## A target-driven molecule design framework.

The following table describes the code and data set used.

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| **“EA”** | |
| name | content |
| **main.m** | Main program of Evolutionary algorithm. |
| **initpop.m** | Code for initializing the population. |
| **binary2decimal.m** | Code for binary and Decimal conversion. |
| **crossover.m** | Code for individual crossover. |
| **mutation.m** | Code for variation. |
| **calobjvalue.m** | Code for calculating fitness function. |
| **selection.m** | Code for individual selection. |
| **best.m** | Code for calculating the optimal individual. |
| **A.mat** | A trained model for predicting polarizability. |
| **beta.mat** | A trained model for predicting first-order hyperpolarizability |
| **U.mat** | A trained model for predicting dipole moment. |
| **E.mat** | A trained model for predicting HOMO-LUMO gap. |
| **“NN”** | |
| **a.m** | Bayesian neural network code for predicting polarizability. |
| **beta.m** | Bayesian neural network code for predicting first-order hyperpolarizability. |
| **E.m** | Bayesian neural network code for predicting HOMO-LUMO gap. |
| **U.m** | Bayesian neural network code for predicting dipole moment. |

Note: All codes of Evolutionary algorithm should be placed in the same folder when used.

The code we use is run in matlab R2021a on window 11. The matlab program used needs to download the neural fitting toolbox.