Supporting information for

In silico identification of potential thyroid hormone system disruptors among chemicals in human serum and chemicals with high exposure index

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S2
**S1. Dataset preparation**

*Thyroid peroxidase (TPO):* the TPO inhibition dataset was taken from Friedman et al.\(^1\) and in this study, 1074 ToxCast chemicals were screened in a single-concentration using the Amplex UltraRed TPO assay for their potential to inhibit TPO. In brief, the screening revealed 314 potent TPO inhibitors that elicited more than 20% decrease in maximal TPO activity. They were then divided into 3 categories; “highly selective”, “low selective” and “non-selective” as defined by Friedman et al.\(^1\) and then the non-selective compounds decreasing TPO activity by less than 22% were removed to obtain a more specific dataset with TPO inhibitors.

*Iodothyronine deiodinases 1, 2, 3 (DIOs):* datasets for inhibition of three deiodinases (DIO1, DIO2 and DIO3) were taken from Olker et al\(^2\). In this work, 1800 chemicals from the ToxCast database were screened for chemicals potency to inhibit DIO1, DIO2 and DIO3 in single-concentration experiments. The 240 potent inhibitors were tested in a concentration-response mode. Putative deiodinase inhibitors were defined as those confirmed in concentration-response screening and those showing more than 20% inhibition in the single concentration screening.

*Sodium/iodide symporter (NIS).* Data for NIS inhibition was taken from Wang et al\(^3\), who screened 293 unique chemicals selected from the ToxCast Phase I library in the Radioactive Iodide Uptake (RAIU) assay. The library contains environmental contaminants, mostly pesticides and antimicrobials. After the initial single concentration testing, full dose-response experiments for 136 chemicals were performed in which 90 were eliminated due to cytotoxicity.
S2. Information on Human Blood Data Base (HBDB) and Swedish Product Register (SE-PR) lists

HBDB: The HBDB used in the current study is an in-house database described in details elsewhere\(^4\). It consists of 440 anthropogenic organic chemicals found in human blood world-wide, reported in studies published between 2000-2020. 419 compounds with clearly defined structures and which could be processed with RDkit were used for the prediction in this study. Pharmaceuticals, endogenous compounds and metals are not included in the HBDB and neither articles written in other languages than English or Swedish. SMILES, CAS number, and other identifiers were collected for all chemicals. The database is not considered exhaustive, as individual chemical names could have been foreseen with the general search terms used (we refer to the original publication by Engelhardt et al.\(^4\) for the details). The chemicals detected in blood HBDB mainly consists of nonpolar chemicals with 83% halogenated structures and 69% aromatic structures, out of which 11% are phenolic. The chemical groups in the HBDB are listed in Table S3.

SE-PR: Anyone manufacturing or importing products to Sweden have to provide information on chemicals and chemical products to the Swedish Chemicals Agency. The information is stored in the SE-PR, containing information on e.g., quantity, product category and sector of use, and if the product is available to consumers. To be able to predict the potential of the chemicals in products to reach different human and environmental media, an exposure index (EI) was developed and applied to the SE-PR\(^5\). The target exposure matrices in the EI includes surface water, soil, air, sewage treatment plant and human (occupational and consumer). The calculation of the index utilizes use categories, quantities, consumer availability, hazard labelling, and number of products containing the compound. An evaluation of the calculation resulted in a slightly updated calculation and is described in detail elsewhere\(^6\). The SE-PR dataset used here contains organic chemicals with the highest exposure index to consumers (>6), and consists of 937 individual entries.
Table S1. Performance of thyroid-specific conformal prediction models with significance levels (SL) of 0.02, 0.05, 0.15 and 0.3. nAp, nIAp, nBp, nEp – number of compounds predicted as “active”, “inactive”, “both”, and “empty”; TPR – true positive rate; FPR – false positive rate; TDR(A, B) – true discovery rate for “active” and “both” regions; NPV – negative predictive value

| Model                  | SL  | nA test* | nIA test* | validity actives | validity inactives | efficiency actives | efficiency inactives | active  | inactive | both  | empty  | TPR  | FPR  |
|------------------------|-----|----------|-----------|------------------|-------------------|-------------------|---------------------|---------|----------|-------|--------|------|------|
| TRHR antagonists       | 0.02| 10       | 1331      | 1.00             | 0.98              | 0.30              | 0.02                | 28      | 0.11     | 0     | NA     | 1313 | 0.01 |
|                        |     |          |           |                  |                   |                   |                     | 0       | NA       | 0     | 0.30   | 0.30 | 0.02 |
|                        | 0.05| 10       | 1331      | 1.00             | 0.96              | 0.30              | 0.04                | 53      | 0.06     | 0     | NA     | 1288 | 0.01 |
|                        |     |          |           |                  |                   |                   |                     | 0       | 0.30     | 0     | 0.30   | 0.04 | 0.04 |
|                        | 0.15| 10       | 1331      | 0.90             | 0.87              | 0.80              | 0.74                | 179     | 0.04     | 811   | 1.00   | 351  | 0.01 |
|                        |     |          |           |                  |                   |                   |                     | 0       | 0.70     | 0     | 0.70   | 0.13 | 0.13 |
|                        | 0.3 | 10       | 1331      | 0.90             | 0.65              | 1.00              | 0.92                | 248     | 0.04     | 982   | 1.00   | 0    | NA   |
|                        |     |          |           |                  |                   |                   |                     | 0       | 0.70     | 0     | 0.70   | 0.13 | 0.13 |
| TSHR agonist           | 0.02| 54       | 1224      | 1.00             | 0.99              | 0.33              | 0.21                | 35      | 0.51     | 234   | 1.00   | 1009 | 0.04 |
|                        |     |          |           |                  |                   |                   |                     | 0       | 0.33     | 0     | 0.33   | 0.01 | 0.01 |
|                        | 0.05| 54       | 1224      | 0.98             | 0.96              | 0.56              | 0.42                | 82      | 0.35     | 467   | 1.00   | 729  | 0.03 |
|                        |     |          |           |                  |                   |                   |                     | 0       | 0.54     | 0     | 0.54   | 0.04 | 0.04 |
|                        | 0.15| 54       | 1224      | 0.93             | 0.86              | 0.80              | 0.75                | 216     | 0.18     | 747   | 0.99   | 315  | 0.03 |
|                        |     |          |           |                  |                   |                   |                     | 0       | 0.72     | 0     | 0.72   | 0.14 | 0.14 |
|                        | 0.3 | 54       | 1224      | 0.80             | 0.63              | 0.98              | 0.93                | 322     | 0.14     | 869   | 0.99   | 0    | NA   |
|                        |     |          |           |                  |                   |                   |                     | 0       | 0.81     | 0     | 0.81   | 0.23 | 0.23 |
| TSHR antagonist        | 0.02| 42       | 1258      | 1.00             | 0.99              | 0.31              | 0.27                | 29      | 0.45     | 323   | 1.00   | 948  | 0.03 |
|                        |     |          |           |                  |                   |                   |                     | 0       | 0.31     | 0     | 0.31   | 0.01 | 0.01 |
|                        | 0.05| 42       | 1258      | 0.95             | 0.95              | 0.60              | 0.53                | 88      | 0.26     | 608   | 1.00   | 604  | 0.03 |
|                        |     |          |           |                  |                   |                   |                     | 0       | 0.55     | 0     | 0.55   | 0.05 | 0.05 |
|                        | 0.15| 42       | 1258      | 0.86             | 0.85              | 0.83              | 0.91                | 217     | 0.13     | 969   | 0.99   | 114  | 0.06 |
|                        |     |          |           |                  |                   |                   |                     | 0       | 0.69     | 0     | 0.69   | 0.15 | 0.15 |
|                        | 0.3 | 42       | 1258      | 0.26             | 0.57              | 0.67              | 0.85                | 195     | 0.13     | 905   | 1.00   | 0    | NA   |
|                        |     |          |           |                  |                   |                   |                     | 0       | 0.60     | 0     | 0.60   | 0.14 | 0.14 |
| DIO1                   | 0.02| 41       | 304       | 0.98             | 0.99              | 0.24              | 0.19                | 13      | 0.69     | 55    | 0.98   | 277  | 0.11 |
|                        |     |          |           |                  |                   |                   |                     | 0       | 0.22     | 0     | 0.22   | 0.01 | 0.01 |
|                        | 0.05| 41       | 304       | 0.98             | 0.94              | 0.34              | 0.43                | 31      | 0.42     | 113   | 0.99   | 201  | 0.13 |
|                        |     |          |           |                  |                   |                   |                     | 0       | 0.32     | 0     | 0.32   | 0.06 | 0.06 |
|                        | 0.15| 41       | 304       | 0.90             | 0.87              | 0.71              | 0.74                | 64      | 0.39     | 191   | 0.98   | 90   | 0.13 |
|                        |     |          |           |                  |                   |                   |                     | 0       | 0.61     | 0     | 0.61   | 0.13 | 0.13 |
| Model | SL | nA test* | nIA test* | validity actives | validity inactives | efficiency actives | efficiency inactives | active nAp | TDR.A | inactive nIAp | NPV | nBp | TDR.B | both empty | TPR | FPR |
|-------|----|---------|----------|-----------------|-------------------|-------------------|-------------------|-----------|-------|-------------|-----|-----|-------|------------|-----|-----|
| 0.3   | 41 | 304     | 0.61     | 0.63            | 0.88              | 0.92              |                   | 96        | 0.31  | 220         | 0.97| 0   | NA    | 29         | 0.73| 0.22|
| DIO2  | 0.02| 55    | 290      | 1.00            | 0.98              | 0.22              | 0.26              | 18        | 0.67  | 70          | 1.00| 257 | 0.17  | 0          | 0.22| 0.02|
|       | 0.05| 55    | 290      | 1.00            | 0.94              | 0.35              | 0.46              | 35        | 0.54  | 116         | 1.00| 194 | 0.19  | 0          | 0.35| 0.06|
|       | 0.15| 55    | 290      | 0.95            | 0.84              | 0.64              | 0.74              | 77        | 0.42  | 174         | 0.98| 94  | 0.21  | 0          | 0.58| 0.16|
|       | 0.3 | 55    | 290      | 0.75            | 0.62              | 0.93              | 0.94              | 118       | 0.38  | 205         | 0.97| 0   | NA    | 22         | 0.82| 0.25|
| DIO3  | 0.02| 59    | 286      | 1.00            | 0.96              | 0.20              | 0.20              | 23        | 0.52  | 47          | 1.00| 275 | 0.17  | 0          | 0.20| 0.04|
|       | 0.05| 59    | 286      | 0.95            | 0.95              | 0.39              | 0.37              | 35        | 0.57  | 95          | 0.97| 215 | 0.17  | 0          | 0.34| 0.05|
|       | 0.15| 59    | 286      | 0.88            | 0.85              | 0.69              | 0.66              | 76        | 0.45  | 154         | 0.95| 115 | 0.16  | 0          | 0.58| 0.15|
|       | 0.3 | 59    | 286      | 0.71            | 0.69              | 0.97              | 0.98              | 120       | 0.35  | 216         | 0.93| 3   | 0.33  | 6          | 0.71| 0.27|
| NIS   | 0.02| 8     | 33       | 1.00            | 1.00              | 0.00              | 0.00              | 0         | NA    | 0           | NA | 41  | 0.20  | 0          | 0.00| 0.00|
|       | 0.05| 8     | 33       | 1.00            | 0.94              | 0.13              | 0.06              | 3         | 0.33  | 0           | NA | 38  | 0.18  | 0          | 0.13| 0.06|
|       | 0.15| 8     | 33       | 1.00            | 0.82              | 0.50              | 0.48              | 10        | 0.40  | 10          | 1.00| 21  | 0.19  | 0          | 0.50| 0.18|
|       | 0.3 | 8     | 33       | 1.00            | 0.61              | 1.00              | 0.97              | 21        | 0.38  | 19          | 1.00| 1   | 0.00  | 0          | 1.00| 0.39|
| TPO   | 0.02| 59    | 139      | 0.98            | 0.99              | 0.20              | 0.16              | 13        | 0.85  | 21          | 0.95| 164 | 0.29  | 0          | 0.19| 0.01|
|       | 0.05| 59    | 139      | 0.92            | 0.96              | 0.61              | 0.33              | 37        | 0.84  | 45          | 0.89| 116 | 0.20  | 0          | 0.53| 0.04|
|       | 0.15| 59    | 139      | 0.90            | 0.86              | 0.80              | 0.71              | 60        | 0.68  | 85          | 0.93| 53  | 0.23  | 0          | 0.69| 0.14|
|       | 0.3 | 59    | 139      | 0.76            | 0.68              | 0.98              | 0.99              | 87        | 0.53  | 108         | 0.89| 0   | NA    | 3          | 0.78| 0.29|
| TTR   | 0.02| 18    | 27       | 1.00            | 1.00              | 0.44              | 0.00              | 8         | 1.00  | 0           | NA | 37  | 0.27  | 0          | 0.44| 0.00|
|       | 0.05| 18    | 27       | 0.94            | 1.00              | 0.78              | 0.74              | 13        | 1.00  | 21          | 0.95| 11  | 0.36  | 0          | 0.72| 0.00|
| Model     | SL | nA test* | nIA test* | validity actives | validity inactives | efficiency actives | efficiency inactives | active nA | TDR.A | inactive nIA | NPV | nBp | TDR.B | empty | TPR | FPR |
|-----------|----|----------|-----------|------------------|-------------------|--------------------|---------------------|-----------|-------|------------|-----|------|-------|-------|-----|-----|
|           | 0.15 | 18 | 27 | 0.94 | 0.70 | 1.00 | 0.89 | 19 | 0.89 | 23 | 0.96 | 0 | NA | 3 | 0.94 | 0.07 |
|           | 0.3  | 18 | 27 | 0.61 | 0.33 | 0.83 | 0.67 | 14 | 1.00 | 19 | 0.95 | 0 | NA | 12 | 0.78 | 0.00 |
| TRβ agonist | 0.02 | 7  | 1313 | 1.00 | 0.98 | 0.29 | 0.02 | 23 | 0.09 | 0 | NA | 1297 | 0.00 | 0 | 0.29 | 0.02 |
|           | 0.05 | 7  | 1313 | 1.00 | 0.96 | 0.43 | 0.04 | 50 | 0.06 | 0 | NA | 1270 | 0.00 | 0 | 0.43 | 0.04 |
|           | 0.15 | 7  | 1313 | 1.00 | 0.88 | 0.43 | 0.13 | 154 | 0.02 | 21 | 1.00 | 1145 | 0.00 | 0 | 0.43 | 0.12 |
|           | 0.3  | 7  | 1313 | 0.57 | 0.74 | 0.86 | 0.83 | 340 | 0.01 | 752 | 1.00 | 228 | 0.00 | 0 | 0.43 | 0.26 |
| TRβ antagonist | 0.02 | 64 | 1001 | 1.00 | 0.99 | 0.20 | 0.15 | 23 | 0.57 | 145 | 1.00 | 897 | 0.06 | 0 | 0.20 | 0.01 |
|           | 0.05 | 64 | 1001 | 0.98 | 0.97 | 0.34 | 0.43 | 52 | 0.40 | 399 | 1.00 | 614 | 0.07 | 0 | 0.33 | 0.03 |
|           | 0.15 | 64 | 1001 | 0.95 | 0.89 | 0.78 | 0.78 | 162 | 0.29 | 664 | 1.00 | 239 | 0.06 | 0 | 0.73 | 0.11 |
|           | 0.3  | 64 | 1001 | 0.73 | 0.64 | 0.91 | 0.90 | 212 | 0.25 | 747 | 0.99 | 0 | NA | 106 | 0.83 | 0.16 |
Table S2. General CP models performance (all tested SLs). nAp, nIAp, nBp, nEp – number of compounds predicted as “active”, “inactive”, “both”, and “empty”; TPR – true positive rate; FPR – false positive rate; TDR(A, B) – true discovery rate for “active” and “both” regions; NPV – negative predictive value

| Model            | SL   | nA test* | nIA test* | validity actives | validity inactives | efficiency actives | efficiency inactives | active nAp | TDR_A | nIAp | NPV | empty nBp | TDR_B | nEp | FPR  |
|------------------|------|----------|-----------|------------------|-------------------|-------------------|---------------------|------------|-------|------|------|-----------|-------|-----|------|
|                  |      |          |           |                  |                   |                   |                     |            |       |      |      |           |       |     |      |
| **AHR agonists** | 0.01 | 150      | 1118      | 0.99            | 0.99              | 0.25              | 0.31                | 48          | 0.75  | 330  | 1.00 | 890       | 0.13  | 0   | 0.24 |
|                  | 0.02 | 150      | 1118      | 0.99            | 0.98              | 0.41              | 0.50                | 87          | 0.69  | 532  | 1.00 | 649       | 0.14  | 0   | 0.40 |
|                  | 0.05 | 150      | 1118      | 0.97            | 0.95              | 0.61              | 0.65                | 147         | 0.59  | 675  | 0.99 | 446       | 0.13  | 0   | 0.58 |
|                  | 0.1  | 150      | 1118      | 0.93            | 0.90              | 0.82              | 0.79                | 224         | 0.50  | 785  | 0.99 | 259       | 0.10  | 0   | 0.75 |
|                  | 0.15 | 150      | 1118      | 0.92            | 0.85              | 0.92              | 0.92                | 292         | 0.43  | 880  | 0.99 | 96        | 0.13  | 0   | 0.84 |
|                  | 0.2  | 150      | 1118      | 0.89            | 0.79              | 1.00              | 0.98                | 328         | 0.41  | 919  | 0.98 | 0        | NA    | 21 | 0.89 |
|                  | 0.25 | 150      | 1118      | 0.73            | 0.67              | 0.90              | 0.91                | 287         | 0.43  | 861  | 0.99 | 0        | NA    | 120| 0.83 |
|                  | 0.3  | 150      | 1118      | 0.60            | 0.52              | 0.83              | 0.82                | 243         | 0.47  | 797  | 0.99 | 0        | NA    | 228| 0.77 |
| **CAR agonist**  | 0.01 | 173      | 1088      | 1.00            | 0.99              | 0.20              | 0.34                | 42          | 0.81  | 366  | 1.00 | 853       | 0.16  | 0  | 0.20 |
|                  | 0.02 | 173      | 1088      | 0.98            | 0.98              | 0.35              | 0.45                | 74          | 0.77  | 476  | 0.99 | 711       | 0.16  | 0  | 0.33 |
|                  | 0.05 | 173      | 1088      | 0.94            | 0.96              | 0.60              | 0.64                | 133         | 0.70  | 664  | 0.98 | 464       | 0.15  | 0  | 0.54 |
|                  | 0.1  | 173      | 1088      | 0.89            | 0.91              | 0.82              | 0.81                | 223         | 0.55  | 803  | 0.98 | 235       | 0.13  | 0  | 0.71 |
|                  | 0.15 | 173      | 1088      | 0.84            | 0.86              | 0.93              | 0.94                | 283         | 0.47  | 903  | 0.97 | 75        | 0.16  | 0  | 0.77 |
|                  | 0.2  | 173      | 1088      | 0.79            | 0.77              | 0.98              | 0.96                | 306         | 0.45  | 911  | 0.97 | 0        | NA    | 44 | 0.80 |
|                  | 0.25 | 173      | 1088      | 0.64            | 0.61              | 0.88              | 0.87                | 260         | 0.50  | 836  | 0.97 | 0        | NA    | 165| 0.75 |
|                  | 0.3  | 173      | 1088      | 0.54            | 0.48              | 0.82              | 0.79                | 226         | 0.55  | 771  | 0.98 | 0        | NA    | 264| 0.72 |
| **CAR antagonist** | 0.01 | 29       | 936       | 1.00            | 0.99              | 0.14              | 0.01                | 11          | 0.36  | 0    | NA    | 954       | 0.03  | 0  | 0.14 |
|                  | 0.02 | 29       | 936       | 1.00            | 0.99              | 0.21              | 0.01                | 16          | 0.38  | 0    | NA    | 949       | 0.02  | 0  | 0.21 |
|                  | 0.05 | 29       | 936       | 0.97            | 0.96              | 0.41              | 0.22                | 46          | 0.24  | 174  | 0.99 | 745       | 0.02  | 0  | 0.38 |
|                  | 0.1  | 29       | 936       | 0.93            | 0.92              | 0.59              | 0.53                | 94          | 0.16  | 420  | 1.00 | 451       | 0.03  | 0  | 0.52 |
|                  | 0.15 | 29       | 936       | 0.90            | 0.88              | 0.72              | 0.69                | 130         | 0.14  | 536  | 0.99 | 299       | 0.03  | 0  | 0.62 |
|                  | 0.2  | 29       | 936       | 0.76            | 0.83              | 0.90              | 0.82                | 181         | 0.10  | 617  | 0.99 | 167       | 0.02  | 0  | 0.66 |
|                  | 0.25 | 29       | 936       | 0.69            | 0.78              | 1.00              | 0.96                | 230         | 0.09  | 701  | 0.99 | 34        | 0.00  | 0  | 0.69 |
|                  | 0.3  | 29       | 936       | 0.69            | 0.62              | 1.00              | 0.91                | 203         | 0.10  | 676  | 0.99 | 0        | NA    | 86 | 0.69 |
| **PPAR-delta agonist** | 0.01 | 17      | 1192      | 1.00            | 0.98              | 0.12              | 0.02                | 21          | 0.10  | 0    | NA    | 1188      | 0.01  | 0  | 0.12 |
|                  | 0.02 | 17      | 1192      | 1.00            | 0.97              | 0.12              | 0.03                | 37          | 0.05  | 0    | NA    | 1172      | 0.01  | 0  | 0.12 |
| Model                  | SL | nA test* | nIA test* | validity actives | validity inactives | efficiency actives | efficiency inactives | active nAp | TDR.A | nIAp | NPV | nBp | both efficiency | empty nEp | TPR | FPR |
|------------------------|----|----------|-----------|------------------|--------------------|--------------------|--------------------|-------------|-------|------|-----|-----|----------------|-----------|-----|-----|
|                        |    |          |           |                  |                    |                    |                    |             |       |      |     |     |                |           |     |     |
| PPARD antagonist       | 0.05 | 17 | 1192 | 1.00 | 0.95 | 0.35 | 0.11 | 70 | 0.09 | 67 | 1.00 | 1072 | 0.01 | 0 | 0.35 | 0.05 |
|                        | 0.1 | 17 | 1192 | 0.94 | 0.90 | 0.59 | 0.55 | 131 | 0.07 | 530 | 1.00 | 548 | 0.01 | 0 | 0.53 | 0.10 |
|                        | 0.15 | 17 | 1192 | 0.94 | 0.84 | 0.71 | 0.74 | 199 | 0.06 | 700 | 1.00 | 310 | 0.02 | 0 | 0.65 | 0.16 |
|                        | 0.2 | 17 | 1192 | 0.88 | 0.80 | 0.82 | 0.88 | 256 | 0.05 | 807 | 1.00 | 146 | 0.02 | 0 | 0.71 | 0.20 |
|                        | 0.25 | 17 | 1192 | 0.71 | 0.74 | 0.94 | 0.98 | 306 | 0.04 | 882 | 1.00 | 12 | 0.00 | 9 | 0.76 | 0.25 |
|                        | 0.3 | 17 | 1192 | 0.59 | 0.58 | 0.88 | 0.89 | 250 | 0.05 | 824 | 1.00 | 0 | NA | 135 | 0.71 | 0.20 |
| PPARG agonist          | 0.01 | 13 | 1151 | 1.00 | 0.99 | 0.23 | 0.01 | 9 | 0.33 | 0 | NA | 1155 | 0.01 | 0 | 0.23 | 0.01 |
|                        | 0.02 | 13 | 1151 | 1.00 | 0.99 | 0.31 | 0.01 | 17 | 0.24 | 0 | NA | 1147 | 0.01 | 0 | 0.31 | 0.01 |
|                        | 0.05 | 13 | 1151 | 1.00 | 0.95 | 0.31 | 0.05 | 57 | 0.07 | 0 | NA | 1107 | 0.01 | 0 | 0.31 | 0.05 |
|                        | 0.1 | 13 | 1151 | 1.00 | 0.90 | 0.54 | 0.23 | 118 | 0.06 | 148 | 1.00 | 898 | 0.01 | 0 | 0.54 | 0.10 |
|                        | 0.15 | 13 | 1151 | 1.00 | 0.85 | 0.69 | 0.53 | 183 | 0.05 | 435 | 1.00 | 546 | 0.01 | 0 | 0.69 | 0.15 |
|                        | 0.2 | 13 | 1151 | 0.92 | 0.80 | 0.85 | 0.68 | 241 | 0.04 | 553 | 1.00 | 370 | 0.01 | 0 | 0.77 | 0.20 |
|                        | 0.25 | 13 | 1151 | 0.92 | 0.75 | 0.92 | 0.82 | 301 | 0.04 | 654 | 1.00 | 209 | 0.00 | 0 | 0.85 | 0.25 |
|                        | 0.3 | 13 | 1151 | 0.92 | 0.71 | 1.00 | 0.94 | 350 | 0.03 | 743 | 1.00 | 71 | 0.00 | 0 | 0.92 | 0.29 |
| PPARG antagonist       | 0.01 | 39 | 1222 | 1.00 | 0.99 | 0.18 | 0.01 | 16 | 0.44 | 0 | NA | 1245 | 0.03 | 0 | 0.18 | 0.01 |
|                        | 0.02 | 39 | 1222 | 1.00 | 0.98 | 0.28 | 0.03 | 31 | 0.35 | 15 | 1.00 | 1215 | 0.02 | 0 | 0.28 | 0.02 |
|                        | 0.05 | 39 | 1222 | 1.00 | 0.96 | 0.51 | 0.23 | 72 | 0.28 | 228 | 1.00 | 961 | 0.02 | 0 | 0.51 | 0.04 |
|                        | 0.1 | 39 | 1222 | 1.00 | 0.91 | 0.59 | 0.47 | 128 | 0.18 | 467 | 1.00 | 666 | 0.02 | 0 | 0.59 | 0.09 |
|                        | 0.15 | 39 | 1222 | 1.00 | 0.86 | 0.67 | 0.64 | 197 | 0.13 | 614 | 1.00 | 450 | 0.03 | 0 | 0.67 | 0.14 |
|                        | 0.2 | 39 | 1222 | 0.95 | 0.82 | 0.79 | 0.80 | 251 | 0.12 | 756 | 1.00 | 254 | 0.03 | 0 | 0.74 | 0.18 |
|                        | 0.25 | 39 | 1222 | 0.85 | 0.77 | 0.92 | 0.94 | 316 | 0.09 | 865 | 0.99 | 80 | 0.04 | 0 | 0.77 | 0.23 |
|                        | 0.3 | 39 | 1222 | 0.69 | 0.68 | 0.92 | 0.97 | 333 | 0.09 | 883 | 0.99 | 1 | 0.00 | 44 | 0.77 | 0.25 |
| PPARG antagonist       | 0.01 | 69 | 1057 | 1.00 | 0.99 | 0.19 | 0.06 | 26 | 0.50 | 54 | 1.00 | 1046 | 0.05 | 0 | 0.19 | 0.01 |
|                        | 0.02 | 69 | 1057 | 1.00 | 0.98 | 0.20 | 0.20 | 37 | 0.38 | 190 | 1.00 | 899 | 0.06 | 0 | 0.20 | 0.02 |
|                        | 0.05 | 69 | 1057 | 0.97 | 0.95 | 0.33 | 0.42 | 70 | 0.30 | 396 | 0.99 | 660 | 0.07 | 0 | 0.30 | 0.05 |
|                        | 0.1 | 69 | 1057 | 0.93 | 0.90 | 0.54 | 0.64 | 133 | 0.24 | 582 | 0.99 | 411 | 0.08 | 0 | 0.46 | 0.10 |
|                        | 0.15 | 69 | 1057 | 0.83 | 0.86 | 0.78 | 0.79 | 195 | 0.22 | 689 | 0.98 | 242 | 0.06 | 0 | 0.61 | 0.14 |
|                        | 0.2 | 69 | 1057 | 0.77 | 0.81 | 0.94 | 0.92 | 253 | 0.19 | 781 | 0.98 | 92 | 0.04 | 0 | 0.71 | 0.19 |
|                        | 0.25 | 69 | 1057 | 0.70 | 0.74 | 0.97 | 0.97 | 277 | 0.18 | 820 | 0.98 | 1 | 0.00 | 28 | 0.72 | 0.21 |
|                        | 0.3 | 69 | 1057 | 0.62 | 0.57 | 0.93 | 0.87 | 232 | 0.21 | 755 | 0.98 | 0 | NA | 139 | 0.70 | 0.17 |
| PXR agonist            | 0.01 | 301 | 897 | 0.99 | 0.99 | 0.19 | 0.28 | 62 | 0.87 | 244 | 0.99 | 892 | 0.27 | 0 | 0.18 | 0.01 |
| Model | SL | nA test* | nIA test* | validity actives | validity inactives | efficiency actives | efficiency inactives | active nAp | TDR.A | inactive nIAp | NPV | both nBp | TDR.B | empty nEp | TPR | FPR |
|-------|----|----------|-----------|-----------------|------------------|-------------------|-------------------|----------|------|-------------|-----|----------|------|----------|-----|-----|
| 0.02  | 301| 897      |           | 0.98            | 0.99             | 0.32              | 0.37              | 105      | 0.88 | 327         | 0.98| 766      | 0.27 | 0        | 0.31| 0.01|
| 0.05  | 301| 897      |           | 0.95            | 0.96             | 0.53              | 0.58              | 181      | 0.81 | 503         | 0.97| 514      | 0.27 | 0        | 0.49| 0.04|
| 0.10  | 301| 897      |           | 0.90            | 0.90             | 0.80              | 0.82              | 298      | 0.71 | 679         | 0.96| 221      | 0.28 | 0        | 0.70| 0.10|
| 0.15  | 301| 897      |           | 0.84            | 0.85             | 0.96              | 0.95              | 375      | 0.64 | 763         | 0.94| 60       | 0.20 | 0        | 0.80| 0.15|
| 0.20  | 301| 897      |           | 0.76            | 0.73             | 0.96              | 0.94              | 376      | 0.64 | 755         | 0.94| NA       | 0    | NA       | 67  | 0.80|
| 0.25  | 301| 897      |           | 0.59            | 0.59             | 0.84              | 0.86              | 332      | 0.67 | 691         | 0.96| NA       | 0    | NA       | 175 | 0.74|
| 0.30  | 301| 897      |           | 0.47            | 0.46             | 0.77              | 0.78              | 295      | 0.72 | 636         | 0.97| NA       | 0    | NA       | 267 | 0.70|
Figure S1. Efficiency, true discovery rate of “active” prediction region (TDR.A), true positive rate (TPR) and false positive rate (FPR) of general toxicity models
Table S3. Chemical groups present in the database of chemicals found in human blood (HBDB). PCB – polychlorinated biphenyl; PFAS – Per- and polyfluoroalkyl substances; PAH – polycyclic aromatic hydrocarbon

| Compound group                     | Number of compounds |
|------------------------------------|---------------------|
| PCBs                               | 165                 |
| PFAS                               | 41                  |
| Pesticides                         | 40                  |
| Flame retardants                   | 33                  |
| Dioxin and Furans                  | 21                  |
| Phenols                            | 17                  |
| PAHs                               | 14                  |
| Industrial bulk chemicals          | 13                  |
| PCB metabolites                    | 12                  |
| Pesticide metabolites              | 10                  |
| Brominated flame retardant metabolites | 9              |
| UV-filters                         | 9                   |
| Phthalate metabolites              | 7                   |
| Phthalates                         | 7                   |
| Halogenated alkanes                | 5                   |
| Parabens                           | 4                   |
| Personal care products             | 4                   |
| Flame retardant metabolites        | 3                   |
| Tobacco smoke                      | 2                   |
| UV-filter metabolites              | 2                   |
| Personal care product metabolites  | 1                   |
Figure S2. The number of chemicals predicted/known to potentially disrupt thyroid hormone system via general toxicity MIEs in the Human Blood database (HBDB, A) and the activity distribution (B); and in the Swedish Product Register (SE-PR, C, D) with SL=0.1. Light green and light orange colors represent compounds confirmed inactive/active (known) in the model training data, dark colors represent the newly predicted chemicals and gray color represent chemicals not given certain predictions (those predicted both or empty)
Figure S3. The number of thyroid-specific models (A) and general toxicity models (B) among phthalates found in the HBDB that have been predicted/known active/inactive. Light green and light orange colors represent compounds confirmed inactive/active in the model training data, dark colors represent the newly predicted chemicals and grey color represent chemical not given certain prediction (chemical predicted both or empty). BBzP – Benzyl butyl phthalate; DBP – Dibutyl phthalate; DEHP – Di(2-ethylhexyl) phthalate; DEP – Diethyl phthalate; DNOP – Di(2-ethylhexyl) phthalate; MBP – Monobutyl phthalate; MeHHP – Mono-2-ethyl-5-hydroxyhexyl phthalate; MEHP – Mono(2-ethylhexyl) phthalate; MEOHP – Mono(2-ethyl-5-oxohexyl)phthalate; MiBP – Isobutyl hydrogen phthalate; MMP – Monomethyl phthalate; MOP – Mono-n-octyl phthalate
Figure S4. The number of thyroid-specific models (A) and general toxicity models (B) among parabens in the HBDB that have been predicted/known active/inactive. Light green and light orange colors represent compounds confirmed inactive/active in the model training data, dark colors represent the newly predicted chemicals and grey color represent chemical not given certain prediction (chemical predicted both or empty)
Figure S5. The number of thyroid-specific models (A) and general toxicity models (B) that bisphenols identified in the HBDB has been predicted/known active/inactive in. Light green and light orange colors represent compounds confirmed inactive/active in the model training, dark colors represent the newly predicted chemicals and grey represents chemicals not given certain prediction (chemicals predicted both or empty). BPA – bisphenol A; BPF – bisphenol F; BPS – bisphenol S; TBBPA – tetrabromobisphenol A; BPC – bisphenol C; BPE – bisphenol E; BPG – bisphenol G; BPM – bisphenol M; BPP – bisphenol P; BPZ – bisphenol Z; BPFL – bisphenol Fl; BPBP – bisphenol BP
**Table S4.** Compounds from the HBDB and the SE-PR list that were predicted to be active by at least 9 thyroid-specific CP models

| Dataset | CAS      | DTXSID               | Name                                                                 |
|---------|----------|----------------------|----------------------------------------------------------------------|
| HBDB    | 923925-51-3 | DTXSID301009365      | 2,4-dibromo-5-(2,4,5-tribromophenoxy)phenol                          |
| HBDB    | 297742-10-0 | DTXSID40616008       | 2,3,5-Tribromo-6-(2,4-dibromophenoxy)phenol                          |
| HBDB    | 105064-07-3 | DTXSID10903992       | 2,3,5-Tribromo-4-(2,4-dibromophenoxy)phenol                          |
| HBDB    | 111863-67-3 | DTXSID50433647       | CHEMBL362761                                                          |
| HBDB    | 602326-22-7 | DTXSID90797013       | 2,3-Dibromo-4-(2,4-dibromophenoxy)phenol                             |
| HBDB    | 602326-23-8 | DTXSID60454863       | Phenol, 2,5-dibromo-4-(2,4-dibromophenoxy)-                           |
| HBDB    | 79755-43-4 | DTXSID60229856       | 3,5-Dibromo-2-(2,4-dibromophenoxy)phenol                             |
| HBDB    | 80246-25-9 | DTXSID50903991       | 2,4-Dibromo-6-(2,4-dibromophenoxy)phenol                             |
| HBDB    | 13595-25-0 | DTXSID7065548        | Phenol, 4,4’-[1,3-phenylenebis(1-methylethylene)]bis-                |
| HBDB    | 2167-51-3  | DTXSID0058693        | Bisphenol P                                                           |
| HBDB    | 149589-59-3 | DTXSID50904125       | 2,2’,3,4,4’,5-Hexachloro[1,1’-biphenyl]-3-ol                          |
| HBDB    | 158076-69-8 | DTXSID00166372       | 2,2’,3,4,4’,5,5’-Heptachloro-3-biphenylol                            |
| HBDB    | 158076-62-1 | DTXSID10166368       | (1,1’-Biphenyl)-4-ol, 2,2’,3,3’,4,5-hexachloro-                        |
| HBDB    | 145413-90-7 | DTXSID60163004       | (1,1’-Biphenyl)-4-ol, 2,2’,3,4,5,5’-hexachloro-                      |
| HBDB    | 158076-68-7 | DTXSID40166371       | (1,1’-Biphenyl)-4-ol, 2,2’,3,4,5,5’-heptachloro-                     |
| HBDB    | 54284-55-8  | DTXSID90202637       | (1,1’-Biphenyl)-3-ol, 2,2’,4,5,5’-hexachloro-                        |
| HBDB    | 158076-64-3 | DTXSID80166370       | 2,2’,3,4,5,5’,6-heptachloro[1,1’-biphenyl]-3-ol                      |
| HBDB    | 190317-24-9 | DTXSID901009363      | 2,3,3’,5,5’,6-heptachloro[1,1’-biphenyl]-4-ol                        |
| HBDB    | 37853-59-1  | DTXSID1024627        | 1,2-Bis(2,4,6-tribromophenoxy)ethane                                 |
| HBDB    | 1844-01-5   | DTXSID70283308       | 4,4’-Dihydroxytetraphenylmethane                                     |
| HBDB    | 943913-15-3 | DTXSID20873415       | 6:2/8:2 Fluorotelomer phosphate diester                              |
| HBDB    | 1895-26-7   | DTXSID30172360       | 12:2 Fluorotelomer phosphate diester                                 |
| HBDB    | 29082-74-4  | DTXSID2021074        | Octachlorostyrene                                                    |
| HBDB    | 189084-64-8 | DTXSID4052689        | 2,2’,4,4’,6-Pentabromodiphenyl ether                                 |
| HBDB    | 366791-32-4 | DTXSID50573491       | 1,2,3-Tribromo-5-(3,4-dibromophenoxy)benzene                         |
| HBDB    | 182677-30-1 | DTXSID60872265       | 2,2’,3,4,5’,5’-Hexabromodiphenyl Ether                               |
| HBDB    | 63387-28-0  | DTXSID30881107       | 1,2,3,4,5-Pentabromo-6-(2,3,4,5-tetrabromophenoxy)benzene            |
| HBDB    | 437701-79-6 | DTXSID30451985       | BDE-207                                                              |
| HBDB    | 437701-78-5 | DTXSID40556652       | 2,2’,3,3’,4,5,5’,6,6’-nonabromodiphenyl ether                       |
| HBDB    | 189084-62-6 | DTXSID90873922       | 2,3’,4’,6-Tetabromodiphenyl Ether                                    |
| HBDB    | 93703-48-1  | DTXSID80877030       | BDE-77                                                               |
| HBDB    | 182346-21-0 | DTXSID4052685        | 2,2’,3,4,4’-Pentabromodiphenyl ether                                 |
| HBDB    | 60348-60-9  | DTXSID9030048        | 2,2’,4,4’,5-Pentabromodiphenyl ether                                 |
| HBDB    | 84852-53-9  | DTXSID2052732        | 1,1’-Oxybis[2,3,4,5,6-pentabromobenzene]                              |
| HBDB    | 35065-30-6  | DTXSID2073481        | 2,2’,3,3’,4,4’,5-Heptachlorobiphenyl                                |
| HBDB    | 52663-71-5  | DTXSID4073540        | 2,2’,3,3’,4,4’,6-Heptachlorobiphenyl                                |
| HBDB    | 52663-74-8  | DTXSID7074167        | 2,2’,3,3’,4,5,5’-Heptachlorobiphenyl                                |
| HBDB    | 38411-25-5  | DTXSID4074142        | 2,2’,3,3’,4,5,6-Heptachlorobiphenyl                                |
| HBDB    | 40186-70-7  | DTXSID9074147        | 2,2’,3,3’,4,5,6-Heptachlorobiphenyl                                |
| HBDB    | 52663-70-4  | DTXSID2074164        | 2,2’,3,3’,4,5,6-Heptachlorobiphenyl                                |
| HBDB    | 52663-67-9  | DTXSID2074162        | 2,2’,3,3’,5,5’,6-Heptachlorobiphenyl                                |
| HBDB    | 52663-64-6  | DTXSID0073538        | 2,2’,3,3’,5,6,6’-Heptachlorobiphenyl                                |
| SBDB      | DTXSID          | Description                                      |
|-----------|-----------------|--------------------------------------------------|
| 35065-29-3| DTXSID6038299   | 2,2',3,4,4',5,5'-Heptachlorobiphenyl              |
| 74472-47-2| DTXSID8074235   | 2,2',3,4,4',5,6'-Heptachlorobiphenyl              |
| 60145-23-5| DTXSID9074191   | 2,2',3,4,4',5,6'-Heptachlorobiphenyl              |
| 52663-69-1| DTXSID7074163   | 2,2',3,4,4',5,6'-Heptachlorobiphenyl              |
| 74472-48-3| DTXSID3074236   | 2,2',3,4,4',6,6'-Heptachlorobiphenyl              |
| 39635-31-9| DTXSID4074144   | 2,3',4,4',5,5'-Heptachlorobiphenyl                |
| 41411-64-7| DTXSID3074151   | 2,3',4,4',5,6'-Heptachlorobiphenyl                |
| 74472-50-7| DTXSID3074238   | 2,3',4,4',5,6'-Heptachlorobiphenyl                |
| 69782-91-8| DTXSID30867845  | 2,3',4,5,5',6'-Heptachlorobiphenyl                |
| 52663-78-2| DTXSID1074171   | 2,2',3,4,4',5,6-Octachlorobiphenyl               |
| 127-54-8  | DTXSID30281401  | 2,2-Bis(4-hydroxy-3-isopropylphenyl)propane      |
| 35822-46-9| DTXSID1052034   | 1,2,3,4,6,7,8-Heptachlorodibenzodioxin           |
| 67562-39-4| DTXSID8052350   | 1,2,3,4,6,7,8-Heptachlorodibenzo[b,d]furan       |
| 55673-89-7| DTXSID9052216   | 1,2,3,4,7,8,9-Heptachlorodibenzofuran            |
| 57117-44-9| DTXSID2069155   | 1,2,3,6,7,8-Hexachlorodibenzofuran               |
| 72918-21-9| DTXSID9052470   | 1,2,3,7,8,9-Hexachlorodibenzo[b,d]furan          |
| 60851-34-5| DTXSID3052276   | 2,3,4,6,7,8-Hexachlorodibenzo[b,d]furan          |
| 116806-76-9| DTXSID60151527 | 1,1'-Biphenyl, 2,2',3,4',5,6-hexachloro-4-\((methylsulfonyl)\)- |
| 207122-15-4| DTXSID3052692  | 2,2',4,5,6'-Hexabromodiphenyl ether              |
| 35854-94-5| DTXSID10873929  | 2,2',4,6,6'-Hexabromodiphenyl Ether              |
| 207122-16-5| DTXSID8052693  | 2,2',3,4,5,6'-Heptabromodiphenyl ether           |
| 446255-39-6| DTXSID3074789  | BDE-196                                          |
| 117964-21-3| DTXSID9074775  | BDE-197                                          |
| 337513-72-1| DTXSID7074749   | BDE-203                                          |
| 3268-87-9 | DTXSID4025799   | Octachlorodibenzo-p-dioxin                       |
| 39001-02-0 | DTXSID3052062   | Octachlorodibenzo furan                         |
| 35694-08-7 | DTXSID5074139   | 2,2',3,3',4,4',5,5'-Octachlorobiphenyl          |
| 42740-50-1 | DTXSID3074157   | 2,2',3,3',4,4',5,6'-Octachlorobiphenyl          |
| 33091-17-7 | DTXSID0074134   | 2,2',3,3',4,4',6,6'-Octachlorobiphenyl          |
| 68194-17-2 | DTXSID1074204   | 2,2',3,3',4,5,5',6-Octachlorobiphenyl           |
| 52663-75-9 | DTXSID2074168   | 2,2',3,3',4,5,5',6'-Octachlorobiphenyl          |
| 52663-73-7 | DTXSID2074166   | 2,2',3,3',4,5,6,6'-Octachlorobiphenyl           |
| 40186-71-8 | DTXSID4074148   | 2,2',3,3',4,5,6,6'-Octachlorobiphenyl           |
| 2136-99-4  | DTXSID0074132   | 2,2',3,3',5,5',6,6'-Octachlorobiphenyl          |
| 52663-76-0 | DTXSID7074169   | 2,2',3,4,4',5,5',6-Octachlorobiphenyl           |
| 74472-53-0 | DTXSID2074241   | 2,3',3,4,4',5,5',6-Octachlorobiphenyl           |
| 40186-72-9 | DTXSID50865989  | 2,2',3,3',4,4',5,5',6-Nonachlorobiphenyl        |
| 52663-79-3 | DTXSID6074172   | 2,2',3,3',4,4',5,6,6'-Nonachlorobiphenyl        |
| 52663-77-1 | DTXSID6074170   | 2,2',3,3',4,5,5',6,6'-Nonachlorobiphenyl        |
| 2051-24-3  | DTXSID4047541   | Decachlorobiphenyl                               |
| 7426-07-5  | DTXSID90225265  | 2,3,4,5-tetrachloro-6-hydroxy-N-phenylbenzamide |
| 24949-31-3 | DTXSID00903986  | 2,6-Dibromo-3-(2,4-dibromophenoxy)phenol         |
| 602326-21-6| NA              | 4'-OH-BDE 17                                     |
| 1578186-46-5| NA             | 6:2/14:2 diPAP                                   |
| 52969-11-4 | DTXSID70165175  | 2,3,6-Trichloro-4-(3,4-dichlorophenyl)phenol      |
| 70648-26-9 | DTXSID6029915   | 1,2,3,4,7,8-Hexachlorodibenzofuran               |
| SE-PR      | DTXSID20893830  | Pigment Red 264                                  |
| SE-PR | 1709-70-2 | DTXSID6027428 | Ionox 330 |
| SE-PR | 6706-82-7 | DTXSID50879809 | Solvent Yellow 29 |
| SE-PR | 67990-27-6 | DTXSID5052383 | C.I.Solvent Yellow |
| SE-PR | 68259-05-2 | DTXSID00887313 | Benzoic acid, 3,3’-[(2,5-dimethyl-1,4-phenylene)bis[iminocarboxyl](2-hydroxy-3,1-naphthalenediyi)-2,1-diazenediyi]bis[4-methyl-, 1,1’-bis(2-chloroethyl) ester |
| SE-PR | 81-77-6 | DTXSID2026280 | Vat Blue 4 |
| SE-PR | 3520-72-7 | DTXSID6052031 | Benzidine orange |
| SE-PR | 5590-18-1 | DTXSID4052219 | 3,3’-(1,4-Phenylenediimino)bis(4,5,6,7-tetrachloro-1H-isoindol-1-one) |
| SE-PR | 68310-04-3 | DTXSID1052406 | 2-[(4-Dodecylphenylazo)-4-(2,4-xylylazo)resorcinol |
| SE-PR | 65087-00-5 | DTXSID0052334 | 2,4-Bis[(4-dodecylphenylazo)resorcinol |
| SE-PR | 125-20-2 | DTXSID2051633 | 3,3-Bis(4-hydroxy-5-isopropyl-o-tolyl)phthalide |
| SE-PR | 980-26-7 | DTXSID2052655 | C.I. Pigment Red 122 |
| SE-PR | 4151-51-3 | DTXSID9063320 | Tris(4-isocyanatophenyl) thiophosphate |
| SE-PR | 1745-89-7 | DTXSID1061942 | 4,4’-Isopropylidenebis(2-allylphenol) |
| SE-PR | 355-49-7 | DTXSID40188997 | Perfluorohexadecane |
| SE-PR | 6358-30-1 | DTXSID2036293 | 8,18-Dichloro-5,15-diethyl-5,15-dihydrodiindolo[3,2-b:3′,2′-m]triphenodioxazine |
| SE-PR | 4378-61-4 | DTXSID8044674 | C.I. Vat Orange 3 |
| SE-PR | 15890-25-2 | DTXSID5027776 | Antimony diamyldithiocarbamate |
| SE-PR | 5567-15-7 | DTXSID1021453 | C.I. Pigment Yellow 83 |
| SE-PR | 6358-85-6 | DTXSID1021451 | C.I. Pigment Yellow 12 |
| SE-PR | 4424-06-0 | DTXSID8025913 | C.I. Pigment Orange 43 |
| SE-PR | 13001-39-3 | DTXSID4065317 | Benzonitrile, 2,2’-(1,4-phenylenedi-2,1-ethenediyi)bis- |
| SE-PR | 28983-56-4 | DTXSID90889705 | Methyl Blue |
| SE-PR | 5521-31-3 | DTXSID9029273 | C.I. Pigment Red 179 |
| SE-PR | 128-80-3 | DTXSID9044376 | D & C Green No. 6 |
| SE-PR | 2786-76-7 | DTXSID7029243 | C.I. Pigment Red 170 |
| SE-PR | 56358-10-2 | DTXSID30866555 | 2-Naphthalenamine, N-(2-ethylhexyl)-1-[2-[3-methyl-4-[2-[3-methylphenyl]diazenyl]phenyl]diazenyl]- |
| SE-PR | 6428-31-5 | DTXSID3064356 | C.I. Direct Black 19, disodium salt |
| SE-PR | 30125-47-4 | DTXSID2067539 | C.I. Pigment Yellow 138 |
| SE-PR | 6417-50-1 | DTXSID4064345 | 1,4-Benzenedicarboxamide, N,N'-bis[5-(benzoylamino)-9,10-dihydro-9,10-dioxo-1-anthracenyl]- |
| SE-PR | 59656-20-1 | DTXSID9069344 | 1,3,4-Thiadiazole, 2,5-bis(tert-dodecylthio)- |
| SE-PR | 4051-63-2 | DTXSID2052079 | Pigment Red 177 |
Figure S6. Chemical space of HBDB and SE-PR investigated with principal component analysis (PCA). Dimensionality is reduced to 2 dimensions explaining 35% of the total variation in the data. Compounds from HBDB and SE-PR lists predicted to be active with 90% confidence level in at least 9 thyroid-specific models are shown as orange and violet diamonds, respectively. All other compounds from the lists are shown in green and olive. Notably the most predicted active chemicals from both sets are dissimilar, HBDB actives (orange diamonds) are forming a cluster with a couple of exceptions. Most active compounds from SE-PR (violet diamonds) in general tend to separate from the rest SE-PR compounds (light-green circles).
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