

Sample cassette tracking system in macromolecular crystallography beamlines at the Photon Factory

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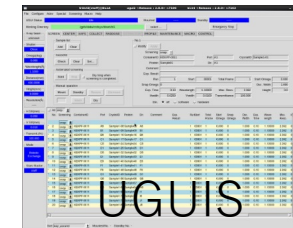
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Institute of Particle and Nuclear Studies, High Energy Accelerator Research Organization

MX beamlines at the Photon Factory

All 5 beamlines are equipped

- Sample changer
- High precision diffractometer
- Pixel array detector

A common control software



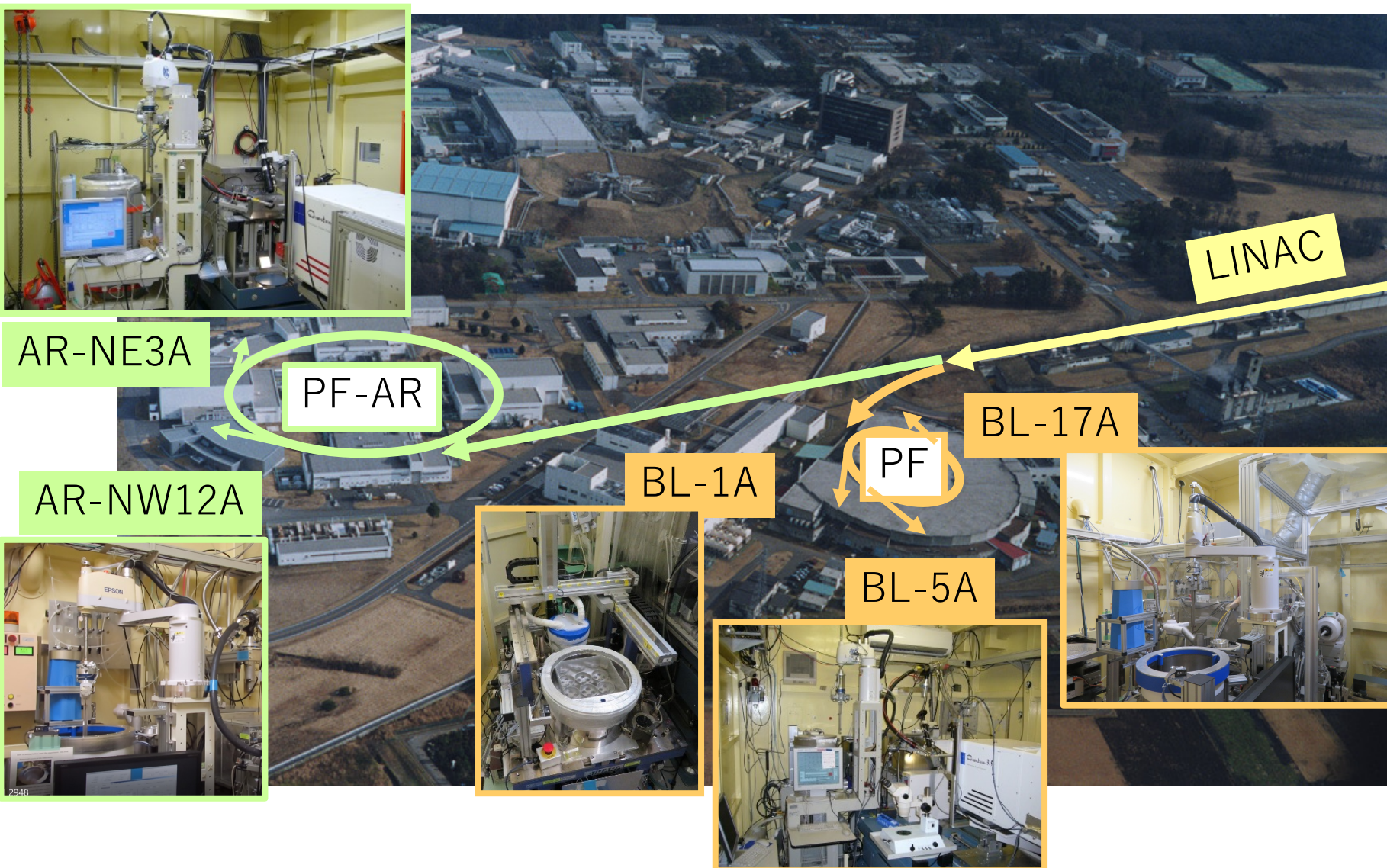
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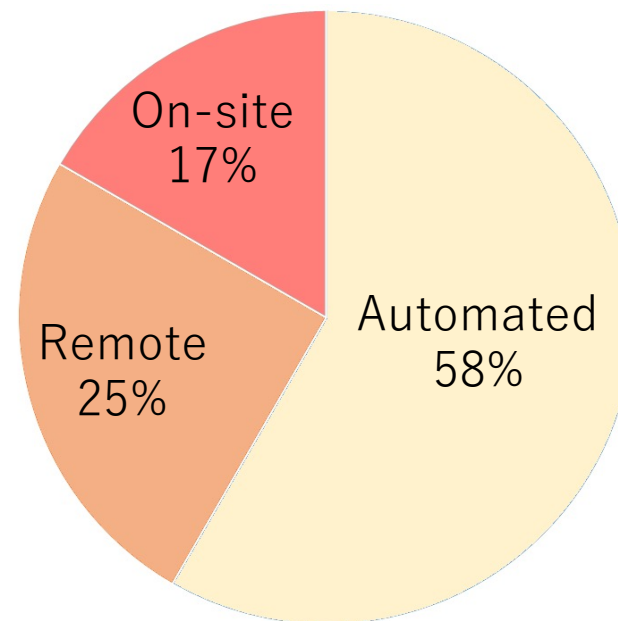
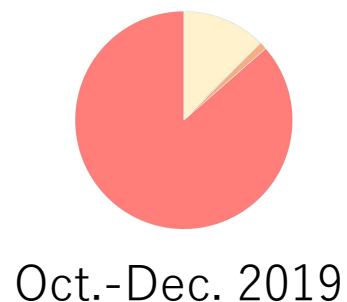


All beamlines supports

- *X-ray centering-based automated unattended measurements*
- *Remote interactive experiments with NoMachine*



Impact of COVID-19 pandemic in PF MX BLs



Jun. 2020

Currently, 75 % of beamtime are automated or remote.

Beamtime allocation (June 2020)

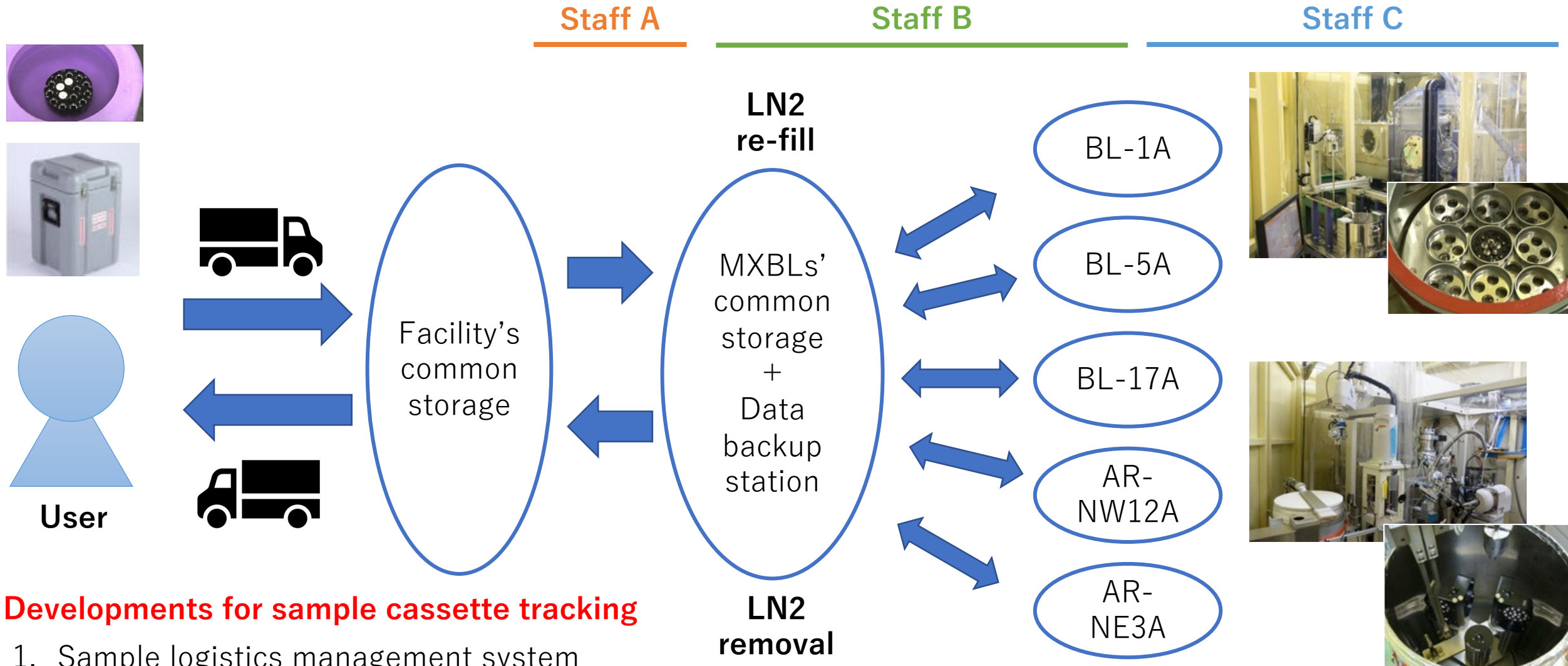
	PF-MODE	BL1A		BL5A		BL17A	
		10:00 - 17:30	18:00 - 1:30	9:30 - 17:00	17:30 - 1:00	9:30 - 17:00	17:30 - 1:00
6/17 Wed	A	S	調整	S	調整	S	調整
	B	S	調整	S	調整	S	調整
	C	S	調整	S	調整	S	調整
6/18 Thu	A	S	調整	I	第	18G621	大沼 貴之
	B	S	調整	I	第 / 予	S	調整
	C	S	調整	S	調整	I	J
6/19 Fri	A	I	大 / 予	I	杏	I	J / 予
	B	19G038	阿部 郁朗	Ra	ラビッド		
	C	S	調整				
6/20 Sat	A	20RP-04	松垣 直宏	19G100	高妻 孝光	I	アステラス
	B			BINDS	BINDS		
	C						
6/21 Sun	A			18G505	藤城 貴史		
	B			19G104	玉田 太郎		
	C			S	調整		
6/22 Mon	A	I	旭	19G681	本田 真也	19G004	森田 洋行
	B	19G625	寺脇 慎一	18G614	藤本 瑞	19G008	富田 耕造
	C	20G099	西野 達哉	20G056	田上 俊輔	19G027	中村 照也
6/23 Tue	A	19G081	千田 俊哉	19G136	矢嶋 俊介	19G592	河合 聡人
	B	18G522	森田 洋行	19G535	松井 崇	18G523	横山 英志
	C	19G510	禾 晃和	18G645	田中 伊知朗	19G063	竹内 恒
6/24 Wed	A	18G559	田之倉 優	19G508	殿塚 隆史	19G045	中村 顕
	B	19G587	久保田 智巳	19G080	宮原 郁子	18G521	小沼 剛
	C	19G509	松村 洋寿	18S2-002	佐藤 文菜	19G051	佐藤 宗太
6/25 Thu	A	X	N/A	X	N/A	X	N/A
	B	X	N/A	X	N/A	X	N/A
	C	S	調整	S	調整	S	調整
6/26 Fri	A	I	杏	Ra	ラビッド	19G148	山田 太郎
	B	20G010	阿部 郁朗			I	アステラス
	C	19G096	前仲 勝美				
6/27 Sat	A	19G077	大西 康夫	19G149	片柳 克夫		
	B	19G150	姚 関	19G097	宮崎 剛垂		
	C	19G502	沼田 倫征	19G669	工藤 紀雄		
6/28 Sun	A	19G025	田上 貴祥	18G648	林 郁子	I	アステラス
	B	18G613	星野 忠次	19G154	菱木 麻美		
	C	S	伏信 進也	19G099	夏目 亮		
6/29 Mon	A	I	ベ / 大	18S2-002	佐藤 文菜	19G512	海野 昌喜
	B	19G639	山崎 和彦	19G048	長江 雅倫	19G001	原 幸大
	C	S	調整	19G076	木平 清人	I	J
6/30 Tue	A	I	第	18G689	尾高 雅文	I	J / 予
	B	19G530	藤橋 雅宏	19G015	櫻庭 春彦	S	調整
	C	20G023	喜田 昭子	19G578	五十嵐 圭日子	S	調整

Result of the increase of automated and remote experiments

Many samples are arrived every day.
Any mistake is fatal for its experiment.



Sample logistics



Developments for sample cassette tracking

1. Sample logistics management system
2. Automatic Uni-puck identification by the sample changer

Sample logistics management system

Shipping information	
Beamtime	2020-10-26 09:30 - 2020-10-26 17:00
Beamline	BL-1A
Proposal No.	19G081
Shipper	Contact person (*)
	Affiliation
	Position
	Email (*)
	Email(confirm) (*)
	Phone number (*)
	Zip code (*)
	Address (*)
Date	Shipping
	Expected arrival
	Receipt
Contents of the shipment	DryShipper
	HDD
Comment	

Apply

Close

PDF file by
email



Sample logistics management system

A BL staff reads the QR code and updates the status on each step .

The status is managed by database and shared by all BL staffs.

Beamtime term	Sample	Fatal mistake
Jun. 2020 (w/o the system)	52	1
Oct. – Dec. 2020 (with the system)	148	0

premo.kek.jp/RCM-Web/action/xmlviewer/executeTemplateWithParam.html

PRemo - List of shipment

PRemo
PF Remote Monitoring system

Filter (Status)
☒ None ☒ Shipping ☒ Receipted ☒ Returned ☐ Closed

Filter (Beamline)
☒ BL-1A ☒ BL-5A ☒ BL-17A ☒ AR-NW12A ☒ AR-NE3A

Filter (Style, Type)
☐ On-site ☐ Industrial use

Sort key 1
Beamtime (Start) ☒ A → Z ☐ Z → A

Sort key 2
- ☐ A → Z ☐ Z → A

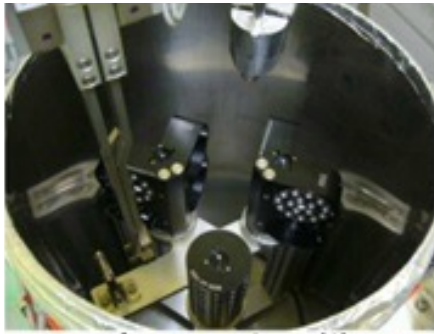
Reload

Beamtime	Beamline	Proposal number	Spokesperson	Chemical form	Status							
	Style	User id	Contact person		Shipping	Exp. arrival	Receipt	Backup	Set up	Experiment	Clear up	Return
02-22 09:30 - 02-22 17:00	BL-17A Remote	2019G008 tomita	富田 耕造 富田耕造	Uploaded	02-18	02-19 (Fri)	02-19	Doing	02-19	02-22	02-23	02-23
02-22 18:30 - 02-23 01:30	BL-5A Automated	2019G656 shomura	庄村 康人 庄村康人	Uploaded	02-17	02-18 (Thu)	02-18	Doing	02-19	02-23	02-23	02-23
02-23 01:30 - 02-23 09:00	BL-1A Automated	2019G510 nogi	禾 晃和 禾 晃和	Uploaded	02-18	02-19 (Fri)	02-19	02-23	02-19			02-23
02-23 09:30 - 02-24 09:00	BL-17A Automated	Rapid miwa	丹羽 隆介 海老原佳奈	Uploaded	02-18	02-18 (Thu)	02-19		02-22		02-24	02-24
02-23 09:30			丹羽 隆介									

Status								
Shipping	Exp. arrival	Receipt	Backup	Set up	Experiment	Clear up	Return	Close
02-18	02-19 (Fri)	02-19	Doing	02-19	02-22	02-23	02-23	

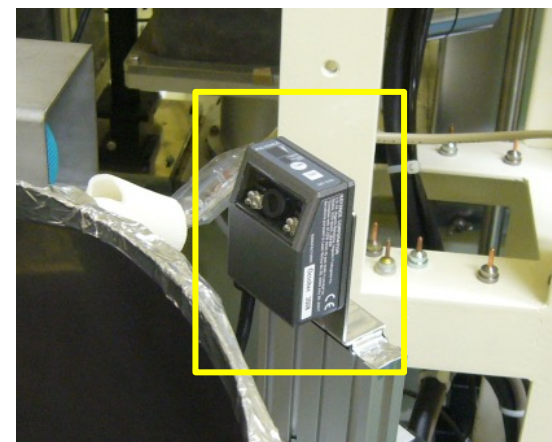
02-26 17:00	Automated	senda	千田美紀	Uploaded	02-24	02-24 (Wed)	02-24		02-24	02-26	02-26	03-01	
02-26 10:00 - 02-27 09:30	AR-NE3A Automated	Rapid tyokoyama	横山 武司 横山武司	Uploaded	02-24	02-25 (Thu)	02-25	Doing	02-25	02-26	03-01	03-01	
02-26 10:30 - 02-26 18:00	AR-NW12A Remote	2019G136 yajima	矢嶋 俊介 矢嶋 俊介	Uploaded	02-24	02-25 (Thu)	02-25	03-01			02-26	03-01	
02-26 17:30 - 02-27 09:00	BL-1A Remote	2020G016 mizutani	村田 武士 鈴木花野	Uploaded	02-24	02-25 (Thu)	02-25	03-01	02-25	02-26	02-26	03-01	
02-26 17:30 - 02-27 01:00	BL-17A Automated	2019G095 hokudai	前仲 勝実 Shunsuke Kita	Uploaded	02-22	02-24 (Wed)	02-24	03-01	02-26	02-27	03-01	03-01	
02-27 09:30 - 02-27 17:00	BL-1A Remote	2020G563 tanokura	田之倉 優 宮川拓也	Uploaded	02-25	02-26 (Fri)	02-26	03-01	02-26	02-27	02-27	03-01	
02-27 09:30	BL-17A	2019G071	千田 俊哉	Uploaded	02-26	02-26 (Fri)	02-24		02-26	02-27	03-01	03-01	

Uni-puck identification by a 2D barcode pin

PAM-HC (BL-1A)	PAM (other 4 BLs)
	
	
9 Uni-pucks	12 Uni-pucks or 3 SSRL cassettes



[BarcodeList]
 C0203AO608:SEN003
 C0203AO621:SEN004
 C0203AO628:SEN005
 C0203AO630:CPS1656



The sample changer reads the barcode of the pin and identify Uni-puck ID and position in the Dewar automatically.

Current problem

- Readout error
- Time consuming
(>20 mins for 12 pucks)

Summary

- Photon Factory has five MX beamlines.
- 75 % of beamtime are automated unattended measurements or remote interactive experiments.
- Sample cassette tracking is necessary for automated or remote beamtime operation.
- We have developed sample logistics management system.
- A 2D barcode pin is used for Uni-puck identification.
- We are working on RFID for a fast and robust Uni-puck identification.

Acknowledgements



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Thank you for your attention!