



How to Order Compounds from infiniSee xREAL

Important Information

Your privacy is important to us. Per default, **your query is not exported** with the results. Be sure the feature is not switched on during export for ordering (see Page 2).

To receive a 10% discount on your order from the xREAL Space, you need to export your search results from infiniSee xREAL.

1. Check molecules you are interested in. If you want to order compounds from several searches and modes, collect your molecules of interest in the Analyzer Mode and export them at the same time.
2. Go to 'Export checked results' and select 'Export Results as...' and select "Molecules files (*.sdf)".
3. Send the exported file to Enamine via libraries@enamine.net to receive your quote.

The screenshot displays the infiniSee xREAL software interface. At the top, there is a 'Query' section with 'unnamed' and 'Results' tabs. Below this, a 'Result Summary' box shows search parameters: Query (unnamed), Found Molecules (100), and From (xREAL_2024-07). To the right, 'Used Parameters' includes Maximum Number of Results (100), Minimum Similarity (0.10), and Fingerprint (ECFP4). Further right, 'Search Session Info' shows the user (Alexander Neumann), start time (13:27 2024-08-19), duration (00:01:57), and version (6.2.0).

A red box highlights the 'Export Results as...' menu option, which is open, showing sub-options: 'Export Results as...', 'Export Results per Space Source...', and 'Copy to Clipboard as SMILES'. Below the menu, a table of search results is visible. The table has columns for '#', 'Similarity', 'Space', 'Name', 'MW', and 'LogP'. The first six rows are visible, with the first row having a similarity of 1.000 and the sixth row having a similarity of 0.859. Red arrows point to the first, second, and fifth rows of the table. At the bottom of the interface, a 'Matching' section shows two chemical structures with a score of 1,000 and 0.571.

| # | Similarity | Space | Name | MW | LogP |
|---|------------|---------------|---------------|--------|------|
| 1 | 1.000 | xREAL_2024-07 | m_22b...54062 | 495.63 | 1.3 |
| 2 | 0.884 | xREAL_2024-07 | m_22b...22586 | 465.58 | 4.6 |
| 3 | 0.871 | xREAL_2024-07 | m_22b...40590 | 479.60 | 4.4 |
| 4 | 0.861 | xREAL_2024-07 | m_22b...34682 | 495.63 | 1.3 |
| 5 | 0.859 | xREAL_2024-07 | m_22b...14310 | 481.58 | 3.2 |
| 6 | 0.859 | xREAL_2024-07 | m_22b...60648 | 497.64 | 3.5 |



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Per default, your query molecule is masked and therefore not exported during export.

Yet, if you have turned it on during a session, it is also possible to turn it back off.

Got to 'System' > 'Export'

| Molecule | # | Similarity % | Specs | Name | MW | LogP | TPSA |
|----------|-------|---------------|---------------|-------------|--------|------|------|
| | 1 | 1.000 | vREAL_2024-07 | m_22b_54962 | 495.63 | 1.76 | 88.7 |
| | 0.884 | vREAL_2024-07 | m_22b_22986 | 465.58 | 4.02 | 84.2 | |
| | 0.871 | vREAL_2024-07 | m_22b_40350 | 479.60 | 4.41 | 84.2 | |
| | 0.861 | vREAL_2024-07 | m_22b_34882 | 495.63 | 1.76 | 88.7 | |
| | 14310 | 481.58 | 3.26 | 93.5 | | | |
| | 20648 | 497.64 | 3.97 | 84.2 | | | |

Green in 'Mask Query' means SMILES of the query will not be exported with the results.

Red means, the exported file will contain the respective query molecule SMILES as a column to each entry.

| Molecule | # | Similarity % | Specs | Name | MW | LogP | TPSA |
|----------|-------|---------------|---------------|-------------|--------|------|------|
| | 1 | 1.000 | vREAL_2024-07 | m_22b_54962 | 495.63 | 1.76 | 88.7 |
| | 0.884 | vREAL_2024-07 | m_22b_22986 | 465.58 | 4.02 | 84.2 | |
| | 0.871 | vREAL_2024-07 | m_22b_40350 | 479.60 | 4.41 | 84.2 | |
| | 0.861 | vREAL_2024-07 | m_22b_34882 | 495.63 | 1.76 | 88.7 | |
| | 14310 | 481.58 | 3.26 | 93.5 | | | |
| | 20648 | 497.64 | 3.97 | 84.2 | | | |