Graphical user interface, chart

Description automatically generated

Graphical user interface, chart

Description automatically generated

*Figure 1. Predicted HSPs in scatter plots against experimental HSP for (A) the 87 molecules and (B) the 193 molecules. The dashed lines indicate the ideal fit.*

*Table 1 The measures of regression and error taken from a paper [14] from Sanchez et al in red and in black from separate experimentation.*

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Dataset | Target | Approach | MAE | RMSE | R2 |
| solvents n=193 from GitHub [1] | δd | KernelRidge | 0.80 | 1.22 | 0.56 |
|  | Lasso | 0.91 | 1.44 | 0.39 |
| solvents n=193 |  | Lasso | 0.68 | 0.94 | 0.32 |
| solvents n=87 |  | Lasso | 0.98 | 1.52 | 0.56 |
|  |  |  |  |  |  |
| solvents n=193 from literature [14] | δp | KernelRidge | 2.46 | 3.70 | 0.50 |
|  | Lasso | 2.80 | 4.34 | 0.31 |
| solvents n=193 |  | Lasso | 1.93 | 2.66 | 0.54 |
| solvents n=87 |  | Lasso | 2.49 | 3.55 | 0.67 |
|  |  |  |  |  |  |
| solvents n=193 from literature [14] | δh | KernelRidge | 2.25 | 3.16 | 0.70 |
|  | Lasso | 2.66 | 3.56 | 0.62 |
| solvents n=193 |  | Lasso | 1.55 | 1.96 | 0.77 |
| solvents n=87 |  | Lasso | 1.91 | 2.78 | 0.86 |