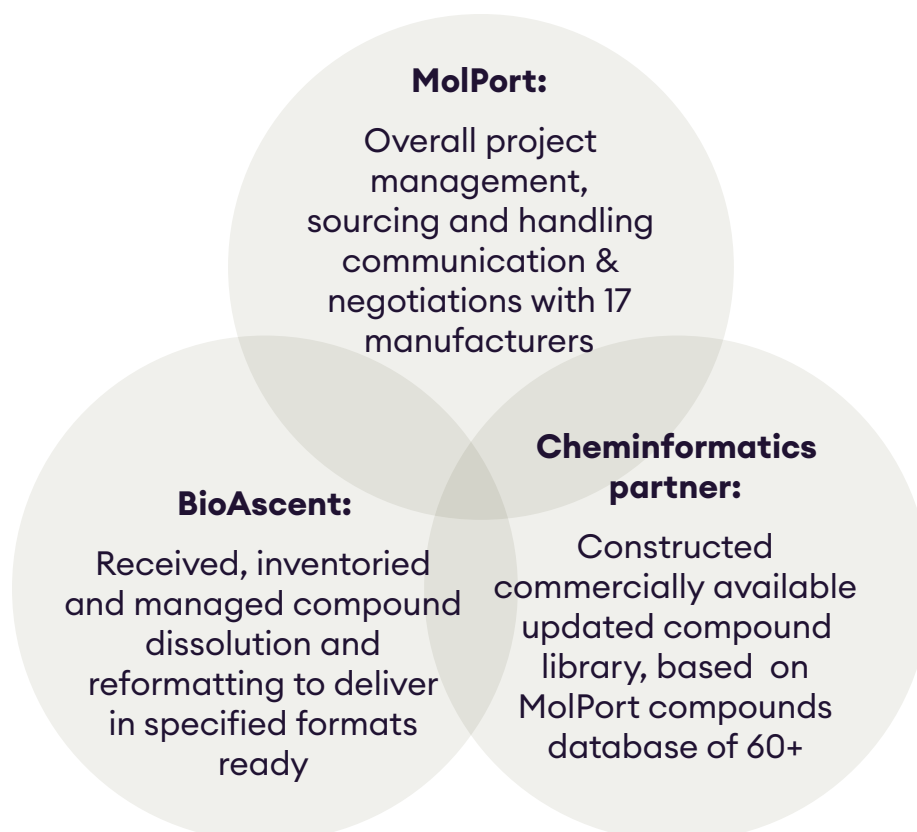


**Case study** **146 000 compound library acquisition**

**Successfully solved an extensive screening library acquisition problem, on time, within budget, and delivered samples ready for screening**

**Overview:**

The customer is in a leading drug development partnership targeting a specific therapeutic area. They were working with drug discovery services company BioAscent and other cheminformatics experts to design and acquire a 100,000 (initially)-compound library for screening.

**Approach:****Outcome:**

MolPort exceeded the customer's expectations, sourced and received the 143,531 ordered compounds in different formats, handled the logistics to deliver the samples as per customer requirements: a) solid, b) dry film (2µmole) in matrix 2D barcoded tubes, c) in solution in 384 well plates (200µL at 10mM in 100% DMSO).

## Rapid, Cost-effective Library Expansion in the Search for new effective drugs.

### Summary

The customer is in product development partnership in specific drug research. The customer was working with drug discovery services company BioAscent and consulted with cheminformatics experts to acquire a 100K compound library for screening.

After trying to locate and source the desired compounds from individual manufacturers, the customer turned to MolPort for advice and assistance in simplifying the compound selection and acquisition process. Access to MolPort's 7.8M database of commercially available compounds coupled with its expertise in compound ordering and logistics enabled the customer to select an expanded compound library for the same budget. MolPort successfully delivered 99.4% of the compounds in the required amounts and formats within the four-week deadline.

### Situation

As part of its drug discovery activities, the customer had a long-standing research partnership with BioAscent. The customer and BioAscent engaged with cheminformatics experts to design and acquire a 100K compound library for screening. The optimum screening library design was created using joint expertise in cheminformatics and compound analysis.

Once the library was designed, the customer opted to contact the 17 selected compound suppliers individually to enquire about sample availability, delivery schedules, and pricing. This proved to be a time-consuming administrative overhead, and the customer was not sure whether they were selecting the most cost-effective and reliable suppliers who would be able to deliver the specified compounds with the required purity, in the right format, on time, and within budget.

At this point in the project, BioAscent suggested the customer to work with MolPort. MolPort used experience and expertise in compound acquisition and logistics to benchmark the various initial offers from the suppliers whom the customer had contacted.

### Solution

MolPort coordinated cooperation between all project participants and provided access to its 7.8M commercially available compound database so that they could construct a new compound library. MolPort's experience in dealing with multiple suppliers helped the cheminformatic partners to focus on selected suppliers who would be able to meet the project's required timeframe. MolPort also suggested making contingency plans to deal with likely cancellations or other non-delivery issues. Together with the customer, they increased the compound selection to 115K, out of which 100K would be delivered for sure.

Once the partner had finalized the compound set, MolPort started to negotiate with the 17 selected suppliers to agree the terms and conditions of the compound library supply. As a result of smooth sourcing project flow customer decided to increase the compound library size by more than 45% to a new total of 146K compounds.

With full agreement and a sign contract between the customer, BioAscent, and the cheminformatics partner, MolPort ordered the compound set, and handled the logistics to deliver 99.4% of the compounds to BioAscent within the required four-week timeframe.

### Outcome

MolPort sourced and received the 143,531 ordered compounds in different formats, handled the logistics to deliver the samples as per customer requirements: a) solid, b) dry film (2µmole) in matrix 2D barcoded tubes, c) in solution in 384 well plates (200µL at 10mM in 100% DMSO).

BioAscent received, inventoried, and managed the compound dissolution and reformatting to deliver the following formats ready for screening in the various assays:

- 3 x 384-well plates Mother Plate (20µL at 10mM, columns 23-24 empty);
- 1 x 384-well PP HDW (28µL at 10mM, columns 1-2 and 23-24 empty);
- 3 x 384-well acoustic plates (5µL at 10mM, columns 23-24 empty);
- 3 x 1536-well acoustic plates (5µL at 10mM, columns 45-48 empty);
- 3 x 384-well Assay Ready Plates (columns 23-24 empty);
- 1 x 1536-well Assay Ready Plate (columns 45-48 empty).

By placing their trust in the excellent collaboration between MolPort and BioAscent, the customer was happy to find reliable partners who successfully delivered the project on time, with additional benefits:

- MolPort and BioAscent cooperation provided the customer with a single point of contact to cover all aspects of the project including access to data, compound acquisition, and compound management. This streamlined and simplified communication ensured consistency and increased project's efficiency.
- MolPort's expertise and experience in compound sourcing, dealing with multiple chemical suppliers, and ability to negotiate cost-effective pricing for bulk orders helped the customer acquire 43% more compounds.
- MolPort's and BioAscent's deep expertise in compound sourcing, logistics and sample management ensured that 99% of the required compound library was delivered and received on time for planned screening.

If you are facing compound sourcing challenges and are looking for an efficient and cost-effective solution that will save you time and overhead, and let you focus on science rather than administration, please contact us to see how we can help.