



BIOLOGICAL
CRYSTALLOGRAPHY

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Supporting information for article:

ISPyB for BioSAXS, the gateway to user autonomy in solution scattering experiments

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S1. Mobile access

The ISPYBB web interface provides easy access to the information in the database from different places and different platforms. Recently, the incorporation of HTML5 technology allows ISPYBB pages to be accessed using mobile technology (both iOS and android) – allowing greater convenience for an increasingly connected user community. Users can prepare experiments; monitor their sample shipment; or view summary pages of the data collections from any device of their choice from any location with an internet connection (Ginn et al., 2013).

S2. Ancillary tools for Beamline Staff

In order to take full advantage of the logged experiments beamline staff tools have been provided to aid diagnostics and ensure reliability.

S2.1. Data mining

Data logging increases efficiency at all stages of an experiment (preparation, acquisition and analysis) by presenting the important information in an intuitive way. Integrating ISPyB for BioSAXS gives additional indirect benefits to the users. With the 'Data mining' tool beamline staff are informed of how the user community is using the beamline and how the beamline is performing. This allows feedback to ensure reliability and data quality, rapid response in case of problems and improved anticipation of the real needs of the community for future developments. Some essential feedback for beamline managers is shown in Figure S2.

S2.2. Logger

The ISPyB logger is a tool for developers, system administrators and beamline staff. It allows them to diagnose a problem even before users are aware of its existence. A typical example is shown in Figure S3, the view which highlights logins; communication between programs, which has highlighted a computer switched off and facilitated an immediate restart preventing data loss; errors, which has enabled the development team to be deploying the bug fixes when the local contact called to highlight an issue. The view also highlights time consuming methods among other statistics, allowing the developers to focus on issues directly affecting experiments. Any time saved diagnosing problems is of direct benefit to the users and monitoring of how the systems is used under real conditions enables optimisation giving reliability and proactively preventing lost time.

S3. Technical specifications

ISPyBB is written in Java J2EE and uses the JBoss Application Server (<http://jboss.org/jbossas>). It combines Struts Model-View-Controller (MVC) Web Application Framework (<http://struts.apache.org>) and pure JavaScript using the library Ext JS (www.sencha.com) which corresponds to HTML5 standards. The end-user interface is a pure web-based application that is

accessible from any compatible browser. At the ESRF the database used for ISPyBB is MySQL (<http://www.mysql.com>) which is an open-source relational database and distributed under the terms of the GNU General Public License. At the DLS the database used is Oracle (<http://www.oracle.com>). ISPyBB uses ejb3s with Hibernate and/or ejbql as an object-relational mapping tools for the Java language, providing a framework for mapping an object-oriented model to a relational database.

In BioSAXS experiments the data visualization is crucial for interpreting the results. For ISPyBB a set of visualizations and plots has been developed. Once results have been analyzed by the online data analysis pipeline EDNA (Incardona et al, 2009), the ISPyBB database is populated through the web services and the user interface makes such results accessible in real time. For data visualization it has extended the use of Java Applets or other technologies like Flash or Silverlight where the installation of third-party plugging of software is necessary. However, in ISPyBB all data representation is carried out by the browser avoiding the need of installing external software taking the advantage of using HTML5 standard including SVG (Scalar Vector Graphics) and WebGL (Web Graphics Library). A current limitation is that HTML5 based applications can be run only in computers with recent graphics cards and with compatible web browsers.

S3.1. Sustainability

ISPyB is anticipated to be in long term use at multiple sites and therefore maintenance and support of the technologies used is of issue. The GUI has been developed using an inheritance-based design in order to move from one library to another in the case it becomes necessary in the future to move away from extJS. The database structure is in principle not restricted and already is adapted for use with Oracle and Mysql databases. Oracle has committed that MySQL will remain open source until 2015. However, there is no guarantee after this. For the facilities using a MySQL DataBase, the adaptation to Oracle already exists and switching should therefore be less difficult. Additionally a good choice could be MariaDB (<https://mariadb.com/kb/en/mariadb-versus-mysql-compatibility/>) which is a drop-in replacement to MySQL. When matching the versions of MySQL and MariaDB we would simply need to uninstall MySQL and install MariaDB which should require minimal effort.

Macromolecules

Multiple Select

Macromolecule	Buffer Conditions
MES6	6.80 mg/ml 1x ⚠
	11.50 mg/ml 1x ✓
	19.10 mg/ml 1x ⚠
HEPES	4.30 mg/l
	8.10 mg/l
	16.10 m
TRIS9	4.00 mg/ml 1x ✓
	9.60 mg/ml 1x ⚠
	16.80 mg/ml 1x ⚠
TRIS8	6.30 mg/l
	8.80 mg/l
	16.80 m
NAA4	4.20 mg/ml 1x ⚠
	8.10 mg/ml 1x ⚠
	14.70 mg/ml 1x ⚠
NAAS	3.80 mg/l
	8.30 mg/l
	16.30 m
TEST	6x 0.00 mg/ml 6x ⚠
	1.00 mg/ml 1x ⚠
BWATER	1.00 mg/ml 1x ⚠
	17x 6.80
TBS2	2.70 mg/l
	3.00 mg/l
	3.40 mg/l
	17x 6.80

A
 Good quality measurements
 Probably valid with manual processing
 More n...

(a)



(b)

Figure S1 Mobile view using Safari on iPhone a) Explore results, b) Data collection.

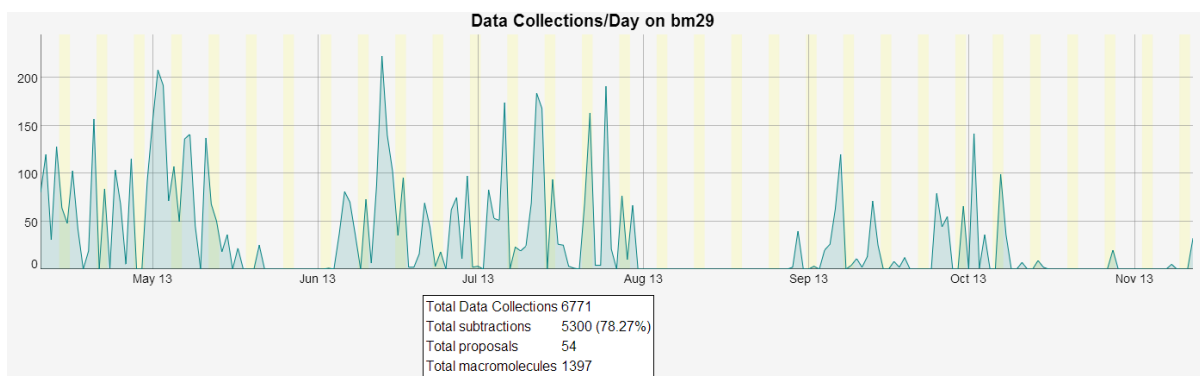


Figure S2 Examples of 'Data mining' table for beamline managers, Data Collections per day table displays productivity of the beamline.

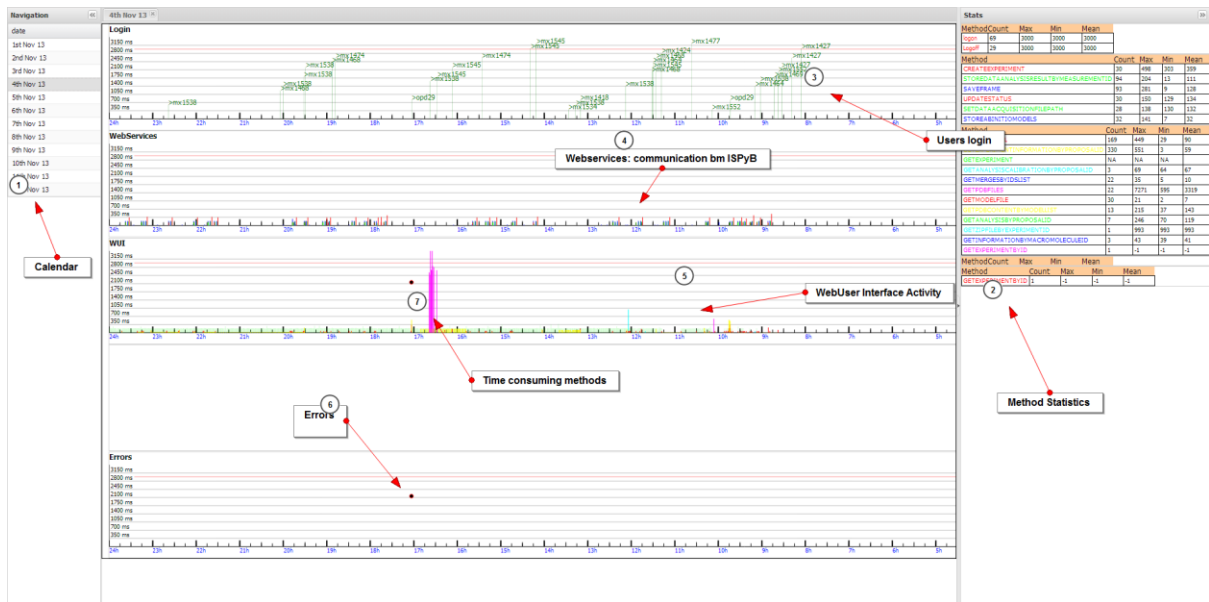


Figure S3 Example for the use of the logger tool for monitoring our webservices. 1) Calendar to select dates to view, 2) statistics of methods used, 3) User login times, 4) times for Beamline ISPyB communications 5) User activate on Web interface, 6) Errors (highlighting problems which needs to be fixed), 7) time consuming methods (in need of further optimisation).

ISPyB
Information System for Protein Crystallography Beamlines

Prepare Experiment

Lab-contacts Shipping Prepare Experiment Data Acquisition Explore Your Results Feedback Home

Macromolecules
Buffers

Name: *II. - Temperature Series, flow, viscosity and transmission change* [Download Source File](#)
 Type: *TEMPLATE*
 Date: *Jan 13, 2014 2:56:38 PM*

Comments: [BsxCube] Generated from BsxCube

Measurements Specimens Requirements

Specimen			Parameters					Comments	
Macromo.	Conc.	Buffer	Exp. Temp.	Vol. Load	Trans.	Wait T.	Flow		
C2	1.000	B1	4.00 C	40.00 μ l	100 %	0 s	yes	low	<input type="button" value="REMOVE"/>
A	1.000	B Plate: [2, A-9]	6.00 C	40.00 μ l	80 %	0 s		medium	<input type="button" value="REMOVE"/>
C1	1.000	B Plate: [2, A-9]	6.00 C	40.00 μ l	90 %	0 s	yes	low	<input type="button" value="REMOVE"/>
A	1.000	B Plate: [2, A-9]	6.00 C	40.00 μ l	90 %	0 s	yes	medium	<input type="button" value="REMOVE"/>
A	1.000	B Plate: [2, A-9]	6.00 C	40.00 μ l	90 %	0 s	yes	low	<input type="button" value="REMOVE"/>
A	1.000	B Plate: [2, A-9]	6	40	90	0	<input checked="" type="checkbox"/>	medi	<input type="button" value="REMOVE"/>
A	1.000	B Plate: [2, A-9]	6.0	<input type="button" value="Update"/>	<input type="button" value="Cancel"/>		yes	low	<input type="button" value="REMOVE"/>
C1	1.000	B Plate: [2, A-9]	6.00 C	40.00 μ l	100 %	0 s	yes	low	<input type="button" value="REMOVE"/>
C2	1.000	B Plate: [2, A-9]	6.00 C	40.00 μ l	100 %	0 s	yes	low	<input type="button" value="REMOVE"/>
C1	1.000	B Plate: [2, A-9]	6.00 C	40.00 μ l	100 %	0 s	yes	low	<input type="button" value="REMOVE"/>
A	1.000	B Plate: [2, A-9]	6.00 C	40.00 μ l	100 %	0 s	yes	low	<input type="button" value="REMOVE"/>
C2	1.000	B1	6.00 C	40.00 μ l	100 %	0 s	yes	low	<input type="button" value="REMOVE"/>
A	1.000	B Plate: [2, A-9]	8.00 C	40.00 μ l	100 %	0 s		medium	<input type="button" value="REMOVE"/>
C2	1.000	B1	8.00 C	40.00 μ l	100 %	0 s	yes	low	<input type="button" value="REMOVE"/>
C2	1.000	B1	10.00 C	40.00 μ l	100 %	0 s	yes	low	<input type="button" value="REMOVE"/>

(a)

ISPyB
Information System for Protein crystallography Beamlines

Prepare Experiment

Lab-contacts | Home | Shipping | Prepare Experiment | Data Acquisition | Explore Your Results | Feedback

Macromolecules
Buffers

Name : C4u 50 [Download Source File](#)
 Type : TEMPLATE
 Date : Nov 29, 2013 10:46:23 AM

Comments: [BsxCube] Generated from BsxCube [EDIT]

Measurements | Specimens | Requirements

Macromolecule	Buffer	Conc.	Vol. Well	Plate	Row	Well
Buffers						
	Hepes50c		240.00 μ l	2	C	11
	Hepes50d		960.00 μ l	2	D	9
C4c 50						
C4c 50	Hepes50d	0.300 mg/ml	40.00 μ l	3	H	3
C4c 50	Hepes50d	0.300 mg/ml	40.00 μ l	3	H	2
C4c 50	Hepes50d	0.300 mg/ml	40.00 μ l	3	H	1
C4c 50	Hepes50d	0.500 mg/ml	40.00 μ l	3	H	5
C4c 50	Hepes50d	0.500 mg/ml	40.00 μ l	3	H	6
C4c 50	Hepes50d	0.500 mg/ml	40.00 μ l	3	H	4
C4c 50	Hepes50d	0.800 mg/ml	40.00 μ l	3	H	8
C4c 50	Hepes50d	0.800 mg/ml	40.00 μ l	3	H	9
C4c 50	Hepes50d	0.800 mg/ml	40.00 μ l	3	H	7
C4c 50	Hepes50d	1.060 mg/ml	40.00 μ l	3	H	11
C4c 50	Hepes50d	1.060 mg/ml	40.00 μ l	3	H	12
C4c 50	Hepes50d	1.060 mg/ml	40.00 μ l	3	H	10
C4u 50						

1.- Deep Well

A	○	○	○	○	○	○	○	○	○	○	○
B	○	○	○	○	○	○	○	○	○	○	○
C	○	○	○	○	○	○	○	○	○	○	○
D	○	○	○	○	○	○	○	○	○	○	○
E	○	○	○	○	○	○	○	○	○	○	○
F	○	○	○	○	○	○	○	○	○	○	○
G	○	○	○	○	○	○	○	○	○	○	○
H	○	○	○	○	○	○	○	○	○	○	○

2.- 4 x (8 + 3) Block

A	○	○	○	○	○	○	○	○	○	○	○
B	○	○	○	○	○	○	○	○	○	○	○
C	○	○	○	○	○	○	○	○	○	○	○
D	○	○	○	○	○	○	○	○	○	○	○
E	○	○	○	○	○	○	○	○	○	○	○
F	○	○	○	○	○	○	○	○	○	○	○
G	○	○	○	○	○	○	○	○	○	○	○
H	○	○	○	○	○	○	○	○	○	○	○

3.- 96 Well plate

A	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○
B	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○
C	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○
D	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○
E	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○
F	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○
G	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○
H	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○	○

Plate Types | Auto Fill | Empty | Zoom In

(b)

ISPyB
Information System for Protein crystallography

Prepare Experiment

Lab-contacts Home Shipping Prepare Experiment Data Acquisition Explore Your Results Feedback

Macromolecules
Buffers

Name: C4u 50 [Download Source File](#)
Type: TEMPLATE
Date: Nov 29, 2013 10:46:23 AM
Comments: [BsxCube] Generated from BsxCube

Measurements Specimens Requirements

Tip
Estimated volume is the maximum volume required. Depending on the order of your measurements you may use less. Click on create stock solutions if you plan to ship these stock solutions

Estimation of required Volume

Go to Shipment

Specimen	Estimated Volume	Stock Solution
C4c 50 + Hepes50d	480.00 μ l	<input type="button" value="NEW STOCK SOLUTION"/>
C4u 50 + Hepes50c	120.00 μ l	<input type="button" value="NEW STOCK SOLUTION"/>
Hepes50c	240.00 μ l	<input type="button" value="NEW STOCK SOLUTION"/>
Hepes50d	960.00 μ l	<input type="button" value="NEW STOCK SOLUTION"/>

(c)

Figure S4 Prepare Experiment table: a) list of measurements created, b) specimen list with its locations in sample changer, c) sample requirements window.

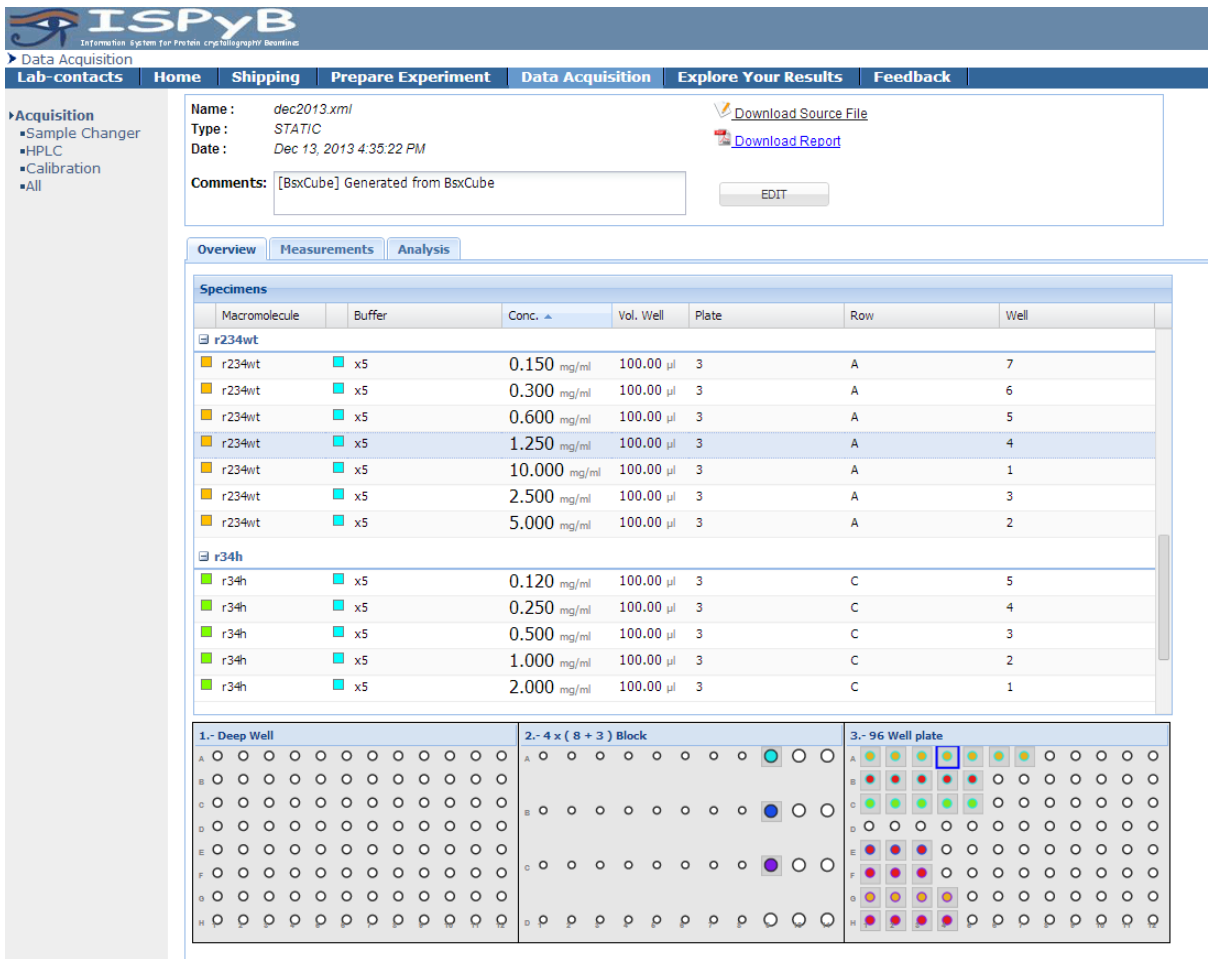
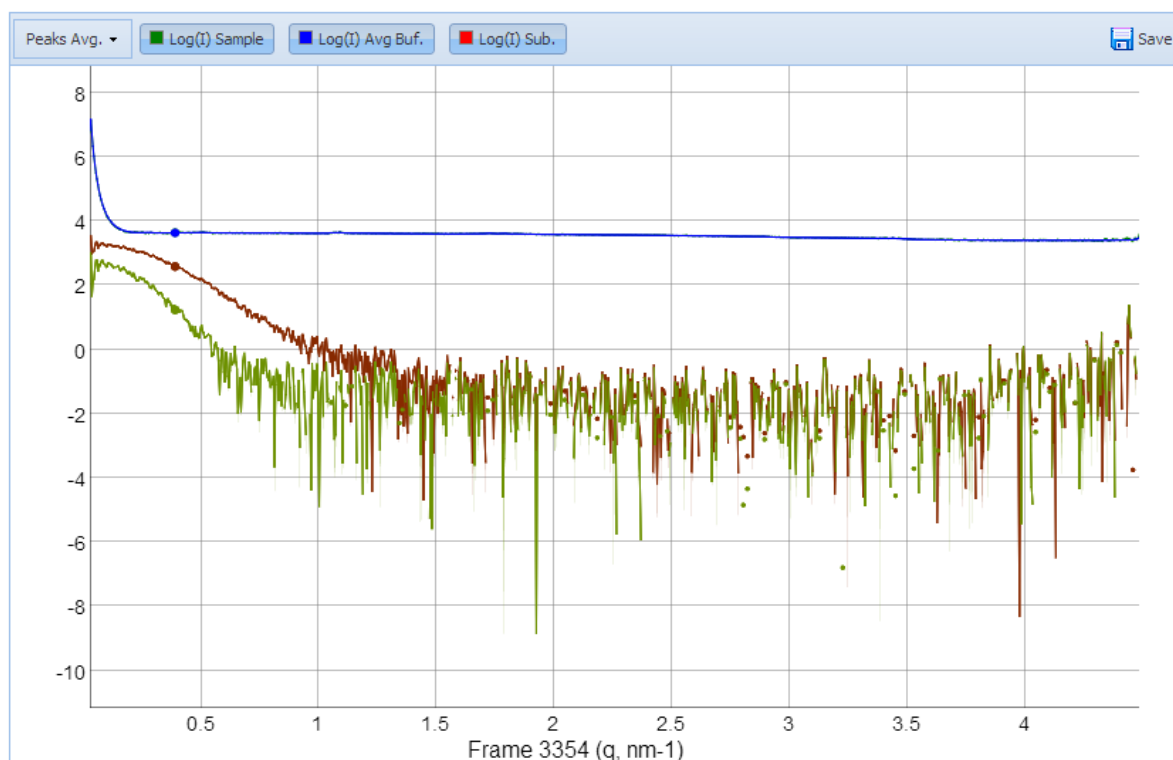
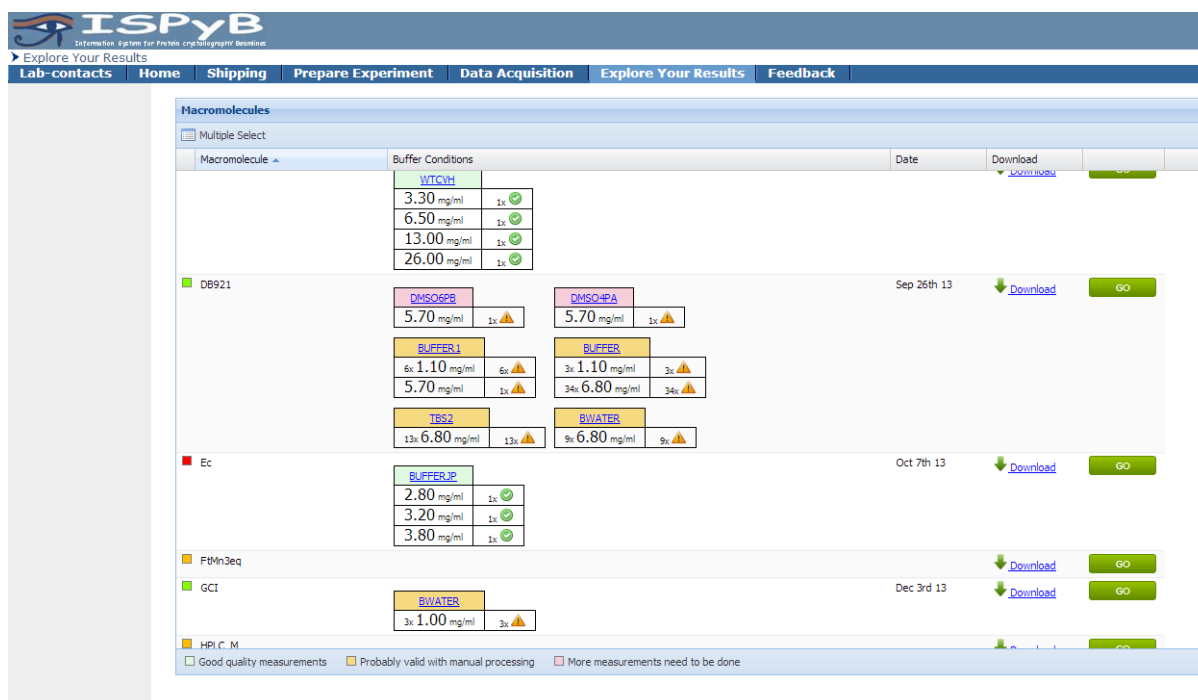


Figure S5 Summary of each experiment showing the samples to be measured and their locations in the sample changer.



(a)



(b)

Figure S6 a) 1D plot of the scattering data for the merged files produced by the auto processing, blue averaged buffer used for subtractions, Brown and green show the merged profiles for the peaks detected. b) File manager, shows the peaks detected and the frames used as well as a download option for each peak.

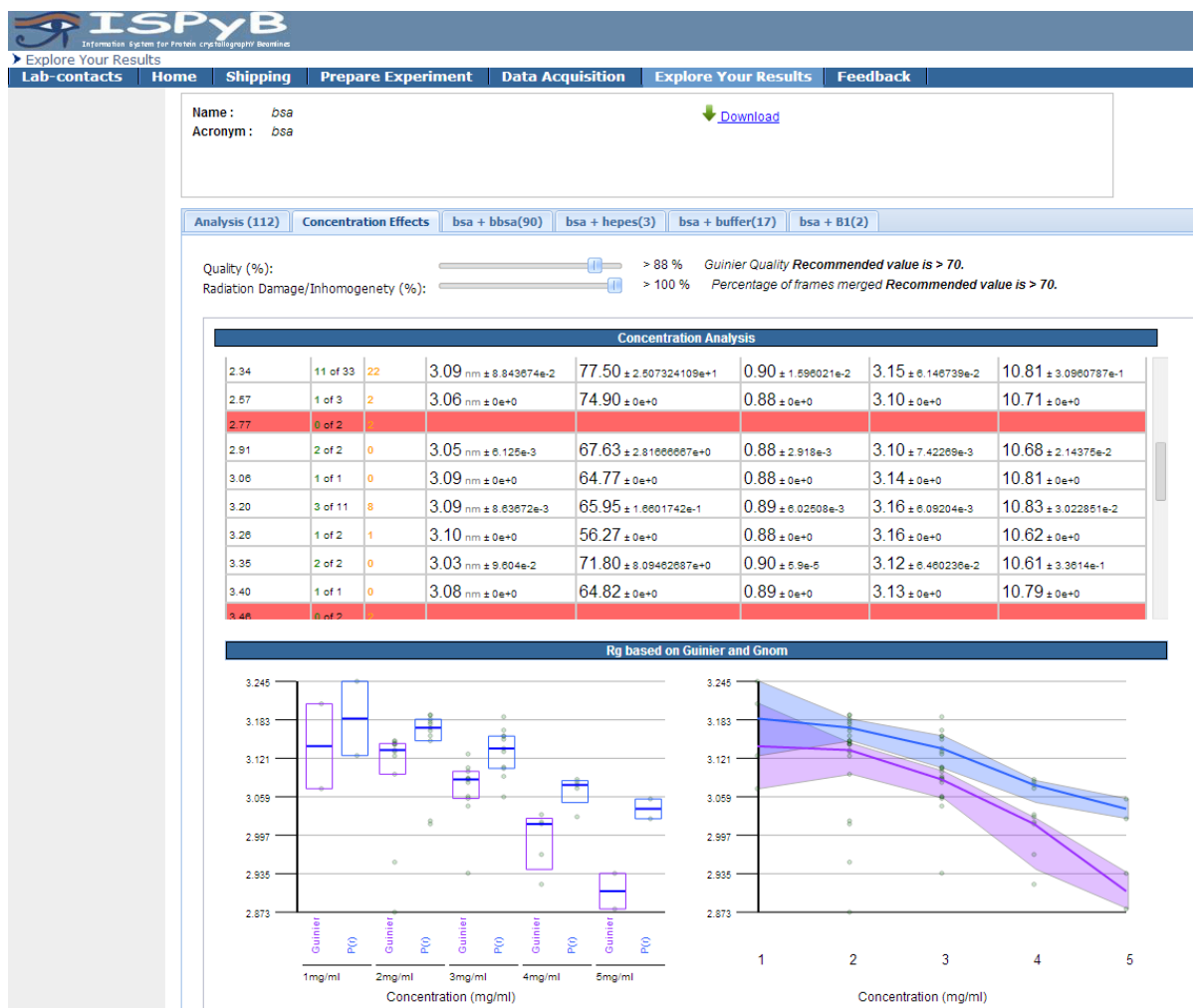


Figure S7 *Explore Your Results* table: a) general view of all measured compounds, b) Concentration Effects window for a given macromolecule.

Supplementary References

Ginn, H., Mostefaoui, G.K., Levik, K., Grimes, J.M., Walsh, M.A., Ashton, A. & Stuart, D.I. (2013) *CCP4 Newsletter on protein crystallography*, **49**, 20-24