Supporting Informatiion

Transfer Learning-Enhanced Multi-Target QSRR  
Modeling  
  
Priyanka Kumari, Madureira Sanches Ribeiro Guilherme,Pratyush  
Choudhary,Thomas Van Laethem,Marianne Fillet, Phillipe hubert, Pierre-Yves Sacre, and Cedric hubert \*  
Department of Pharmacy, Laboratory of Pharmaceutical Analytical Chemistry,CIRM, Liege, Belgium, 4000  
;Laboratory for the Analysis of Medicines, CIRM, Liege, Belgium , 4000  
¶Northwestern University, Illinois, USA, 60208  
E-mail: [priyanka@student.uliege.be](mailto:priyanka@student.uliege.be); [hubert.cedric@uliege.be](mailto:hubert.cedric@uliege.be)  
  
---------------------------------------------------------------------------------------------------------------------------

**Table S1: Hyperparameters for the MLP model**

|  |  |
| --- | --- |
| **Hyperparameter** | **Value** |
| FC layer | 5 |
| FC Units | 1000, 500, 200, 100, 1 |
| Dropout rate | 0.1 |
| Learning rate | 1e-4 |

Based on the lipophilicity change over pH: we hv 2 groups of compounds (Group 1 having net charge and Group 2 , having no net charge). Below is their classification:

**Table S2: Compound classification based on comparison with pKa**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Compounds** | **pH 2.7** | **pH 3.5** | **pH 5.0** | **pH 6.5** | **pH 8.0** | **Class** | **pKa** |
| **Group 1: Charged** | | | | | | | |
| **3-aminobenzoic acid** | base | base | acid | acid | acid | acid-base | Acidic:4.81, Basic:3.27 |
| **Carteolol** | base | base | base | base | base | base | Acidic:13.41,14.19, Basic:9.76 |
| **Gallic Acid** | neutral | acid | acid | acid | acid | acid | Acidic: 3.94, 9.04, 11.17. 14.8 |
| **Mandelic Acid** | neutral | acid | acid | acid | acid | acid | Acidic: 3.84, 13.57 |
| **Niacinamide** | base | base | neutral | neutral | neutral | base | Acidic : 13.39, Basic: - 1.25, 3.63 |
| **Papaverine** | base | base | base | base | neutral | base | Basic: 6.03 |
| **Phenylacetic Acid** | neutral | neutral | acid | acid | acid | acid | Acidic : 4.55 |
| **Procainamide** | base | base | base | base | base | base | Acidic: 15.75 Basic: 3.32, 9.04 |
| **Verapamil** | base | base | base | base | base | base | Basic: 9.68 |
| **Group 2 : Neutral (No net Charge)** | | | | | | | |
| **Coumarin** | neutral | neutral | neutral | neutral | neutral | neutral | -- |
| **Danthron** | neutral | neutral | neutral | neutral | neutral | neutral | Acidic: 7.89,8.54 |
| **Dibenzothiophene** | neutral | neutral | neutral | neutral | neutral | neutral | -- |
| **Estradiol** | neutral | neutral | neutral | neutral | neutral | neutral | Acidic: 10.33 Basic: -0.88 |
| **Ethylbenzene** | neutral | neutral | neutral | neutral | neutral | neutral | -- |
| **Eugenol** | neutral | neutral | neutral | neutral | neutral | neutral | Acidic: 9.94 |

**Figure S1 : Error Variations for group of compounds along the pH**  
**x-axis:** Specific compounds within each group , **y-axis**: The error values.  
Different coloured bars (blue, orange, green, and light blue) represent different median values (Median\_M1, Median\_M2, Median\_M3, and Median\_M4) for each compound corresponding to four models(ST\_WTL(M1), ST\_TL(M2), MT\_WTL(M3), MT\_TL(M4)).   
Error bars: the standard error in the measurements.

**Table S3: Result comparison with SVM model**

**(Single target models for each target and calculated the mean)**

|  |  |
| --- | --- |
| **Hyperparameter** | **Value** |
| C | 0.01 |
| Degree | 2 |
| **Model Performance** | |
| MSE | 48.45 |
| R2 | 0.14 |

A blue and white bar graph

Description automatically generated

**Figure S2: SHAP Summary plot for Multitarget QSRR(M4) for Target1- Retention time at pH 2.7**

A blue and white bar graph

Description automatically generated

**Figure S3: SHAP Summary plot for Multitarget QSRR(M4) for Target2- Retention time at pH 3.5**

A blue and white bar chart

Description automatically generated

**Figure S4: SHAP Summary plot for Multitarget QSRR(M4) for Target3- Retention time at pH 5.0**

A blue and white bar graph

Description automatically generated

**Figure S5: SHAP Summary plot for Multitarget QSRR(M4) for Target4- Retention time at pH 6.5**

A blue and white bar graph

Description automatically generated

**Figure S6: SHAP Summary plot for Multitarget QSRR(M4) for Target5- Retention time at pH 8.0**