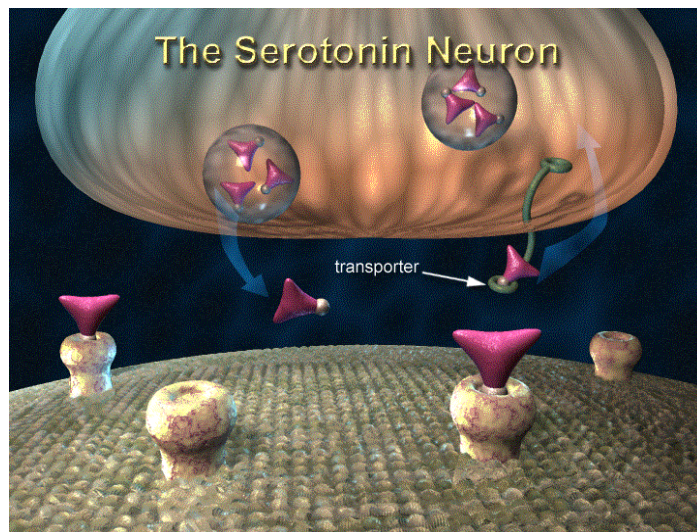


## Transporter Inhibitor Databases

Chemical Biological and Pharmacological Information of Transporter inhibitors from International Journals, US and International Patents have been curated and a unique database is now available in various formats like in ISIS/Base DB, SD, XML and Oracle. This database can also be made available for any set of Transporter super families. The database will be licensed on a non-exclusive basis.

### Each individual Record consists of:

- 2D/3D molecular structure with Mol. wt. & Formula, IUPAC and generic Name, SMILES
- Title, Authors, Company Address,
- Reference of the Patent or Journal,
- Compound number / Example number, GVK\_ID
- Bioassay with details of units, quantitative biological activity, types of targets along with their isomeric or mutated forms,
- Cell specification if it is cell based assay.
- ADME parameters
- Any anomalies are observed

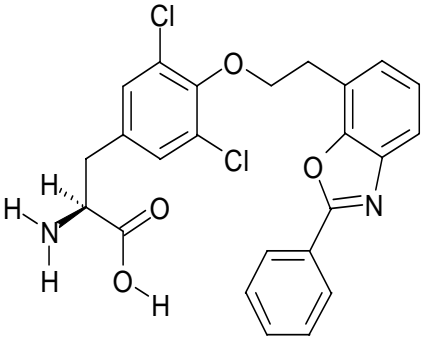


All structures listed in tables/text with activity data are generated from articles and patents have been curated to indicate the chemical space explored for each family of targets. Details of **Assay method, Source-Name, Source-Code, Official gene name of protein, Locus\_Id, Multiple Loci, Locus reference, values of the target, units of measurement and activity value** are also curated. The database can be further customized to suit any specific requirements or additional data.

### The databases could be effectively used:

- Easy query using any one or more number of fields or their logical combinations
- Structure, sub-structure, and similarity based query
- Easy export of the database or retrieved results to an SD or RD files, ChemFinder, excel sheet, MSAccess or Oracle databases
- Pharmacophore hypothesis, analogue (3D-QSAR) and structure based drug design and virtual screening.

**Sample Record**

Structure		Activity						
<p>Structure</p> 		*fmla_Structure	<b>C<sub>24</sub>H<sub>20</sub>Cl<sub>2</sub>N<sub>2</sub>O<sub>4</sub></b>					
		*mol.weight_Structure	<b>471.3440</b>					
		Structure Name	<b>(S)-2-Amino-3-(3,5-dichloro-4-[2-(2-phenyl-benzooxazolyl)-ethoxy]-phenyl)-propionic acid</b>					
		SMILES	<b>NC(Cc1ccc(Cl)c(Cl)c1)C(=O)OCCOc2ccc(Oc3ccccc3n2)cc4ccccc4</b>					
		Title	<b>1) AROMATIC AMINO ACID DERIVATIVES AND MEDICINAL COMPOSITIONS</b>					
		inventor	<b>1) ENDO, Hitoshi; KANA, Yoshikatsu; TSUJIHARA, Kenji; SAITO, Kunio</b>					
		company_address	<b>1) ENDO, Hitoshi [JP/JP]; 229-0022 1-23-7 Kanagawa (JP).</b>					
		claim/example	<b>1) Example 23</b>					
Platform_Name	Journal/Patent	GVK_ID	REF_ID	reference				
<b>Transporter</b>	Patent	<b>1434965</b>	<b>1508</b>	<b>WO 03/066574 A1</b>				
S_No	Journal	Year	Volume	Issue	Start_page	End_page	PubMed_Id	
1	WO 03/066574 A1	2003						
bioassay 1) Aromatic amino acid derivative as L-type amino acid transporter inhibitor : Useful in treatment of cancer								
Derivative	Target	Agonist/Antagonist/Inhibitor	Therapeutic_use	Binding_Site				
Aromatic amino acid	L-type amino acid transporter	Inhibitor	Cancer					
remarks								
Final	Error_4	Success	Error_3	Reviewer_2	Error_2	Reviewer_1	Error_1	Curator
		222 <input checked="" type="checkbox"/>						

Structure			Activity						
GVK_ID 1434965		reference WO 03/066574 A1				claim/example 1) Example 23			
protein\cell\anim	Source_name	Source_code	official_name	Locus_ID	MultipleLoci	Locus_Ref	assay_type	Assay_no	REFER
L-type amino acid transporter 1		Human	SLC7A5	8140			B		1
L-type amino acid transporter 2		Human	SLC7A8	23428			B		1
L-type amino acid transporter 2		Human	SLC7A8	23428			B		1
protein	Activity Type	Activity UOM	Activity Prefix	Activity Value	SD	enzyme/cell_assay			REFERENCE
L-type amino acid transporter 1	IC50		<	1.0000000000		Inhibition of leucine uptake by L-type amino acid transporter 1 in human upon incubation at 37 degree C for 10 minutes			1
L-type amino acid transporter 2	IC50		>	100.0000000000		Inhibition of leucine uptake by L-type amino acid transporter 2 in human upon incubation at 37 degree C for 10 minutes			1
L-type amino acid transporter 2	Selectivity		=	100.0000000000		Selectivity for human L-type amino acid transporter 2 to that of L-type amino acid transporter 1 for leucine uptake inhibition			1
Target_class	Family	Subfamily	Sub_subfamily	PDB_ID	Standard_name	Alias	Other_names	P/S	REFERENCE
Transporters	Solute carrier family 7	Heteromeric amino acid transporter			solute carrier family 7 (cationic amino acid transporter, y+ system), member 5	4F2LC, CD98, D16S469E, E16, LAT1, MPE16, hLAT1		P	1
remarks									

## Other Databases

**Our other database products include:**

- **MCD** -Medchem Database consisting of biologically active compounds from journals.
- **CCD**—Compounds with pharmacokinetic, dynamic properties in various levels of clinical trials
- **DD** – Pharmacokinetic and dynamic properties of all the FDA approved drugs.
- **PCD** – Pre-clinical Pharmacokinetic, dynamic and Metabolite information of compounds.
- **MBT** - Proven or established mechanism of toxicity for ‘drug like’ compounds.
- **TXD** - Different Toxicities information of pharmacologically active compounds.
- **NPD** - Bio-active Natural Products and semi-synthetic compounds curated from Journals.

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