

Disclosing incoherent sparse and  
low-rank patterns inside  
homologous GPCR tasks for better  
modelling of ligand bioactivities

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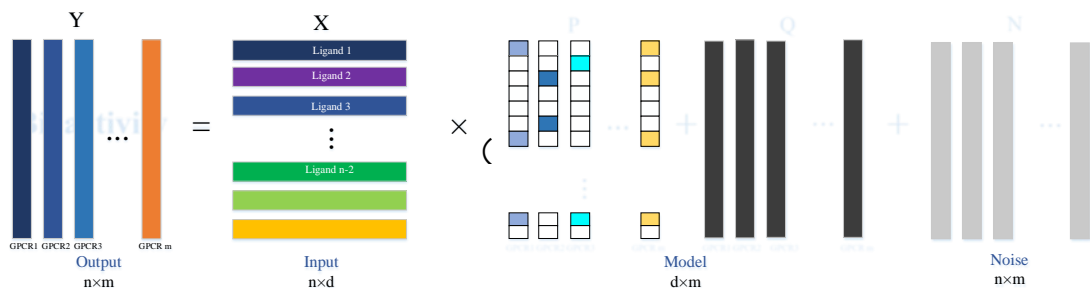
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# Problems & Ideas

- Accurately modelling and interpreting ligand bioactivities for new and potential drug targets in G protein-coupled receptors (GPCRs)
  - the lack of labeled training samples
- Ideas: A multi-task regression learning with incoherent sparse and low-rank patterns (MTR-ISLR) to model ligand bioactivities
  - introducing homologous GPCR tasks
  - the low-rank constraint catching the underlying relationship among homologous GPCR tasks
  - the entry-wise sparse constraint discovering essential discriminative substructures of each GPCR task

# Main Contributions

- Schematic of MTR-ISLR



$$\min_{Z, P, Q \in \mathbb{R}^{n \times m}} \sum_{j=1}^m \sum_{i=1}^{n_j} L(z_j^T x_i^j, y_i^j) + \gamma \|P\|, \quad s.t., \quad Z = P + Q, \|Q\|_* \leq \tau.$$

- Web page

**MTR-ISLR (Multi-task Regression Learning with Incoherent Sparse and Low-rank Patterns)**

— for Better Modelling of Ligand Bioactivities

Examples of compounds from GPCR Library having pharmacophore similarity to Ambrisentan and bearing scaffolds that are bioisosteric to the spiro-piperidine-indane privileged fragment (via examine.net)

MTR-ISLR (multi-task regression learning with incoherent sparse and low-rank patterns) is a novel method to precisely model and interpret bioactivities of ligand molecules by combining homologous GPCRs. MTR-ISLR was examined on a set of thirty-one representative GPCRs datasets that cover nine subfamilies of human GPCRs. The results demonstrate that the combination of homologous GPCRs in learning bioactivities of ligands can effectively improve the performance and interpretation of models by utilizing similar information of interaction and ligand samples cross these GPCR proteins. This is of great significance for understanding GPCR-ligand interaction and developing new drugs targeting GPCRs.

**Reference:**  
Junsheng Wu, et al. *Disclosing incoherent sparse and low-rank patterns inside homologous GPCR tasks for better modelling of ligand bioactivities*. Submitted.

**Download:**  
Source Code of MTR-ISLR Program

**MTR-ISLR Online Server:**

**G Protein-Coupled Receptor:**  
5-hydroxytryptamine receptor 1F (P30010)

Copy and paste your compound (up to 10) below in [SMILES strings](#).

Or you can upload [files](#) with the SMILES strings.

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