



ENZYME INHIBITOR LIGAND-SET™

Product Number **L 6787**

Storage Temperature $-20\text{ }^{\circ}\text{C}$

Product Description

The Enzyme Inhibitor LIGAND-SET™ is a set of 80 small organic ligands which inhibit a variety of enzymes. These ligands are arrayed in a standard 96-well plate format; each well has a capacity of 1 ml.

This set can be used for screening new drug targets, for guiding secondary screens of larger, more diverse libraries and for standardizing and validating new screening assays.

Enzyme inhibitors are used in a variety of instances to block the actions of specific types of enzymes, whether *in vivo* or *in vitro*. The majority of the inhibitors provided here block certain protein serine-threonine kinases, tyrosine kinases, and protein phosphatases that phosphorylate or dephosphorylate intracellular proteins, thereby increasing or decreasing their activity. Also included are monoamine oxidase inhibitors, that mediate the α deamidation of the monoamine neurotransmitters to aid in their degradation and elimination. This Ligand-Set also includes inhibitors of nitric oxide synthase, reverse transcriptase, alkaline phosphatase, phosphodiesterases, and cyclooxygenase.

Components/Reagents

The Enzyme Inhibitor LIGAND-SET™ contains 2 mg of each ligand per well. Stock solutions can be readily prepared by adding 1 ml of DMSO to each well. The set also comes with a diskette containing a structure database, or SD file, and a Microsoft Excel file containing the catalog number, name, rack position and pharmacological characteristics of each ligand. The following is a listing of all the enzyme inhibitors included:

A-165	Rp-cAMPS triethylamine
A1784	Aminopterin
A2169	3'-Azido-3'-deoxythymidine
A-230	gamma-Acetylinic GABA
A-253	(±)-AMT hydrochloride
A4669	Acyclovir

Product Information

A6011	Acetazolamide
A7795	H-9 dihydrochloride
A8003	Allopurinol
B7283	Benserazide hydrochloride
B8132	S(-)-p-Bromotetramisole oxalate
B8279	Ro 20-1724
C-108	2-Cyclooctyl-2-hydroxyethylamine hydrochloride
C-126	S(-)-Carbidopa
C2932	Chelerythrine chloride
C3930	Calmidazolium chloride
C4042	Captopril
C6506	(±)-p-Chlorophenylalanine
D-103	(±)-2,3-Dichloro-alpha-methylbenzylamine hydrochloride
D-131	3,5-Dinitrocatechol
D-210	4,5-Dianilinophthalimide
D2926	Diphenyleneiodonium chloride
D5519	Diacylglycerol kinase inhibitor I
D6899	Diclofenac sodium
D9751	2,4-Diamino-6-hydroxypyrimidine
E-114	erythro-9-(2-Hydroxy-3-nonyl)adenine hydrochloride
E8375	(-)-Physostigmine
F-124	Furafylline
F6513	Fusaric acid
G1274	HA-1004 hydrochloride
G6649	Genistein

H4759	Hydrochlorothiazide
H9382	3-Hydroxybenzylhydrazine dihydrochloride
I2142	KN-62
I4883	(±)-Ibuprofen
I7016	H-7 dihydrochloride
I7378	Indomethacin
I7627	Iproniazid phosphate
I8021	L-N6-(1-Iminoethyl)lysine hydrochloride
I8768	L-N5-(1-Iminoethyl)ornithine hydrochloride
K1003	Ketoconazole
L9908	LY-294,002 hydrochloride
M-003	R(-)-Deprenyl hydrochloride
M-182	MDL 12,330A hydrochloride
M3127	S-Methylisothiourea hemisulfate
M3778	Clorgyline hydrochloride
M4659	Milrinone
M7033	NG-Monomethyl-L-arginine acetate
M7628	DL-alpha-Methyl-p-tyrosine
M9656	H-8 dihydrochloride
N1392	Nialamide
N-161	NPC-15437 dihydrochloride
N-194	NS-398
N2001	Neostigmine bromide
N-211	NS 2028
N5501	NG-Nitro-L-arginine
N7778	7-Nitroindazole
O0886	Olomoucine
O3636	ODQ
P-106	3-Phenylpropargylamine hydrochloride

P-215	PD 098,059
P3510	Papaverine hydrochloride
R-106	Ro 16-6491 hydrochloride
R-107	Ro 41-1049 hydrochloride MAO-A inhibitor
R-108	Ro 41-0960
R6520	Rolipram
S0758	Sulfaphenazole
S-145	SKF 91488 dihydrochloride
S-153	SQ 22536
S5890	Sanguinarine chloride
T-173	Thiocitrulline
T-175	1-(2-Trifluoromethylphenyl)imidazole
T-182	Tyrphostin A9
T3932	AG 1295
T7883	Trimethoprim
U-120	U0126
U6756	U-73122
U6881	U-73343
V8261	(±)-gamma-Vinyl GABA
Z0878	Zaprinast

Preparation Instructions

To create a new database in ISIS™/BASE :

- Open ISIS™/BASE.
- Choose **File>New database**.
- Enter **Enzyme Inhibitor** or a preferred name in the File name field.
- Click **Save**.

The “Create Database” window will now be open.

- Enter **Catnum** for the Field name.
- Choose **Variable text** from the drop down window of the Type field.
- Click **Add**.
- Repeat the above steps for the following:

Field name	Type
Name	Variable text
Position	Variable text
Action	Variable text
Class	Variable text
Selectivity	Variable text
SecName	Variable text
Description	Variable text

- Enter **Structure** for the Field name.
- Choose **Structure** from the drop down window of the Type field.
- Enter ***Structure** for the External name.
- Click **Add**.
- Click **Save**.

The main ISIS™/BASE window will now be open.

To create the Form:

- Click on the “Draw a box” button (second button down on the left of the screen).
- Move the mouse to the bottom left hand corner and draw a box, ½ inch high, the length of the screen by clicking on the left mouse button and dragging the mouse across the screen. (see figure below)
- Above this box, draw another ½ inch high box the length of the screen. (see figure below)
- Above this box, draw a third ½ inch high box the length of the screen. (see figure below)
- Above these long boxes draw 3 ½ inch high x 3 inch wide boxes. (see figure below)
- Above these 3 boxes, draw another three the same size. (see figure below)
- Draw a final box to fit the remaining space of the screen above these boxes. (see figure below)



Double click on the top box. This will open the Box properties window.

- Click on **Structure**.
- Click **OK**.
- Repeat the same steps, clicking on the appropriate field name for the appropriate box:

Box	Field name
First small box	ID
Second small box	Catnum
Third small box	Position
Fourth small box	Action
Fifth small box	Class
Sixth small box	Selectivity
First long box	Name
Second long box	SecName
Bottom long box	Description

- Choose **File>Save form**.
- Enter Enzyme Inhibitor or preferred name.
- Click **OK**.

Importing an SD file:

- Click **Update**.
- Choose **File>Import>SD File**. **NOTE:** For MAC users, you must hold down the **option key** while choosing **File>Import>SD File**. If you do not, the Enzyme Inhibitor.sdf will not be visible in the import window.

- Enter **Enzyme Inhibitor.sdf** (Located on the floppy diskette provided with the plate).
 - Click **Open**.
The Import SD File window will now be open.
 - Click on **Add a new record including structure**, on both sides of the table.
 - Click **OK**.
- The database is now ready to use.

Storage/Stability

Store plate –20 °C with cap strips firmly in place. Plate cover should only be removed when plate is in use to prevent loss of caps strips.

SMS 8/00

Sigma brand products are sold through Sigma-Aldrich, Inc.

Sigma-Aldrich, Inc. warrants that its products conform to the information contained in this and other Sigma-Aldrich publications. Purchaser must determine the suitability of the product(s) for their particular use. Additional terms and conditions may apply. Please see reverse side of the invoice or packing slip.