Optimizing Reagent Selection

This module introduces new users to Reagent Selector. Participants create shopping lists of reagents from known suppliers for use in a synthetic or combinatorial chemistry workflow, collect compounds from in-house inventories, and use ISIS substructure searching query features to optimize the design of an appropriate reagent core.

Course Objectives

The participant will be able to:

- Create a reagent core to search for reagents
- Use ISIS query features to create a refined reagent core
- Refine a reagent list by filtering, clustering, and sorting
- Determine whether selected reagents are available in-house
- Create a shopping list of reagents to be ordered from suppliers

Prerequisites

None

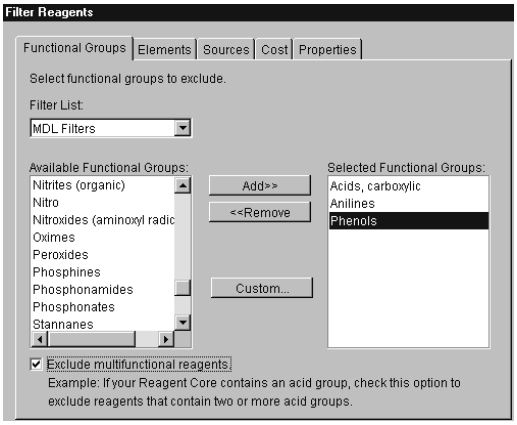
Note: This course does not teach in-depth structure searching. For such skills, see Molecule Searching.

Course Length

1/2 day

Examples from the Class

Filtering reagents based on functional groups



Using ISIS query features to refine a reagent core