# Can deep learning do better? [6]

**Table 5**

Prediction performance and standard deviations using 10- fold cross validation on the Solubility Challenge Dataset (125 molecules)

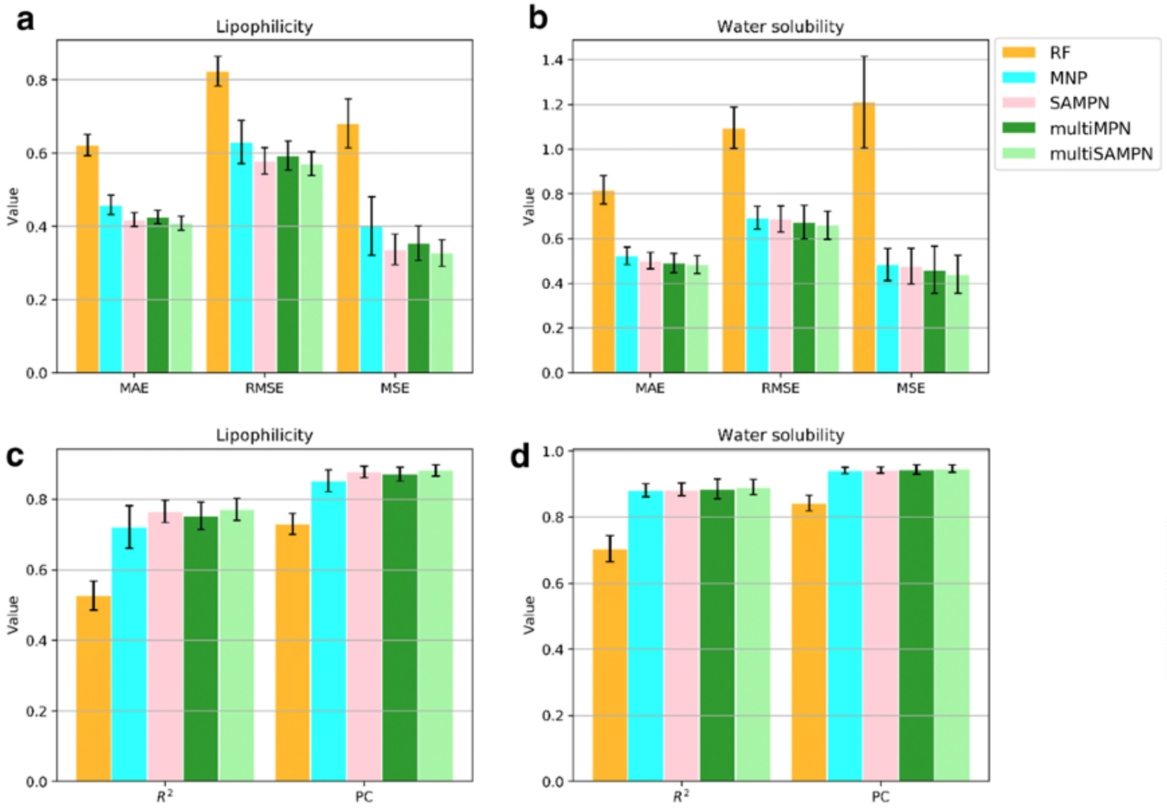
| Models | $R^2$ | std $R^2$ | RMSE | std RMSE | AAE | std AAE |
|---|---|---|---|---|---|---|
| UG-RNN | 0.32 | 0.03 | 1.41 | 0.12 | 1.08 | 0.10 |
| UG-RNN-LogP | 0.45 | 0.04 | 1.27 | 0.13 | 1.03 | 0.11 |
| UG-RNN-CR-LogP | 0.44 | 0.09 | 1.28 | 0.18 | 1.03 | 0.16 |
| UG-RNN-Huusk | 0.43 | 0.02 | 1.16 | 0.03 | 0.93 | 0.03 |
| UG-RNN-Huusk-Sub | 0.48 | 0.02 | 1.11 | 0.03 | 0.84 | 0.01 |
| UG-RNN-LogP-Huusk | 0.54 | 0.02 | 1.00 | 0.03 | 0.82 | 0.03 |
| UG-RNN-LogP-Huusk-Sub | 0.60 | 0.02 | 0.94 | 0.02 | 0.71 | 0.02 |
| UG-RNN-CR-LogP-Huusk | 0.62 | 0.03 | 0.96 | 0.06 | 0.83 | 0.06 |
| UG-RNN-CR-LogP-Huusk-Sub | 0.67 | 0.03 | 0.90 | 0.06 | 0.74 | 0.05 |
| NN-Sol-Chal[11] | 0.40 | - | 1.51 | - | - | - |
| MLR-Sol-Chal[11] | 0.51 | - | 0.95 | - | 0.77 | - |
| New *in silico* consesus[11] | 0.60 | - | 0.90 | - | 0.68 | - |

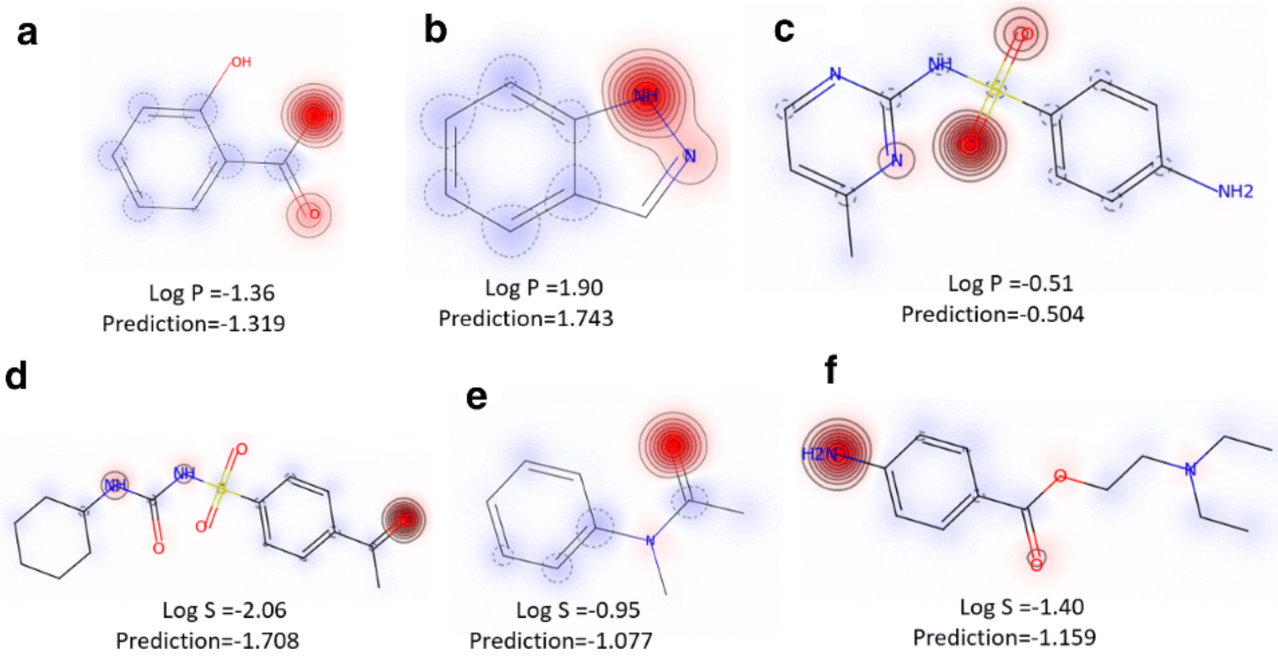
Better than simple neural network, but worse than MLR

Huusk results are based on more data.
Sub results use different solubility values.

In summary, deep learning can do better if there is more data.

# Opening the black box?




Recent deep learning method seems to perform well in solubility prediction and also highlights moieties that contribute to (red) or detract from (blue) solubility. See Ref. [7].