	 LLDPEmysample.tri 	
	\$	olsenlab	3 SANS	F127_merged.txt	
	\$	AFRL-VaiaProject	 Binary Polymer Solutio 		
Share a thought	ø	CRIPT_Test			001004

Figure 1-17

CRI0085

5. Select Edit (9) and select Edit collaborators (10).

¢ RIPT	Name	✓ Search materials				Q~ Q DAbout O-
My CRIPT Browse ~ Q. Advanced Search Featured		CRIPT ID d877eecc-c2 verification for instruc	manual b7-4b7f-8aca-62c40ce3b70b @ tion manual ▲ Materials 屬 Files			9 € CD ± + 12 + 1 ✓ Edit ▼ CD ± + 12 + 1 ✓ Edit T Collaborators Edit collaborators Edit collaborators Edit collaborators Edit collaborators
Help		Showing 1-1 of 1	Collection			
			Name ţ	👌 Experiments 📬	■ Inventory ⁺ ₄	Project 1,
			Sample manual			Sample manual
🍕 Share a thought		at Sample manual		© 2022 MIT All Rights Reserved		Created Nov. 16, 2022, 9:25 p.m. by sheld Updated Nov. 16, 2022, 9:25 p.m. by sheld

Figure 1-18

- 6. Name (11) will be autogenerated from the Project or user can enter a new name for the group.
- 7. Check the Public option box (12) if user wishes to make this access group visible to the community. For more information, see "Non-public change" on page 1-16.
- 8. Description (13) allows user to specify details about the project.
- 9. Enter ORCID iD (14) of the collaborator to be added, select add user icon (15), and select Submit (16).

NOTE: If the ORCID iD contains any letters, they must be in lowercase.

Searc	h materials	🖍 Edit group	×		
	CRIPT ID 44e05545-fd26-4e7c-b099-55a1622d22da 12	Name* Sample Valid group name			
	Showing 1-1 of 1 User	Public Description (optional) Add a description to this access group	11		
	sheld	Search for user by ORCID 10000-30000-30000-30000 Enter a valid 16-digit ORCID	-44	19-249	
		Group members (1)	*	16	
			Close Submit		CDIO04

Figure 1-19

{ **CRIPT** }

CRI0074

EDIT PROJECT

1. Select Browse drop-down (1) and select Projects (2).

¢ RIPT	Name v Search materials	67~ Q. (1) About (1) -
KRIPT My CRIPT My CRIPT Browse Projects Collections Collections Collections Collections Collections Advanced Search Featured Help	Name Search materials Image: Constraint of the search materials in the search materials of CRIPT, you car: Cluick Tips for Getting Started Image: Constraint of the search materials and consearch materials and constraint	<image/> <image/> <section-header><section-header><section-header><section-header><section-header><section-header><section-header><section-header><section-header><section-header><section-header><section-header><section-header><section-header><section-header><section-header><section-header><section-header><section-header><section-header><section-header></section-header></section-header></section-header></section-header></section-header></section-header></section-header></section-header></section-header></section-header></section-header></section-header></section-header></section-header></section-header></section-header></section-header></section-header></section-header></section-header></section-header>
	(0 2022 M/T (All Rights Reserved	
Share a thought		
	E ! (00	CRI000

Figure 1-20

2. Select the project to be edited (3).

¢RIPT Name	✓ Search materials			G~~ Q ⓓ About €
My CRIPT	📱 Proje	ects		New project
III Browse -	My recent p	projects		
Q Advanced Search	Sample	e 3 👜 📱 Sample 2	a sample 1 a 3	
Featured	No files	No files O collections	Rofiles	
🖺 Help	Showing 1-	15 of 24 Projects		88 1
		Name 1	🛅 Collections 😘	le Files 1.
		Sample 3		
	. 6	Sample 2		
		sample 1		
	6	SDK test project	Tutorial Examples	ec.bd, nmr.bd
	6	Test Project Almon	Almon Collection	
	6	DMREF-Redox		
	6	CRIPT Examples	Tutorial	
	6	Expo2022	1 Expo2022	(3) example_template_v0
	6	CRIPT_1	CRIPT test	
	6	waldow_lab	1 test_synthesis1	
	6	Weak bond network toug	RAFT networks toughe	
	6	Strong-weak	Strong-weak test colle	
	6	OlsenLab_rubberrecycling	Polyethylene Grafting	
	6	Alexis private project test	Polyethylene Grafting	1 LLDPEmysample.tri
📫 Share a thought	6	olsenlab	(1) SANS	F127_merged.txt
			F : 4.04	CF

Figure 1-21

3. Select Edit (4).

4. Select Edit project (5).

	ne 🗸 Searc	:h materials				©∼ Q B About ⊖ -
My CRIPT Browse Advanced Search	CRIPT ID verificatio	ample r d877eecc-c2b7 on for instructic	manual Manual			€ CD ± + CD + ▲ Cdit • Edit project Control Control
Featured	🖻 Co	llections 1	🛦 Materials 🖷 File	S		5 Delete this project
Help	Showin	g 1-1 of 1 (Collection			
			Name 1	🛓 Experiments 🐛	🖬 Inventory 📬	Project 🖞
		â	Sample manual			Sample manual
₩C Share a thought	🚉 Samp	ole manual		© 2022 MIT All Rights Reserved		Created Nov. 16, 2022, 9:25 p.m. by sheld Updated Nov. 16, 2022, 9:25 p.m. by sheld
						CRI0074

Figure 1-22

- 5. Users can edit the manual Name (6), project description (7), and non-public change (8). For more information on non-public change, see "Non-public change" on page 1-16.
- 6. Select Save (9) to save changes.

NOTE: New projects are private by default and can only be viewed and modified by collaborators that are associated with the project.

ERIPT Editor	ck to CRIPT			(8)	Cancel Save : i
6	Sample manual			non-public (change)	Delete
\bigcirc	Sample manual				
	verification for instruction n	nanual	h	9	
	🖪 Collections (0) 👗 Ma	aterials (0) 🛛 🖷 Files (0)	Save		↔ New Collection
	Name	Description		Contents	
≪ € Share a thought					
			Figure 1-23		CRI0072



INITIAL SETUP

NON-PUBLIC CHANGE

- 1. Navigate to Edit project. For more information, see "Edit project" on page 1-14.
- 2. Select public (1) to make project visible to public.
- 3. Select Check box (2) to accept permission to continue.
- 4. Select Confirm (3) to save choice.



DELETE A PROJECT

1. Select Browse drop-down (1) and select Projects (2).

<complex-block><complex-block>• Control Control</complex-block></complex-block>	CRIPT Name	✓ Search materials_	©~ Q. ● About ● -
<form> Control Control Co</form>	My CRIPT	Hello, user! Cuick Tips for Getting Started	From the CRIPT blog Love ChemDraw? Hate ChemDraw? Ether way. CRIPT will work for you!
L toes How You Can Help A Mote Our Early Adopter Community Image: Community	Collections Experiments Materials Data References	Set display name + visibility in the CNPT user directory in \bigoplus Account Settings Create and manage us. Access Groups with your colleagues and collaborators Use the sidebar to browse \bigoplus collections, \bigoplus Experiments, and more Tell us what you think using the built-in feedback channels To upload you own data, you can use our Excel template + parser or Python SDK. Please visit the Docs Hub to learn more about these and other resources.	An integrated under the CRFT structure editor and here it can integrate with your Chemichan endities. If I Can CRIPT, So Can You Harry feech (Diana Lab, MIT)
I returne In the Pipeline In the Pipeline Witt the blog > 0 2022 MT M Rights Reservel	Users Advanced Search	How You Can Help ~ A Note to Our Early Adopter Community ~	Wby a naturative experimentation was convinced that learning BigSMLES and using CGRT are worthink endeavori. Collaboration at MONET, an NSF Center + ERIPT
© 2022 M/T Al Rights Reserved	 Featured Help 	In the Pipeline \checkmark	Sighen Calg MONET. Data University) How a Nighly collaborative polymer research center can benefit from sharing data through a platform such as CRIPT. Visit the blog I
© 2022 MT All Rights Reserved			
© 2022 MT AN Rights Reserved			
₩ ² Share a thought		© 2022 MTT (All Rights Reserved	
	₩ ² Share a thought		00/202

Figure 1-25

2. Select the project to be deleted (3).

¢RIPT Name ~	Search materials			g~ Q BAbout e-	
My CRIPT	Project	S	0	New project	I
Q Advanced Search	Sample 3	Sample 2 B Notice	a sample 1 a 3		
Featured	0 collections	0 collections	២ 0 collections		
🗎 Help	Showing 1-15 o	f 24 Projects		H 1 2	
		Name %	Collections %	@ Files %	
	□ ê	Sample 3			
	□ ê	Sample 2			
		sample 1			
	\$	SDK test project	Tutorial Examples	ec.bt, nmr.bt	
	٩	Test Project Almon	Almon Collection		
	\$	DMREF-Redox			
	٩	CRIPT Examples	Tutorial		
	٢	Expo2022	① Expo2022	(3) example_template_v0	
	٩	CRIPT_1	CRIPT test		
	٩	waldow_lab	1 test_synthesis1		
	٢	Weak bond network toug	RAFT networks toughe		
	٢	Strong-weak	Strong-weak test colle		
	٩	OlsenLab_rubberrecycling	Polyethylene Grafting		
	٩	Alexis private project test	Operation Polyethylene Grafting	1LDPEmysample.tri	
H: Share a thought	٢	olsenlab	SANS	127_merged.txt	
			Figure 1.00	CRI	0014

Figure 1-26



INITIAL SETUP

- 3. Select Edit (4).
- 4. Select Delete this project (5).

¢ RIPT	Name	✓ Search	n materials				۲ ۹ ۹ ۲ ۹ ۲ ۲ ۹ ۲ ۲ ۹ ۲ ۲ ۹ ۲ ۲ ۲ ۲ ۲ ۲
 My CRIPT Browse Advanced Search 		CRIPT ID d	ample r 1877eecc-c2b7 n for instructio	manual ∵4b7f-8aca-62c40ce3b70b @ n manual			Image: Constraint of the second s
* Featured		🖪 Coll	lections 1	🔺 Materials 🛛 🖷 Files			Delete this project
🗎 Help		Showing	g 1-1 of 1 C	Collection			
				Name 📬	≙ Experiments ∿	🖀 Inventory 📬	Project 😘
			â	Sample manual			Sample manual
		조 Sample manual			© 2022 MIT All Rights Reserved		Created Nov. 16, 2022, 9:25 p.m. by sheld Updated Nov. 16, 2022, 9:25 p.m. by sheld
in onare a thought							CRI0074

Figure 1-27

5. Enter ORCID iD (6) and select Confirm (7). For more information, see "Locate ORCID iD" on page 1-19. *NOTE:* If the ORCID iD contains any letters, they must be in lowercase.

	Delete project	×
b60439ed11 🗖	To confirm, please enter your ORCID iD.	ancel Confirm
🖷 Files		
		00000

Figure 1-28

CRI0088

LOCATE ORCID ID

1. Select Account drop-down (1) and select Account Settings (2).

CRIPT Name	✓ Search materials				(1) ² Q Q-
 My CRIPT Browse * Projects Collections Experiments 	Sample CRIPT ID d877eecc-c2 verification for instruct Collections	manual b7-4b7f-8aca-62c40ce3b70b 🕤 ion manual			
 Inventories Materials Data References 	Showing 1-1 of 1	Collection			
:2: Users		Name 1		Inventory 1:	Project 1
Q Advanced Search		sample manual	U sample		Sample manual
 Featured Help 					
	🚢 Sample manual				Created Nov. 16, 2022, 9:25 p.m. by sheld Updated Nov. 16, 2022, 9:25 p.m. by sheld
			© 2022 MIT All Rights Reserved		
📢 Share a thought					

Figure 1-29

2. ORCID iD (3) location is shown.

Share a thought			Figure 1-30	CR10089
			© 2022 MIT All Rights Reserved	
		Email user@domain.org		
	(3)	CRIPT ID fd00f000-0b0a-0b0b-b0dc-a0c000cd00a0		
Help	~ /	ORCID © 0000-0000-0000x		
Featured		Profile visibility Visible in CRIPT user directory (default)		
Q Advanced Search		Display name sample user		
Browse *		Sample User		
My CRIPT		O Account settings		Edit account settings
¢ RIPT	Name 🗸	Search materials		



CREATE A COLLECTION

Each project within CRIPT holds both materials and collections. Collections are groupings of data that represent publishable units of research (i.e. one paper). Collections are the organizational level used to make data viewable to the public. All collections are by default non-public; the general public cannot view the users collection until it is made public at the project level. For more information, see "Non-public change" on page 1-16.

1. Select Browse drop-down (1) and select Collections (2).

	Hello, user! • 0000-0000 0000-0000	From the CRIPT blog
III Browse	Quick Tips for Getting Started	Love ChemDraw? Hate ChemDraw? Either way. CRIPT will work for you!
Projects Collections Collections Collections Amaterials Collect References Amaterials Collect References Amaterials Collect C	With the brand new user interface of CRIPT, you care: • Set display name + visibility in the CRIPT user directory in ④ Account Settings: • Create and manage au, Access Groups with your colleagues and collaborators • Use the sidebar to horwas @ Collections, § Experiments, and more • Reli <i>us what</i> you <i>think</i> using the built-in feedback channels • To upload you own data, you can use our Excel template + parser or Python SDK. Please visit the ⑤ Docs Hub to learn more about these and other resources:	Exhibition Frames CEIIIe La MATT An integrate with your ChemOne voorkfors. If I Can CRIPT, So Can You (CRIPT) Kong Seeth (Stern Lah, MT) Way Seeth (Stern Lah, MT) Way and the operimentation was convided that learning BigSMULES and using
Q. Advanced Search	How You Can Help	CRIPT are worthwhile endeavors.
Featured	A Note to Our Early Adopter Community In the Pipeline	Stephen Graig MONT. Duke University
🗎 Help		How a highly collaborative polymer research center can benefit from sharing data through a platform such as CRIPT. visit the blog ⇒
	© 2022 MIT (A) Rights Reserved	
		CRI0007

Figure 1-31

2. Select New collection (3).

3
B
1 📓 Inventory 1 📲 Project 1
nerization 1 Tutorial Materials SDK test project
Test Project Almon
A Katsumata Project
Polymeth Katsumata Project
Inear_polymer_3pdb (AFRL-VaiaProject
xperiment MuckleyTestProject
nerization 1 Tutorial Materials CRIPT Examples
.2, expt_3 CTV
.2, expt_3 CTV
.2, expt.3 CTV
OlsenLab_BCD8
ting via 8 Alexis private project test
OlsenLab_rubberrecycling
R5, R6, R OlsenLab_sustainablepoly
2022 MIT All Rights Reserved
nts olyr BM of F olyr xpt xpt sraf R4, ©

Figure 1-32

- 3. Enter Name (4) for New Collection.
- 4. Enter Description (5) for New Collection and select Create (6) to save.

CRIPT Editor	ack to CRIPT				C	ancel Create : ()
(4) (5)	Sample manual Sample manual Construction	New Collection	â no	n-public		
	Experiments () 👗 Inventori	es () Description	Create	Contents	• New Experiment	
₩ Share a thought		I	Figure 1-33			CRI007

EDIT A COLLECTION

1. Select Browse drop-down (1) and select Collections (2).

	Hello, user! occorrection	From the CRIPT blog
III Browse -	Quick Tips for Getting Started	Love ChemDraw? Hate ChemDraw? Either way, CRIPT will work for you! *********************************
Projects Collections Collections Collections Anterials Collections References LA Users Q. Advanced Search	With the brand new user interface of CRIPT, you cars: • Set display name - visibility in the CRIPT user directory in @ Account Settings: • Create and manage a Access Society with your colleagues and collaborators • Use the diable to borous @ Collections, @ Experiments, and more • Rit us what you chink using the built-in feedback channels To upload you own data, you can use our Excel template + parser or Python SDIC. Please visit the @ Docs Hub to learn more about these and other resources. How You Can Help	Additional Forester (Store Les Strif) Additional Storester (Store Les Strif) Additional Storester (Storester Storester and Nove it can integrate with your Cereminate unotificate Additional Storester (Storester Storester S
Featured	A Note to Our Early Adopter Community	Center
🗎 Help	In the Pipeline	Stephen Craig (MONST. Duke University) How a highly collaborative polymer research center can benefit from sharing data
	@ 2022 MT [All Rights Reserved	visit the blog →
		CEI000

Figure 1-34



INITIAL SETUP

2. Select collection to be edited (3).

¢ RIPT	Name 🗸	Search materi	als				@~ Q (About
My CRIPT Browse Advanced Search Featured		My re	cent col Sample experiments inventories nple	a of 15 Collections			() #
E neib				Name 1	₫ Experiments %	■ Inventory %	Project %
			â	Sample			Sample
			0	Tutorial Examples	 Anionic Polymerization 	1 Tutorial Materials	SDK test project
			٩	Almon Collection			Test Project Almon
			\$	MKJ Test Upload	ATRP of PBMA		Katsumata Project
			\$	Practice Atom Transfer Ra	Synthesis of Polymeth		Katsumata Project
			٢	Binary Polymer Solution P		B linear_polymer_3pdb (AFRL-VaiaProject
			٩	MuckleyTestCollection	 MuckleyTestExperiment 		MuckleyTestProject
			0	Tutorial	 Anionic Polymerization 	 Tutorial Materials 	CRIPT Examples
			٩	CTV_rubber_recycling_2	16 expt_1, expt_2, expt_3		сти
			٩	CTV_rubber_recycling_1	<pre>(10) expt_1, expt_2, expt_3</pre>		CTV
			٩	CTV_rubber_recycling	<pre>(16) expt_1, expt_2, expt_3</pre>		CTV
			\$	Block Copolymer Phase Be			OlsenLab_BCDB
			٩	Polyethylene Grafting_take2	Opposite the second		Alexis private project test
			\$	Polyethylene Grafting			OlsenLab_rubberrecycling
			٢	Original_Polyester	(172) R2, R3, R4, R5, R6, R		OlsenLab_sustainablepoly
Share a thought					© 2022 MIT All Rights Reserved		051004

Figure 1-35

3. Select Edit (4) and select Edit collection (5).

CRIPT Name	✓ Search materials				(2) Q About Q
 My CRIPT Browse - Advanced Search Featured Help 	Sample manual > Samp Sample m CRIPT ID d74c015e-bb25 verification for instruction Experiments Showing 1-1 of 1 Ex	le manual hanual 4ef5-a4c8-1757e7e476e6 @ manual Inventories periment			€ Co € + € + Co Collection 5 Collection
		Name t	Processes ↑	() Data 斥	E Collection 1,
		Sample	 Sample 		Sample manual
₩¢ Share a thought	🕰 Sample manual		© 2022 MIT All Rights Reserved		Created Nov. 18, 2022, 4:12 p.m. by sheld Updated Nov. 18, 2022, 4:12 p.m. by sheld
			Figure 1-36		CRI0086

- 4. Users can edit the collection name (6) and collection description (7).
- 5. Select Save (8) to save changes.

CRIPT Editor	ck to CRIPT							Cancel	Save	: 6	
6 7	Sample manual Sample manual verification for instruction manual					👫 Sample manual	盲 Delete				
	🖾 Expe	riments (1)	ories (0)	Save •	8		+ New Experiment				
	ô	Name Sample	Description verification for manual		Contents	ita					
₩ : Share a thought											
										CF	210087

Figure 1-37

DELETE A COLLECTION

1. Select Browse drop-down and select Collections.

¢ RIPT	Name V Search materials	07~ Q 🛈 About 😬 -
CRIPT My CRIPT Frowse Projects Collections Collections Katerials Collections References Luses C. Advanced Search Featured Help	Yeard materials Image: Search materials Image: S	<image/> <image/> <section-header><section-header><section-header><section-header><section-header><section-header><section-header><section-header><section-header><section-header><section-header><section-header><section-header><section-header><section-header><section-header><section-header><section-header><section-header><section-header><section-header></section-header></section-header></section-header></section-header></section-header></section-header></section-header></section-header></section-header></section-header></section-header></section-header></section-header></section-header></section-header></section-header></section-header></section-header></section-header></section-header></section-header>
	© 2022 MIT (All Rights Reserved	
🐗 Share a thought		
	Figure 1-38	CRI000



INITIAL SETUP

2. Select Collection to be deleted (3).

CRIPT Name	✓ Search materials	at			وت م About 😁
My CRIPT My CRIPT Srowse Advanced Search Featured	My recer San the two sample Showing	nt collections	3)		■ #
B Help		Name 14	₫ Experiments %	Inventory %	Project %
		Sample			Sample
		S Tutorial Examples	 Anionic Polymerization 	 Tutorial Materials 	SDK test project
		S Almon Collection			Test Project Almon
		S MKJ Test Upload	1 ATRP of PBMA		Katsumata Project
		Practice Atom Transfer Ra	Synthesis of Polymeth		Katsumata Project
		Binary Polymer Solution P		Iinear_polymer_3pdb (AFRL-VaiaProject
		MuckleyTestCollection	MuckleyTestExperiment		MuckleyTestProject
		S Tutorial	 Anionic Polymerization 	Tutorial Materials	CRIPT Examples
		CTV_rubber_recycling_2	(16) expt_1, expt_2, expt_3		CTV
		CTV_rubber_recycling_1	(6) expt_1, expt_2, expt_3		CTV
		CTV_rubber_recycling	(6) expt_1, expt_2, expt_3		CTV
		Block Copolymer Phase Be			OlsenLab_BCDB
		Polyethylene Grafting_take2	O Polymer Grafting via B		Alexis private project test
		Polyethylene Grafting			OlsenLab_rubberrecycling
		Original_Polyester	(772) R2, R3, R4, R5, R6, R		OlsenLab_sustainablepoly
₩ Share a thought			@ 2022 MIT All Rights Reserved		



- 3. Select Edit (4).
- 4. Select Delete this collection (5).

¢ RIPT	Name	✓ Search	materials				©~~ Q	_
My CRIPT		Sample ma	nual 🕨 Sampl	e manual				1)
Browse -		CRIPT ID di verification	mple m 74c015e-bb25 for instruction	anual 4ef5-a4c8-1757e7e476e6 manual	6 1			
 Featured Help 		✿ Expe	eriments 🕦	Inventories			Delete this collection	
		Showing	1-1 of 1 Exp	periment				
				Name 1		() Data 14	🛅 Collection 💈	
			â	Sample	(1) Sample		Sample manual	
		よ Sample	: manual		© 2022 MT (All Rights Reserved		Created Nov. 18, 2022, 412 p.m. by sheld Updated Nov. 18, 2022, 412 p.m. by sheld	
∯ද Share a thought								

Figure 1-40

{ **CRIPT** }

5. Enter ORCID iD (6) and select Confirm (7). For more information, see "Locate ORCID iD" on page 1-19. *NOTE:* If the ORCID iD contains any letters, they must be in lowercase.

	Delete collection
101 04-0 0020-7-010 F	Deleting this collection will remove all of its contents (Experiments, Data, and Files) permanently. Are you sure you wish to proceed? To confirm, please enter your ORCID iD.
Inventories	(D) XXXX-XXXX-XXXX Cancel Confirm

Figure 1-41

HELP MENU

1. Help menu (1) provides many different resources to assist users in getting the most out of the CRIPT platform. Most features of the help menu can be accessed from the CRIPT Home Page or the CRIPT Landing Page.

¢ RIPT	Name ~	Search materials		Q~~ Q. 🚯 About 😁 -
My CRIPT		Hello, user! e concentration		From the CRIPT blog
Browse -		Quick Tips for Getting Started	^	Love ChemDraw? Hate ChemDraw? Either way, CRIPT will work for you!
Projects Collections Experiments Materials Data References Users		With the brand new user interface of CRIPT, you can: • Set display name + visibility in the CRIPT user directory in 🕒 Account Settings • Create and manage ±4. Access Groups with your colleagues and collaborators • Use the idebart to rowe 🖀 Collections, § La pointemist. Jaim more • Tell us what you think using the built-in feedback channels • Tell us what you think using the built-in feedback channels To upload you own data, you can use our Excel template + parser or Python SDK. Please visit the 👔 Docs Hub to learn more about these and other resources.		International Information Control (LASS) Informa
Q Advanced Search		How You Can Help	~	CRIPT are worthwhile endeavors.
E Conturned	(1)	A Note to Our Early Adopter Community	~	Center
Help	\cup	In the Pipeline	\sim	Stephen Craig (MONET, Duke University) How a highly collaborative polymer research center can benefit from sharing data
		© 2522 MT All Rights Reserved		visit the blog ≯
No. Share a thought				CBI0007

Figure 1-42

INITIAL SETUP



Figure 1-43

CRI0024

Python SDK

Instructions and examples for programmatic integration with CRIPT via the CRIPT python package cript.py. For more information, see *Python SDK*.

Browsable API

Self-documenting JSON-based CRIPT data explorer (requires login).

Controlled vocabulary

List of controlled vocabulary used in the CRIPT data model.

Ingestion tools

Repository of software for organizing and uploading data to CRIPT.

CRIPT Manual

Tips and videos for getting around the CRIPT application interface.

Excel Uploader

Upload user data to CRIPT in tabular form using the Excel template. For more information, see "Excel Uploader" on page 2-2.

Frequently asked questions (FAQs)

Answers to common questions about the CRIPT platform.

Data model

Manuscript that describes the CRIPT data model.

CRIPT blog

Community-driven educational content for polymer informatics.

Terms and Conditions

Rights and obligations of CRIPT and its community of users.

SHARE A THOUGHT

- 1. The Share a thought button (1) allows the user to provide user feedback on the CRIPT platform. The feedback collected is used to refine the CRIPT platform experience to better serve the users. Any feedback is greatly appreciated by the CRIPT platform administrators and programmers. The Share a thought button can be found in the lower left of most pages while navigating through the CRIPT web app.
- 2. Select the type of feedback from the drop-down (2).
- 3. Optional: you can select how you feel, rate the importance, and urgency.
- 4. Optional: you can describe your feedback in more details.
- 5. Optional: you can choose to submit your feedback anonymously, or uncheck it if you wish to be contacted and discuss your suggestions with the CRIPT team.
- 6. Select Submit (3) to send feedback.

CRIPT Name ~ Sear	rch materials	₩c Share a thought ×	Q~ Q. O About ⊖ -
My CRIPT	Ø My CRIPT	Which type of feedback would you like to share?	
III Browse -	Use the links below to navigate through your CRIPT projects.	Interface layout V	
Q Advanced Search	> 🖬 Sample	How does this item make you feel? (optional)	
Featured		frustrated conflused neutral content excited	
🖺 Help		How would you rate its importance? (optional)	
		minor major	
		How would you rate its urgency? (optional)	
		eventual immediate	
		How does this item align with your expectations for it? (optional)	
		far below far above	
		Description (optional)	
		Describe your feedback in more detail	
		Keep my feedback anonymous (uncheck if you are open to being contacted by the CRIPT team)	
1			
			CRI0025

Figure 1-44

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Chapter 2

Excel Uploader

USING EXCEL UPLOADER

REQUIRED DOWNLOADS

Uploading data to CRIPT using the Excel Uploader requires the following:

- Download the Excel Template.
- Download the CRIPT Excel Uploader executable.
- · Locate and record the user specific API token.

EXCEL TEMPLATE

- 1. Navigate to CRIPT Home > Help > Excel Uploader > CRIPT Excel Template, or use the following hyperlink "CRIPT Excel Template".
- 2. Download file and save to a known working location.
- 3. For information on using the template, see "Excel Template" on page 2-12.

CRIPT EXCEL UPLOADER EXECUTABLE

- 1. Navigate to CRIPT Home > Help > Excel Uploader > CRIPT Excel Uploader executable or use the following hyperlink "CRIPT Excel Uploader executable".
- 2. Download file and save to a known working location.
- 3. For information on using the Excel Uploader, see "Excel Uploader" on page 2-2.

EXCEL UPLOADER

1. Locate the saved CRIPT Excel Uploader file and run the file. *NOTE:* All fields must be filled out before upload can begin.

HOST

Host (1) indicates the CRIPT instance that you want to upload your data to, whether that is CRIPT or a private instance.

For most users, the Host will be **criptapp.org**.

NOTE: This field will need to be entered.

Example: Host: criptapp.org

However, if any user wants to connect to their own private instance of CRIPT, they can easily do that by changing the host to whatever URL they are using.



(\$) CRIPT Excel Uploader - version 0.6.0 — 🗆	×
CRIPT Excel Uploader	
Host: criptapp.org	
Om API Token: Token 012345e678910b111213a14151617181b9202122 O	
Project Name: My Project Name	
Collection Name: My Collection Name	
Excel File: Excel absolute file path	
Your data will be uploaded as non-public	
Upload	
Please refer to our <u>documentation</u> on how to fill out this screen	
	CRI00

Figure 2-1

{ **CRIPT** }

API TOKEN

The API Token is needed to authenticate the user before saving data.

1. On the CRIPT home page, select the user icon (1) and Security settings (2).

¢ RIPT	Name 🖌 Sea	h materials		
My CRIPT		Hello, User! © 0000-0000-0000-0000 Quick Tips for Getting Started	^	From the CRIPT blog
Q Advanced Search		With the brand new user interface of CRIPT, you can: • Set display name + visibility in the CRIPT user directory in ④ Account Settings • Create and manage a.k. Access Groups with your colleagues and collaborators • Use the sidebar to browse ⊕ Cilciticns, § Experiments, and more • Rif us what you thrink using the built-in feedback channels To upload you own data, you can use our Excel template + parser or Python SDK: Please visit the ⑤ Docs Hub to lean How You Can Help A Note to Our Early Adopter Community	n more about these and other resources. \sim \sim	Character Alexandree A
		In the Pipeline	ved	bythen olgo yb00tf Duk (bw/m) Hore a helpo denotive polymer research center can benefit from sharing data through a platform such as CNIF. Visit the blog →
₩ ² Share a thought				CR10028

Figure 2-2

2. Select the Copy button (3) next to the API Token (4) to copy it to the clipboard.

¢ RIPT	Name Y Sear	ch materials					0~ (ک 🚯 Abou	t 0-
My CRIPT		Security s	ettings nd access groups.						
Q Advanced Search		API Token Always keep your API toke	n private!	4					
🖺 Help	3	Use your API token to conn	ct to CRIPT using the CRIPT SE	>K or through HT requests by includ	ing the full token in your Authorization HTTP h	ader. If your token is compromised, you can generate a new one.	Ø	C Regenerate A	IPI token
	•	Use access goups to control	who can make changes to obj	ects in the CRIPT database.					
		Showing 1-3 of 3 Acc	ess groups						88
				Name 14		± Members ∿			
			ê	Sample 2_1		8 sheld, tzurcher			
			â	sample 1		2 sheld, tzurcher			
			©	Sample		Sheld, tzurcher			
₩ ² Share a Hought					© 2022 MT Al Right Reserved				
									CRI0032

Figure 2-3

EXCEL UPLOADER

3. Paste API Token into the API Token field (5).

NOTE: The word "Token" in front of the random characters is part of the token as well.



	(CRIPT Excel Uploader - version 0.6.0 — 🗆 🗙
	CRIPT Excel Uploader
	Host: criptapp.org
(5)	Or API Token: Token 012345e678910b111213a14151617181b9202122 ●
\odot	Project Name: My Project Name
	Collection Name: My Collection Name
	Excel File: Excel absolute file path
	Your data will be uploaded as non-public
	Upload
	Please refer to our <u>documentation</u> on how to fill out this screen

Figure 2-4

PROJECT

A Project can be thought of as a bunch of folders with each containing experiments that contribute to a single project. A Project is needed for the software to know which project these experiments are for, and each Collection belongs to a Project. For more information, see "Create a Project" on page 1-10.

- 1. Navigate to the Projects tab within CRIPT.
- 2. Locate and select the project associated with the data to be uploaded.
- 3. Copy the Project name (1).

¢RIPT Name ~	Search materials			67~ Q 🚯 About 🔒 -
My CRIPT Browse ~ Q. Advanced Search	CRIFTID Datakdoso-bif9-4165-addsb-ofec9457a205			co 🎮 🛨 🕲 Public 🚦
Featured	🖻 Collections 🚺 🔺 Materials 🚺 🖷 Files			
🗎 Help	Showing 1-1 of 1 Collection			
	Name %	호 Experiments %	■ Inventory [†] ₄	Project %
	Sample collection			Upload Sample
	<section-header> sample 1</section-header>	© 2022 IAT (Al Rights Reserved		Created Oct. 25, 2022, 3:56 p.m. by sheld Updated Oct. 28, 2022, 7:40 p.m. by sheld
				CRI003
		Figure 2-5		

EXCEL UPLOADER

4. Paste Project name into the Project Name field (2).

Example: Project Name:	Upload Sample
------------------------	---------------

	{{} CRIPT Excel Uploader - version 0.6.0 — — — X
	CRIPT Excel Uploader
	Host: criptapp.org
	• API Token: Token 012345e678910b111213a14151617181b9202122
07	Project Name: My Project Name
	Collection Name: My Collection Name
	Excel File: Excel absolute file path
	Your data will be uploaded as non-public
	Upload
	Please refer to our <u>documentation</u> on how to fill out this screen

Figure 2-6

{ **CRIPT** }

COLLECTION

A Collection can be thought of as a binder filled with experiments. The entire Excel file will become a collection within the CRIPT Platform. For more information, see "Create a Collection" on page 1-20.

- 1. Navigate to the Collections tab within CRIPT.
- 2. Locate and select the collection associated with the data to be uploaded.
- 3. Copy the Collection name (1).

¢RIPT Name	✓ Search materials		©r~ Q.
My CRIPT Browse Q Advanced Search	Sample > Sample		co ► ± ✿ Private : ✓ Edit collection ⊈ Create new experiment
 Featured Help 	No experiments.		Create new inventory Delete this collection
■ Share a thought	tt Sample,2	© 2022 MT (All Rights Reserved	Created Oct. 19, 2022, 6:59 p.m. by sheld Updated Oct. 19, 2022, 6:59 p.m. by sheld
		Figure 0.7	CRI0020

EXCEL UPLOADER

4. Paste Collection name into the Collection Name field (2).



Example: Collection Name: Sample



EXCEL FILE

This field allows the user to search for the file to upload.

1. Select Excel File (1).





EXCEL UPLOADER

- 2. Locate file (2) to be uploaded and select.
- 3. Select Open (3) and the Excel File location will auto populate the field.

This	PC > Desktop > MIT software			ٽ ~		
Organize 🔻 New folder						?
(2)	Name	Date		А	В	
3D Objects	R example template v0-4-2	10/2	1	relation	attribute	
			2	*experiment	*name	
Desktop			3			
Documents			4 A	nionic Polymerization of Styrene	Crude SEC of polystyrene	SE
👆 Downloads			5 A	nionic Polymerization of Styrene	NMR of polystyrene	n
👌 Music			6			+
Pictures			/ 。			+
😽 Videos			9			
Windows (C:)		1	10			
👳 owners (0:)		1	11			\square
programs (P:)		1	12			\square
clients (R:)		1	13			+
shared (St)		1	14			+
			15			
almon enterprise		>	4	material mixture	÷ : •	►
File nan	ne: example_template_v0-4-2			(3) ~	Excel file	\sim
				\sim	Open Cancel	

Figure 2-10

4. Select the Upload button (4).

{\$} CRIPT Exce	l Uploader - version 0.6.0		- 0
		CRIPT Excel Uploader	
=	Host:	criptapp.org	
O	API Token:	Token 012345e678910b111213a14151617181b9202122	0
	Project Name:	My Project Name	
8	Collection Name:	My Collection Name	
	Excel File:	Excel absolute file path	
Your d	ata will be uploaded as	non-public	
(4)		Upload	
Please	refer to our <u>documenta</u>	tion on how to fill out this screen	

Figure 2-11

EXCEL TEMPLATE

COLUMN SETUP

There are two different methods for creating the column structure for data entry.

AUTOFILL

- 1. Open Excel Template.
- 2. The Excel Template will have some of the columns started for reference points.
- 3. Create new columns by using the drop-downs (1).
- **NOTE:** Creating columns requires an understanding of the structure of the individual sheet, see **Chapter 2, "Structure of Excel Sheets"**.





MANUAL ENTRY

- 1. Open Excel Template.
- 2. The Excel Template will have some of the columns started for reference points.
- 3. Unlock the Excel Template by selecting Review (1), and then Unprotect Sheet (2).
- **NOTE:** The sheets do not require a password and are locked to prevent accidentally deleting formulas within the individual cells.





To prevent Data validation problems, do not copy, cut, paste, or drag cells with drop-down data validations into any other cell.

• There are input messages on cells that contain drop-downs to alert the user not to accidentally change.

Please do not copy or paste	
This cells contain data validations.	
To avoid issues please do not copy from, paste on, drag, autofill or bring its validation to any other cell to avoid issues	
	CRI0050

Figure 2-14

STRUCTURE OF EXCEL SHEETS

The first (3) rows define the type of data that will input into a column. Row 4 is used for user instructions and is not used by the program. Row 5 and beyond is used for data input.

te ≪ Format Painter	Calibri B <u>I</u> U	• 11 • • ⊞ • <u>⊅</u> •	A [*] A [×] ∓ ≡ ≫ 20 Wrap Text × Δ ≡ ≡ ≡ ≡	General \$ ~ % 9 %	Good Neutral Check Cell Explanatory	Calculation	insert Delete Forma	∑ AutoSum * ŽV O III Fill × Sort & Find & Analyze ◊ Clear × Finter × Select × Data
Clipboard 15		Font	rs Alignment rs	Number Fa	Styles		Cells	Editing Analysis Adobe
* : ×	$\checkmark = f_X$							
А	в	с	D	E	F	G	н	I.
attribute	attribute	identifiers	identifiers	identifiers	identifiers	property	property	property
*name	notes	cas	names	smiles	bigsmiles	phase	color	molar_mass
								g/mol
		CAS number	additional names	nplified molecular-input line-entry system (SMILE	bigSMILES line notation	phase of matte	risual appearance of substanc	of one mole of a compound; computed from the standard atomic weigh
oluene		108-88-3	methylbenzene; toluene	Cc1ccccc1		liquid	colorless	
styrene		100-42-5	vinylbenzene; phenylethylene; ethenylbenzene; styrer	C=Cc1ccccc1				
-butanol		71-36-3	n-butanol; n-butyl alcohol; 1-butyl alcohol; nBuOH; 1-b	00000				
nethanol		67-56-1	Methyl alcohol; CH3OH; MeOH; methanol	co		liquid	colorless	
olystyrene			poly(styrene); poly(vinylbenzene); polystyrene		[H]{[>][<]C(C[>])clccccc1[<]}C(C	liquid	colorless	
nixture								
omponent1								
component2								
ntermediate_material_	1							

Figure 2-15



ROW 1: CATEGORY

Row 1 (1) defines the characteristic of row 2 (2).

	() A	В	С
1	2 attribute	quantity	identifiers
2	*name	volume	cas
3		ml	
4			CAS number
5	toluene	10	108-88-3
6	styrene	10	100-12-5 CRI003

Figure 2-16

All possible options are:

• attribute

- Defines the nomenclature of the column.
- condition
 - The condition under which the property was found.
 - Some examples include: *temperature, mixing_rate, stirring, and time_duration.*
 - A full list of conditions can be found at the CRIPT Docs hub. Navigate to CRIPT Home > Help > Controlled vocabulary > Condition key, or use the following hyperlink "**Condition controlled vocabulary**".
- identifier
 - Provides the naming method for material in the column.
 - Some examples include: *smiles, bigSmiles, cas, and name.*
 - A full list of material identifiers can found at the CRIPT Docs hub. Navigate to CRIPT Home > Help > Controlled vocabulary > Material identifier key, or use the following hyperlink "Material identifier controlled vocabulary".
- property
 - Describes the characteristic or unit combinations for the property in the column.
 - Some examples include: phase, color, density, and molar_mass.

relation

- · Allows column row to reference another row in a different sheet.
- An example would be to relate attribute (3) *name (4) to relation (5) *mixture (6) on another sheet. For more information on sheets, "See "Individual Excel Sheets" on page 2-17".

1 attribute	attribute	identifiers	identifiers	identifiers	identifiers
2 *name	nouse	Cas	names	smiles	bigsmiles
3		(3)			
4		CAS number	additional names	nplified molecular-input line-entry system (SMILE	bigSMILES line notation
5 toluene	(4)	108-88-3	methylbenzene; toluene	Cc1ccccc1	1
6 styrene	9	100-42-5	vinylbenzene; phenylethylene; ethenylbenzene; styre	C=Cc1ccccc1	
7 1-butanol		71-36-3	n-butanol; n-butyl alcohol; 1-butyl alcohol; nBuOH; 1-b	OCCCC	
8 methanol		67-56-1	Methyl alcohol; CH3OH; MeOH; methanol	со	1
9 polystyrene			poly(styrene); poly(vinylbenzene); polystyrene		[H]{[>][<]C(C[>])c1ccccc1[<]}C(C
10 mixture					
11 component1					
12 component2					
13 intermediate_materi	ial_1				
14					
15					
					CRI0044



1	relation	relation
2	*mixture	*material
3		
4	Pick a value from *name column of material sheet that repersents the mixture	6) Pick a value from *name column of material sheet
5	mixture	component1
6	mixture	component2
7		
8		
9		
10		
11		
12		

Figure 2-18

• quantity

- · Column specifies the amount or combinations of quantities.
- The numerical value can be combined with a unit of measure.

ROW 2: COLUMN NAME

Defines the name of the Column and can be edited by the user.

- Columns beginning with " * " are required (eg. *name).
- Columns beginning with "#" will be ignored (eg. #storage).
 - The # columns are a good idea to use if you want to have some notes but don't want them necessarily read or uploaded to CRIPT.
- Some sheets have drop-downs' for row 2. After selecting an option, row 1, row 3, and row 4 are automatically populated with the correct information.
- **NOTE:** Some sheets have drop-downs for row 2. After selecting an option, row 1, row 3, and row 4 are automatically populated with the correct information.
- **NOTE:** As the controlled vocabulary is updated, it is very possible that the drop-down options and autofill can become outdated.
- Each Excel sheet has rows 1, 3, and 4 locked for protection.
 - This is because rows 1, 3, and 4 contain formulas that if accidentally deleted or overwritten would break the autofill feature.
 - The sheets are protected without a password and can be easily unprotected.



CRI0045

EXCEL UPLOADER

Nesting Headers in Row 2

Nesting can be defined as having a combination of names.

Combined names are separated by a colon ": ".

- Example: density at a certain temperature.
 - · density:temperature
- Example: uncertainty of a material property condition.
 - · density:temperature:uncertainty
- **NOTE:** Nesting "data" column values should derive from the "*name " column of the data sheet. For more information, see "Individual Excel Sheets".
- **NOTE:** Nesting "citation", column values should derive from the "*name " column of the Citation sheet. For more information,See "Individual Excel Sheets" on page 2-17.

ID

The Id feature is used to allow for multiple measurements through time. With Id it is possible to take several measurements through an experiment, and later use nesting to record more details.

If there are multiple densities throughout time and we want to show each of their temperatures (or any other condition), we can use an Id field to differentiate between the different temperatures. We denote an Id with brackets and a number inside such as [1] or [2]. The Id is used to identify distinct properties/conditions of the same type.

1. To identify two density measurements at two different temperatures, we could create the following column headers: [1]density (1), [1]density:temperature (2), [2]density (3), [2]density:temperature (4).

D	E	F	G
	2	3	4
[1]density	[1]density:temperature	[2]density	[2]density:temperature
0.87	20	1	30
		a /a	CRI004



ROW 3: UNITS

Defines the units used in the column.

- Some examples include: Celsius, g/ml.
- A full list of supported units can be found at: https://github.com/hgrecco/pint/blob/master/pint/default_en.txt, or use the following hyperlink "supported units".

ROW 4: INSTRUCTIONS

Many columns contain instructions on row 4. These clarify the data that should go in that column after the value for row 2 is picked.

{ (CRIPT }

ROW 5 AND BEYOND: USER INPUT

These rows are used to enter user data.

- Some columns allow for more than a single value. List values must use a semicolon "; " as a separator.
- · Example of inputting multiple funders.

attribute
funding
list of your funders (e.g, funder1; funder2; funder3)
 funder 1; funder 2; funder 3; funder4
Figure 2-20

INDIVIDUAL EXCEL SHEETS

The Excel Template is comprised of 10 individual sheets in the sheet line (1) for specific characteristics. These are separated into two colored categories. Orange categories (2) are required and Grey categories (3) optional.

NOTE: Sheets can not be renamed, but can be removed. The optional column's not needed can be left blank or deleted.

material	mixture component	process	prerequisite process	process ingredient	process product	process equipment	data	citation	

Figure 2-21

MATERIAL SHEET

The material sheet is used to input the materials at the beginning of the experiment (ingredients), and the material that occurs as a result of the experiment (process product).

1. Enter material's unique name in the first available row (1).

NOTE: Each material entered must be unique and can not be duplicated.

2. Generate new column category (2) as needed for additional information. See "Column setup" on page 2-12.

File Home Insert	Page Layout Formu	las Data <u>Review</u> View Help Acrobat					모 Comments 🗠 Share 👻			
abc III III III III IIII IIII IIIIIIIIII										
A		D	E	F	G	Н	I 🔺			
1 attribute	attribute tifiers	identifiers	identifiers	identifiers	property	property	property			
2 *name	notes cas	names	smiles	bigsmiles	phase color		molar_mass			
3							g/mol			
4	CAS number	additional names r	nplified molecular-input line-entry system (SMILE	bigSMILES line notation	shase of matt	ersual appearance of substanc	of one mole of a compound; computed from the standard atomic weights			
5 toluene	108-88-3	methylbenzene; toluene	Cc1ccccc1		liquid	colorless				
6 styrene	100-42-5	vinylbenzene; phenylethylene; ethenylbenzene; styre	C=Cclcccccl							
7 1-butanol	71-36-3	n-butanol; n-butyl alcohol; 1-butyl alcohol; nBuOH; 1-bu	occcc							
8 methanol	67-56-1	Methyl alcohol; CH3OH; MeOH; methanol	co		liquid	colorless				
9 polystyrene		poly(styrene); poly(vinylbenzene); polystyrene		[H]{[>][<]C(C[>])c1ccccc1[<]}C(C	liquid	colorless				
10 mixture										
11 component1										
							CRI0052			



MIXTURE COMPONENT SHEET (OPTIONAL)

This sheet defines the components of the mixture materials.

- 1. The mixture value (1) is derived from the "*name" column of the material sheet that represents the mixture.
- 2. The material value (2) is derived from the "*name" column of the material sheet.



Figure 2-23

EXPERIMENT SHEET

This sheet defines the experiment.

- 1. Attribute name (1) should be a unique name to describe the experiment.
- 2. Notes (2) are used to add additional information regarding the experiment.
- 3. Funding (3) lists the funders for the project.

NOTE: When entering more then 1 funder, a semicolon "; " must be used to separate the names.

C5	▼ : × √ f _x	funder 1; funder 2; funder 3			•
	А	В	С		
1	attribute	attribute	attribute		
2	*name	1 notes	2 funding	(3)	
3		\checkmark	ک		
4	unique name	regular text	list of your funders (e.g, funder1;	; funder2; funzer3)	
5	Anionic Polymerization of Styrene		funder 1; funder 2; funder 3		
6				Ctrl) -	
7					
8					
9					
10					
11					
12			0		V
3	material mixture co	omponent experiment pr	prerequisite process p	process ingredient process pro	
Rea	dy 🕅 Accessibility: Investigate				Ⅲ Ⅲ − − + 100%
					CRI0054

Figure 2-24

{ (CRIPT }

PROCESS SHEET

Define the processes of each experiment.

- 1. Experiment value (1) is derived from the "*name" column of the experiment sheet.
- 2. Name (2) is a unique name for the process.
- 3. Type (3) is selected from the name column of Process Type file found at CRIPT Home > Help > Controlled vocabulary > Process type, or use the following hyperlink "Process Type".
- 4. Keywords (4) is selected from the name column of Process keywords found at CRIPT Home > Help > Controlled vocabulary > Process keyword, or use the following hyperlink "Process keywords".
- 5. Description (5) describes the process.
- 6. Notes (6) allows user to enter notes regarding process.





- 7. Equipment (7) is selected from the list of equipment found at CRIPT Home > Help > Controlled vocabulary > Equipment key, or use the following hyperlink "equipments".
- 8. Columns H and beyond are customizable. Some examples would include.
 - Process property temperature (8) is selected from the list of Process property found at CRIPT Home > Help > Controlled vocabulary > Process property key, or use the following hyperlink "process property".
 - Condition time_duration (9), is selected from the list of Condition Keys at CRIPT Home > Help > Controlled vocabulary > Process property key, or use the following hyperlink "process property".

1	attribute	property	condition	property
2	equipment	temperature	time_duration	enthalpy_activation
3		degC	min	J/mol
4	you can have a list of equipments	7 Temperature 8	vent occurred (also see time_dur) an	halpy of activation, molar ba
5		25	30	
6		25	30	
7		25	30	
8				
9				
10				CBI0062

Figure 2-26

PREREQUISITE PROCESS SHEET

Define the immediate prerequisites for each process.

- 1. Process (1) is derived from the "*name" column of the process sheet.
- 2. Prerequisite (2) is derived from the "*name" column of the process sheet.

NOTE: Each prerequisite must be from the previous process.

Fi	e Home	Insert	Page Layout	Formul	as Data	Review	View	Help	Acro	bat									
a Spe	DC == [Iling Thesaurus Wo Sta Proofing	123 orkbook atistics	Check Accessibility ~ Accessibility	j Smart Lookup Insights	Translate	Show Changes Changes	New Commen	t C	Previous Comment Commer	Next Comment	Show Comments	Notes Votes	Protect Sheet	Protect Workbool	Allow Edi k Ranges Protect	t Unshare Workbook	Hide Ink ~		
B9	B9 \checkmark : $\times \checkmark f_x$																		
	Α								В										
1				relat	ion					relation									
2				*pro	cess					*prerequisite									
3													Ľ						
4			Pick value from	n *name c	olumn of pr	ocess sheet					1	Pick vo'ae	from *nd	ame colu	mn of pro	cess sheet			
5	Anionic of Styren	ne - 2	/							Anionico	of Styrene -	1/							
6	Anionic of Styren	ne - 3								Anionic o	of Styrene -	2							
7																			ĥ
8																			
																		CRI00)56

Figure 2-27

PROCESS INGREDIENT SHEET

Define the ingredients for each process and their respective quantities.

- 1. Process (1) is derived from the "*name" column of the process sheet.
- 2. Material (2) is derived from the "*name" column of the material sheet.
- 3. Keyword (3) is selected from the list of ingredients found at CRIPT Home > Help > Controlled vocabulary > Ingredient keyword, or use the following hyperlink "Ingredient keyword".
- 4. Columns D and beyond are customizable. Some examples would include.
 - Quantity mole (4) is selected from the list of quantity values found at CRIPT Home > Help > Controlled vocabulary > Quantity key, or use the following hyperlink "Quantity key".

0	4 * : X fx = HYPERLINK("https://criptapp.org/keys/ingredient-keyword/","pick from Name column of ingredients") *												
1	A	В	с	D	E	F	G	^					
1	relation	relation	attribute	quantity	quantity	quantity							
2	*process (1)	*material (2)	*keyword (3)	mole	4 mass	volume							
3				mmole	kg	ml							
4	Pick value from *name column of process sheet	Pick value from *name colv in of material sheet	pick from Name column in ingredients										
5	Anionic of Styrene - 1	toluene	solvent			10							
6	Anionic of Styrene - 2	styrene	monomer		0.455								
7	Anionic of Styrene - 3	methanol	workup										
8	Anionic of Styrene - 3	intermediate_material_1	workup										
9													
10													
11	1												
12	2												
	material mixture component	experiment process prerequisite process	process ingredient process product p	+ : •				Þ					

Figure 2-28

PROCESS PRODUCT SHEET

This sheet describes the resulting product after completing a process.

- 1. Process (1) is derived from the "*name" column of the process sheet.
- 2. Material (2) is derived from the "*name" column of the material sheet.

As \checkmark \times \checkmark $f_{\rm x}$ Anionic of Styrene - 2	*
A B 1 relation 2 *process 3 *material 4 Pick value from *name column of rocess sheet Pick value from *name column of rocess sheet	
5 Anionic of Styrene - 2 intermediate_material_1 6 Anionic of Styrene - 3 polystyrene 7	
10 11 12 ▶ material mixture component experiment process process ingredient process product p ⊕ :	¥
	CR10058

Figure 2-29

PROCESS EQUIPMENT SHEET

Define the equipment used in a process.

- 1. Process (1) is derived from the "*name" column of the process sheet.
- 2. Key (2) is selected from the list of equipment found at CRIPT Home > Help > Controlled vocabulary > Equipment key, or use the following hyperlink "Equipment key".
- 3. Description (3) describes the type of equipment.
- 4. Citation (4) is derived from the "*name" column of the citation sheet.
- 5. Condition temperature (5) is selected from the list of conditions found at CRIPT Home > Help > Controlled vocabulary > Condition key, or use the following hyperlink "Condition key".

A	5 👻 : 🔀 🗸 🏑 🏂 Anionic of Styrene	-1			*
4	А	В	с	D	E
1	relation	attribute	attribute	relation	Condition
2	*process	*key	description	citation	(5) temperature
3	\bigcirc		<u> </u>	4	J degt
4	Pick value from *name column of process sheet	pick from Name column of equipments		Pick value from *name columy of citation sheet	Temperature
5	Anionic of Styrene - 1	glass_rbf	Glass round bottom flask	Ref1	
6					
7					
8					
9					
10					
	more process prerequisite process	s ingredient process product process equ	ipment data citation 🕂	: •	Þ
					CRI0059

Figure 2-30

EXCEL UPLOADER

DATA SHEET

This sheet defines the data files you want to upload to CRIPT, such as a CSV file from a robot, an image, or any other type of file.

- 1. Experiment (1) is derived from the "*name" column of the experiment sheet.
- 2. Name (2) is a unique name for the experiment.
- 3. Type (3) is selected from the list of data types found at CRIPT Home > Help > Controlled vocabulary > Data type, or use the following hyperlink "Data type".
- 4. Source (4) can either be a path to a local file on your computer or a url to a website.
- 5. Sample_preparation (5) is derived from the "*name" column of the process sheet.





CITATION SHEET

This sheet can be used to reference any sources used in the experiments that you want to cite in CRIPT.

1. Required columns are the title (1) and Digital object identifier (doi) (2). Optional information can be added in the additional columns.

abc Spelling Thesaurus Workbook Statistics	Check Smart Accessibility ~	Translate Show Changes	New Delete Previous N Comment Comment Com	lext Show Notes U	Unprotect Protect Allow Edit Unsha Sheet Workbook Ranges Workbo	re Hide					
Proofing	Accessibility Insights	Language Changes	Comments	Notes	Protect	Ink					~
A5 • : ×	√ <i>f</i> ∗ Ref1										~
4	A	В	С	D	E	F	G	н	1	J	
1 attr	ribute	attribute	attribute	attribute	attribute	attribute	attribute	attribute	attribute	attribute	
2 *t		*doi	2 authors	journal	publisher	year	volume	issue	pages	issn	
3			\sim								
4 5 Ref1	_/	doi:/1	Brad;	journal	o'reilly media	2022	11	943		test	tes
6											
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8											_
9											
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12											
1 process	prerequisite process	process ingredient	process product process equi	inment data citation							
, process	prerequisite process	processingredient	process produce process equi							CRI	0061

Figure 2-32

Chapter 3

Python SDK

QUICKSTART

PREREQUISITES:

- Python version 3.9 or higher
- Internet access
- API Token. For more information, See "API Token" on page 2-3

INSTALLATION

- 1. Download and install Python version 3.9 or higher.
- 2. Open the command prompt by selecting the Windows icon and type "CMD".
- 3. Enter "pip install cript" to the command line (1) and press enter.



Figure 3-1

CONNECT TO CRIPT

1. Enter "python" at cursor (1) and press enter.

Command Prompt	_		×
			^
C:\WINDOWS\System32>pip install cript			
Requirement already satisfied: cript in c:\users\sheld\appdata\local\programs\python\python310\lib\site-pa	ckages	(0.6.	0)
Requirement already satisfied: beartype>=0.10.4 in c:\users\sheld\appdata\local\programs\python\python310\ ges (from cript) (0 11 0)	lib\sit	te-pac	ka
Requirement already satisfied: pint>=0.19.2 in c:\users\sheld\appdata\local\programs\python\python310\lib\ (from cript) (0.20.1)	site-pa	ackage	s
Requirement already satisfied: requests>=2.27.1 in c:\users\sheld\appdata\local\programs\python\python310\ ges (from cript) (2.28.1)	lib\sit	te-pac	ka
Requirement already satisfied: globus-sdk>=3.7.0 in c:\users\sheld\appdata\local\programs\python\python310 ages (from cript) (3.14.0)	\lib\si	ite-pa	ick
Requirement already satisfied: pyjwt[crypto]<3.0.0,>=2.0.0 in c:\users\sheld\appdata\local\programs\python \site-packages (from globus-sdk>=3.7.0->cript) (2.6.0)	\pythor	n310\l	ib
Requirement already satisfied: cryptography!=3.4.0,>=3.3.1 in c:\users\sheld\appdata\local\programs\python \site-packages (from globus-sdk>=3.7.0->cript) (38.0.3)	\pythor	n310\l	ib
Requirement already satisfied: charset-normalizer<3,>=2 in c:\users\sheld\appdata\local\programs\python\py te-packages (from requests>=2.27.1->cript) (2.1.1)	thon316	0\lib\	si
Requirement already satisfied: idna<4,>=2.5 in c:\users\sheld\appdata\local\programs\python\python310\lib\ (from requests>=2.27.1->cript) (3.4)	site-pa	ackage	s
Requirement already satisfied: urllib3<1.27,>=1.21.1 in c:\users\sheld\appdata\local\programs\python\pytho packages (from requests>=2.27.1->cript) (1.26.12)	n310\li	ib∖sit	e-
Requirement already satisfied: certifi>=2017.4.17 in c:\users\sheld\appdata\local\programs\python\python31 kages (from requests>=2.27.1->cript) (2022.9.24)	0\lib\s	site-p	ac
Requirement already satisfied: cffi>=1.12 in c:\users\sheld\appdata\local\programs\python\python310\lib\si rom cryptography!=3.4.0.>=3.3.1->globus-sdk>=3.7.0->cript) (1.15.1)	te-pack	kages	(f
Requirement already satisfied: pycparser c:\users\sheld\appdata\local\programs\python\python310\lib\sit om cffi>=1.12->cryptography!=3.4.0,>=3.2 1 globus-sdk>=3.7.0->cript) (2.21)	e-packa	ages (fr
C:\WINDOWS\System32>python			~



- 2. Open text editor (Microsoft Notepad shown).
- 3. Copy and paste the example code into notepad to modify.

host = "<endpoint_hostname>" # e.g., criptapp.org token = "<your_api_token>" cript.API(host, token)

- 4. Modify the host line (1) with the application programming interface (API) destination.
- 5. Modify the token line (2) with the user token. See "API Token" on page 2-3.

File Edit Format View Help	
<pre>inport cript host = "criptapp.org"1 token = "Token 5d357051969ef9f4390dc1896aff0cff44852bcc" cript.API(host, token)</pre>	2)
	OBIOOCO

Figure 3-3

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{ (CRIPT }

- 6. Copy and paste modified host line from Notepad to the command prompt cursor (3) and press enter.
- 7. Copy and paste modified token line from Notepad to the command prompt cursor (4) and press enter.
- 8. Copy and paste cript.API line from Notepad to the command prompt cursor (5) and press enter.
- 9. Confirm connected to API site (6).

NOTE: Each line must be entered individually.

Command Prompt - python -	×]
Requirement already satisfied: globus-sdk>=3.7.0 in c:\users\sheld\appdata\local\programs\python\python310\lib\site- ages (from cript) (3.14.0)	pack ^	•
Requirement already satisfied: requests>=2.27.1 in c:\users\sheld\appdata\local\programs\python\python310\lib\site-p ges (from cript) (2.28.1)	acka	
Requirement already satisfied: cryptography!=3.4.0,>=3.3.1 in c:\users\sheld\appdata\local\programs\python\python310 \site_packages (from globus-sdk>=3.7.0->cript) (38.0.3)	\lib	
Requirement already satisfied: pyjwt[crypto]<3.0.0,>=2.0.0 in c:\users\sheld\appdata\local\programs\python\python310 \site_packages (from globus-sdk>=3.7 e>cript) (2.6.0)	\lib	
Requirement already satisfied: urllib3<1.27,>=1.21.1 in c:\users\sheld\appdata\local\programs\python\python310\lib\s nackages (from requests>=2.27.1->cript) (1.26.12)	ite-	
Requirement already satisfied: idna<4,>=2.5 in c:\users\sheld\appdata\local\programs\python\python310\lib\site-packa	ges	
Requirement already satisfied: certifi>=2017.4.17 in c:\users\sheld\appdata\local\programs\python\python310\lib\site	-pac	
Requirement already satisfied: charset-normalizer<3,>=2 in c:\users\sheld\appdata\local\programs\python\python310\li te-nackages (from requests)=2 27 1->crint) (2 1 1)	b∖si	
Requirement already satisfied: cffi>=1.12 in c:\users\sheld\appdata\local\programs\python\python310\lib\site-package	s (f	
Requirement already satisfied: pycparser in c:\users\sheld\appdata\local\programs\python\python310\lib\site-packages om cffi>=1.12->cryptography!=3.4.0,>=3.3.1->globus-sdk>=3.7.0->cript) (2.21)	(fr	
C:\WINDOWS\System32>python		
Type "help", "copyright", "credits" or "license" for more information.		
<pre>>>> import cript >>> host = "criptapp.org"3</pre>		
>>> token = "Token 5d357051970ef9f4390db1896aff0cff44852bcc"		
Connected to https://criptapp.org/api6	~	
	CRI0	067

Figure 3-4

SAMPLE TASKS

The sample tasks are excellent templates to be used to record data. Replace sample tags in quotes with the name that applies to the project.

Create a node:

Create a Project and Collection node.

```
proj = cript.Project(name="MyProject")proj.save()
```

coll = cript.Collection.create(project=proj, name="MyCollection")

Create an Experiment node.

```
expt = cript.Experiment(
    collection=coll,
    name="Anionic Polymerization of Styrene with SecBuLi"
)
expt.save()
```

NOTE: The use of create() here, instantiates and saves the object at the same time.

PYTHON SDK

Update a node:

Update the Project and Collection node created above.

```
proj.name = "OurProject"
proj.save()
```

coll.update(name="OurCollection")

NOTE: The use of update() here, updates and saves a node at the same time.

Delete a node:

Delete the Collection node created above.

coll.delete()

Get an existing node:

Get the official CRIPT Project node.

```
proj = cript.Project.get(name="CRIPT")
```

Get the official styrene Material node via name.

styrene = cript.Material.get(project=proj.uid, name="Styrene")

Get the official styrene Material node via UID.

styrene = cript.Material.get(uid="<material_uid>")

Get the official styrene Material node via URL.

```
styrene = cript.Material.get(url="<material_url>")
```

Get Material nodes:

Get an existing Inventory node from the database.

uid = "134f2658-6245-42d8-a47e-6424aa3472b4"

- inv = cript.Inventory.get(uid=uid, get_level=1)
- **NOTE:** Get_level is set to 1 so that the Material nodes are auto-generated. This parameter defaults to 0, but can be set to any integer.

Notice that the Material node objects have been auto-generated.

type(inv.materials[0])
<class 'cript.data_model.nodes.material.Material'>

Run a search query:

Search for Material nodes with a molar mass of less than 10 g/mol.

```
res = cript.Material.search(
    properties = [
        {
            "key": "molar_mass",
            "value__lt": 10,
            "unit": "g/mol"
        }
    ]
)
```

Page through the results.

res.json()	# View the raw JSON for the query
res.objects()	# Generate objects for the current page
res.next_page()	# Flip to the next page
res.previous_page	e() # Flip to the previous page

Upload a file:

User will need a Project and Data node to upload a file.

```
proj = cript.Project.get(uid="<project_uid>")
data = cript.Data.get(uid="<data_uid>")
```

Create a File node that points to a local file.

```
path = "path/to/local/file"
f = cript.File(project=proj, source=path)
file.save()
```

Download a file:

Download the file that was uploaded above.

```
path = "path/to/local/file"
f.download_file(path=path)
```

NOTE: The default path for a download is in the current directory.

PYTHON SDK

Create a Process node:

```
prcs = cript.Process(
    experiment=expt,
    name="Anionic of Styrene",
    type = "multistep",
    description = "In an argon filled glovebox, a round bottom flask was filled with 216 ml of dried toluene. The "
        "solution of secBuLi (3 ml, 3.9 mmol) was added next, followed by styrene (22.3 g, 176 mmol) to "
        "initiate the polymerization. The reaction mixture immediately turned orange. After 30 min, "
        "the reaction was quenched with the addition of 3 ml of methanol. The polymer was isolated by "
        "precipitation in methanol 3 times and dried under vacuum."
    )
    prcs.save()
```

Add Ingredient nodes to the Process node:

Get the Material nodes from the Inventory node.

```
solution = inv['SecBuLi solution 1.4M cHex']
toluene = inv['toluene']
styrene = inv['styrene']
butanol = inv['1-butanol']
methanol = inv['methanol']
```

Define Quantity nodes indicating the amount of each Ingredient.

```
initiator_qty = cript.Quantity(key="volume", value=0.017, unit="ml")
solvent_qty = cript.Quantity(key="volume", value=10, unit="ml")
monomer_qty = cript.Quantity(key="mass", value=0.455, unit="g")
quench_qty = cript.Quantity(key="volume", value=5, unit="ml")
workup_qty = cript.Quantity(key="volume", value=100, unit="ml")
```

Create Ingredient nodes for each:

```
initiator = cript.Ingredient(
  keyword="initiator",
  material=solution,
  quantities=[initiator_qty]
)
solvent = cript.Ingredient(
  keyword="solvent",
  material=toluene,
  quantities=[solvent qty]
)
monomer = cript.Ingredient(
  keyword="monomer",
  material=styrene,
  quantities=[monomer_qty]
)
quench = cript.Ingredient(
  keyword="quench",
  material=butanol,
  quantities=[quench_qty]
)
workup = cript.Ingredient(
  keyword="workup",
  material=methanol,
  quantities=[workup qty]
)
```

Add Ingredient nodes to the Process node:

prcs.add_ingredient(initiator) prcs.add_ingredient(solvent) prcs.add_ingredient(monomer) prcs.add_ingredient(quench) prcs.add_ingredient(workup)

Add Condition nodes to the Process node:

```
temp = cript.Condition(key="temperature", value=25, unit="celsius")
time = cript.Condition(key="time_duration", value=60, unit="min")
prcs.add_condition(temp)
prcs.add_condition(time)
```

Add Property node to the Process node:

```
yield_mass = cript.Property(
    key="yield_mass",
    value=0.47,
    unit="g",
    method="scale"
)
prcs.add_property(yield_mass)
```



PYTHON SDK

Create a Material node (process product):

Instantiate the node.

```
polystyrene = cript.Material(project=proj, name="polystyrene")
```

Add Identifier nodes.

```
names = cript.ldentifier(
    key="names",
    value=["poly(styrene)", "poly(vinylbenzene)"]
)
bigsmiles = cript.ldentifier(
    key="bigsmiles",
    value="[H]{[>][<]C(C[>])c1ccccc1[<]}C(C)CC"
)
chem_repeat = cript.ldentifier(key="chem_repeat", value="C8H8")
polystyrene.add_identifier(names)
polystyrene.add_identifier(chem_repeat)
polystyrene.add_identifier(bigsmiles)</pre>
```

Add Property nodes.

```
phase = cript.Property(key="phase", value="solid")
color = cript.Property(key="color", value="white")
```

polystyrene.add_property(phase)
polystyrene.add_property(color)

Save the Material and add it to the Process node as a product.

```
polystyrene.save()
prcs.add_product(polystyrene)
```

Save the Process node.

prcs.save()

Create a File node and upload a file:

Instantiate a File node and associate it with the Data node created above.

```
path = "path/to/local/file"
f = cript.File(project=proj, source=path)
```

NOTE: The source field should point to a file on the local filesystem.

NOTE: Depending on the file size, there could be a delay while the checksum is generated.

Upload the local file by saving the File node. Follow all prompts that appear.

api.save(f)

Create a Data node:

```
sec = cript.Data(
    experiment=expt,
    name="Crude SEC of polystyrene",
    type="sec_trace",
)
```

Add the uploaded File to the Data node.

sec.add_file(f)
sec.save()

Associate a Data node with a Property node:

Create one more Property node for polystyrene.

mw_n = cript.Property(key="mw_n", value=5200, unit="g/mol")

Add the Data node to the new Property node.

mw_n.data = sec

Add the new Property node to polystyrene, then save it.

polystyrene.add_property(mw_n)
polystyrene.save()

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