

BrightnESS²

Bringing Together a Neutron Ecosystem for Sustainable Science with ESS

H2020-INFRADEV-3-2018-1

Grant Agreement Number: 823867

brightness²

Deliverable

D 4.5 Service Catalogue including price list with three use cases

1. Project Deliverable Information Sheet

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5. Executive Summary

This delivery is a catalogue and price list that is related to the delivery D4.4 “*Processes and procedures for targeted access routes*”. There will be references to the different access routes and to other similar facilities’ way of defining their services, prices and deduction models.

The services are divided in to three different levels to cover the full range of possibilities, from pure measurement to a potential “door-to-door” service.

Different principal pricing models are explained and applied to provide an overview of analysed opportunities at existing facilities.



6. Service Catalogue

Based on the input collected through interviews with facilities and industry representatives, a range of supplied and demanded services have been identified. Services can be provided on three different levels:

- **Level 1** is concerned with providing industry with access to beamtime and delivering data as the core product of ESS. This service will be provided directly from ESS.
- **Level 2** is concerned with additional assistance around the measurement, that can help to make them more accessible to non-expert users. They include feasibility tests, optimisation of the measurement design, analysis and counselling. These services can be provided by the ESS, through a dedicated industry unit or beamline scientists, or by Research Technology Organisations (RTO), mediator companies, industry platforms, etc.
- **Level 3** is concerned with outreach to new industry users and increasing the awareness of industrial application and value-creation from neutron analyses. Activities on this level are expected to be covered by either the ESS general budget and/or by funding agencies through collaborative project applications. They are therefore not covered in the price calculation examples.

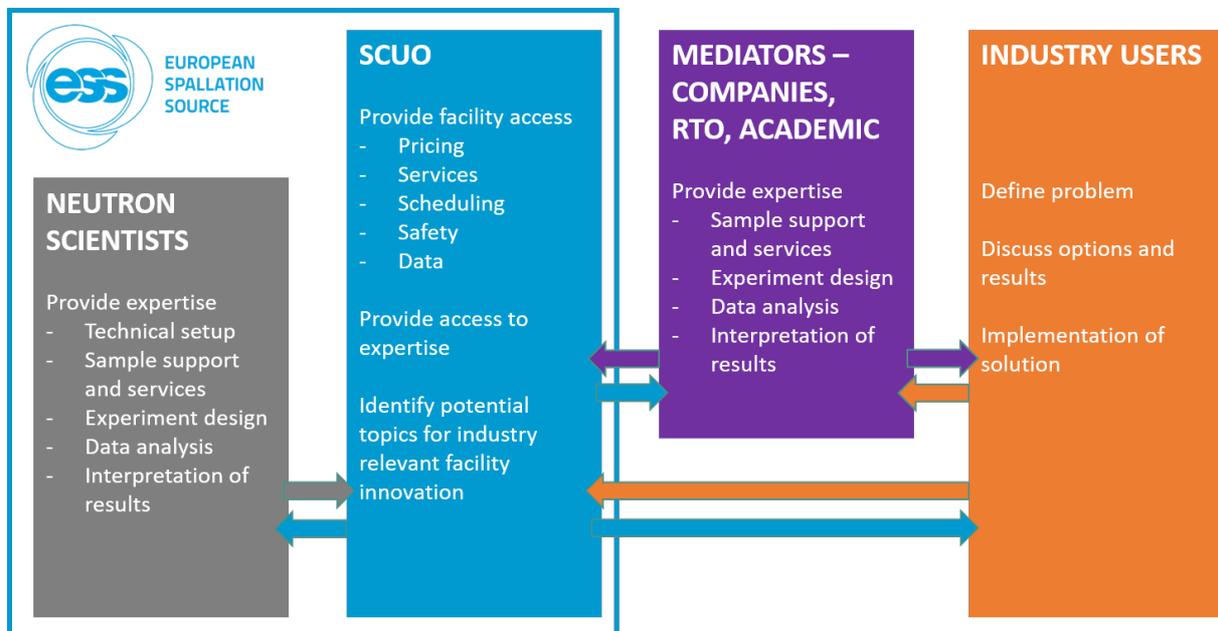


Figure 1 The ESS Model for industry use

Services for each of the three levels are presented in the table below. For each service, it is also noted which resources are required if ESS wishes to run them.

Level 1 services	Required resources	Available input/resources
Industry Proprietary Access	Price structure / list	Examples in next chapter
	Standard agreement (and modified version for mail-in)	Input for terms and conditions in report D4.4: The service should include instrument setup, data reduction as needed, on-call assistance in case of instrument issues, initial data storage up to a given time limit. The agreement must be determined by the legal department in collaboration with SCUO.
	Data storage	Storage by DMSC of proprietary data until full transfer to the company is confirmed, up to a year. Must be clearly labelled by 'confidential' or even under restricted access.
	Sample declaration system	Use general user SCUO software – with option for non-disclosure or labelling of information as confidential
	Safety assessment system	Use general user SCUO software – with option for non-disclosure or labelling of information as confidential
	Form for detailed description of sample handling and disposal	Use general user SCUO software – with option for non-disclosure or labelling of information as confidential
	Sample shipping system	Under construction as part of the general user SCUO software
	Optional NDA	Covering any information on that must be shared for safety assessment and sample handling (see above). The agreement must be determined by the legal department in collaboration with SCUO.
	Staff for beamline setup, on-call duty and assistance with data reduction	Input for requirements covered in report D4.4. Staff can be SCUO staff or beamline staff.
	Site access system, incl. lab access	Should be part of a general system for user site access and welcome function.
	Open slots and general wiggle room in schedule, especially for instruments of particular industrial relevance	Input for requirements covered in report D4.4: Aim for access availability within a month. Administered by SCUO.
	Invoice system	Decide if this is handled by SCUO or a financial office

Data collection for mail-in measurements	Staff dedicated to data collection and extended sample handling	Input for requirements covered in report D4.4. Staff capabilities: - Expertise in using a range of different instruments SCUO staff or beamline staff.
Deuteration services	Price structure/list	Could be set per mg material Set for a specified number of expressions/crystallisation attempts/etc., based on estimate of time consumption Is thought to be offered in connection with a neutron experiment, either through peer-review or proprietary
	Staff available for communicating with industry and performing deuteration and/or crystallisation of (bio-)molecules	DEMAX facility with the relevant staff capabilities within chemical synthesis, protein expression, crystal growth, etc.

Table 1: Level 1 services

The Quick Access route can also prove to be very useful for industry, especially for feasibility tests. Some decisions must be made:

- What is the allowed extent of a Quick Access measurement or experiment?
- Can Quick Access be run under an NDA?
- If it is run under an NDA, will it go under the mail-in IPA route?

Level 2 services	Required resources	Available input/resources
Measurement design	Staff dedicated to discussion with industry users and preparation for their measurement/experiment	Input for requirements covered in report D4.4. Staff capabilities: - an eye for industry service - connections to and insight into a range of beamlines - insight into complementary techniques and methods SCUO staff, beamline staff, or external mediators.
Data analysis	Staff allocated to analyse the data – often orders of magnitude more time	- Expertise in a range of different neutron techniques - Communication with industry SCUO staff, beamline staff, or external mediators.

	consuming than the data acquisition	
Data analysis Data interpretation	Data analysis software and tools	Continuous communication between SCUO, beamline staff, and DMSC regarding needs and options.
	Staff allocated to meet and discuss with industry in several iterations and prepare reports	Input for requirements covered in report D4.4. Staff capabilities: - Expertise in a range of different neutron techniques - Insight into the industrial sample and problem - Communication with industry SCUO staff, beamline staff, or external mediators.
Counselling	Staff allocated to collaborate with industry	Input for requirements covered in report D4.4. Staff capabilities: - Insight into relevant industrial areas/sectors - Understanding of the importance of the given problem and the modes of work of the company - Overview of alternative solutions to problem, incl. neutrons and other - Communication with industry SCUO staff, beamline staff, or external mediators.
Matchmaking	Staff available for discussing with industry and setting up connections to other relevant collaborators	Input for requirements covered in report D4.4. Staff capabilities: - Relevant connections in the academic and industrial eco-system - an eye for industry needs - insight into technical possibilities SCUO staff, beamline staff, or external mediators.
Development of proposals	Staff available for assisting with proposals, when industry use of the general peer-reviewed access is relevant	Input for requirements covered in report D4.4. Staff capabilities: - Connections to a range of beamlines and insight into their capabilities - Insight into complementary techniques and methods - Communication with industry SCUO staff, beamline staff, or external mediators.
Technology adaption	Staff for construction of industry-relevant beamline sample environment	Input for requirements covered in report D4.4. Staff capabilities: - An eye for industry needs, and time for thorough discussions

		<ul style="list-style-type: none"> - Connections to a range of beamlines and insight into their capabilities - Insight into complementary techniques and methods SCUO staff, beamline staff, or external mediators.
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Table 2: Level 2 services

Level 3 activities	Required resources	Available input/resources
Increase of awareness and industry outreach	Staff for outreach and communication	Input for requirements covered in report D4.4. Staff capabilities: <ul style="list-style-type: none"> - Communication with industry and the general public - News stories - Participation in industry meetings, conferences, etc. Covered by SCUO and the communication dept.
	Program for funding of industry case measurements	High value for use in communication towards industry, political and funding agencies, and the general public. Managed by the SCUO. Requires funding through ESS or an external program.
	Participation in projects and networks for a specific field, sector, or technique, including or targeted towards industry	<ul style="list-style-type: none"> - Increase of awareness and application of neutron techniques - Training programs for industry in relevant subjects or techniques Managed by the SCUO. Requires funding through ESS or an external program.

Table 3: Level 3 activities

7. Price list

A price list or model should enable the setting of a price for a specific service a priori. In cases where it is not possible to give a fixed price, maybe because the extent of the work is not possible to determine, it should be possible to give an estimate, or to share the price model with the customer so that it is clear to them before entering a commitment.

According to the service catalogue, services might be provided at three different levels. Services and activities on level 3 are expected to be covered by either the ESS general budget and/or by funding agencies through collaborative project applications. Services on levels 1 and 2 are commercial and should be covered by the industry customers and are discussed individually below. The general principle, as also described in the European Charter for Access to Research Infrastructures, is that the full cost should be covered by the industry user, ensuring that a company is not indirectly subsidised. This cost, however, might be defined in different ways according to the different price calculations below. Also, rates for staff must be set to avoid under-pricing in competition with private service providers or mediators.

7.1. Price calculations for access to beamtime – Level 1 services

For level 1, the facility services are associated with providing beamtime and data. It is suggested that ESS follows the other comparable facilities, in including staff for instrument setup, and on-call staff in the beamtime rate. Initial data reduction might also be covered.

Pricing according to full operation costs

The majority of the interviewed facilities calculate the price of beamtime from the running costs of the entire facility. In this way, overhead is included in the price. The calculation of the hourly rate then is:

$$\text{Beamtime hourly rate} = R_{OC} = \frac{\text{Annual facility operation cost at full operation}}{\text{Total amount of beamtime available at full facility operation}}$$

The price is flat for all instruments. The operation costs are determined at full operation, and do therefore not include major construction costs or establishment of new beamlines. If the annual operation cost is calculated based on the actual accounts, it might be based on an average over five years, to avoid sensitivity to fluctuations.

Often there is a minimum amount of beamtime that can be purchased at a given instrument, ranging from 4 to 24 hours, and in some cases, beamtime can only be purchased in quanta of 'shifts' (e.g. 8 hours) or full days.

The hourly rate at 22 instruments at ESS can be estimated from the report *Science Directorate – Work Breakdown Structure during Steady-State Operation* from 2019. Here, the number of beam days for the user programme is set to 3520. Assuming an annual full operation cost of 165 M€, this results in a rate of 47 k€ per day.

Pricing according to beamline construction costs

A suggestion has also been made at the ESS to consider pricing beamtime by the cost of construction of the individual beamline. Here, the dismantling of the beamline could also be taken into account. Staff and overhead costs must then be added separately:



$$\text{Beamtime hourly rate} = \frac{\text{Beamline construction costs}}{\text{Total amount of beamtime during the amortization period}} + n \times \text{beamline staff hourly rate} + \text{Overhead}$$

This model will result in different rates for each beamline and might be more difficult to determine and maintain. Also, it should be noted, that after the amortization period, the value of the instrumentation is set to zero, while it is still in use, and its actual value might not be accounted for.

In the report *Science Directorate – Work Breakdown Structure during Steady-State Operation* from 2019, an additional instrument is estimated to require approximately 9.5 additional fulltime staff. The additional running costs might be estimated to 48 M€ for 22 instruments (the science directorate budget minus investments and user-related costs for reimbursements, PhD-programs, etc.), resulting in 2.2 M€ per year. Adding construction costs of e.g. 12 M€ amortized over 12 years, results in a rate for beamtime of 20 k€ per day. Overhead for other than the science directorate might also be added and could result in a price of 25-30 k€.

Pricing according to value

Since the ‘market’ for neutron analyses is quite small, a market value does not seem to be established. Therefore, beamtime is generally not priced according to the value it creates with the customer, but rather based on the costs, as described above.

For synchrotron facilities, there is a market within the most used techniques, mainly protein crystallography, and here, the prices might be adjusted from the cost price. Either slightly down to be comparable to prices at other facilities, or slightly up if the demand is high and upgrades have been done to the beamline.

For ESS, an actual market based on supply and demand is not expected in the foreseeable future. Furthermore, the awareness of neutron analyses and their potential value-creation is relatively low with most companies. Therefore, it is not possible to price beamtime based solely on its value for the customers. Rather, by logging returning customers it will be possible to assess whether the product value matches the price.

7.2. Price calculations for scientific support and consultancy – Level 2 services

Services based on consultancy must be priced based on an hourly rate including overhead. This might be set as a flat rate, or it might depend on the level of the involved staff.

It should be noted that companies requiring scientific support or consultancy, in most cases need a total, fixed price for a combined task. That is, including any consultancy for sample handling, data collection, data analysis, etc. Therefore, it must be possible to estimate the required time for a specific task and give an offer based on this estimate. If a specific task is particularly difficult to estimate, the required level of flexibility must be included in the agreement and offer.

Price reductions

Some of the tasks included in a service, might be creating value directly for ESS. This provides an option to reduce the price accordingly. At PSI this has been formalized in the following way for projects that are performed as a collaboration with the facility scientists. The level of alignment with PSI interests, here labelled *LA*, is assessed within four different categories and given a value of 0, 25, 50, 75, or 100 %. The four categories are:

- The freedom for the facility to publish the scientific results, LA_{publish}

- The freedom for the facility to use the results, LA_{results}
- The alignment with the facility goals on industry support, impact, and visibility, LA_{impact}
- The return on any investment in equipment, infrastructure, prototypes, or royalties, LA_{invest}

Each of the four are weighted similarly. At PSI, the maximum price reduction is set to 50 %. The reduction is therefore calculated as:

$$\text{Reduction} = 50 \% \times \left(\frac{LA_{\text{publish}} + LA_{\text{results}} + LA_{\text{impact}} + LA_{\text{invest}}}{4} \right)$$

Whether price reductions up to 50 % are sustainable, will depend on how the staff hourly rate is set. If it is set at less than two times the actual staff cost, the cost will not be fully covered at 50 % reduction.

At PSI, since the income from the task is allocated to the beamline's division, the decision of whether a reduction should be offered, is made by the beamline responsible.

Additional setup for full door-to-door service

As a part on the BrightnESS² project, ESS has initiated logistics collaboration initiatives between Research Infrastructures in Europe. Following an initial conference, a RI Logistica working group is founded, and a concept and manifest is taking shape.

All RIs agree that remote access is key in the future and one of the service solutions could be a door-to-door service, where users can select an all-inclusive solution:

- In- and outbound courier sample handling incl. sample packaging and environment during shipping, customs declaration for international shipment
- Insurance while in transit
- Option for remote-access data collection by the company
- Sample storage and handling at the facility

A possible future solution for this kind of service can well be a joint logistics concept and non-profit organisation, that will set up partnerships to be utilised by the RIs when offering their services.

Currently a plan for the future, but with the help from BrightnESS² and projects like ENRITTC, the realisation is actually in focus.

Pricing of such service(s) is currently difficult to determine, but the objective of the RI Logistica is to establish the best possible agreements for execution, on a commercial basis, while still delivering the required quality.

Access to other resources

Whereas access to beamtime is a key service for ESS, rates might also be set for access to other resources, such as the ESS lab for Deuteration and macromolecular Crystallisation, DEMAX. Deuterated material obtained through DEMAX in connection to a measurement or experiment is added to the service catalogue below.

7.1. Verification and revision of the pricing model

After a pricing model has been determined, it must be validated by comparison to services of similar facilities and to commercial service providers. Given that the market for neutron analyses is not large enough to necessarily be driven by supply and demand, this is necessary to avoid under-pricing and



unfair competition, or over-pricing leading to prices that are unacceptable to the users. The prices might be adjusted correspondingly.

Regular revisions of the pricing model and the rates for beamtime, staff, and access to other resources is recommended, maybe every three years.

8. Price list use cases

8.1. Three use examples

On each level, a typical service is identified, and a price is calculated according to the different pricing models presented above.

Level 1 service example

On this level, a typical service provided to a company would be access to 8 hours of beamtime on a given instrument. As described above, this will include the instrument setup, on-call assistance, and potentially basic data reduction. The company will perform the measurements themselves, and either travel to the facility or run the measurements by remote access if this is an option. The invoice will therefore cover:

- 8 hours of beamtime

Level 2 service example

On this level, a typical service provided to a company would be measurement on a couple of samples, here estimated to 8 hours beamtime for comparability to the level 1 service example. Scientific support for data collection, data analysis and a report of the results is estimated to $(4+12+4) = 20$ hours. The invoice will therefore cover:

- Measurement of the described samples, with a price set to that of 8 hours of beamtime
- 20 hours of staff support for data collection, analysis, and reporting

The staff rate should be set to avoid under-pricing in competition with external commercial service providers.

If the project is performed on collaborative terms with the beamline staff, a price reduction might be applied to the staff rates according to the scheme given above. In this example, the levels of alignment are set in the following way:

- It is assumed that the experiment is fully confidential, that the data are not for publication, therefore $LA_{\text{publish}} = 0$
- Given that a company is often only interested in information within their specific field, it is assumed that the facility will be able to use other results that are obtained, therefore $LA_{\text{results}} = 50\%$
- There might be some impact for the facility through being allowed to mention the company as a facility user and customer. Therefore, $LA_{\text{impact}} = 50\%$
- Given that no new development or investment is expected for a company-run experiment, there is no return of investment, therefore $LA_{\text{invest}} = 0$

Following the calculation of the price reduction, this results in a reduction of the staff rate of 12.5 %.

Level 3 service example

On this level, collaboration with a company will be run as an activity rather than a commercial service. Therefore, it should be (co-)funded either through a project, or from the facility. A typical

activity would be a company visit on the ESS site, match-making with potential academic or commercial partners, invitation to the company to participate in projects.

For the price calculation given below, an example has been assumed where a company participates in a project to develop new industry relevant sample environment, and in a program funded case measurement. 20 hours additional staff support is added as a commercial task, prompted by the project collaboration and the case measurement. This scenario could be relevant when a new user is introduced to how a technique might help them, and wishes to expand the value for them by getting access to further expert assistance. The activities are then:

- Development of a sample holder or environment in collaborative project
- 8 hours beamtime for case measurement
- 12 hours staff support for data collection and analysis for case measurement
- 20 hours additional staff support for modification of the sample equipment to the specific company needs, and for data interpretation for further implementation at the company

The development of sample environment is assumed to be funded by project. The 2 hours of beamtime and 6 hours of staff support for a case measurement, is assumed to be funded by an industry access program for new users.

The additional staff support is priced as in level 2. Since the project is performed on collaborative terms with the beamline staff, a price reduction applies according to the levels of alignment set in the following way:

- As the example concerns a case measurement that will be public in one form or another, it is assumed that the results might be up for scientific publication, however only after 3 months delay for review by the company. Therefore, $LA_{\text{publish}} = 50\%$
- Given that a company is often only interested in information within their specific field, it is assumed that the facility will be able to use other results that are obtained, therefore $LA_{\text{results}} = 50\%$
- There might be some impact for the facility through being allowed to mention the company as a facility user and customer. Therefore, $LA_{\text{impact}} = 50\%$
- Given that improvements of the sample equipment is included in this effort, the return of investment in the form of an equipment upgrade is significant and $LA_{\text{invest}} = 50\%$

Following the calculation of the price reduction, this results in a reduction of the staff rate of 25 %.

Price based on ->	A: Operation costs, 15 instruments	B: Operation costs, 22 instruments	B with price reduction	B with full logistics setup
Level 1 service example - 8 hours beamtime (incl. setup, on-call assistance, basic data reduction)	$8 \times R_{OC,15}$	$8 \times R_{OC,22}$	$8 \times R_{OC,15}$	$8 \times R_{OC,15}$ + $P_{\text{logistics}}$
Level 2 service example - 8 hours beamtime - 4 hours data collection assist. - 12 hours data analysis - 4 hours report writing	$8 \times R_{OC,15}$ + $20 \times R_{\text{staff}}$	$8 \times R_{OC,22}$ + $20 \times R_{\text{staff}}$	$8 \times R_{OC,22}$ + $20 \times R_{\text{staff}}$ $\times 0.875$	$8 \times R_{OC,22}$ + $20 \times R_{\text{staff}}$ $\times 0.875$ + $P_{\text{logistics}}$
Level 3 activity/service example - Development of sample holder - 8 hours beamtime for case	Project funded	Project funded	Project funded	Project funded

- 12 hours staff support for data collection and analysis - 20 hours staff support for additional data interpretation	$20 \times R_{\text{staff}}$	$20 \times R_{\text{staff}}$	$20 \times R_{\text{staff}} \times 0.75$	$20 \times R_{\text{staff}} \times 0.75 + P_{\text{logistics}}$
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* Staff rate might be set based on which level of staff is involved, or based on a flat rate. It should be set to not under-price in competition with external commercial service providers.

