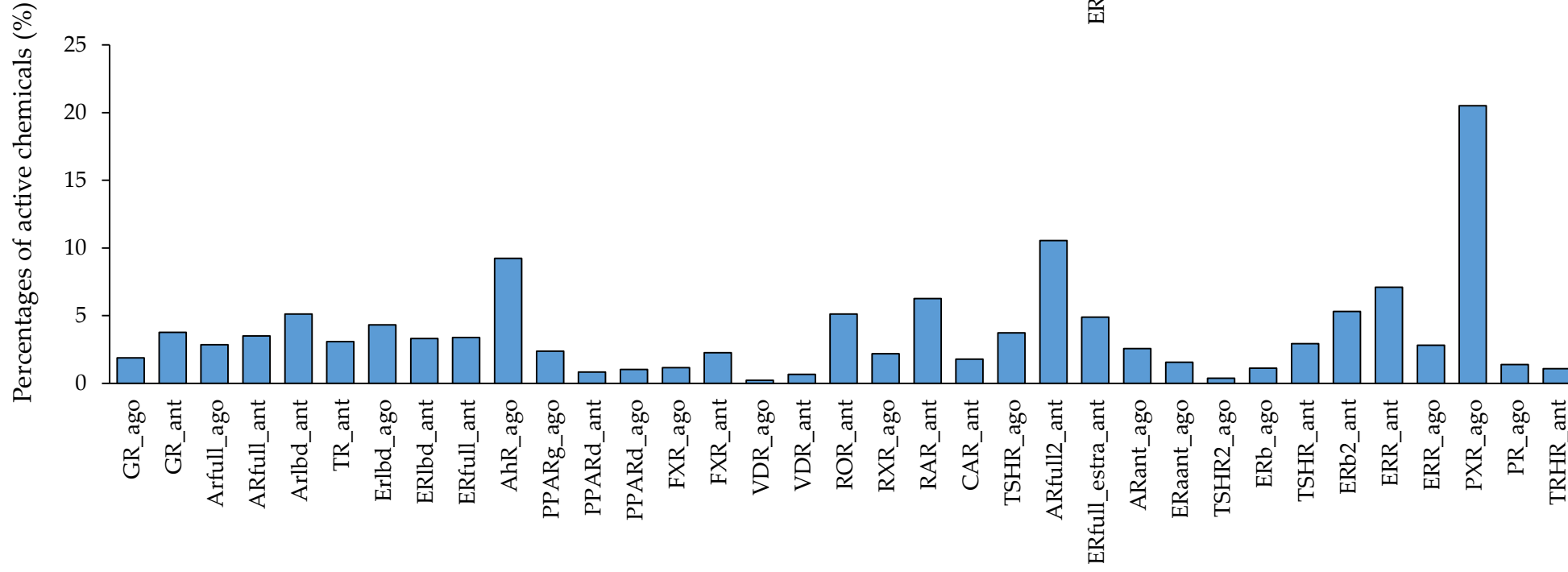


Figure 1

a



b



Supplementary Figure 1

**SMILES**

CC1=CN=C(S1)NC(=O)C2=C(C3=CC=CC=C3S(=O)(=O)N2C)O

**MOE software/CORINA**

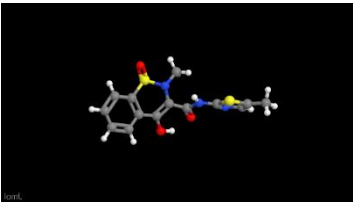
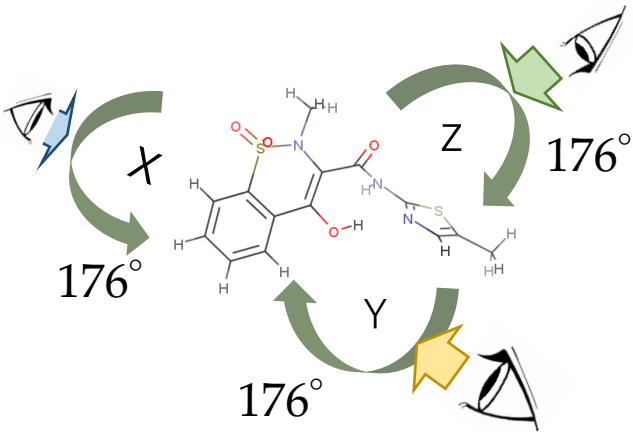
**SDF file**

**DeepSnap**

**png file**

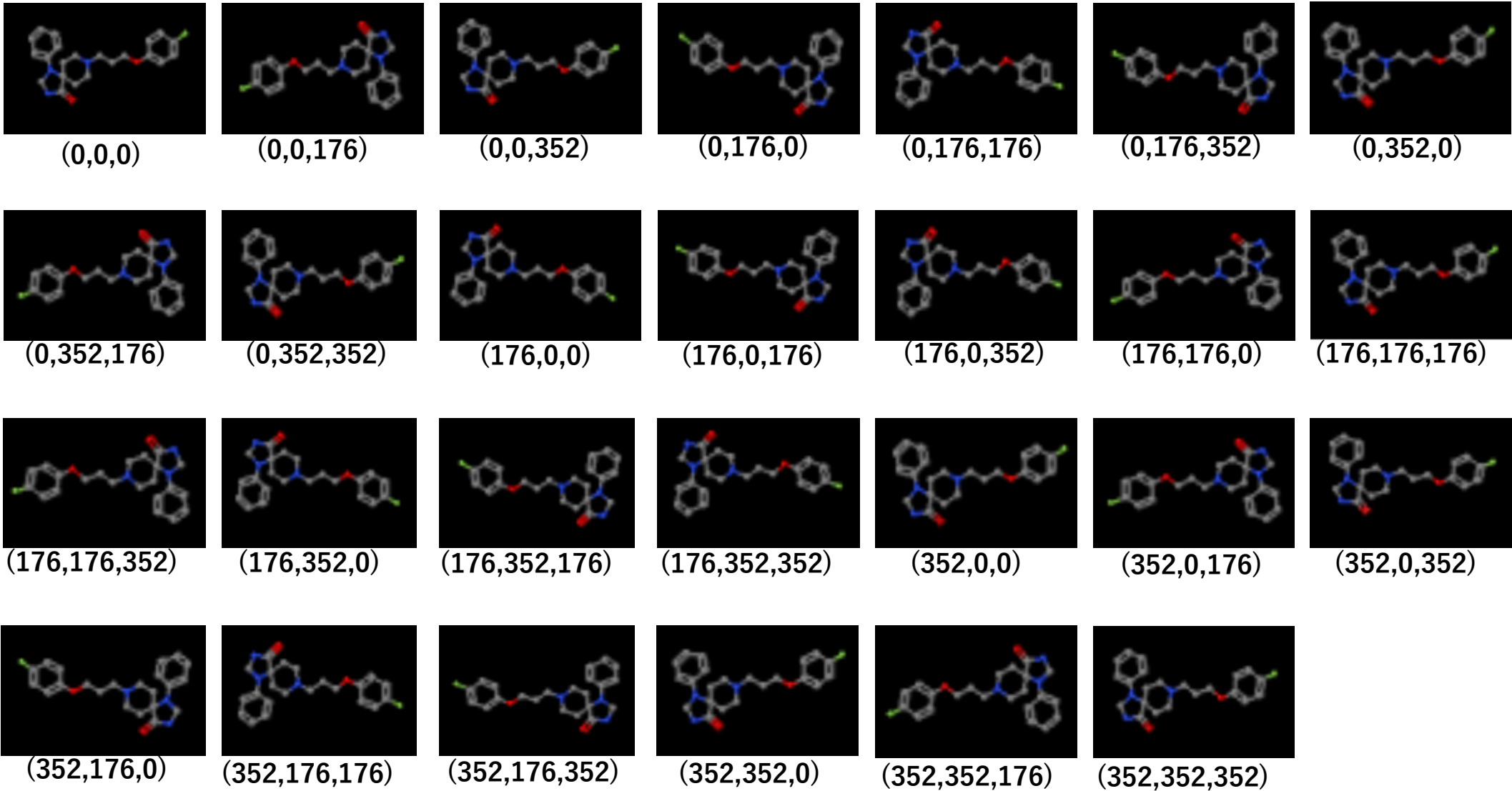
**Deep Learning**

**Prediction Model**

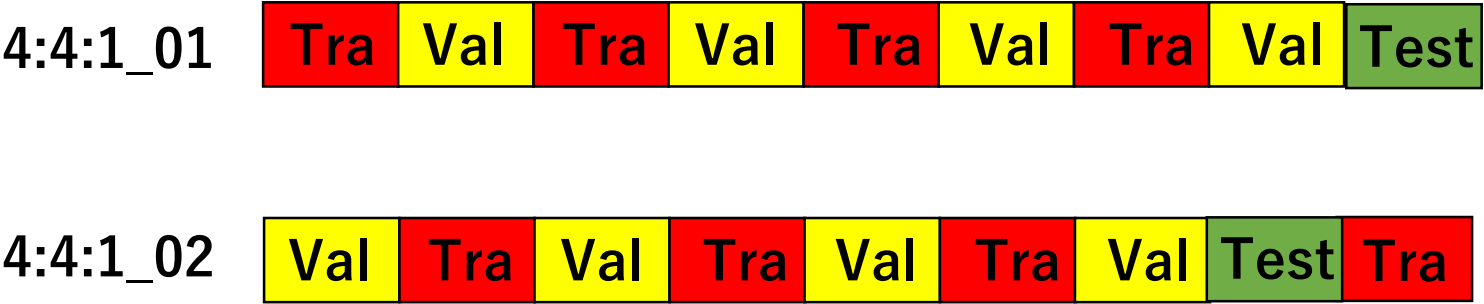


**Train** **Val** **Test**  
( 5 : 5 : 1 )

Figure 2

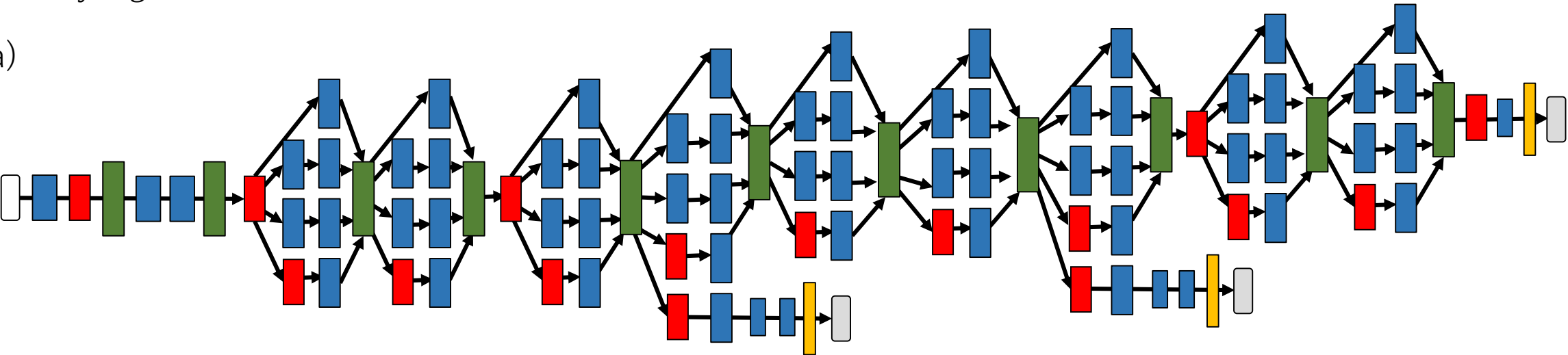


Supplementary Figure 2



Supplementary Figure 3

(a)



input

Convolution

Pooling

Concat/Normalize

SoftmaxActivation

Softmax

(b)

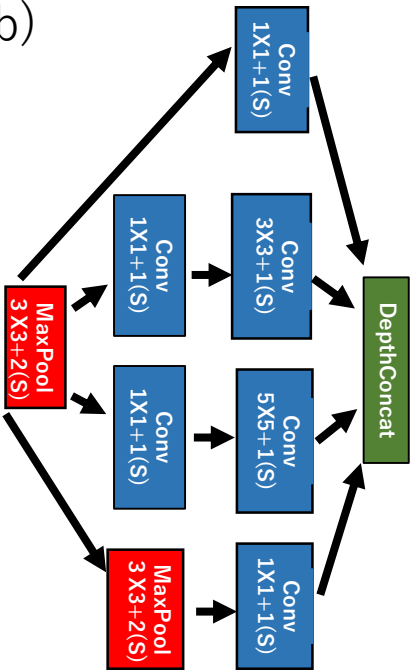
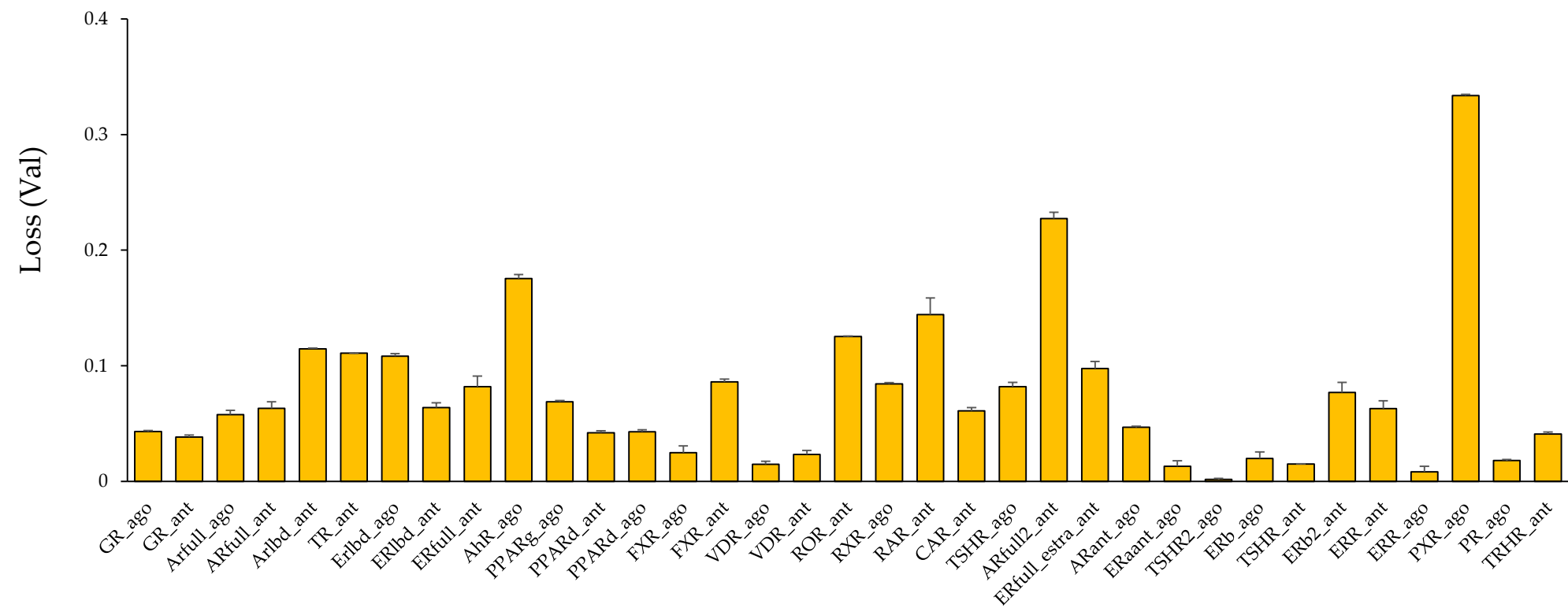


Figure 3



Supplementary Figure 4a

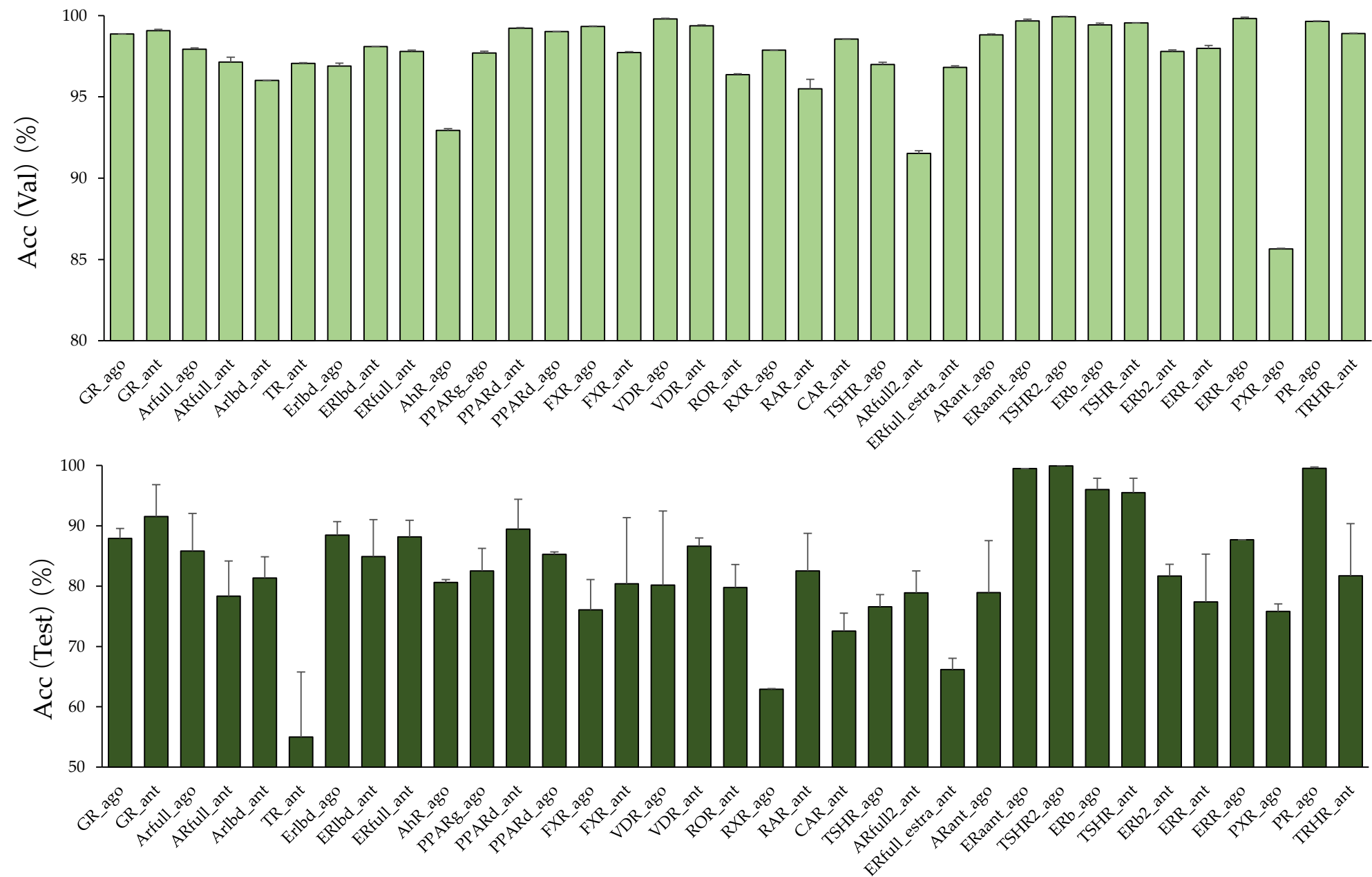
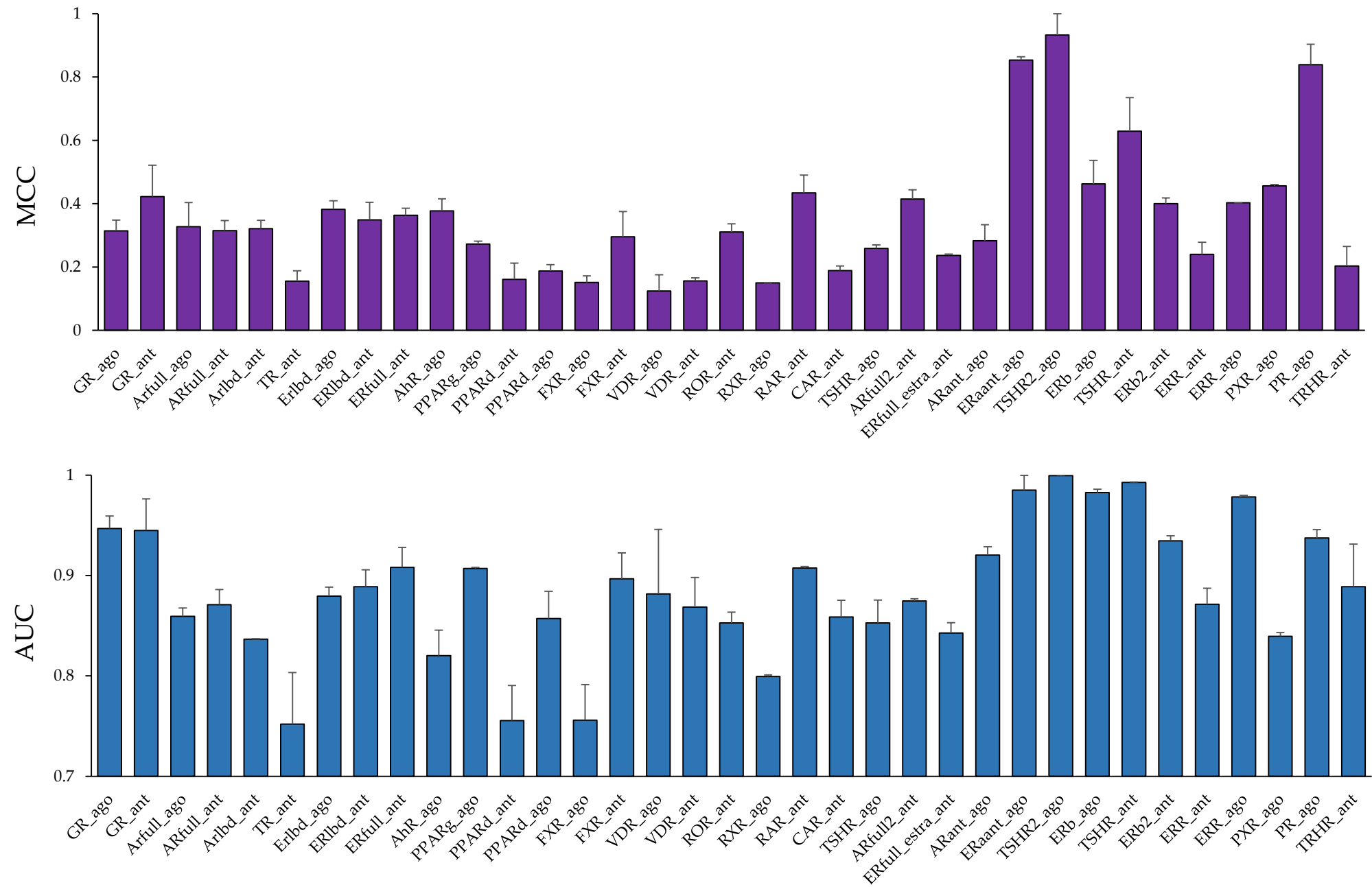


Figure 4



Supplementary Figure 4b

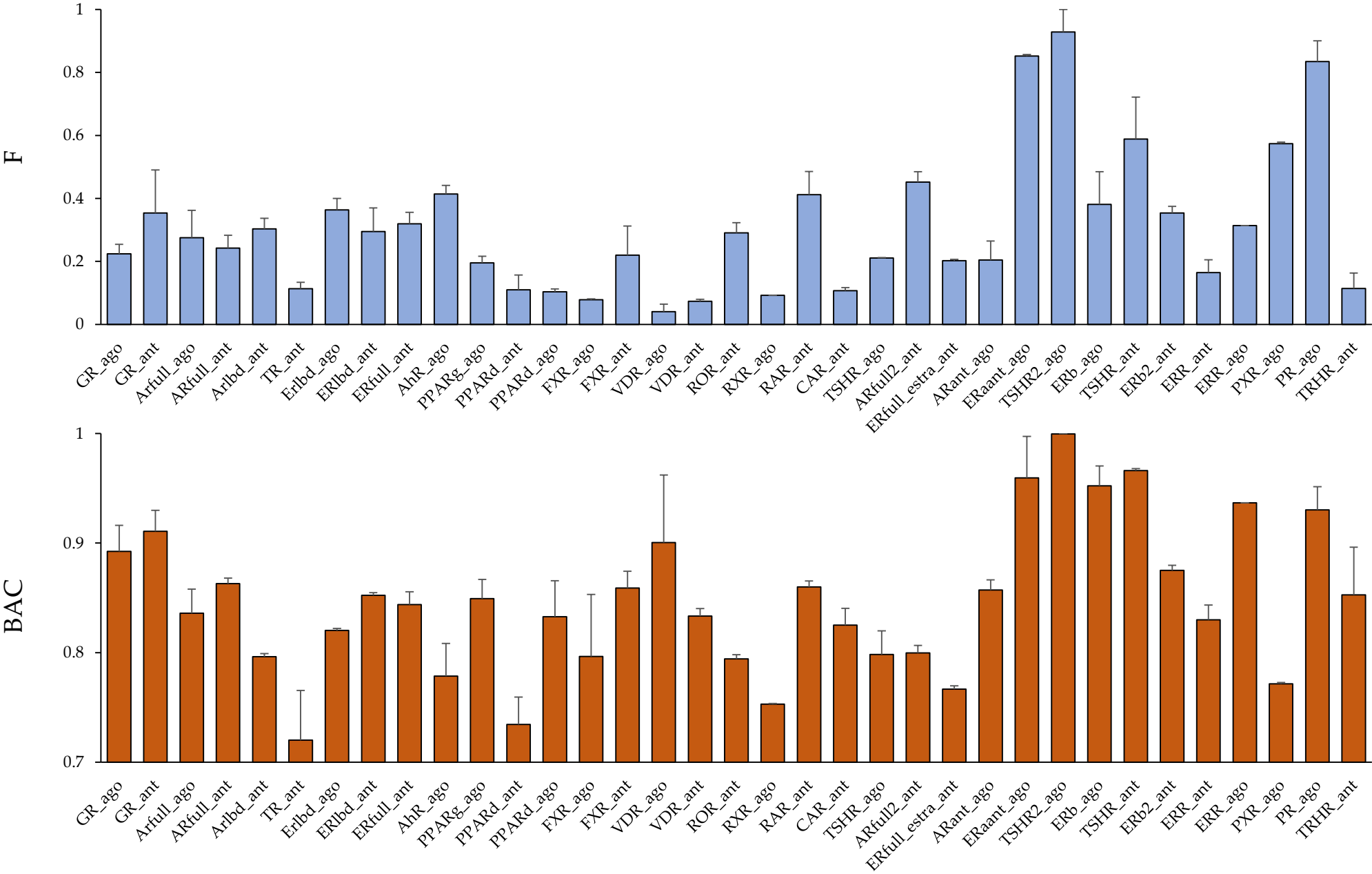
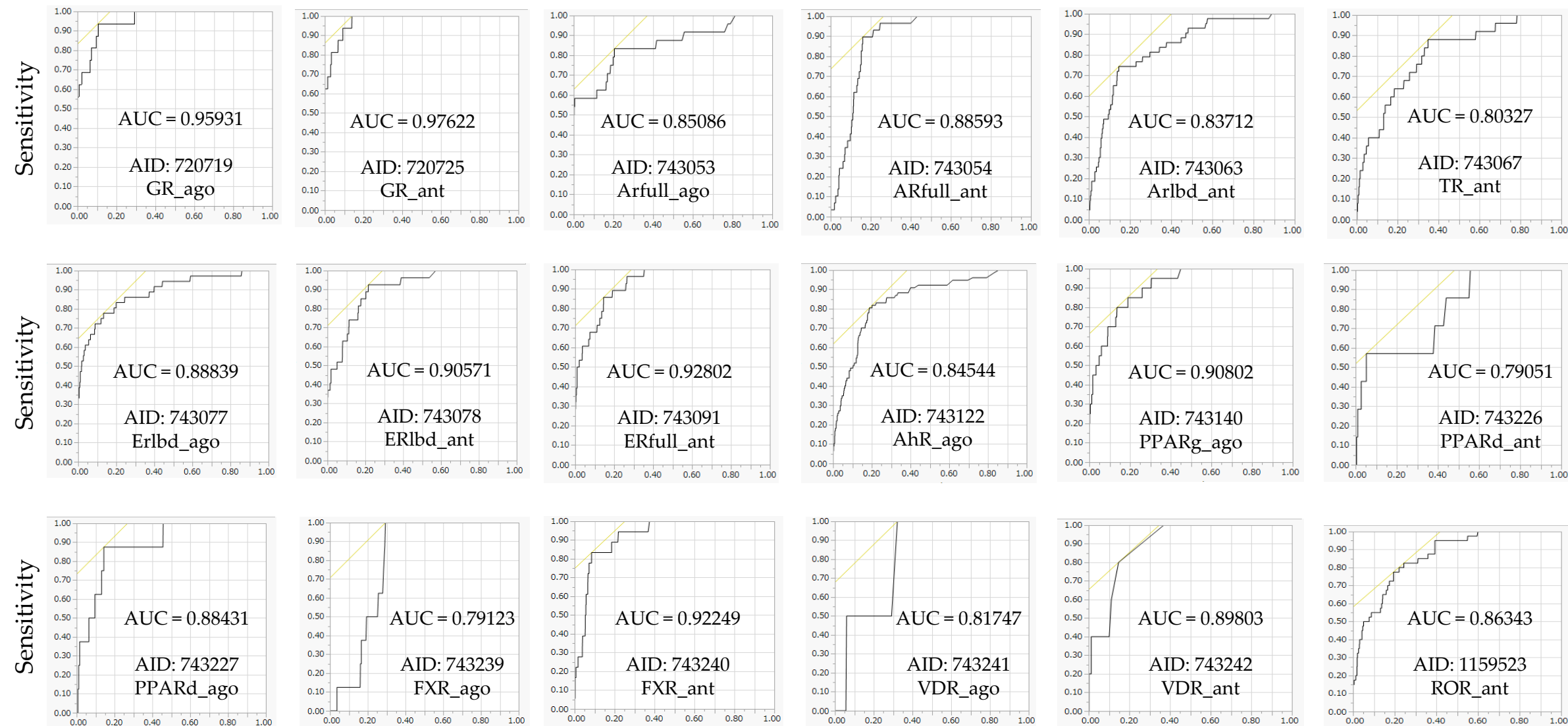
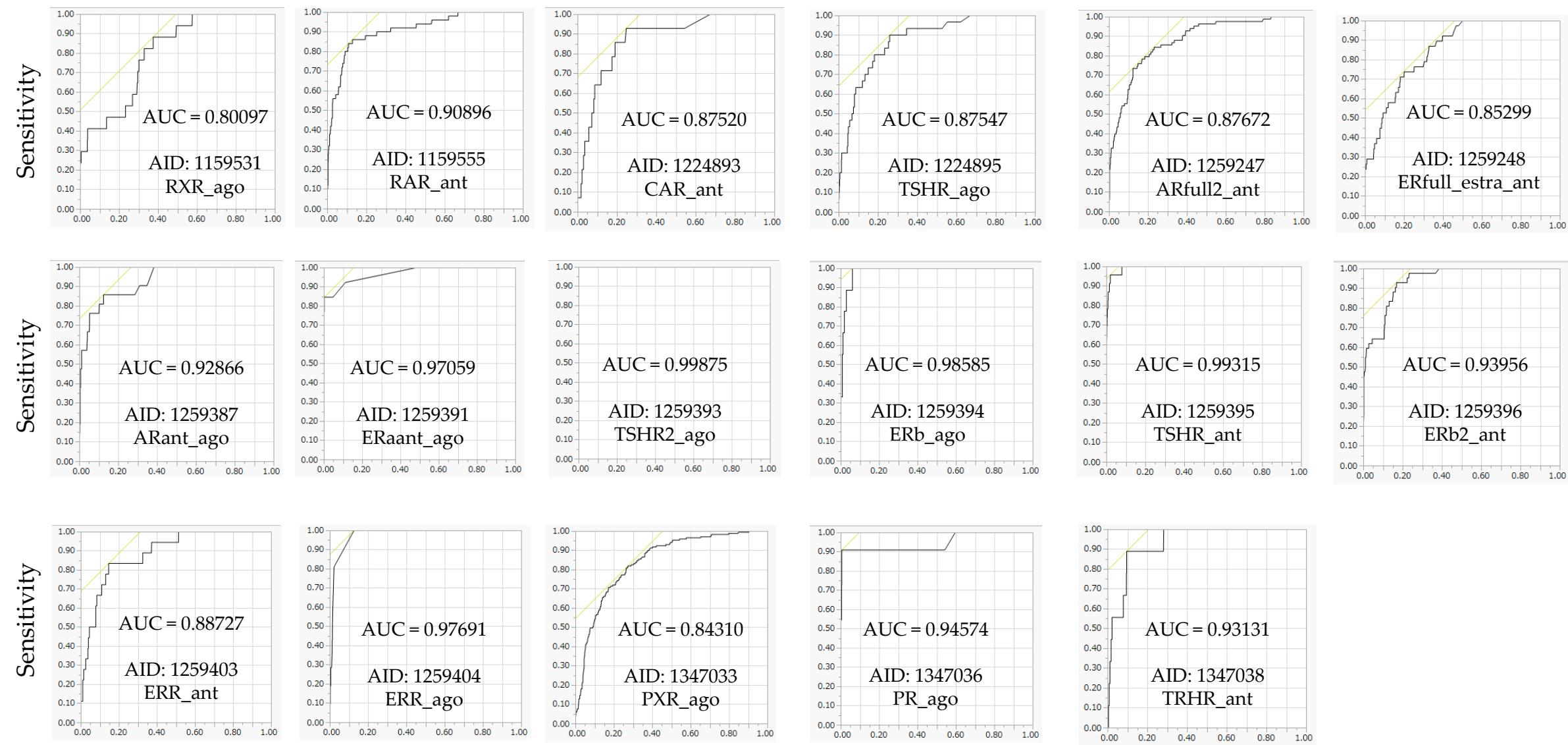


Figure 5



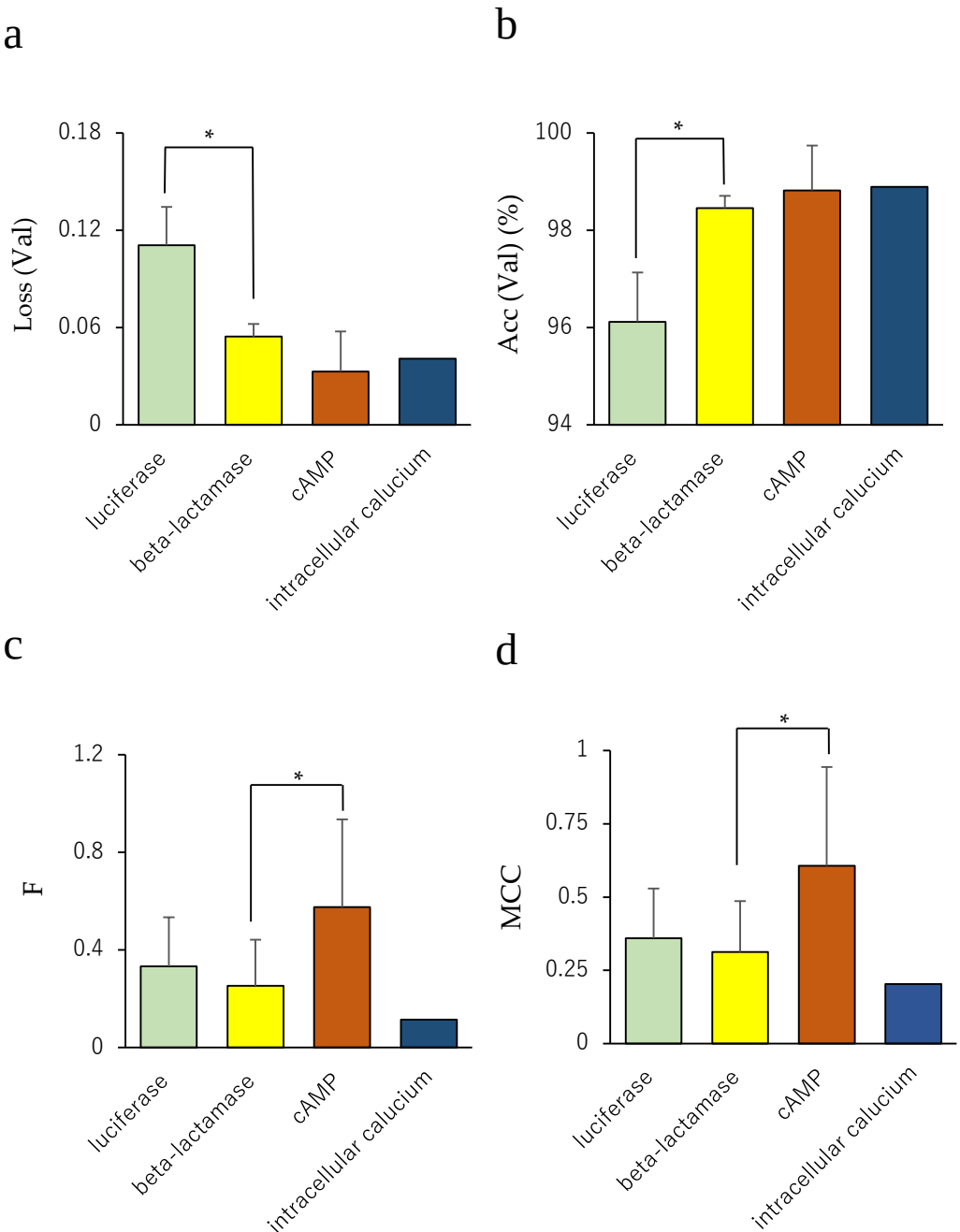
1- Specificity

Figure 5



1- Specificity

Figure 6



Supplementary Figure 5

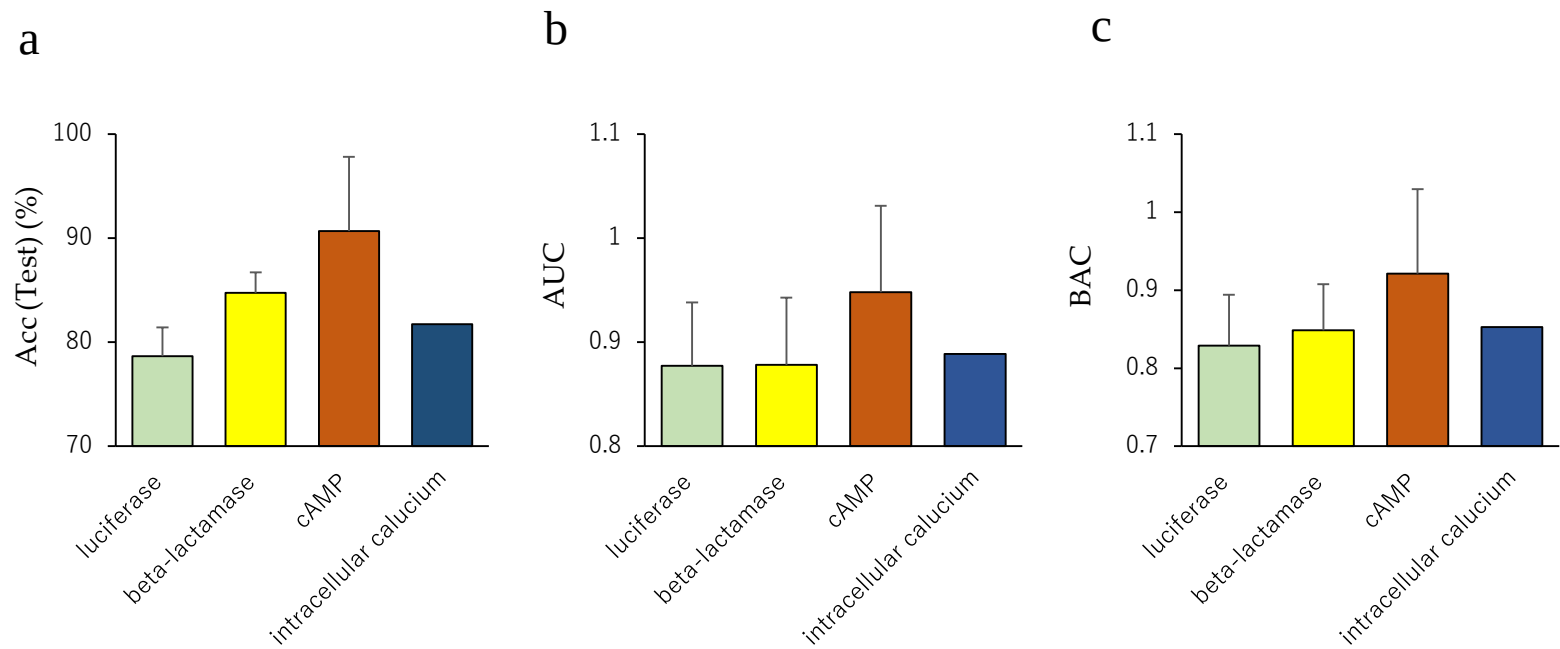


**Table S1.** Nuclear receptors and chemical compounds used in this study.

| PubChem AID | model names      | tra    |          | val    |          | test   |          | total  |          |
|-------------|------------------|--------|----------|--------|----------|--------|----------|--------|----------|
|             |                  | active | inactive | active | inactive | active | inactive | active | inactive |
| 720719      | GR_ago           | 64     | 3313     | 63     | 3314     | 16     | 828      | 143    | 7455     |
| 720725      | GR_ant           | 126    | 3224     | 126    | 3223     | 31     | 806      | 283    | 7253     |
| 743053      | Arfull_ago       | 96     | 3278     | 96     | 3277     | 24     | 819      | 216    | 7374     |
| 743054      | ARfull_ant       | 117    | 3218     | 117    | 3218     | 29     | 805      | 263    | 7241     |
| 743063      | Arlbd_ant        | 171    | 3155     | 170    | 3155     | 42     | 789      | 383    | 7099     |
| 743067      | TR_ant           | 103    | 3230     | 102    | 3230     | 26     | 807      | 231    | 7267     |
| 743077      | Erlbd_ago        | 145    | 3202     | 144    | 3202     | 36     | 801      | 325    | 7205     |
| 743078      | ERlbd_ant        | 111    | 3231     | 111    | 3231     | 27     | 808      | 249    | 7270     |
| 743091      | ERfull_ant       | 113    | 3231     | 113    | 3231     | 28     | 808      | 254    | 7270     |
| 743122      | AhR_ago          | 307    | 3015     | 307    | 3015     | 76     | 754      | 690    | 6784     |
| 743140      | PPARg_ago        | 80     | 3291     | 80     | 3291     | 20     | 823      | 180    | 7405     |
| 743226      | PPARd_ant        | 25     | 3041     | 25     | 3041     | 7      | 760      | 57     | 6842     |
| 743227      | PPARd_ago        | 31     | 3036     | 32     | 3035     | 8      | 759      | 71     | 6830     |
| 743239      | FXR_ago          | 35     | 3032     | 36     | 3031     | 9      | 758      | 80     | 6821     |
| 743240      | FXR_ant          | 69     | 2977     | 69     | 2977     | 17     | 744      | 155    | 6698     |
| 743241      | VDR_ago          | 7      | 3069     | 6      | 3069     | 2      | 767      | 15     | 6905     |
| 743242      | VDR_ant          | 20     | 3045     | 20     | 3044     | 5      | 761      | 45     | 6850     |
| 1159523     | ROR_ant          | 162    | 3000     | 162    | 3000     | 40     | 750      | 364    | 6750     |
| 1159531     | RXR_ago          | 70     | 3122     | 69     | 3122     | 17     | 781      | 156    | 7025     |
| 1159555     | RAR_ant          | 198    | 2968     | 198    | 2968     | 50     | 742      | 446    | 6678     |
| 1224893     | CAR_ant          | 58     | 3148     | 57     | 3148     | 14     | 787      | 129    | 7083     |
| 1224895     | TSHR_ago         | 119    | 3076     | 119    | 3076     | 30     | 769      | 268    | 6921     |
| 1259247     | ARfull2_ant      | 333    | 2824     | 333    | 2823     | 83     | 706      | 749    | 6353     |
| 1259248     | ERfull_estra_ant | 155    | 3025     | 155    | 3024     | 39     | 756      | 349    | 6805     |
| 1259387     | ARant_ago        | 82     | 3126     | 82     | 3126     | 21     | 781      | 185    | 7033     |
| 1259391     | ERaant_ago       | 50     | 3160     | 50     | 3160     | 12     | 790      | 112    | 7110     |
| 1259393     | TSHR2_ago        | 12     | 3210     | 12     | 3209     | 3      | 802      | 27     | 7221     |
| 1259394     | ERb_ago          | 36     | 3172     | 35     | 3172     | 9      | 793      | 80     | 7137     |
| 1259395     | TSHR_ant         | 93     | 3106     | 93     | 3106     | 24     | 776      | 210    | 6988     |
| 1259396     | ERb2_ant         | 168    | 3008     | 169    | 3007     | 42     | 752      | 379    | 6767     |
| 1259403     | ERR_ant          | 224    | 2930     | 224    | 2930     | 56     | 733      | 504    | 6593     |
| 1259404     | ERR_ago          | 84     | 2910     | 84     | 2909     | 21     | 727      | 189    | 6546     |
| 1347033     | PXR_ago          | 683    | 2647     | 684    | 2646     | 170    | 662      | 1537   | 5955     |
| 1347036     | PR_ago           | 48     | 3362     | 47     | 3362     | 11     | 841      | 106    | 7565     |
| 1347038     | TRHR_ant         | 37     | 3366     | 37     | 3366     | 9      | 842      | 83     | 7574     |