Preparing a lecture on the Biological Periodic Table
Preparing a lecture on the Biological Periodic Table — “anti-tumor activity” of coordination compounds

Combine search tools to find property data of coordination compounds.

**Search objective**
Find bioactivity data of coordination compounds with one coordination center that have been studied for “anti-tumor” activity.
1. Perform a **Substance search**.

**Reaxys** has a unique database structure that links substance records directly with property information and corresponding references. To accommodate the variety and complexity of coordination compounds, modify the search form with Querylets that search for ligands through formulas.

Click **Add/Remove Fields** to modify the query form to include ligand **Querylets**.
2. Find the **Querylets** for ligands and add them to the query form.

Type in a property type to find relevant **Querylets**. Reaxys helps with **auto-suggest**.

The **exists** Querylet for One-Center Ligands is a quick way to search for all compounds with a single coordination center.

The Querylet **Base Formula (One-Center Ligands)** allows entering a base ligand formula with a single coordination center.

3. The selected Querylets become part of the query form. Click the **exists** check box.

Alternatively, enter a base ligand formula into the **Base Formula** Querylet field. See the **Appendix** for details about the ligand codes used in Reaxys.
4. Add the **Substance Basic Index** Querylet to search for “anti-tumor” activity.

**Substance Basic Index** searches for text terms in substance records. Because each record includes specific property information, this Querylet can be used to retrieve substance records with anti-tumor activity data.

Enter terms relevant to the desired information. Use **left** and **right truncation** (*) to include search terms with common word roots and connect words with **OR** (the semicolon ; is equivalent). Use **Lookup** to browse and search a list of related words and phrases.
5. The search delivers 1834 substances. Each record includes a list of property data.

Information on “anti-tumor” activity appears under the **Bioactivity** link, which includes quantitative and qualitative information on the in vitro efficacy of the compound.

Note: If using Reaxys without a subscription to Reaxys Medicinal Chemistry, the data retrieved by the **Substance Basic Index** Querylet are listed in the substance record under the link **Pharmacological Data**.
6. Review excerpted bioactivity data for the compound and access source documents.

The first compound has antiproliferative properties with an $LC_{50}$ > 100 µM, measured in breast cancer MCF-7 cells.

Tabulated quantitative data are each linked with their corresponding source. Reveal the title and abstract of a source by clicking Title/Abstract. Access the full text or click View citing articles to see citation information in Scopus.
Each entry in the qualitative information summarizes details about an in vitro assays performed with the compound, including targets tested and results obtained.

Two entries list information about the assays performed in the research article that reported the antiproliferative properties of the compound.
APPENDIX — Constructing a ligand formula

A ligand formula for a single-center coordination compound consists of 2 parts:
(a) A metal, which appears at the beginning of the formula
(b) The ligands attached to the metal, each enclosed in brackets {}

The coordinating atoms in each ligand are represented by codes according to the table below. Numbers of atoms are assigned if >1.

<table>
<thead>
<tr>
<th>Code</th>
<th>Atom(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>L</td>
<td>C</td>
</tr>
<tr>
<td>A</td>
<td>B Si Ge</td>
</tr>
<tr>
<td>D</td>
<td>N P As Sb</td>
</tr>
<tr>
<td>Q</td>
<td>O S Se Te</td>
</tr>
<tr>
<td>X</td>
<td>H F Cl Br I At</td>
</tr>
</tbody>
</table>

Special ligand codes: CO CS CN CNS CNO CNR

The metal is Co

The main ligand has 2 nitrogen and 2 oxygen as coordinating atoms, which are coded with D and Q respectively: 
{(2)D(2)Q}

A second ligand has nitrogen as a coordinating atom, which is coded with D: 
{D}

A third ligand has carbon as a coordinating atom, which is coded with L: 
{L}

Ligand formula: Co{(2)D(2)Q}{D}{L}
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