PK-Sim for simulating PBPK for MetraMorpheus

<https://docs.open-systems-pharmacology.org/v/v10/working-with-pk-sim/pk-sim-documentation/pk-sim-expression-data>

human gene database- <http://setup.open-systems-pharmacology.org/>

It should be noted that the current version of the database only describes spatial distribution of active processes in PBPK models. Temporal aspects such as circadian rhythms underlying chronogenetics are not included in the current version of the database. If necessary, such effects may be considered in a corresponding MoBi® model.

To review for different details of the drug pbpk model <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC9963741/>

**Data to be collected as of now:**

Under create compound:

1)Lipophilicity of the LNP(with value origin(VO)-experiment type, source, any paper)

2)Fraction of lnps unbound to any compound in plasma with VO

3)Molecular weight with VO

4)compound type - neutral, acidic or basic

5)solubility, at different pH

(some of the above using online tools)

Under metabolising enzyme:

the job is to find if any of the enzymes is linked in the metabolism pathway of lnps, antibodies…

(similarly if any protein transporter or signalling molecules)

This is the same list of proteins under all three categories( Metabolising enzymes, transport protein,

- ABCB1

- ABCB11

- ABCC2

-ABCC3

-ABCC4

-ABCC5

-ABCC6

-ABCG2

-BCRP

-BSEP

-CYP1A2

-CYP2A6

CYP2B6

-CYP2C19

CYP2C18

CYP2C8

CYP2C9

CYP2B6

CYP2E1

CYP3A4

CYP3A5

CYP3A7

CYP3A4A11

MATE1

MATE2-K

MDR1

MRP 2

MRP 4

MRP 5

MRP 6

NTCP

OAT 1

OAT 2

OAT 3

OAT4

OAT7

OAT -K1

OAT -K2

OATP1A1

OATP1A2

OATP1A4

OATP1B1

OATP1B2

OATP1B3

OATP2B1

OATP4

OATP4C1

OATP-A

OCT1

OCT2

OCTN1

OCTN2

SLC10A1

SLC21A1

SLC22A1

SLC22A11

SLC22A2

SLC22A4

SLC22A5

SLC22A6

SLC22A7

SLC22A8

SLC22A9

SLC47A1

SLC47A2

SLCO1A1

SLCO1A2

SLCO1A3

SLCO1A4

SLCO1B1

SLCO1B2

SLCO1B3

SLCO2B1

SLCO4C1

UGT1A1

UGT1A4

UGT1A6

UGT1A9

UGT2B4

UGT2B7

With the above data, the PBPK simulation can be done.