

Export Data and Structures

What is the quickest way to export a list of drugs, references, or patents? Can I download a SAR table? How do I generate a chemistry report?

With the export features in *Clarivate Analytics Integrity*, you can work offline and use *Integrity* data in meetings and when on the move, share information and include it in presentations, work with information in a preferred format, and easily integrate data with internal data. **Example Scenario:** you are a biochemist developing a compound to treat arthritis. The compound is a small molecule and you would like to explore the competitor landscape and send reports to colleagues with detailed information about the chemistry of similar early-stage compounds in development for the same condition.

Exporting your chemistry report and SAR table:

Creating a chemistry report

Advanced Search | Session History | Clear Form | Start

Product | Structure Search

Lead Compounds | Under Active Development

Condition (Dev. Status) | "Arthritis" | Index AND >

Phase (Dev. Status) | "Preclinical" | Index AND >

Molecular Weight | from 0 to 500 | Index AND >

Records Retrieved: 52 in Drugs & Biologics Search Results

Entry Number	Highest Phase	Code Name	Generic Name	Brand Name	Product Category	Therapeutic Group	Organization
90101	Launched-1985	DL-458IT L-5458 MDL-458 MP-104	Azacort (former INN) Deflazacort (BAN; USA); Emflaza (Rec. INN) Oxazacort	Calcort Deflan Dezacor Emflaza Flantadin	Corticosteroids Steroids	Antiallergy/A Drugs Rheumatoid Treatment of Antiinflammatory Muscular Dys Agents for Allergic Skin Treatment for	Sanofi (Originator) Supernus PTC Therapeutics Guidotti Ludwig- Maximilians- Univ. Muenchen
90195	Launched-1987	DE-019 REV-002 REV-004 REV-005 SA-96	Bucillamine (Rec. INN) Tiobutarit	Rimatil		Treatment of Disease-Mod Rheumatic D Immunosup Therapy of I of Metabolis Osteoarthritis of Rheumatoid Treatment of	Revive Therapeutics AYUMI Pharmaceutical Santen (Originator)

Options: Keep Me Posted, Export Center, Integrity Reports, Full Records, Product List with Structures, Display Milestones, Gateways to Product Development Status, References, Patents, All Related Information via Quick Search, Printer Friendly Format

Records Retrieved: 52 Record(s) Retrieved

Entry Number: 90101 * | Drug Name: Deflazacort | Highest Phase: Launched-1985

Product Category: Corticosteroids, Steroids

Therapeutic Group: Antiallergy/Antiasthmatic Drugs, Antiinflammatory Drugs, Rheumatoid Arthritis, Treatment of Muscular Dystrophy, Agents for Allergic Skin Disorders, Treatment for

Mechanism of Action: [Detailed description]

Organization: Sanofi (Originator), Supernus, PTC, Therapeutics, Guidotti, Ludwig-Maximilians-Univ. Muenchen

Structure Feature Options: [Detailed description]

Standard InChI: 1S/C25H31NO6/c1-13-26-25(20(30)12-31-14(22)16(28)7-8-23(15,3)22(17)19(29)11-24(18,25)4/h4H3/t17-,18-,19-,21+,22+,23-,24-,25+/m0/s1

Standard InChIKey: FBHSPRKOSMHSIF-GRMWWQJSA-N

Entry Number: 90195 * | Drug Name: Bucillamine | Highest Phase: Launched-1987

Product Category: [Detailed description]

Therapeutic Group: [Detailed description]

Mechanism of Action: [Detailed description]

Organization: [Detailed description]

Set up a search in the **Drugs & Biologics Knowledge Area of Integrity**.

From the drop-down menu of the search field, select **Condition (development status)**, **Phase (development status)**, and **Molecular Weight**.

Use **Index** to select "Arthritis" and "Preclinical" for **Condition** and **Phase** respectively, and type in "from 0 to 500" for **Molecular Weight**.

This search will return a records list; the drug records can be viewed by opening the **Options** drop-down menu and selecting **Product List**.

You can review the structures of these compounds by opening the **Options** menu again and selecting **Product List with Structures**.

Tip:

- Did you know that you can export information from more than one Knowledge Area in *Integrity* at the same time?
- Selected reports that combine information from different Knowledge Areas are available in **MS Word Format** via **Integrity Reports**.
- There are currently 12 different types of **Reports** available in *Integrity* depending on the Knowledge Area.

To create **Integrity Report**, open the **Options** menu from the results in **Drugs & Biologics** and select **Integrity Reports**.

Report Type

Product Report

Sales and Intellectual Property

Chemistry Report

Format

Microsoft Word

Report Name: Arthritis

GENERATE

The screenshot shows the 'Drugs & Biologics' application interface. At the top, there is a navigation bar with 'Home', 'Support/Help', 'Query Manager / Alert Center', and 'Reports' (highlighted with a green box). Below the navigation bar, there is a header section with 'Drugs & Biologics' and a 'GO' button. The main content area displays a detailed report for a specific drug, including fields for Name, Category, Mechanism of Action, and Chemical Structure. The report also includes a section for 'Related Organic Syntheses' with chemical reaction schemes.

In the dialog box you can select the type of report you want: in this example, a **Chemistry Report**. Type in the report name and click generate.

To download the report, click on the **Reports** option on the *Integrity* toolbar.

The report is available in **MS Word** format and contains the synthesis schemes for the products where available.

Exporting a SAR table

The screenshot shows the 'Drugs & Biologics' application interface. At the top, there is a navigation bar with 'Drugs & Biologics', 'Biomarkers', 'Literature', 'Organic Synthesis', 'Pharmacokinetics/ Metabolism', 'Companies & Research Institutions', and 'Experimental Models'. Below the navigation bar, there is a 'Filter by Statistics' section with various filters and a table of results. The 'Experimental Pharmacology' section is highlighted with a green box.

From your list of Drug Records in *Integrity* you can now refer again to the **Options** menu and select **All Related Information via Quick Search**.

Click the results in the **Experimental Pharmacology** Knowledge Area. The pharmacology results can be refined further by applying filtering criteria (**Filter by Statistics**).

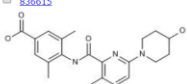
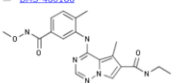
To compare the data based on the same parameter, e.g., **IC50**, click on the **Parameter** tab and select the option for **IC50**.

Next choose the benchmarking criteria, e.g., **Pharmacological Activity** and select the appropriate option (in this example; **TNF-α production inhibition**).

The screenshot shows the 'Records Retrieved' table for 'Experimental Pharmacology'. The table has columns for Drug Name, Biomarker, Mechanism of Action, Experimental Activity, Pharmacological Activity, and Material / Experiment Model. An 'Options' menu is visible on the right side of the table, with 'Structure Activity' highlighted. The table contains several rows of data, including drug names like '835615' and 'BMS-480188'.

The final list of records retrieved can now be viewed as a structure activity report (SAR) table. Click the **Options** pull-down menu and select **Structure Activity**.

The Structure-Activity table can now be exported. By selecting **Export Center** in the **Options** menu, you can select the Export Type; in this example **MS Excel** has been selected.

Drug Name & Structure	Mechanism of Action	Material	Value	Details
 S36615	Signal Transduction Modulators Prostanoid EP4 Receptor Antagonists	Blood, human	0.123 ± 0.001 µM	Ref. 2
			0.123 ± 0.001 µM	Ref. 3
 BMS-480188	Mitogen-Activated Protein Kinase 14 (MAPK14, MAPK p38 alpha) Inhibitors Signal Transduction Modulators TNF-alpha Release Inhibitors	Blood, human Mononuclear cells (blood), human	40 nM 51 nM	Ref. 1 Ref. 2
			51 nM	Ref. 3
			50 nM	Ref. 1
			50.0 nM	Ref. 4

To export the structure activity table, click **Export**.

Tip:

- Did you know that Structure-Activity tables can be exported from the **Experimental Pharmacology** Knowledge Area in a **MS Word**, **MS Excel**, or **ISIS for Excel** format?
- Using the **Export Center** when a Structure-Activity table is created, it is possible to select the Export Type. The information to be included in the table can also be selected here and this is dependent on the Export Type selected.
- By choosing the **Format as Table Data** box, it is possible to merge the **Experimental Activity**, **Pharmacological Activity**, and **Parameter** fields in the Structure-Activity table, eliminating data duplication and improving overall presentation.
- By selecting **ISIS for Excel** for use with an existing ISIS installation it is possible to export chemical structures. When using **MS Excel**, chemical structure images are exported. In addition, chemical structures can be exported as **SMILES** as part of the export when using any of the three Export Types.

Export Center - Experimental Pharmacology Structure Activity Table

This feature allows users to export selected data from Integrity for use in other applications. Up to 2000 records can be exported at a time from this Knowledge Area, either as full pages of records or as selected records (by utilizing the record checkbox feature).

Follow these steps to export data:

- 1) Use the pull-down menu to choose an export format.

Export type: Excel ▼

Format as table data ⓘ

- 2) Check the fields you wish to export for each record.

<input checked="" type="checkbox"/> Experimental Activity	<input checked="" type="checkbox"/> Source
<input checked="" type="checkbox"/> Pharmacological Activity	<input type="checkbox"/> Operator
<input checked="" type="checkbox"/> Parameter	<input type="checkbox"/> Means
<input checked="" type="checkbox"/> Entry Number	<input type="checkbox"/> Var
<input checked="" type="checkbox"/> Drug Name	<input type="checkbox"/> Min Value
<input checked="" type="checkbox"/> Structure image	<input type="checkbox"/> Max Value
<input checked="" type="checkbox"/> SMILES	<input type="checkbox"/> Biomarker
<input checked="" type="checkbox"/> Mechanism of Action	<input type="checkbox"/> System
<input checked="" type="checkbox"/> Material	<input type="checkbox"/> Activity/Effect
<input checked="" type="checkbox"/> Method	<input type="checkbox"/> Target/Condition/Toxicity
<input checked="" type="checkbox"/> String Value	<input type="checkbox"/> Exp Model Name

Check all
Reset all