

Case study 25 000 Focused CNS-targeted Compound Set

One -Stop-Shop (3 partners involved) to Deliver a Focused CNS-targeted 25K Compound Set Within a Limited Budget

Overview:



The customer is in phenotypic screening. Project included design and acquisition of a CNS-targeted 25,000 compound set. The customer was looking for assistance with focused library design, compound sourcing and acquisition, and compound receipt and management.

Approach:

MolPort:

Overall project management, sourcing and handling communication & negotiations with partners and supplier, tracking

BioAscent:

Received, inventoried compound set. Handled the compound management for the customer

Cheminformatics partner:

Constructed focused compound library, based on MolPort stock compounds database

Outcome:

The MolPort-BioAscent-Cheminformatics partner collaborative partnership covered all aspects of the project including access to data for the application of cheminformatics tools for focused library selection, and compound acquisition and management, which helped the customer gain efficiency and reduce cost. Set delivered pre-formulated as 50µL at 10mM concentration in DMSO solution, frozen; in Greiner 384-well plates, 320 samples per plate.

Situation

A cost-conscious European customer contacted MolPort, BioAscent, and Cheminformatics partner with a project to design and acquire a CNS-targeted 25,000 compound set. The customer was looking for assistance with focused library design, compound sourcing and acquisition, and compound receipt and management BioAscent – preferably with a single point-of-contact, and within the constraints of a limited purchasing budget.

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Solution

The details of the project were discussed and confirmed in a conference call with the customer and MolPort and its partners. The key project goals were to select and deliver a high-interest, CNStargeted compound set for a limited budget.

With the project parameters agreed and based on its knowledge of screening compound suppliers and their various pricing, delivery, and reliability characteristics, MolPort suggested focusing the compound selection on a single, preferred supplier.

MolPort provided access to its filter database of commercially available compounds to Cheminformatics partner, so that they could apply their cheminformatics and computational chemistry expertise in selecting a compound set of interest.

MolPort handled the price and delivery negotiations with the preferred supplier, and ordered the compound set to be delivered pre-formulated as 50µL at 10mM concentration in DMSO solution, frozen; in Greiner 384-well plates, 320 samples per plate, with the first and last two columns empty.

BioAscent received and inventoried the compound set and handled the compound management for the customer, so that they were able to proceed immediately to CNS screening.

Outcome

By placing its trust in the MolPort-BioAscent cooperation, the customer found reliable, experienced partners who successfully delivered the project on time.

The MolPort-BioAscent-Cheminformatics partner collaborative partnership covered all aspects of the project including access to data for the application of cheminformatics tools for focused library selection, and compound acquisition and management, which helped the customer gain efficiency and reduce cost.

This cooperation and MolPort's experience in negotiating large compound orders also enabled the customer to obtain the maximum number of high-interest compounds for a limited budget.

If you are facing library selection challenges in your compound acquisition and screening programs, MolPort and its partners can help. MolPort and its library design and compound management partners can quickly understand your requirements, offer expert advice on library and supplier selection, and help negotiate an attractive price to maximize your compound acquisition budget.

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