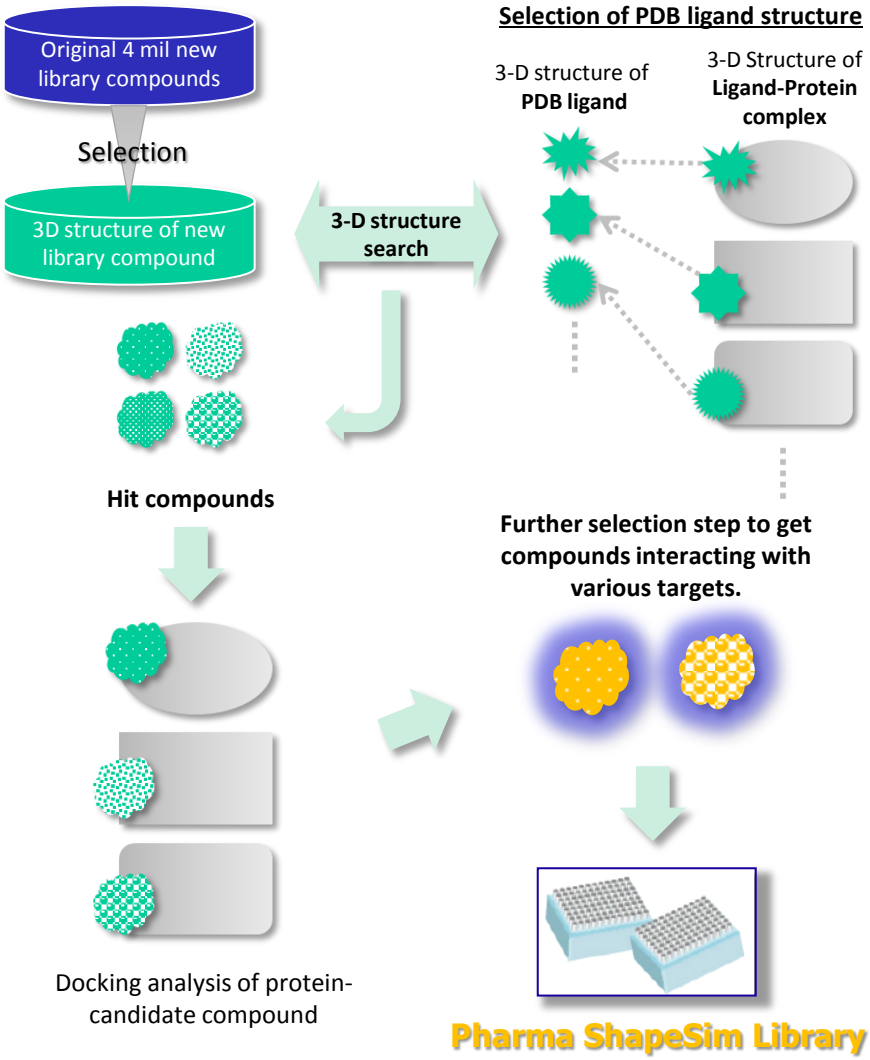
PharmaDesign Original 3D Library

Pharma ShapeSim Library

PharmaDesign selected, synthesized and launched a new library having druggable 3-D structures to support your drug discovery studies.
The “Pharma ShapeSim Library” is designed with novel 3-dimentional matching models from PBD ligands and filtered from 4 million chemical compounds. This library is suitable for phenotype screening, allowing one compound to react with multiple targets.

How to create the Library



Key features

- Selected up to 600 compounds from 4 million chemical library after original selection using 3D structure matching and docking technology.
- All compounds in the library are synthesizable and in stock.
- Available SD file and OEBinary file of all structure information as well as selection path information of PDB ligand docking.
- Designed by PharmaDesign Inc., a specialist of in silico drug designing.

High value subset are also available

- Pharma Shaped Library
  - Phenotype Screening Subset
  - Non-flat Subset

Phenotype screening subset [300]
Compounds that have reactivity with various targets were selected so they are suitable for phenotype screening.

Non-flat subset [140]
We picked compounds with spherical-like structure and with fCsp3 = 0.45 -0.65 in order to mimic the complexity of a drug. fCsp3 is the number of sp3 hybridized carbon / total number of carbon

Worldwide distribution network

United States / Canada
Oakwood Products, Inc.
730 Columbia Hwy.N, Estill,
SC 29172 U.S.A.
TEL +1 404 247 8745 / +1 800 467 3386
FAX +1 803 739 6957
www.oakwoodchemical.com
Email: requests@oakwoodchemical.com

United Kingdom / Europe
Fluorochem Ltd.
Unit 14
Graphite Way, Hadfield, Derbyshire
SK13 1QH United Kingdom
TEL +44 1457 860 111
FAX +44 1457 892 799
www.fluorochem.co.uk

Apollo Scientific Limited
Whitefield Rd, Bredbury, Stockport, Cheshire,
SK6 2QR United Kingdom
TEL +44 161 406 0505
FAX +44 161 406 0506
www.apolloscientific.co.uk

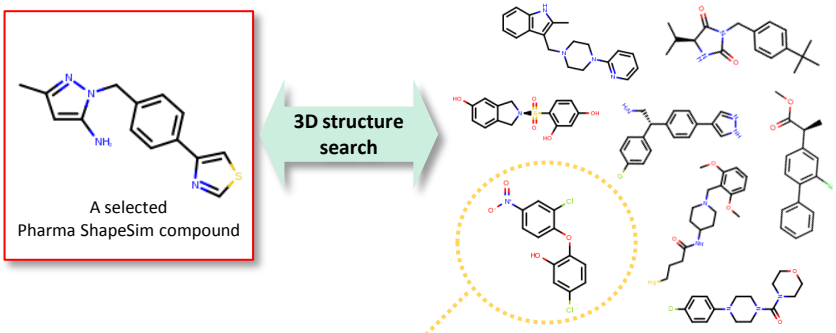
Singapore
Scientific Hub Services (SHS) Pte Ltd.
3 Science Park Drive, #02-12/25 The Franklin,
Office Suite 2 Singapore Science Park I,
118223 Singapore
TEL +65 9850 2655
FAX +65 6640 1351
www.sci-hub.com

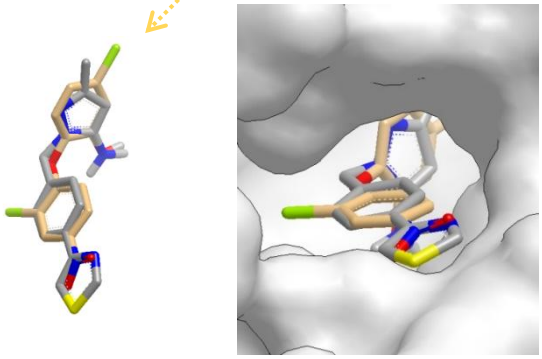
China
Seiko Trading Shanghai Co.,Ltd.
3C, 315 Guangyuan Road, Shanghai
200030 China
TEL +86 21 6090 5268
FAX +86 21 6090 5269
www.seikonet.cn

KISHIDA

KISHIDA CHEMICAL Co.,Ltd. | **E** shiyaku@kishida.co.jp | **W** soyaku.kishida.co.jp
11-8, 2-chome Shin-ohashi, Koto-ku 135-0007 Tokyo Japan | TEL +81-3-5625-5595 FAX +81-3-5625-5596

One Example of Pharma ShapeSim Library



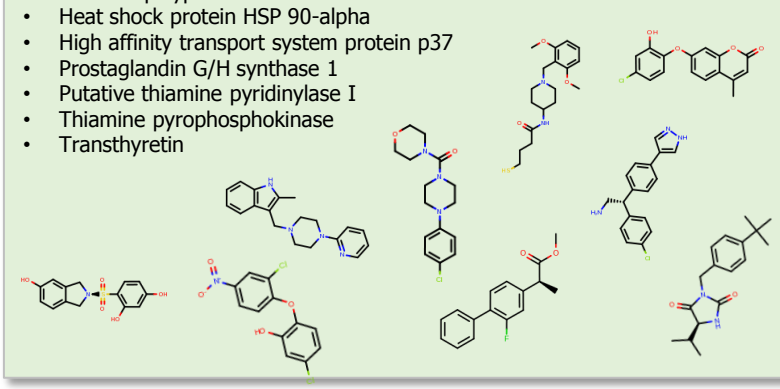


Left: A selected compound (gray colored) has similar 3D structure (but different 2D structure) with PDB ligand (**ROCS = 1.40**[1], **MACCS = 0.23**[2]). Right: Similar docking placement of the protein target in a pocket (**POSIT = 0.75**[3])

1) **ROCS index** showing similarity of 3D structure, range from 0 to 2 (complete match)
2) **MACCS index** showing similarity of 2D structure formula, range from 0 to 1 (highest similarity)
3) **POSIT index** showing compatibility of structure after docking, >0.5 indicates enough compatibility.

16 representative proteins targeted for 38 PBD ligands

- [Pyruvate dehydrogenase (acetyl-transferring)] kinase isozyme 2
- 2'-hydroxybiphenyl-2-sulfinate desulfinase
- ABC-type transport system
- Acidic mammalian chitinase
- Aldo-keto reductase family 1 member C3
- Beta-secretase 1
- cAMP-dependent protein kinase catalytic subunit alpha
- Dehydrosqualene synthase
- Enoyl-ACP reductase
- Genome polyprotein
- Heat shock protein HSP 90-alpha
- High affinity transport system protein p37
- Prostaglandin G/H synthase 1
- Putative thiamine pyridinylase I
- Thiamine pyrophosphokinase
- Transthyretin



SPECIFICATION

- Product name: Pharma ShapeSim Library
- Catalog code: PSS01
- Number of compounds: 600 compounds
  - Full set (600)
  - Mini set (300)
  - Phenotype screening subset (300)
  - Non-flat sublet (140)
- Standard volume: 1mg or 2mg
- Compound form: Solid (contains oily form)
- Purity: > 90 %
- Packaging: 96 well plate format
- Storage condition: Cool and dark place

PACKAGING

- Compounds in micro tube in racks (80 compounds each rack)
- Physical property data of the compound, information about PDB ligands and target which is used for compound selection and in silico docking data : SD File format, OEBinary format, CD-ROM

NOTIFICATION

- Compounds are typically shipped in powder form however some are liquid, oil or high viscosity.
- Please be careful when opening the vial cap. Compounds might be stuck to the reverse side of the vial cap due to vibration during delivery.
- This product is for research use only.
- For further technical details and sales pricing, lead time, please contact your local distributor or Kishida Chemical (shiyaku@kishida.co.jp).

PharmaDesign Inc.

PharmaDesign Inc. is a selective Genomic Drug Discovery venture company founded by professionals on bioinformatics and rational drug design. PharmaDesign contributes to the health and welfare of people by devoting its latest genomic drug discovery technique to develop innovative and specialized medicines. PharmaDesign Inc. has developed the Pharma ShapeSim Library with disclosing an agreement with Kishida Chemical for global sales and marketing distribution.

W | www.pharmadesign.co.jp

KISHIDA

KISHIDA CHEMICAL Co.,Ltd. | E shiyaku@kishida.co.jp | W soyaku.kishida.co.jp
11-8, 2-chome Shin-ohashi, Koto-ku 135-0007 Tokyo Japan | TEL +81-3-5625-5595 FAX +81-3-5625-5596