USER GUIDE

This guide summarizes the major steps of the compound selection and ordering process in Mcule. For more information you can check our online user guide at doc.mcule.com. If you have any questions, feel free to contact us at support@mcule.com.

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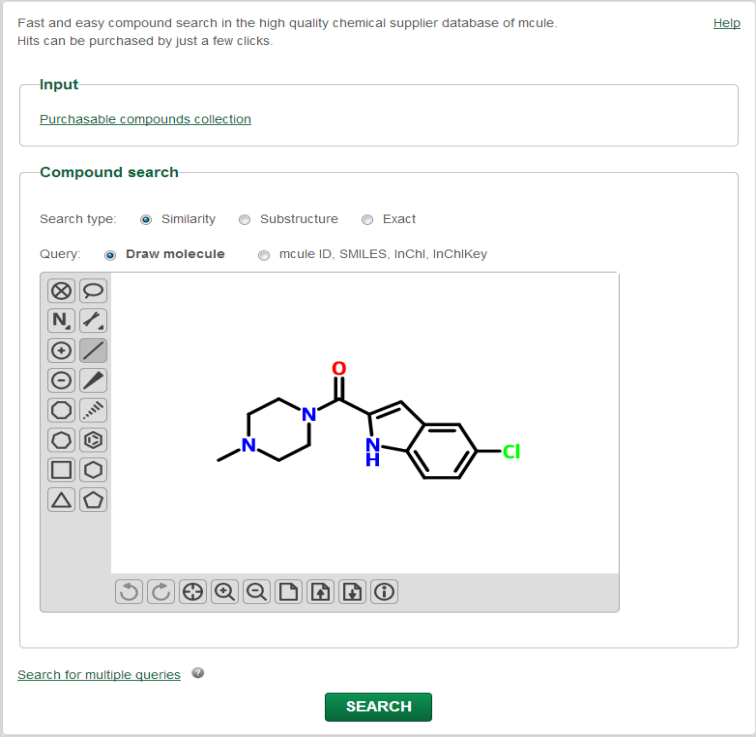
1. BASIC COMPOUND SELECTION

The "Purchasable compounds collection" of Mcule contains over 5 million unique structures and 10 million purchasable products. To keep our database as up-to-date as possible we have developed batch and live handlers that can automatically update stock availability information for millions of products per day. This makes the Mcule database the most up-to-date database of screening compounds currently available. Our compound registration system (Mcule Advanced Curation) includes over 80 steps and 150 substeps including normalization, preparation steps and structural checks. This unique registration system filters out the majority of problematic structures including drawing errors and stereochemical problems. To search this large chemical space we have developed efficient and fast searching tools to help you finding the right compounds for your drug discovery project. Below we list the various searching options you can select in Mcule.

1.1. FIND CHEMICALS / SINGLE QUERY: mcule.com/search

You can use this option to quickly find specific compounds/chemicals or close analogs of a single query compound in the Mcule database.



Exact, Similarity and Substructure searches

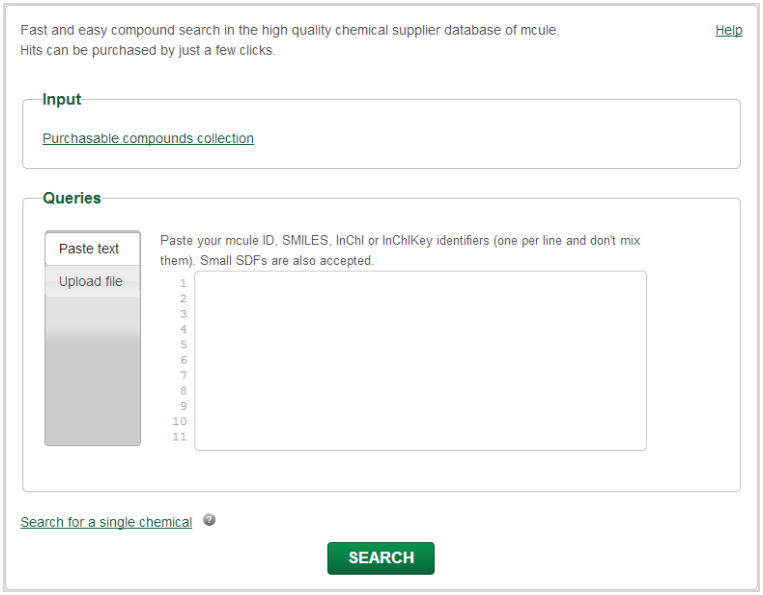
Search by **SMILES, InChI, InChIKey, Mcule ID** or use ChemWriter (Javascript drawer) to specify your query

Searching in **over 5M purchasable compounds** (Mcule database)

1. BASIC COMPOUND SELECTION

1.2. FIND CHEMICALS / MULTIPLE QUERIES EXACT: mcule.com/search/multi

With this option you can run exact searches with multiple query molecules. It can be useful for ordering a set of ligands e.g. virtual screening hits. You can paste or upload structures in multiple formats, such as Mcule IDs, InChI or SMILES strings, InChIKeys and even SDF files and use them as queries in the search.



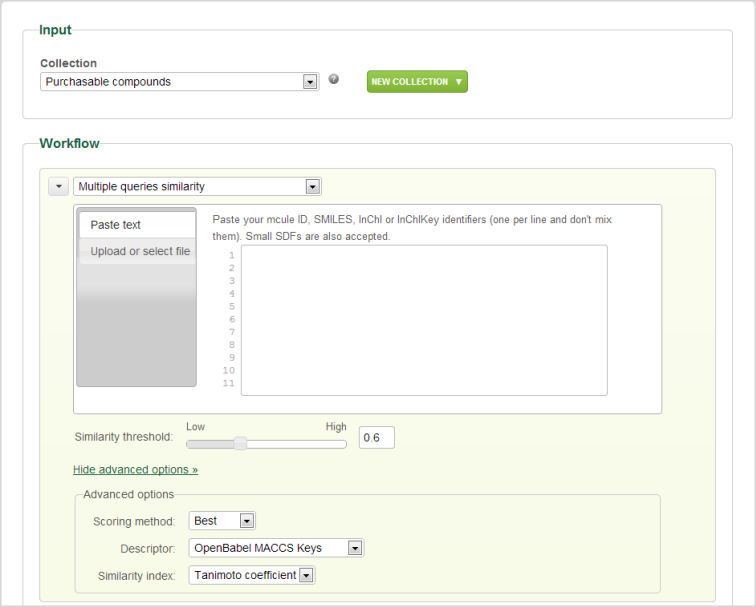
Search for multiple compounds and collect hits in a **single collection**

Paste or upload queries in multiple formats (SMILES, InChI, InChIKey, Mcule ID, SDF)

1. BASIC COMPOUND SELECTION

1.3. FIND CHEMICALS / MULTIPLE QUERIES SIMILARITY: mcule.com/search/screen/?template=multiple-queries-similarity

If you have multiple hits containing common structural elements (e.g. multiple analogs of the same scaffold), it makes sense to include all your hits in a single search as multiple queries. Depending on the scoring method used, the searching algorithm will retrieve hits that are most similar to your query molecules. *Best scoring method* will retrieve the similarity score to the most similar query molecule. *Average scoring method* will calculate an average similarity score to all query molecules.



Search for the **closest analogs** of multiple compounds (e.g. **HTS** and **virtual hits**)

Multiple fingerprints

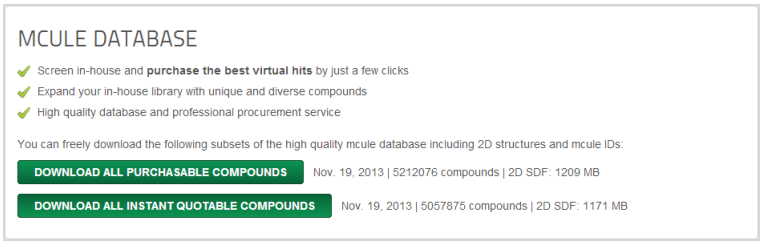
Best and average scoring methods

Paste or upload queries in multiple formats

1. BASIC COMPOUND SELECTION

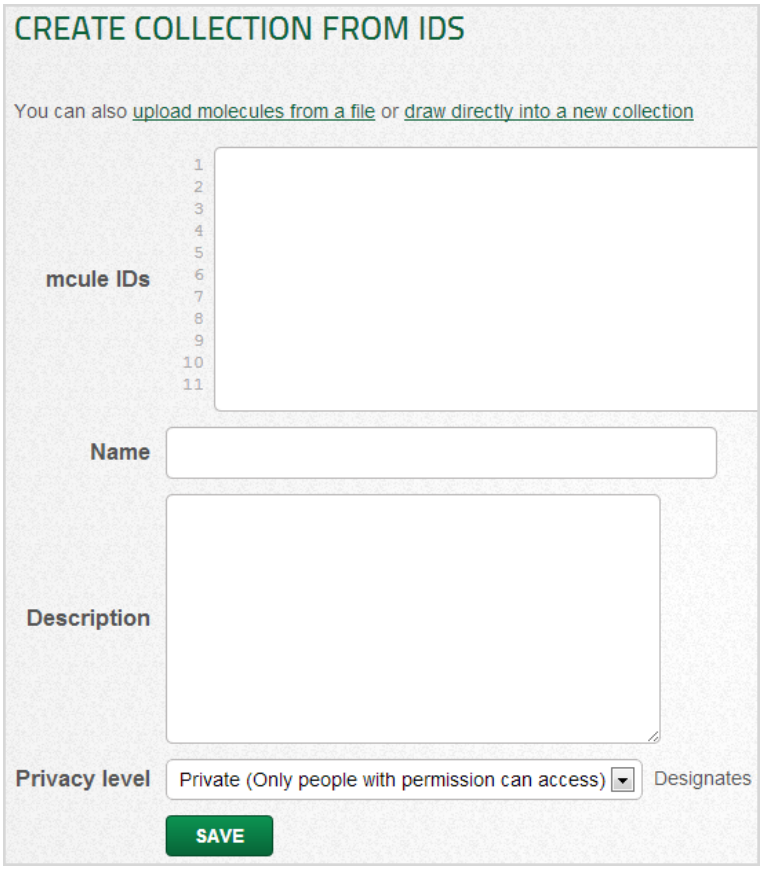
1.4. FIND CHEMICALS / MCULE ID LIST: mcule.com/collection/create/from-ids

Searching for Mcule IDs is the most straightforward and effective way to retrieve a set of molecules from the Mcule database. For example, if you have downloaded the Purchasable compounds collection from our Database Download page, and you want to come back for purchasing some compounds, you can paste Mcule IDs in the below form. All exported SDF files that you download from Mcule contain the corresponding Mcule IDs as a separate SDF field. If you have both a list of Mcule IDs and SDF, it is preferable to use the Mcule ID to retrieve compounds, as it more clearly identifies the structures.



Download the Mcule database:

mcule.com/database



Mcule db is curated by **MAC**:

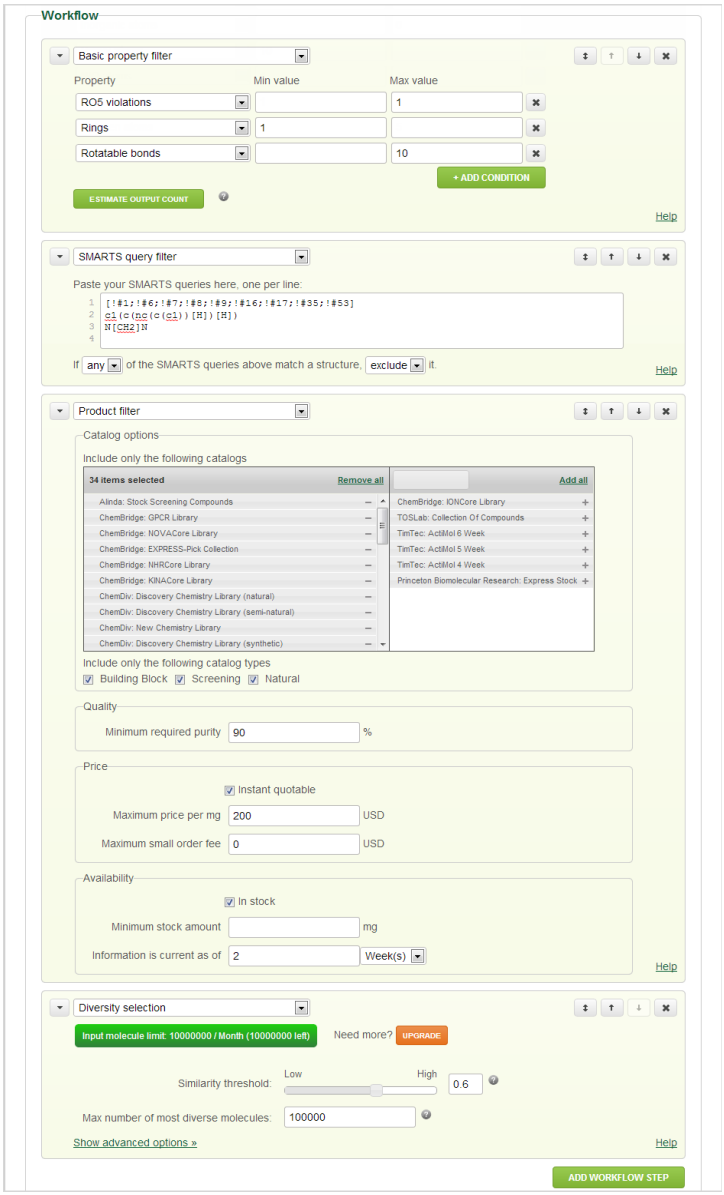
doc.mcule.com/doku.php?id=regsys

Process the database in-house and **come back** with a hit list **to order** or **post-process**

Paste Mcule IDs and create a collection **in seconds**

2. SMART COMPOUND SELECTION: mcule.com/search/screen

The Mcule technology revolutionizes compound selection either for virtual screening or for screening library design. The Workflow Builder can be used to build custom screening and filtering workflows by putting together powerful and advanced cheminformatic and molecular modeling tools like LEGO bricks. It can be used to run structure-based and ligand-based virtual screening workflows and the best hits can be purchased by just a few clicks. It enables the design of screening libraries based on various properties including chemical diversity (large-scale diversity selection) and supplier information (e.g. purity, available stock amount, delivery time, etc.).



Build **fully customized** workflows to filter the Mcule database

Filter by **molecular modeling** (Docking, FTrees Visual Similarities) and **cheminformatic** tools (Phys-chem properties, SMARTS, etc.)

Large-scale **diversity selection**

Use the **Product filter** to include / exclude products based on supplier information (catalogs, prices, stock availability, purity, etc.)

All results and query workflows are **stored** and can be adjusted any time

Uploaded compounds can be also processed

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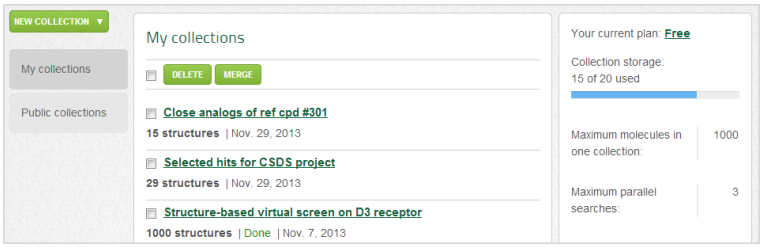
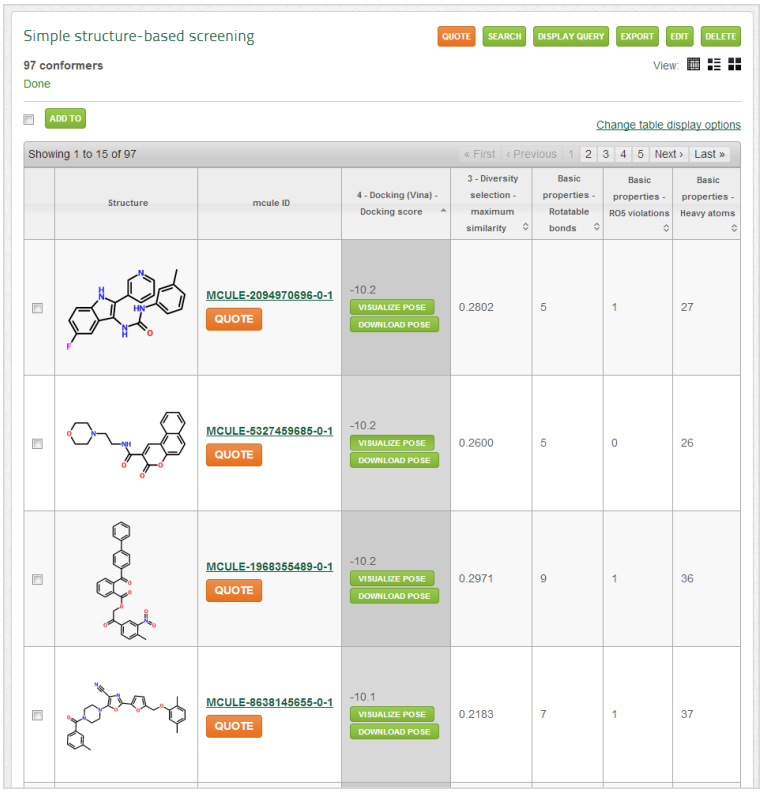
3. COMPOUND COLLECTION MANAGEMENT: mcule.com/collection

In Mcule you can select particular compounds either manually or by using the basic and advanced (smart) searching tools and store them in *collections*. The owner of a collection can set its privacy level to *Private* (only users with permission can get access), *Unlisted* (only people who know the specific URL of the collection can get access), or *Public* (accessible for everybody). Your search results (set of molecules and associated information) are also automatically stored in collections. Not only the search results but the queries are saved as well, so that you can go back and refine your queries until you get the optimal search results. Molecule collection can be stored, deleted, modified, merged, imported, exported and shared with your colleagues. Collections can be visualized in multiple ways together with associated data such as various properties, search and calculation results. Tables can be quickly sorted by these properties. Uploaded compounds are also stored in collections and can be used as input for any searches (all associated data incl. phys-chem properties will be automatically generated).



Search results are stored as **collections** along with the queries



Store, modify, delete, merge, import, export and **share** collections

Unite hit lists and place a **single order**

Multiple views (table, list, grid)

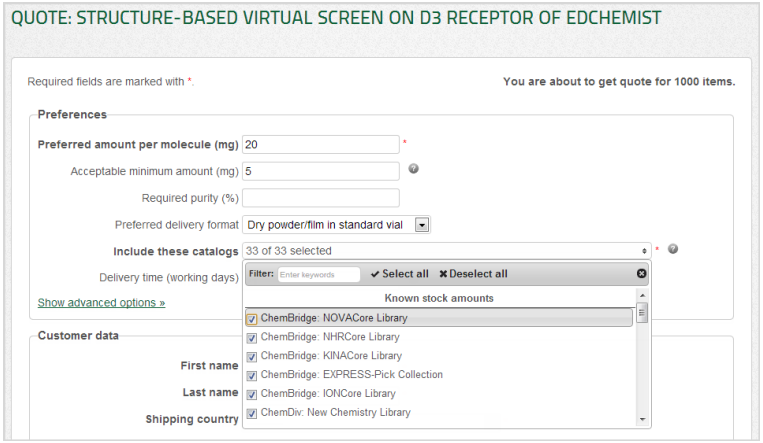
Display properties, **fast sorting**

4. COMPOUND ORDERING

The Mcule database contains over 5 million unique purchasable compounds and 10 million corresponding products. All these compounds can be purchased by clicking on the orange Quote buttons placed next to particular compounds or in the top right corner of collections. Then you can provide basic information required for quote calculation in the Quote form and depending on your price plan you will be able to choose between Instant Quote and Next-Day Quote. If you select Instant Quote, the best price and fastest delivery quotes will be calculated on-the-fly. You can then fine-tune these quotes based on *Effective price*, stock availability and purity information. After you finalized your quote, you can save it and export it in PDF or Excel formats. You can go back any time when you are ready to place the order. Optionally, you can specify a Purchase Order number and upload a PO file issued by your company / institution. After you placed the order, you can track its status online.

4.1. QUOTE FORM

In the quote form you can specify the preferred and the acceptable minimum amounts per compound. For example, if you would like to order 20 mg but at least 5 mg of a compound, then you should set these values as preferred and acceptable minimum, respectively. You can also set the minimum required purity for the products. Please note that for most screening compounds the guaranteed minimum purity is 85-90-95%, depending on the catalogs. You can request the compounds in standard or custom vials (powders) or plates (DMSO solutions). Our recent development now allows to implement any customer-defined formatting option to Instant Quote and we can implement it for you in a few days. To enable custom delivery formats in Instant Quote, please contact us at support@mcule.com. In the Quote form, you can also specify which catalogs should be included / excluded in the quote calculation. Catalogs are grouped based on stock availability information: *Known stock amounts* refers to at least weekly updated information, while for *Stock* catalogs, high availability rate is guaranteed but current amounts are not provided by the supplier. The maximum delivery time (in working days) can be also set.



Select **preferred** and **acceptable amounts**

Select **delivery / reformatting options** (company-specific formats can be implemented)

Select / discard **supplier catalogs** from quotation

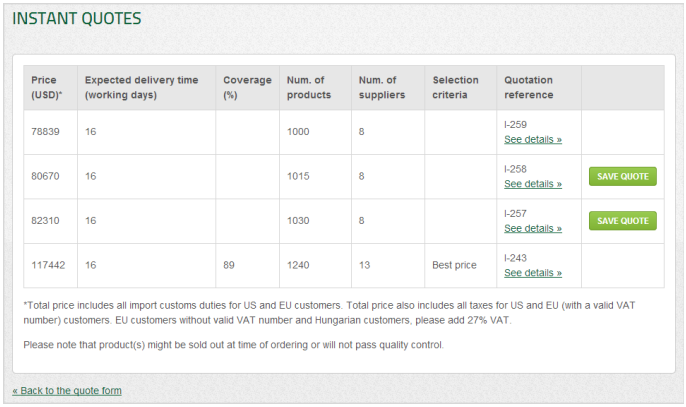
4. COMPOUND ORDERING

4.2. INSTANT QUOTE: mcule.com/quote/list

Instant Quote utilizes a unique price optimization algorithm which calculates the best price and fastest delivery quotes by comparing and optimizing compound prices, supplier discounts, small order fees, delivery costs, customs duties and reformatting options. Since the same compound is typically available from multiple suppliers and there are many parameters to consider during quote generation, the manual price and delivery time optimization could be very challenging even for a relatively small order: the number of possible quotes for 10 compounds each available from 5 suppliers, would be 5^{10}. Additionally, requesting stock availability information is time-consuming especially when the information has to be requested by email.

Our unique quote generation algorithm first automatically checks the stock availability for your selected suppliers. For almost 6M products we have access to the supplier's current stock levels that makes Instant Quote generation particularly reliable.

In the next step, our robust optimization algorithm finds the best product matches by minimizing the total price and the delivery time. Instant Quote generation typically takes 1-2 minutes even for thousands of compounds. After the optimization algorithm finishes the generated quotes will appear in the Quote list view.


INSTANT QUOTES

Price (USD)*	Expected delivery time (working days)	Coverage (%)	Num. of products	Num. of suppliers	Selection criteria	Quotation reference	
78839	16		1000	8		I-259 See details »	
80670	16		1015	8		I-258 See details »	SAVE QUOTE
82310	16		1030	8		I-257 See details »	SAVE QUOTE
117442	16	89	1240	13	Best price	I-243 See details »	

*Total price includes all import customs duties for US and EU customers. Total price also includes all taxes for US and EU (with a valid VAT number) customers. EU customers without valid VAT number and Hungarian customers, please add 27% VAT.

Please note that product(s) might be sold out at time of ordering or will not pass quality control.

« Back to the quote form

Best price and **Fastest delivery** quotes generated in 1-2 minutes

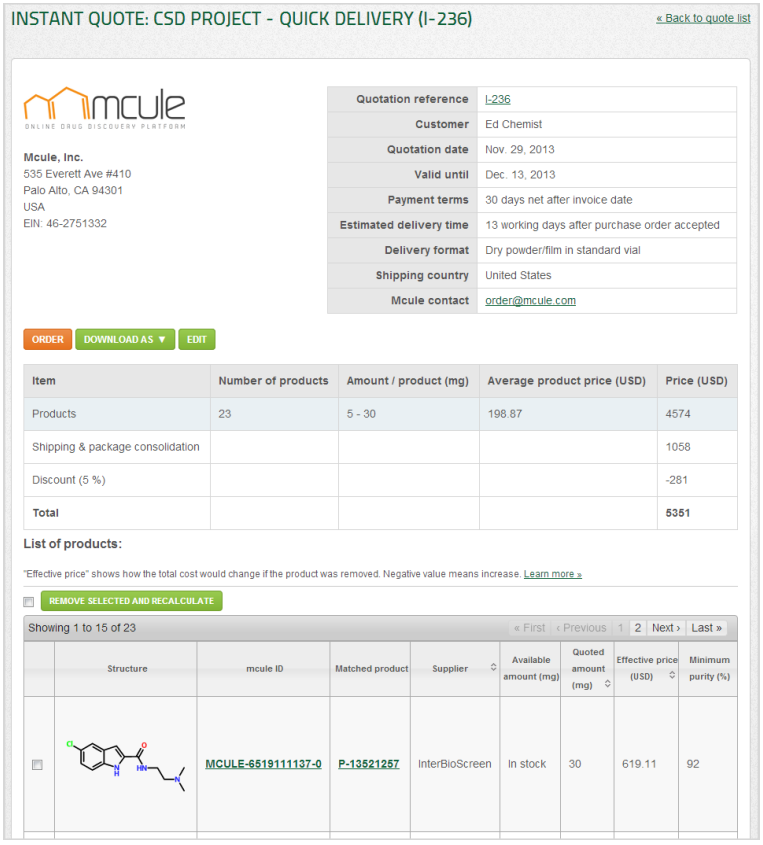
Automatic optimization of product prices, small order fees, delivery costs, customs duties, reformatting costs and bulk ordering discounts

Quote list view shows a short summary of the generated quotes

4. COMPOUND ORDERING

4.2. INSTANT QUOTE: mcule.com/quote/list

After analyzing the summary table in Quote list view, you can click on “See details” to see the break down of the total price of the individual quotes and most importantly you can fine-tune the quote by excluding compounds based on their effective price, stock availability and purity data. After you selected the products you want to remove, click on the “Remove selected and recalculate” button and a new quote will be generated for the remaining products on-the-fly.

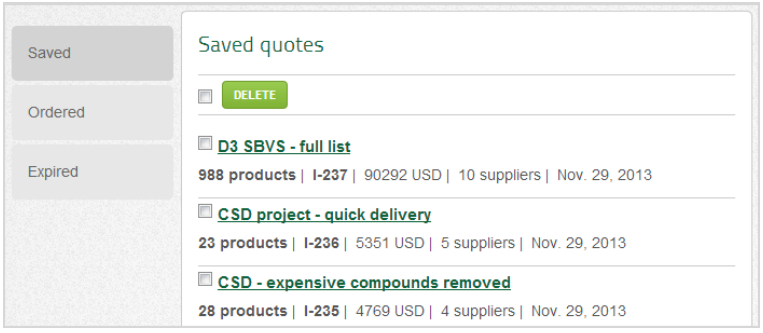


In the Quote list view, click on "See details" to **break down the total price** and analyze the selected products

Download your Instant Quotes in **PDF** or **Excel** formats

Post-process the product list by Effective price (contribution to total price), stock availability and purity

Discard expensive products and **recalculate** the quote **on-the-fly**

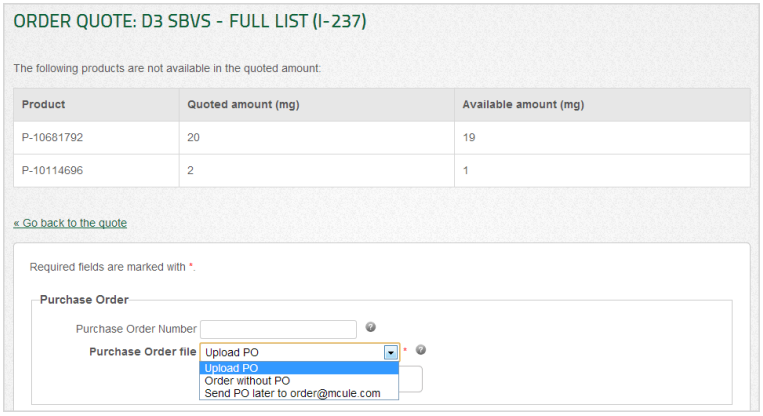


Save, **edit** and organize your Instant Quotes, and place an order by just a few clicks

4. COMPOUND ORDERING

4.3. PLACING AN ORDER

After finalizing your quote, you can place an order by clicking on the orange Order button. Please note that the stock availability of the compounds can change any time. If you go back to a previously saved quote, the stock availability of a compound might have fallen below the acceptable minimum amount. In such a case, the particular product is displayed after clicking on Order. If your quote is older than a few days, we suggest to re-run Instant Quote to make sure you place an order based on the most recently updated stock information. You can specify a PO number which we will use throughout the whole procurement and delivery process. You will be asked to either upload your PO file, send it later or place an order without a PO file. Please note that if you choose to place an order without a PO file, we will start processing your order and any PO files sent to order@mcule.com will be neglected. We also ask for the shipping and billing details, including an EU VAT number for EU customers.



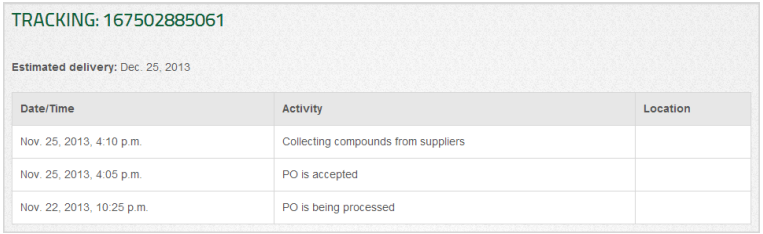
Specify **PO number**

Place an order **completely online** (without emails, phone calls)

Upload or send PO to order@mcule.com

4.4. ORDER TRACKING

After placing an order online, you can track its status by checking its unique URL. You can also request status updates and we will email you when the status of your order gets updated.



Track your orders and get **notifications** when the status of your order gets updated

4. COMPOUND ORDERING

4.5. CUSTOM FORMATTING

You can request custom formatting (custom vials / plates, extra weighting, DMSO solutions, dry ice shipping) and Mcule delivers the compounds as requested. Please note that any customer-defined formatting option can be implemented to our quote calculation algorithm and listed as a new delivery format option in your personal Instant Quote account.

4.6. PACKAGE CONSOLIDATION

Your ordered products will be delivered to you as a single package. You do not need to deal with a lot of chemical suppliers, we collect all products and send you a consolidated package.

4.7. DOOR-TO-DOOR DELIVERY

We provide complete EU and US customs clearance service (customs duties and taxes are paid by Mcule). Mcule does not charge any hidden customs costs to its customers. Additionally, our advanced service enables door-to-door delivery, meaning that you will not be contacted by any customs brokers, just get the package delivered to your door.

If you have any questions, or you need more information please don't hesitate to contact us at support@mcule.com