EUROPEAN SPALLATION SOURCE

Deuteration and Macromolecular Crystallisation Platform

Product List & Sample Shipping

August 2023

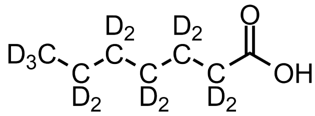
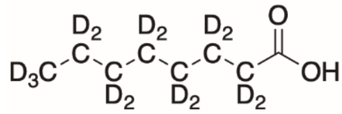
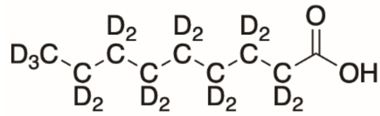
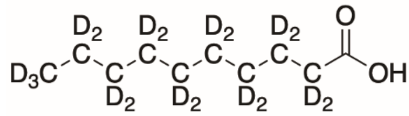
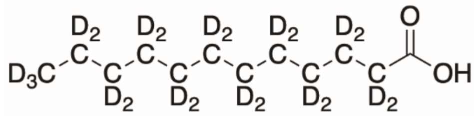
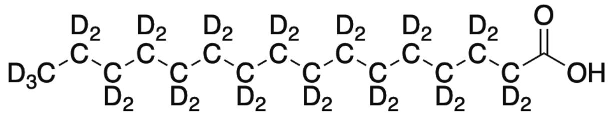
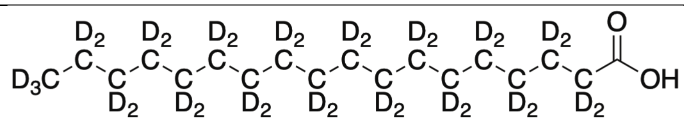
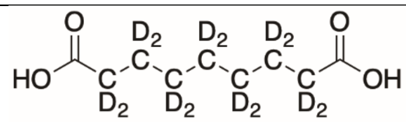
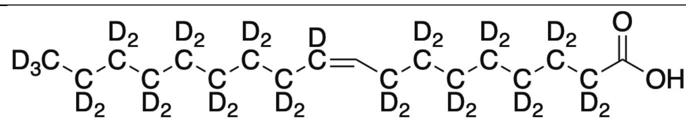
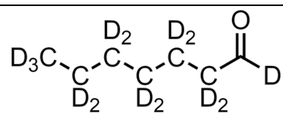
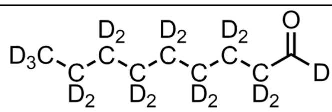
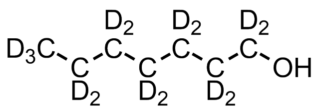
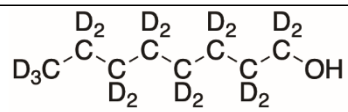
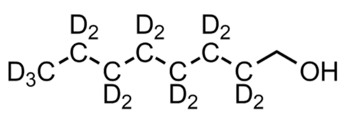
Biological: proteins, biomass, nucleic acids

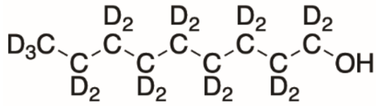
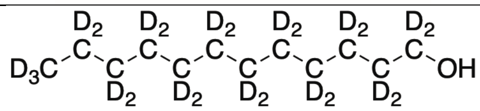
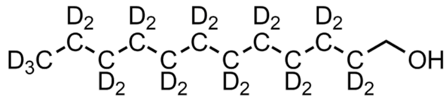
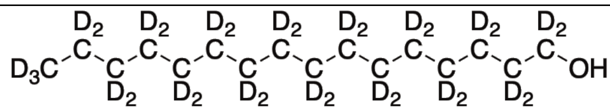
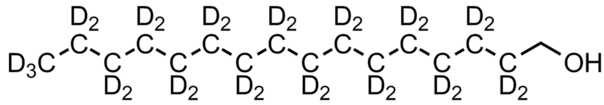
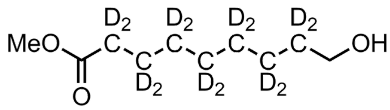
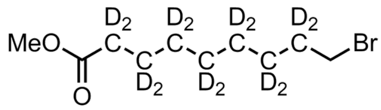
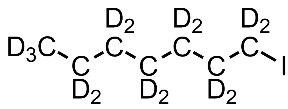
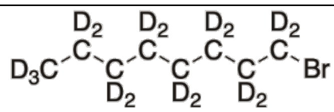
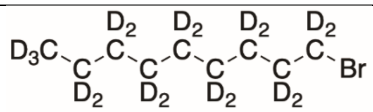
Category
E. coli cell paste (protein expression strains e.g. Tuner DE3, BL21 DE3)
Algal cell paste (*Botryococcus braunii*)
Yeast cell paste (*Pichia pastoris*)
Recombinant proteins with user supplied plasmid (standard strains: Tuner DE3, BL21 etc)
Deuterated plasmid DNA

Biological: purified lipid mixtures

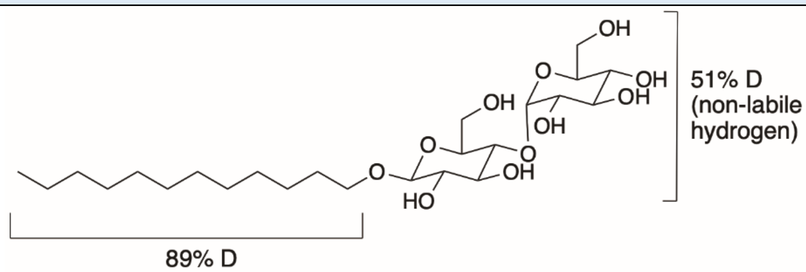
Category
Total lipid extract from yeast (*Pichia pastoris*)
Total phospholipid extract (*Pichia pastoris*)
Feasibility tests for the purification of specific yeast lipid classes (e.g. PC, PE, cardiolipin, ergosterol) from *Pichia Pastoris*

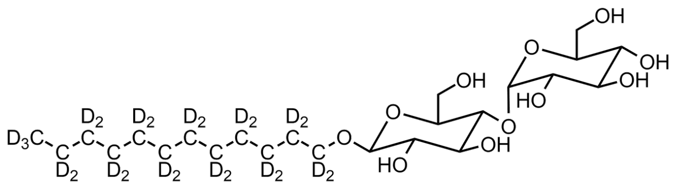
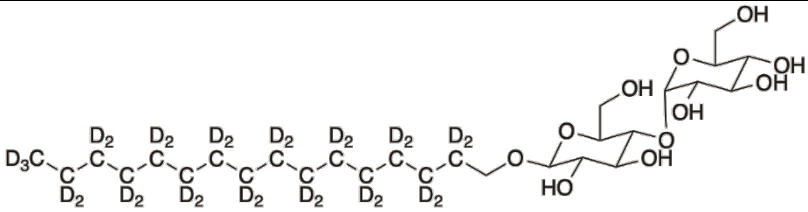
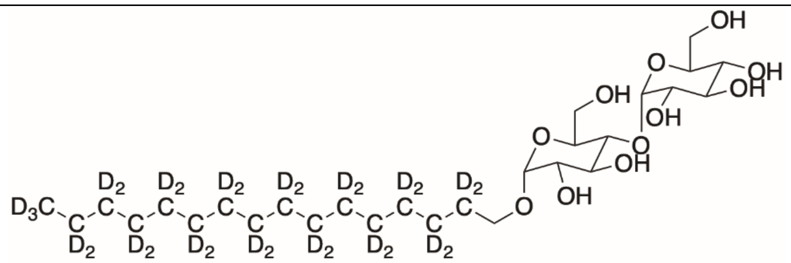
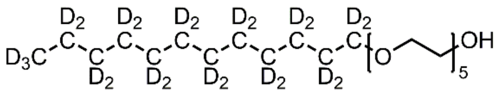
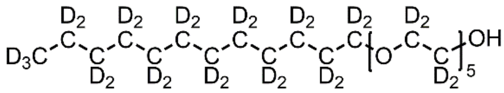
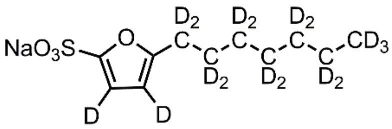
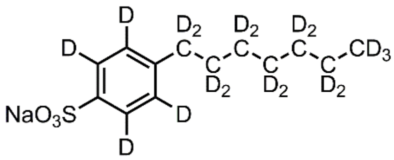
Chemical: carboxylic acids, aldehydes, alcohols, alkyl halides

Compound name	**Chemical structure**
Heptanoic acid-d_{13}	
Octanoic acid-d_{15}	
Nonanoic acid-d_{17}	
Decanoic acid-d_{19}	
Dodecanoic acid-d_{23}	
Hexadecanoic acid-d_{31}	
Octadecanoic acid-d_{35}	
Nonanedioic acid-d_{14}	
Oleic acid-d_{32}	
Heptanal-d_{14}	
Nonanal-d_{18}	
Heptanol-d_{15}	
Octanol-d_{17}	
Octanol-d_{15}	

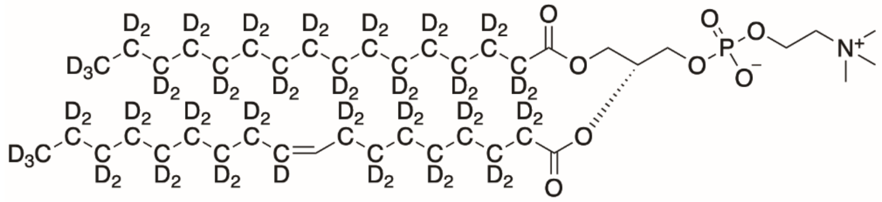
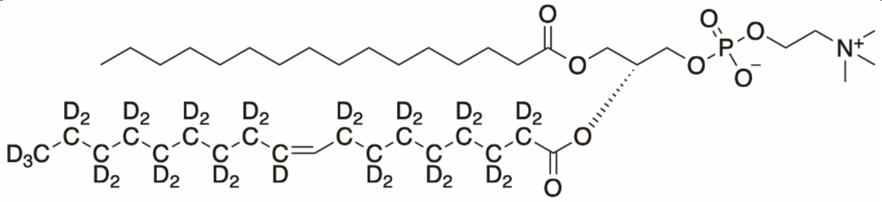
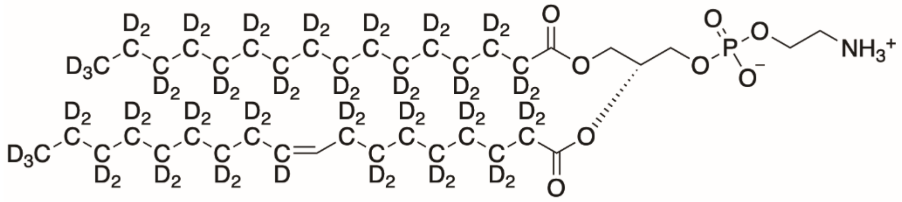
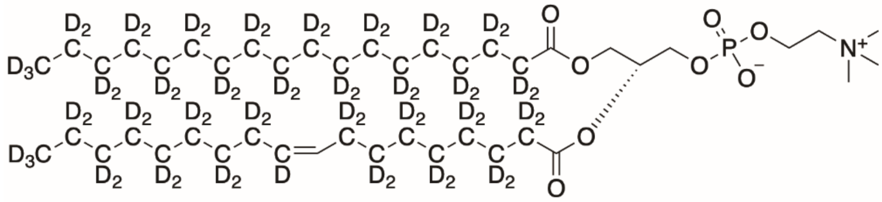
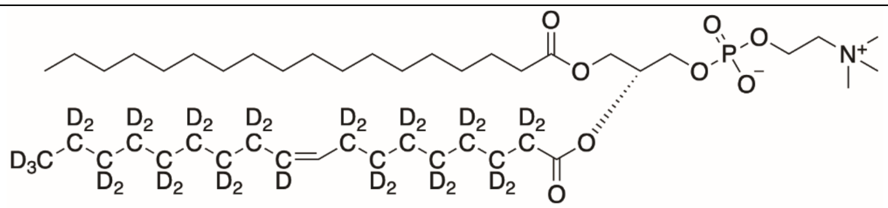
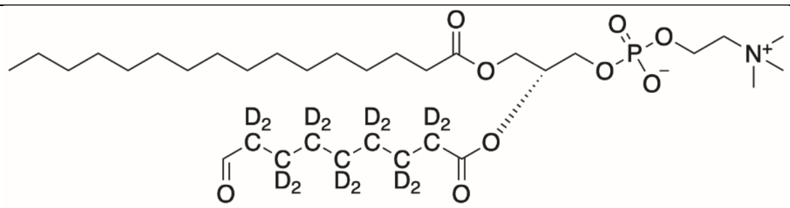
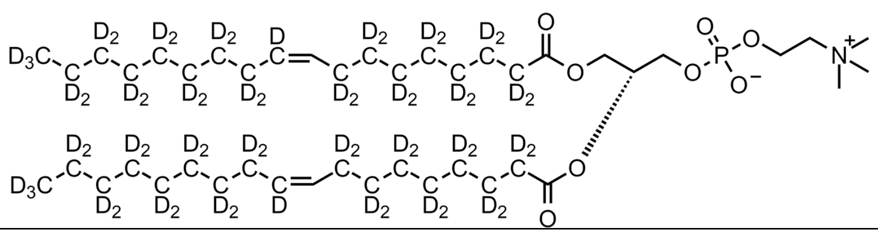
Nonanol-*d*19	
Dodecanol-*d*25	
Dodecanol-*d*23	
Hexadecanol-*d*33	
Hexadecanol-*d*31	
Methyl 9-hydroxynonanoate-*d*14	
Methyl 9-bromononanoate-*d*14	
1-Iodoheptane-*d*15	
1-Bromooctane-*d*17	
1-Bromononane-*d*19	

Chemical: surfactants

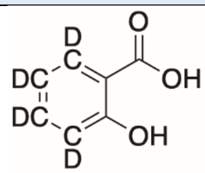
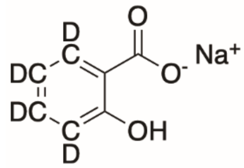
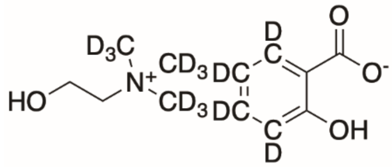
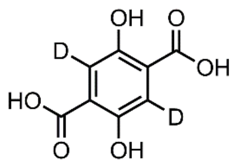
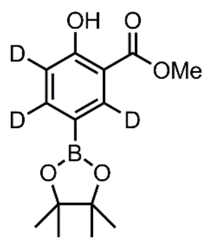
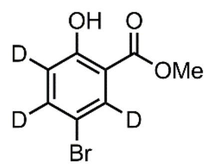
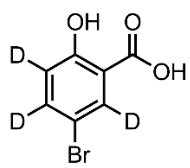
Compound name	**Chemical structure**
n-Dodecyl-β-D-maltopyranoside (alkyl chain 89% deuterated; headgroup 51% deuterated)	

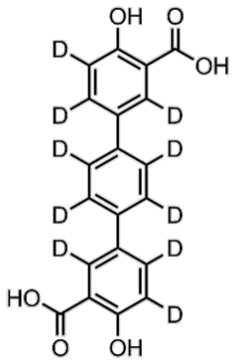
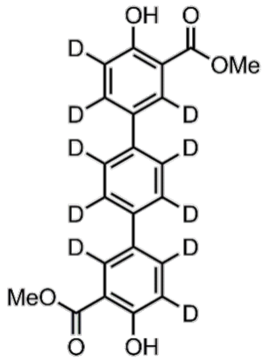
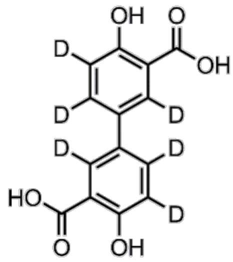
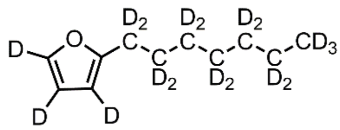
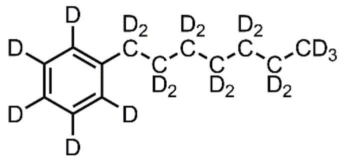
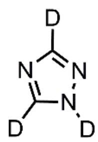
n-Dodecyl-β-D-maltopyranoside-d_{25}	
n-Hexadecyl-β-D-maltopyranoside-d_{31}	
n-Hexadecyl-α-D-maltopyranoside-d_{31}	
Pentaethylene glycol monododecyl ether-d_{25}	
Pentaethylene glycol monododecyl ether-d_{45}	
Sodium 5-heptylfuran-2-sulfonate-d_{15}	
Sodium 4-heptylbenzenesulfonate-d_{15}	

Chemical: phospholipids

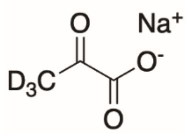
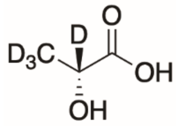
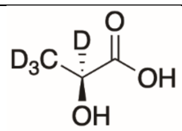
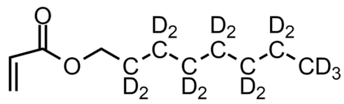
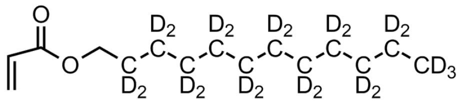
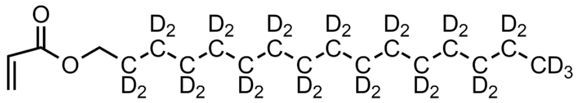
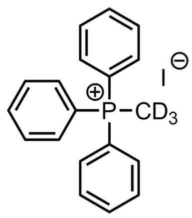
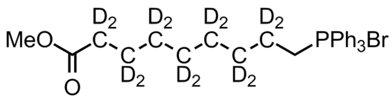
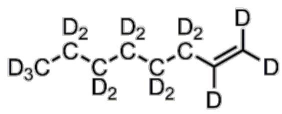
Compound name	Chemical structure
1-Palmitoyl-*d*$_{31}$-2-oleoyl-*d*$_{32}$-*sn*-glycero-3-phosphocholine	
1-Palmitoyl-2-oleoyl-*d*$_{32}$-*sn*-glycero-3-phosphocholine	
1-Palmitoyl-*d*$_{31}$-2-oleoyl-*d*$_{32}$-*sn*-glycero-3-phosphoethanol-amine	
1-Stearoyl-*d*$_{35}$-2-oleoyl-*d*$_{32}$-*sn*-glycero-3-phosphocholine	
1-Stearoyl-2-oleoyl-*d*$_{32}$-*sn*-glycero-3-phosphocholine	
1-Palmitoyl-2-(9-oxononanoyl-*d*$_{14}$)-*sn*-glycero-3-phosphocholine	
1,2-Dioleoyl-sn-glycero-3-phosphocholine-*d*$_{64}$	

Chemical: aromatic & heterocyclic aromatic molecules

Compound name	**Chemical structure**
Salicylic acid-d_4	
Sodium salicylate-d_4	
Choline-d_9 salicylate-d_4	
2,5-Dihydroxyterephthalic acid-d_2	
Methyl 2-hydroxy-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzoate-d_3	
Methyl 5-bromo-2-hydroxybenzoate-d_3	
5-Bromo-2-hydroxybenzoic acid-d_3	

4,4''-dihydroxy-[1,1':4',1''-terphenyl]-3,3''-dicarboxylic acid-d_{10}	
Dimethyl 4,4''-dihydroxy-[1,1':4',1''-terphenyl]-3,3''-dicarboxylate-d_{10}	
4,4'-dihydroxy-[1,1'-biphenyl]-3,3'-dicarboxylic acid-d_6	
2-Heptylfuran-d_{15}	
1-Phenylheptane-d_{15}	
1,2,4-triazole-d_3	

Chemical: miscellaneous

Compound name	Chemical structure
Sodium pyruvate-d_3	
D-Lactic acid-d_4	
L-Lactic acid-d_4	
Octyl acrylate-d_{15}	
Dodecyl acrylate-d_{23}	
Hexadecyl acrylate-d_{31}	
Tetrabutyl ammonium chloride-d_{36}	$N(C_4D_{17})_4Cl$
Methyltriphenylphosphonium iodide-d_3	
9-carbomethoxynonyl-d_{14}-triphenyl phosphonium bromide	
1-Octene-d_{16}	

Crystallisation support:

- Verify protein purity & concentration (SDS-PAGE, UV/Vis or BCA/Bradford assay)
- High-throughput screening in 1-2 μL drops (sitting drop vapour diffusion and/or under-oil batch) against commercial screens.
- Fine-screening and optimization of precipitant conditions with or without temperature control (any temperature between 4 - 37 °C).
- Set-ups for larger drops (20-500μL): sitting drop vapour diffusion, dialysis, under-oil batch
- Support for room temperature capillary mounting of crystals, including final H/D exchange and/or cryo preservation
- Screening with X-rays to verify space group, unit cell and crystal contents (ambient or 100 K)

About DEMAX:

DEMAX is the ESS user support lab that offers chemical and biological deuteration as well as support for protein crystallisation. The DEMAX platform drives a mix of user support & (grant-funded) research activities and produces deuterated materials such as biomass, proteins, lipids and small organic molecules for neutron techniques such as small angle scattering, reflectometry, protein crystallography, spectroscopy, and powder diffraction. Our efforts are aligned to enable high impact science on ESS instruments in life science, soft matter and chemistry.

Don’t hesitate to contact us at demax@ess.eu for more information.

Perishable sample shipping: dry shipper care & handling

General info:

- DEMAX uses dry shippers to send perishable samples. Dry shippers are used for safe transport of samples and are designed to keep your samples at -190 °C for an extended period of time (10 – 21 days if treated properly). These are preferred to dry ice for transport as a correctly prepared dry shipper does *not* fall under dangerous goods regulation.
- We typically will send your samples as overnight express but in case something goes wrong and shipment is delayed, using the dry shipper ensures that your samples arrive unspoiled.
- Please keep the dewar upright and in the shipping container with the foam lid on when not inserting/removing samples. The foam lid has a notch allowing it to slide over the canister rod, please place the lid properly and don't force it if you feel resistance.
- Upon arrival, remove your samples by lifting out the canister seated in the core of the vessel (use insulated gloves or tongs to retrieve your samples from the canister).
- Close up the dry shipper & shipping case and return to us with ordinary freight (any carrier of your choosing – DHL, TNT, Fedex etc). Please include a tracking number and check with your local contact which address to send it to.
- Make sure the "up" arrow and "fragile" sign is visible on the shipping case when attaching shipping labels.
- If you would like to borrow our dry shipper to send your sample on for an experiment, you are welcome to do so. Please ask for permission and also handle the shipper according to the instructions below.

The figure below shows a schematic of the construction of one of these.

What is a dry shipper?

Dry shippers are insulated shipping dewars which consist of LN2-absorption material surrounded by vacuum vessels with multilayer insulation. We use two models, the CX-100 from Taylor-Wharton (panel A, below) and the CY50905 from Thermo Fisher (panel B, below). They have similar storage capacities and both come in a sturdy, protective shipping container. The solid absorbent materials hold liquid nitrogen, keeping the temperature at cryogenic level. When prepared correctly, there is no free-flowing liquid nitrogen to move around, hence avoiding the risk of spilling during transport.

A

B

Do's and don'ts:

- Dropping the dewar can cause damage to the internal structure that will compromise the function of the dry shipper.
- As the liquid nitrogen will evaporate over time, the foam lid should not be forced on or weighted down as this can cause overpressure in the dewar (it needs to vent).
- Keeping it either cold & closed or completely dry between uses, prevents moisture from forming ice crystals (ice/moisture will negatively impact the performance of the vessel).
- If you intend to use it soon, fill it with liquid nitrogen when you receive it to keep it cold until you are ready to ship your samples onwards to your experiment.
- If it will be some days/weeks before using it again or you will not return it to us within a week, please leave it open and let it dry completely between uses.
- If it is "warm" and you want to chill it before sending your perishable sample to a beamtime, please follow the "charging" instructions below.

Cooling down a warm dewar for shipping:

- Wearing the appropriate Personal Protective Equipment (PPE) is strongly recommended when preparing the dry shipper for shipping.
- A "warm" shipper, one standing at room temperature, should not be immediately filled with a large amount of liquid nitrogen as a significant amount of nitrogen gas will be generated as the cold liquid contacts the shipper's warm surfaces.
- Start by slowly and portion-wise pouring in 1-2 liters of liquid nitrogen (cool down the canister as well). Do not fill at this initial stage! The top of the shipper is then closed and the container is allowed to equilibrate for ~ 2 hours.
- After this period, the vessel may be filled with liquid nitrogen & left overnight or up to 24h before shipping. * It is important that the level of liquid nitrogen remain below

the fiberglass neck tube of the vessel and that it not come in contact with the vacuum port which is covered with a black plastic cap.

- At the end of this period, the excess amount of liquid nitrogen remaining in the vessel should be poured off into another vessel before one packs the frozen samples into the cold canister.
- Close with the foam lid and also secure the lid of the shipping case
- Charging is now complete and your dry shipper is ready for pick up!
- We recommend the use of a cart for transferring the heavy-weighted dry shipper from the lab to the pick-up point.

Please reach out to us individually or at demax@ess.eu if you have any questions or queries.