Table 2. Optimized paramters of our hybrid model to reproduce the results for various types of toxicity data sets.

| | | | | | | ptimized paramters o | | produce the results for various | | | | |
|----------------|--|---------|-----------|---------------------------------|----------------------------|----------------------|---|--|-------------------------------------|--|-----------------------------|-------|
| Task NR-ahr | Mini-batch | Epochs | | Network Optimized Activation | Paramters Initilization | Threshold | Features Selection Features Selected | Cross Validation AUROC for Held-out CV | AUROC of Individual Models | nal Test Ensemble Neural Network AUROC | Final tes Random Forrest | |
| NK-anr 1 | iviiii-patch | LPUCHS | 210p-Out | Activation | manization | .meanulu | . catures selected | AONOC IOI NEIG-OUT CV | 0.911 | | .andom rorrest | JVIVI |
| 2 | 32 | 20 | 0.6 | relu | he normal | 1.5*mean | 270 | 0.802233 | 0.912 | 0.919 | | |
| 3 4 | | | | | - | | | | 0.903 0.916 | 0.919 | 0.907 | 0.889 |
| 4 | | | | | | | 1 | | 0.916 | 0.921 | 0.907 | 0.889 |
| | | | | | | | | | | | | |
| NR-ar | Mini-batch | Epochs | Drop-Out | Activation | Initilization | Threshold | Features Selected | AUROC for Held-out CV | AUROC of Individual Models 0.744 | Ensemble Neural Network AUROC | | |
| 2 | 2048 | 20 | 0.1 | alassa alai | h | 1.5*mean | 204 | 0.619164 | 0.743 | 0.744 | | |
| 3 | 2048 | 20 | 0.1 | sigmoid | he_normal | 1.5*mean | 284 | 0.619164 | 0.744 | 0.743 | | |
| 4 | | | | | | | | | 0.744 | 0.743 | 0.638 | 0.730 |
| | | | | | | | | | | | | |
| NR-ar-lbd | Mini-batch | Epochs | Drop-Out | Activation | Initilization | Threshold | Features Selected | AUROC for Held-out CV | AUROC of Individual Models | Ensemble Neural Network AUROC | | |
| 2 | | | | | | | | | 0.882 0.876 | 0.879 | | |
| 3 | 4096 | 20 | 0.9 | relu | he_uniform | 1.2*mean | 365 | 0.769197 | 0.879 | 0.881 | | |
| 4 | | | | | | | | | 0.877 | 0.881 | 0.800 | 0.702 |
| | | | | | | | | | | | | |
| NR-aromatase | Mini-batch | Epochs | Drop-Out | Activation | Initilization | Threshold | Features Selected | AUROC for Held-out CV | AUROC of Individual Models | Ensemble Neural Network AUROC | | |
| 1 | | | | | | | | | 0.794 | | | |
| 3 | 4096 | 20 | 0 | sigmoid | normal | 0.7*mean | 815 | 0.76325 | 0.792 | 0.794 | | |
| 4 | | | | | | | | | 0.790 | 0.794 | 0.792 | 0.782 |
| , <u>u</u> | | | | | | | | | | | | |
| NR-er | Mini-batch | Fnochs | Dron-Out | Activation | Initilization | Threshold | Features Selected | AUROC for Held-out CV | AUROC of Individual Models | Ensemble Neural Network AUROC | | |
| 1 | Willin Butter | Epociis | Diop out | Activation | minimization | Timesinoid | reatures serected | AONOCIO NEIGOGE | 0.823 | | | |
| 2 | 8192 | 40 | 0.2 | relu | he_uniform | 1.7*mean | 292 | 0.689923 | 0.822 | 0.823 | | |
| 3 | | | | | | | | | 0.823 0.818 | 0.823 | 0.778 | 0.791 |
| | | | | Ü | l. | 1 | 1 | | | | | |
| | | - | | | | I= | <u> </u> | | | | | |
| NR-er-lbd 1 | Mini-batch | Epochs | Drop-Out | Activation | Initilization | Threshold | Features Selected | AUROC for Held-out CV | AUROC of Individual Models 0.840 | Ensemble Neural Network AUROC | | |
| 2 | 1024 | 60 | 0.3 | relu | he_uniform | 0.8*mean | 755 | 0.606101 | 0.831 | 0.835 | | |
| 3 | 1024 | 90 | 0.3 | reiu | ne_uniorm | o.o mean | /55 | 0.000101 | 0.832 | 0.836 | 0.300 | 0.200 |
| 4 | | L | 1 | | <u> </u> | 1 | | | 0.834 | 0.836 | 0.768 | 0.786 |
| | | | | | | | | | | | | |
| NR-pparg | Mini-batch | Epochs | Drop-Out | Activation | Initilization | Threshold | Features Selected | AUROC for Held-out CV | AUROC of Individual Models | Ensemble Neural Network AUROC | | |
| 2 | | | | | | | | | 0.864 0.852 | 0.860 | | |
| 3 | 512 | 10 | 0.3 | relu | he_normal | 1*mean | 517 | 0.678438 | 0.857 | 0.858 | | |
| 4 | | | | | | | | | 0.849 | 0.858 | 0.789 | 0.744 |
| | | | | | | | | | Average | 0.836 | 0.782 | 0.775 |
| SR-are | Mini-batch | Epochs | Drop-Out | Activation | Initilization | Threshold | Features Selected | AUROC for Held-out CV | AUROC of Individual Models | Ensemble Neural Network AUROC | | |
| 1 | | | | | | | | | 0.825 | | | |
| 3 | 1024 | 20 | 0.8 | sigmoid | he_normal | 1*mean | 615 | 0.769482 | 0.822 0.825 | 0.827 | | |
| 4 | | | | | | | | | 0.825 | 0.828 | 0.774 | 0.779 |
| | | | | | | | | | | | | |
| CD have | Adial basels | Faraba. | D O-4 | A - 41: 41 | t-lettiet | There should | Footone Colontad | AUDOC 6 U-ld ACV | ALIDOC of tradicidated Associate | F | | |
| SR-hse | Mini-batch | Epocns | Drop-Out | Activation | Initilization | Threshold | Features Selected | AUROC for Held-out CV | AUROC of Individual Models 0.833 | Ensemble Neural Network AUROC | | |
| 2 | 2048 | 20 | 0.4 | relu | he_normal | 0.3*mean | 1028 | 0.774243 | 0.829 | 0.832 | | |
| 3 4 | | | | | - | | | | 0.834 | 0.832 | 0.859 | 0 798 |
| - | | | | | | | 1 | | 0.023 | 0.032 | 0.055 | 0.750 |
| | | | | | | | | | | | | |
| SR-mmp | Mini-batch | Epochs | Drop-Out | Activation | Initilization | Threshold | Features Selected | AUROC for Held-out CV | AUROC of Individual Models 0.955 | Ensemble Neural Network AUROC | | |
| 2 | 1024 | 20 | 0.5 | | h | 0.0* | COF | 0.898425 | 0.953 | 0.959 | | |
| 3 | 1024 | 20 | 0.5 | relu | he_normal | 0.9*mean | 685 | 0.898425 | 0.954 | 0.959 | | |
| 4 | | | | | | | 1 | | 0.953 | 0.958 | 0.978 | 0.916 |
| | | | | | | | | | | | | |
| SR-p53 | Mini-batch | Epochs | Drop-Out | Activation | Initilization | Threshold | Features Selected | AUROC for Held-out CV | AUROC of Individual Models | Ensemble Neural Network AUROC | | |
| 2 | | | | | | | | | 0.874 | 0.876 | | |
| 3 | 512 | 20 | 0.7 | relu | he_normal | 1.7*mean | 223 | 0.665071 | 0.873 | 0.875 | | |
| 4 | | | | | | | | | 0.877 | 0.875 | 0.847 | 0.810 |
| | | | | | | | | | | | | |
| SR-atad5 | Mini-batch | Epochs | Drop-Out | Activation | Initilization | Threshold | Features Selected | AUROC for Held-out CV | AUROC of Individual Models | Ensemble Neural Network AUROC | | |
| 1 2 | 1 | | | | | I | 1 | 1 | 0.819 0.820 | 0.820 | | |
| 3 | 4096 | 20 | 0.1 | relu | he_normal | 1.1*mean | 390 | 0.644897 | 0.820 | 0.820 | | |
| 4 | <u> </u> | L_ | | | | | <u> </u> | <u> </u> | 0.819 | 0.820 | 0.812 | 0.765 |
| | | | | | | | | | Average | 0.862 | 0.854 | 0.814 |
| AM | Mini-batch | Epochs | Drop-Out | Activation | Initilization | Threshold | Features Selected | AUROC for Held-out CV | AUROC of Individual Models | Ensemble Neural Network AUROC | | |
| 1 | | | | | | | | | 0.874 | | | |
| 3 | 1024 | 250 | 0.1 | Sigmoid | he_normal | 1.5*mean | 145 | 0.870 | 0.872 0.872 | 0.880 | | |
| 4 | 1 | | | | | | | | 0.872 | 0.878 | 0.842 | 0.810 |
| | | | | | | | _ | | 5 Fold Cross Validation | 0.879 | 0.831 | 0.815 |
| | | | | | | | | | | · _ | | |
| IGC50 | Mini-batch | Epochs | Drop-Out | Activation | Initilization | Threshold | Features Selected | R^2 for Held-out CV | R^2 of Individual Models | Ensemble Neural Network AUROC | | |
| 1 | | , | | | | | | | 0.804 | | | |
| 2 | 1024 | 400 | 0.1 | Sigmoid>Relu | glorot_normal | 1.5*mean | 117 | 0.805 | 0.805 0.805 | 0.808 | | |
| 3 4 | 1 | | | | | | | | 0.805 | 0.808 | | |
| | • | | | | | | | • | 5 Fold Cross Validation | 0.807 | | |
| | | | | | | | | | | | | |
| LC50 | Mini-batch | Epoche | Dron-Out | Activation | Initilization | Threshold | Features Selected | R^2 for Held-out CV | R^2 of Individual Models | Ensemble Neural Network AUROC | | |
| 1 | January attill | -pouris | J. Sp-Out | Acavation | | comoru | . Julianes selected | A E IOI Held-Out CV | 0.672 | | | |
| 2 | 128 | 40 | 0.3 | Sigmoid>Relu | glorot_normal | 0.1*mean | 857 | 0.678 | 0.661 0.653 | 0.669 | | |
| 3 4 | ł | | | | | | | | 0.653 | 0.678 | | |
| · · | | | | | | | -1 | | 5 Fold Cross Validation | 0.675 | | |
| | | | | | | | | | | | • | |
| 1050 | Mini-batch | Epochs | Dron-Out | Activation | Initilization | Threshold | Features Selected | R^2 for Held-out CV | R^2 of Individual Models | Ensemble Neural Network AUROC | | |
| 1 | ייייייייייייייייייייייייייייייייייייייי | -pouls | s.op-out | Sensarion | anzdUUII | ····conord | . carares selected | 2.01 Held-Out CV | 0.621 | | | |
| 2 | 32 | 200 | 0.6 | Sigmoid>Relu | glorot_normal | 0.1*mean | 817 | 0.613 | 0.626 | 0.621 | | |
| 3 4 | 1 | | | | | | | | 0.625 0.627 | 0.626 | | |
| | 1 | | 1 | | 1 | 1 | 1 | I | 5 Fold Cross Validation | 0.618 | | |
| | | | | | | | | | | | | |
| LC50-DM | Mini-hatet | Epoch | Dron-Cut | Activation | Initilization | Threshold | Features Selected | R^2 for Held-out CV | R^2 of Individual Models | Ensemble Neural Network AUROC | | |
| LC50-DM | Mini-batch | Epochs | ⊅rop-Out | Activation | munization | титемпота | reacures Selected | n-2 for Held-Out CV | R^2 of Individual Models 0.612 | Lisemble Neural NetWork AUROC | | |
| 2 | 128 | 50 | 0.3 | Sigmoid>Relu | glorot_normal | 0.1*mean | 854 | 0.611 | 0.612 | 0.615 | | |
| 3 | 120 | 50 | 0.3 | 5-5-11010≥Netu | 90001 Indition | o.i medii | 0.54 | 0.011 | 0.613 | 0.616 | | |
| 4 | i . | 1 | 1 | | 1 | 1 | 1 | I | 0.614 | 0.616 | | |