ESI Contents

Chapter 2 - Modelling Anion Transport

Folder: C2_AnionTransport

Files:

Experimental_Chemicals_database.xlsx Initial database of compounds following extraction from papers

PAG_dragon_chemical_values.xlsx Experimental values and DRAGON descriptors for original anion transport compounds, excluding duplicates

Chemicals_mechanisms_cleaned.xlsx Additional data on biological action and mechanisms - only for compounds with measured EC_{50} values

logEC50_with_errors.xlsx Excel file containing experimental errors and log(1/EC50) vs ALOGP plot

PAG_2D_structures.zip Structures of anion transporters, individual .mol files

PAG_2D_structures.sdf structures in .sdf format - all compounds in one file

PAG_structures_image.pdf Structures of anion transporters in image format

c3sc51023a_expanded_compounds.sdf Structures of the subset expanded from paper 10.1039/c3sc1023a - Section 2.4.3

Folder: PCA

    2D_Descriptors_PAG_Originalset.csv DRAGON descriptors generated from 2D structures

    2D_Structures_PAG_Originalset.sdf 2D structures of anion compounds (original set)

    3D_Descriptors_PAG_Originalset.csv DRAGON descriptors generated from 3D structures

    3D_Structures_PAG_Originalset.sdf 3D structures of anion compounds (original set)

    PCA_R.nb.html RNotebook containing PCA code and plots

Folder: Model_Fits Files showing fit statistics from various model fits

Chapter 3 - Tambjamine Anion Transporters

Folder: C3_TambAnionTransport

Files:

Compound_structures_2D.zip Tambjamine 2D Compound Structures, individual .mol files

logEC50_with_errors.xlsx Excel file containing experimental errors and log(1/EC50) vs ALOGPs plot

43compounds_DRAGON_descriptors.csv Raw descriptors generated in DRAGON, includes additional synthesised compounds

Tambjamines_dataset_cleaned.csv Dataset from Tambjamine paper[1] contains experimental values, classifiers and descriptors from multiple sources for the 43 tambjamines

4parameter_subset.txt Subset of descriptors used in fit of 4 parameter models.

model_coefficients_CI.xlsx Confidence intervals for selected 2, 3 & 4 parameter models.

model_fit_plots.png Actual vs. predicted plots for selected 2, 3 & 4 parameter models.

Folder: Initial_Models - files for Quesada's models

> **Test_set_cleaned_descriptors.xlsx** 380 descriptors for compounds in test set

> **Training_set_cleaned_descriptors.xlsx** 380 descriptors for compounds in training set

> **Descriptors_original38_modeldescriptors.csv** Descriptors used in initial models, only the original 38 compounds

> **Descriptor_sources.xlsx** Sources for the descriptors generated by Quesada's group

> **fit_all.png** Results of fit all models for the initial modelling

Folder: RCode

> **linear_code_results.r** Code and results for 3 & 4 parameter fits

> **lme4_code_results.r** Code and results for mixed effect linear fits within alkyl R group

> **Tambjamines_New_numbers_classified_cleaned.csv** .csv file used in R code - contains tambjamine descriptors and identifiers

Folder: CombinedQSAR

> **combinedQSAR_structures.sdf** Structures from old_PAG, new_PAG and tambjamine datasets - Section 3.9

> **combinedQSAR_structures.zip** Structures from old_PAG, new_PAG and tambjamine datasets, individual .mol files - Section 3.9

---

[1] Knight, N. J. et al. QSAR analysis of substituent effects on tambjamine anion transporters. Chem. Sci. 7, 1600-1608 (2016).

compounds_noduplicates_Alogps_EC50.xlsx Experimental values and AlogPs for all compounds, no duplicates

compounds_noduplicates_cleaned_descriptors.xls DRAGON descriptors for all compounds, no duplicates

classyfire_compounds_noduplicates.xlsx Classyfire classification groups for all compounds, with counts

Chapter 4 - Data Handling & Visualisation

Folder: C4_DataHandling_Vis

Files:

Example_blog_post_blog3.html Sample blog post in Blog[3] - note links require login

Example_blog_post_LabTrove.html Sample blog post in LabTrove - note links require login

solubility_initial_data.nb.html Example Output from RNotebook

solubility_initial_data.Rmd Example input file to generate RNotebook html output

Folder DataVis

.html and .js files Code for Data Visualisations - see README.txt for the details of each file

Chapter 6 - Remote Experiments

Folder: C6_RemoteExp

Files:

BeerLambertRawdata.m MATLAB script for image processing

BLL_server.js Node.js Code for running BLL server and experiment

troubleshooting.html Troubleshooting page displayed on the website for the students

Folder: views (pages displayed by BLL experiment)

end.ejs Displayed when ending an experiment

experiment.ejs View during experimental run

index.ejs Homepage for experiment

results.ejs Displaying results following an experiment

session_in_use.ejs Displayed if the session is already in use

Folder: styles (contains .css file for experiment)

Folder: sample_data (contains example data from experiment)

Chapter 7 - Smart Lab Interaction

Folder: C7_SmartLab

Files:

node_RED_nodes.json code for nodes, taken from node-RED system

Alexa_Interaction.json interaction model from Alexa developer console

Item_catalog.csv spreadsheet containing catlogue of items