

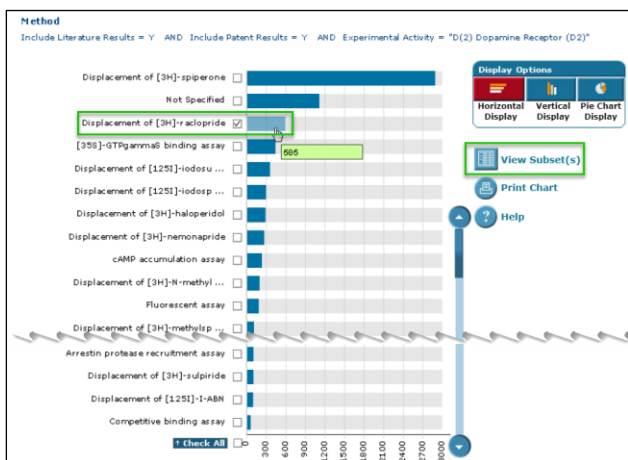
Find compounds with similar experimental activity

Are you investigating a specific target and would like to see compounds that show the highest affinity for this target?

Experimental Activity data within Experimental Pharmacology Knowledge Area of *Clarivate Analytics Integrity* enable you to search experimental data by system, activity/effect, and target/condition/toxicity. Apply advanced filtering tools within *Integrity* to narrow down the results to records with the same experimental methodology for the purposes of comparison. You can also use *Integrity* to gather all related information to those compounds with the highest activity retrieved in your search and link to the Drugs & Biologics Knowledge Area to see the corresponding records. **Example Scenario:** you are a medicinal chemist investigating a specific target, dopamine D2 receptor, with the aim of optimizing a compound for the treatment of psychosis. You would like to see other compounds with similar experimental activity *in vitro* that show high target affinity for the dopamine D2 receptor.

Search for compounds with similar experimental activity:

Data Name	Biomarker	Mechanism of Action	Experimental Activity	Pharmacological Activity	Molecular Weight	Method	Decayrate	Value	Details
D(2) Dopamine Receptor (D2)	Dopamine D(2) receptor affinity	Dopamine D(2) receptor affinity	...	Equipments of [3H]-spiperone	EC-50	> 10 µM	SEL-1
D(1) Dopamine Receptor (D1)	Dopamine D(1) receptor affinity	Dopamine D(1) receptor affinity	...	Equipments of [3H]-spiperone	EC-50	> 10 µM	SEL-1
D(3) Dopamine Receptor (D3)	Dopamine D(3) receptor affinity	Dopamine D(3) receptor affinity	...	Equipments of [3H]-spiperone	EC-50	> 10 µM	SEL-1
D(4) Dopamine Receptor (D4)	Dopamine D(4) receptor affinity	Dopamine D(4) receptor affinity	...	Equipments of [3H]-spiperone	EC-50	> 10 µM	SEL-1
Dopamine Receptor (nonspecified subtype)	Dopamine receptor affinity	Dopamine receptor affinity	...	Equipments of [3H]-spiperone	EC-50	> 10 µM	SEL-1
Duffy Blood Group Antigen	Duffy Blood Group Antigen	Duffy Blood Group Antigen	...	Equipments of [3H]-spiperone	EC-50	> 10 µM	SEL-1
EGF-Like Module-Containing Mucin-Like Hormone Receptor-Like 1	EGF-Like Module-Containing Mucin-Like Hormone Receptor-Like 1	EGF-Like Module-Containing Mucin-Like Hormone Receptor-Like 1	...	Equipments of [3H]-spiperone	EC-50	> 10 µM	SEL-1
Endothelin Receptors	Endothelin Receptors	Endothelin Receptors	...	Equipments of [3H]-spiperone	EC-50	> 10 µM	SEL-1
Formyl Peptide Receptors	Formyl Peptide Receptors	Formyl Peptide Receptors	...	Equipments of [3H]-spiperone	EC-50	> 10 µM	SEL-1
Free Fatty Acid Receptors (FFARs)	Free Fatty Acid Receptors (FFARs)	Free Fatty Acid Receptors (FFARs)	...	Equipments of [3H]-spiperone	EC-50	> 10 µM	SEL-1
Frizzled/Smoothed Receptors	Frizzled/Smoothed Receptors	Frizzled/Smoothed Receptors	...	Equipments of [3H]-spiperone	EC-50	> 10 µM	SEL-1
G Protein-Coupled Receptor 142 (GPR142)	G Protein-Coupled Receptor 142 (GPR142)	G Protein-Coupled Receptor 142 (GPR142)	...	Equipments of [3H]-spiperone	EC-50	> 10 µM	SEL-1
G Protein-Coupled Receptor 172A	G Protein-Coupled Receptor 172A	G Protein-Coupled Receptor 172A	...	Equipments of [3H]-spiperone	EC-50	> 10 µM	SEL-1
G Protein-Coupled Receptor 174 (GPR174)	G Protein-Coupled Receptor 174 (GPR174)	G Protein-Coupled Receptor 174 (GPR174)	...	Equipments of [3H]-spiperone	EC-50	> 10 µM	SEL-1



Go to the **Experimental Pharmacology** Knowledge Area of *Integrity*. Select the **Experimental Activity** field which allows you to search experimental data by system, activity/effect and target/condition/toxicity.

Tip:

- In *Integrity* the **Pharmacological Activity** field contains information referring to the interaction between the drug and the target receptor or enzyme. **Experimental Activity** describes broader, more inclusive information that combines Activity/Effect and Target/Condition/Toxicity subcategories.

To search for target-specific data use the **LookUp** box in the **Index**. In this example, select the general target Dopamine Receptor (D2). The query retrieves the table with experimental pharmacology records.

Tip:

- You can link directly to the target record from the Experimental Pharmacology results list. A hyperlink appears in the record and with one simple click you will be redirected to the record for the Target associated with the data.

The large number of results can be filtered using the **Filter by Statistics** chart options to narrow down the results set. To make the results comparable for the same study method, filter by **Method**.

From the chart select **Displacement of [3H]-raclopride**, a methodology used in binding studies tracking the activity of D2 receptors, then click **View Subset(s)**. This will display a subset of records in the results list that use the same experimental methodology, facilitating comparison.

The results are now all for the same method and, in this case, the activity is already affinity for all records. To further refine the data, select the **Experimental Activity** chart for **System** and click to see only **In Vitro** results.

Tip: There are three Experimental Activity filters that can be used to unify the results: System, Activity/Effect, and Target/Condition/Toxicity

Index Name	Bioassay	Mechanism of Action	Experimental Activity	Pharmacological Activity	Value	Details
13127	SP1	Dopamine D2 Receptor (DRD2) Agonists	D21 Dopamine Receptor (DRD2) affinity, M	Dopamine D2 receptor affinity	93 nM	Ref. 1
13127	SP1	Dopamine D2 Receptor (DRD2) Agonists	D21 Dopamine Receptor (DRD2) affinity, M	Dopamine D2 receptor affinity	78.8 ± 4.10 nM	Ref. 2
13127	SP1	Dopamine D2 Receptor (DRD2) Agonists	D21 Dopamine Receptor (DRD2) affinity, M	Dopamine D2 receptor affinity	80.3 ± 20 nM	Ref. 2
13200	SP1	S-HT2A Receptor Agonists	D21 Dopamine Receptor (DRD2) affinity, M	Dopamine D2 receptor affinity	32 nM	Ref. 5
13200	SP1	S-HT2A Receptor Agonists	D21 Dopamine Receptor (DRD2) affinity, M	Dopamine D2 receptor affinity	32 nM	Ref. 6
13200	SP1	S-HT2A Receptor Agonists	D21 Dopamine Receptor (DRD2) affinity, M	MS mouse fibroblasts transfected with human receptor	13.4 ± 1.00 nM	Ref. 3

To find the compounds with the highest affinity open the **Options** pulldown menu and select **Unify Parameter to Non-Log From** to set all the parameters to the same form for comparison.

Once this is done, click on the **Value Range** filter.

Select the parameter from the dropdown list in the pop-up window. Select **Ki** in this example, then select the unit **M** and click **Go**.

Value
Include Literature Results = Y AND Include Patent Results = Y AND Experimental Activity = "D(2) Dopamine Receptor (D2)"

0 to 1x10 E-14 **View Subset(s)**

1x10 E-14 to 1x10 E-13

1x10 E-13 to 1x10 E-12

1x10 E-12 to 1x10 E-11

1x10 E-11 to 1x10 E-10

1x10 E-10 to 1x10 E-9

1x10 E-9 to 1x10 E-8

1x10 E-8 to 1x10 E-7

1x10 E-7 to 1x10 E-6

1x10 E-6 to 1x10 E-5

1x10 E-5 to 1x10 E-4

1x10 E-4 to 1x10 E-3

1x10 E-3 to 1x10 E-2

1x10 E-2 to 1x10 E-1

1x10 E-1 to 1x10 E0

1x10 E0 to 1x10 E1

1x10 E1 to 1x10 E2

1x10 E2 to 1x10 E3

1x10 E3 to 1x10 E4

1x10 E4 to infinity

Select Parameter & Units

In order to provide a meaningful graphical display of the content you need to filter the selected records down to a single **parameter** and **unit**. Please select a parameter and unit from the lists below:

Ki (346) M (346)

Go

A chart displays with the different ranges of values from which you can select to view only the subsets with the lowest concentration values and therefore the highest affinity. Note that values are presented initially in logarithmic scale.

Tip:

- The values can be changed from logarithmic to **Standard Scale** and back by clicking the button next to the chart.

Working with your data:

Targets & Pathways

Drug & Biologics: 5 RECORDS

Biomarkers: 0 RECORDS

Literature: 3 RECORDS

Organic Synthesis: 0 RECORDS

Pharmacokinetics/Metabolism: 0 RECORDS

Companies & Research Institutions: 0 RECORDS

Experimental Models: 0 RECORDS

Genomics: 0 RECORDS

Patents: 2 RECORDS

Experimental Pharmacology: 8 RECORDS

Clinical Studies: 0 RECORDS

Disease Briefings: 0 RECORDS

Entry Number: 70124 Drug Name: **Spiroperidol** Highest Phase: Launched-1969

Product Category: Butyrophenones, Antipsychotic Drugs

Therapeutic Group: Antipsychotic Drugs

Mechanism of Action: Signal Transduction Modulators, Dopamine D2 Receptor (DRD2) Antagonists

Organization: Janssen (Originator), Eisai

Standard InChI: 1S/C23H26FN3O2/c24-19-10-8-18(9-11-19)21(28)7-4-14-26-15-12-23(13-16-26)22(29)25-17-27(23)20-5-2-1-3-6-20/h1-3,5-6,8-11H,4,7,12-17H2,(H,25,29)

Standard InChIKey: DKGZKTPJOSAWFA-UHFFFAOYSA-N

Entry Number: 90645 Drug Name: **Nemonapride** Highest Phase: Launched-1991

Product Category: Butyrophenones, Antipsychotic Drugs

Therapeutic Group: Antipsychotic Drugs

Mechanism of Action: Signal Transduction Modulators, Dopamine D2 Receptor (DRD2) Antagonists

Organization: Astellas Pharma (Originator), Nigma-Lerads

Standard InChI: 1S/C21H26ClN3O2/c1-14-18(9-10-25(14)13-15-7-5-4-6-8-15)24-21(26)16-11-17(23)19(23-21)12-20(16)27-3/h4-8,11-12,14,16,23H,9-10,13H2,1-3H3,(H,24,26)/t14,18-/m/1/s1

Standard InChIKey: KRVOJCLBAAKS1-RDXWAMCSA-N

Now that you have the compounds with the highest affinity you can view the details of these by opening **Options** pulldown menu and selecting **All Related Information Via Quick Search** and linking to the **Drug & Biologics Knowledge Area**, where you can view drug records for competitor compounds.

To see the structure, select **Options** and **Product List With Structures**.

If you have any questions please contact us at: DTStraining@clarivate.com