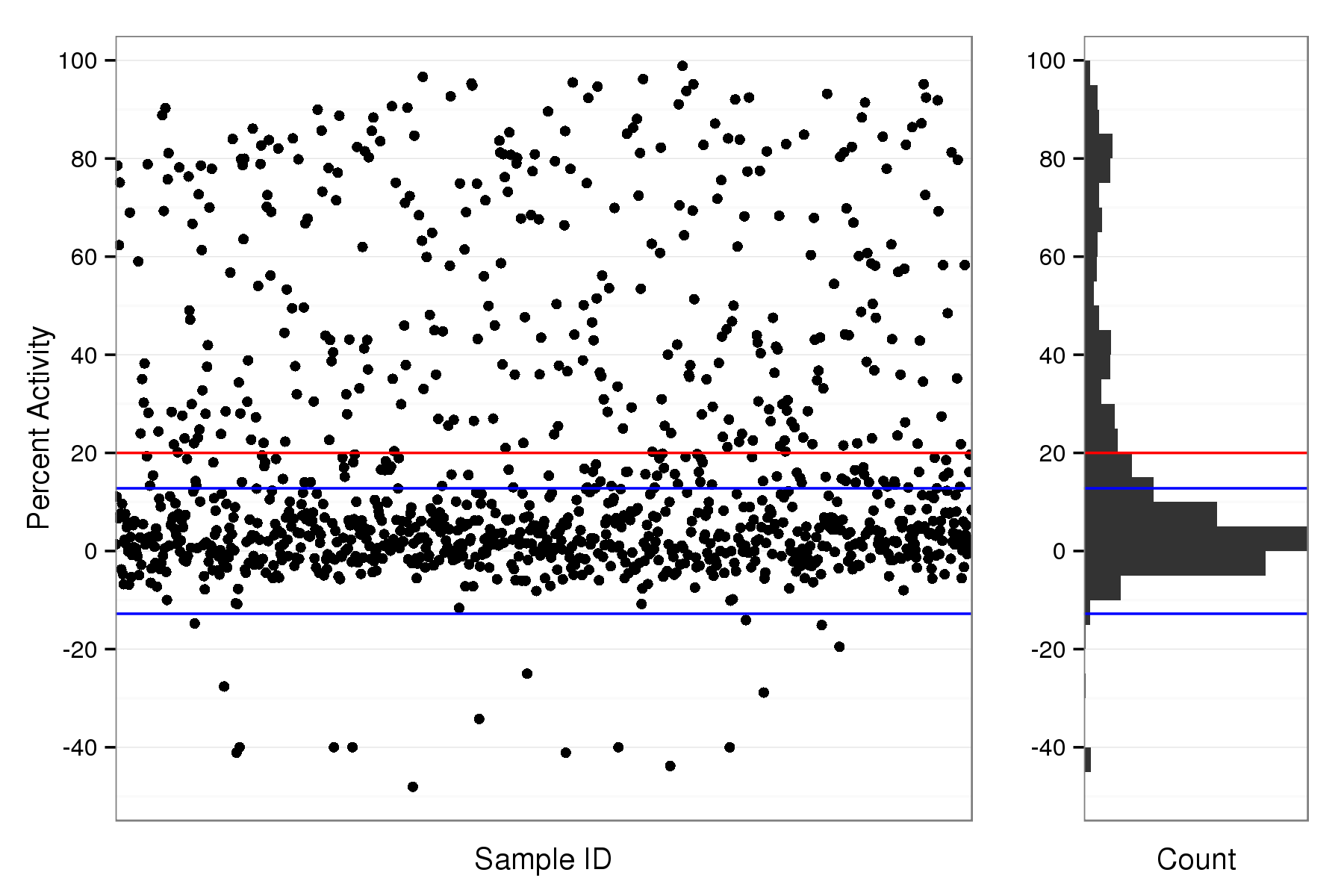


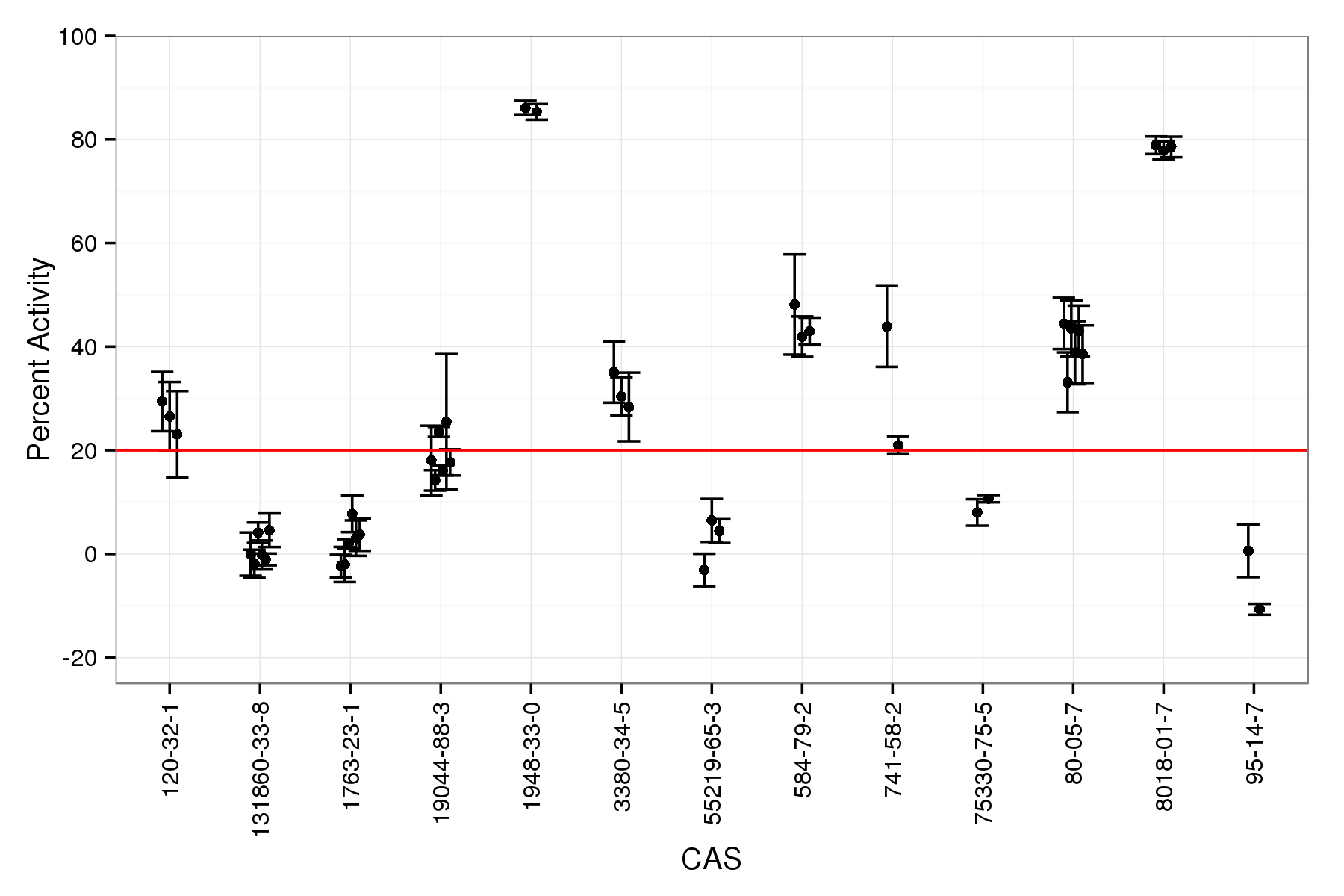
Figure 1. A network view of known potential MIEs for thyroid disruption. Several putative AOPs for thyroid hormone disruption are integrated into a combined AOP network. Given significant perturbation at each step, molecular-initiating events (MIEs) (left) proceed to key events (middle), and then to adverse outcomes (right). MIEs with related assays available in ToxCast are highlighted in green. TPO inhibition, and the key events of the AOP connecting TPO inhibition to adverse neurological outcomes, are highlighted in blue (Zoeller and Crofton, 2005). Other adverse outcomes related to thyroid hormone perturbation are also shown, including hearing loss, altered amphibian metamorphosis, and rodent thyroid tumors (Crofton and Zoeller, 2005; Pickford, 2010; McClain 1989).

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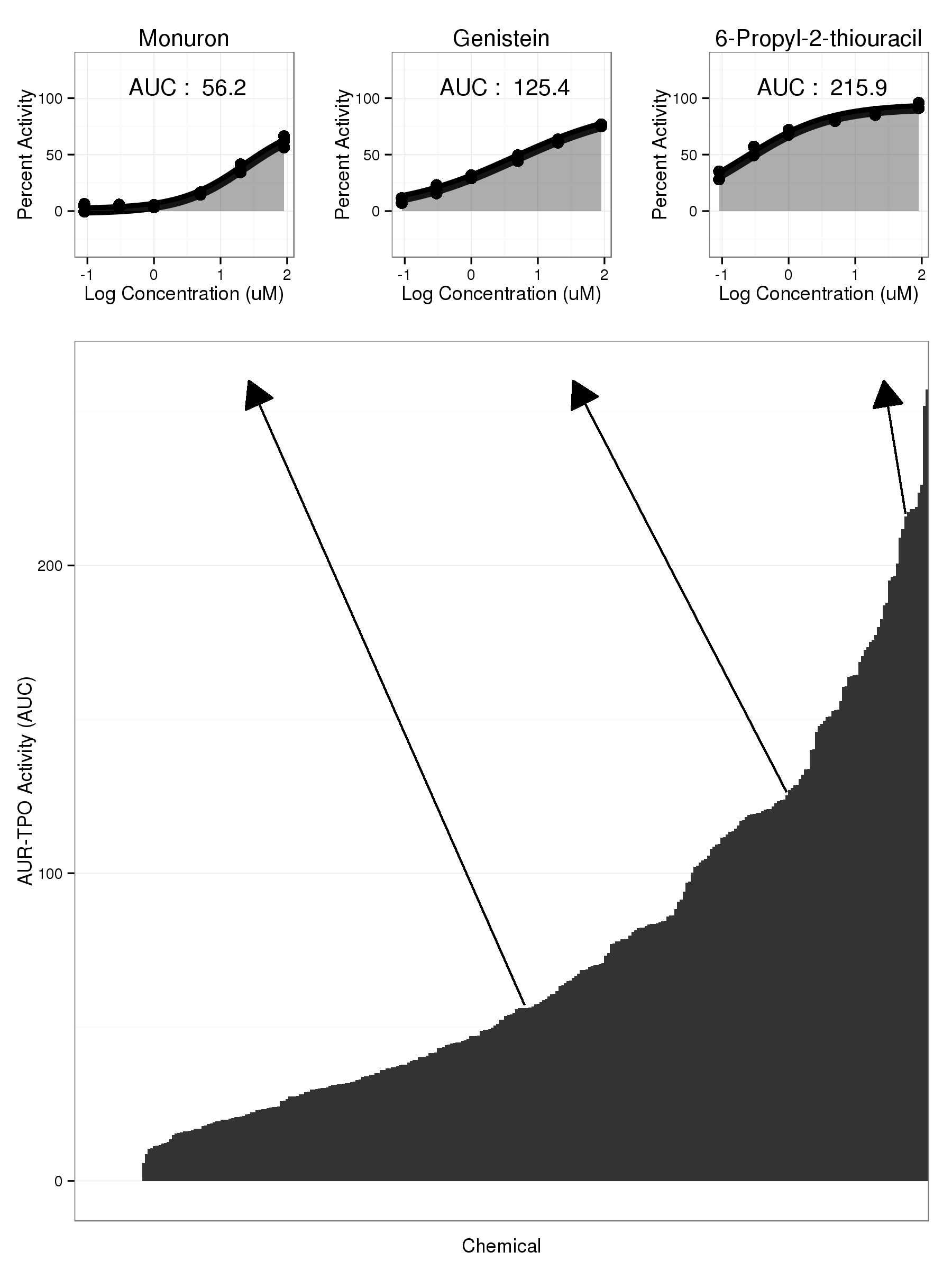
### Figure 2. The tiered screening approach to identity, stratify and confirm TPO inhibitors. 1,074 unique ToxCast chemicals were initially screened using a single, high concentration to identify potential TPO inhibitors. Chemicals testing positive in the single concentration screen were retested in concentration-response for TPO inhibition. A cytotoxicity and luciferase inhibition assay were employed in parallel to identify possible sources of nonspecific assay signal loss, enabling stratification of roughly 300 putative TPO inhibitors based upon selective AUR-TPO activity. The TPO inhibition activities of 150 chemicals were compared across the AUR-TPO and guaiacol oxidation assays to confirm the activity profiles of putative TPO inhibitors.



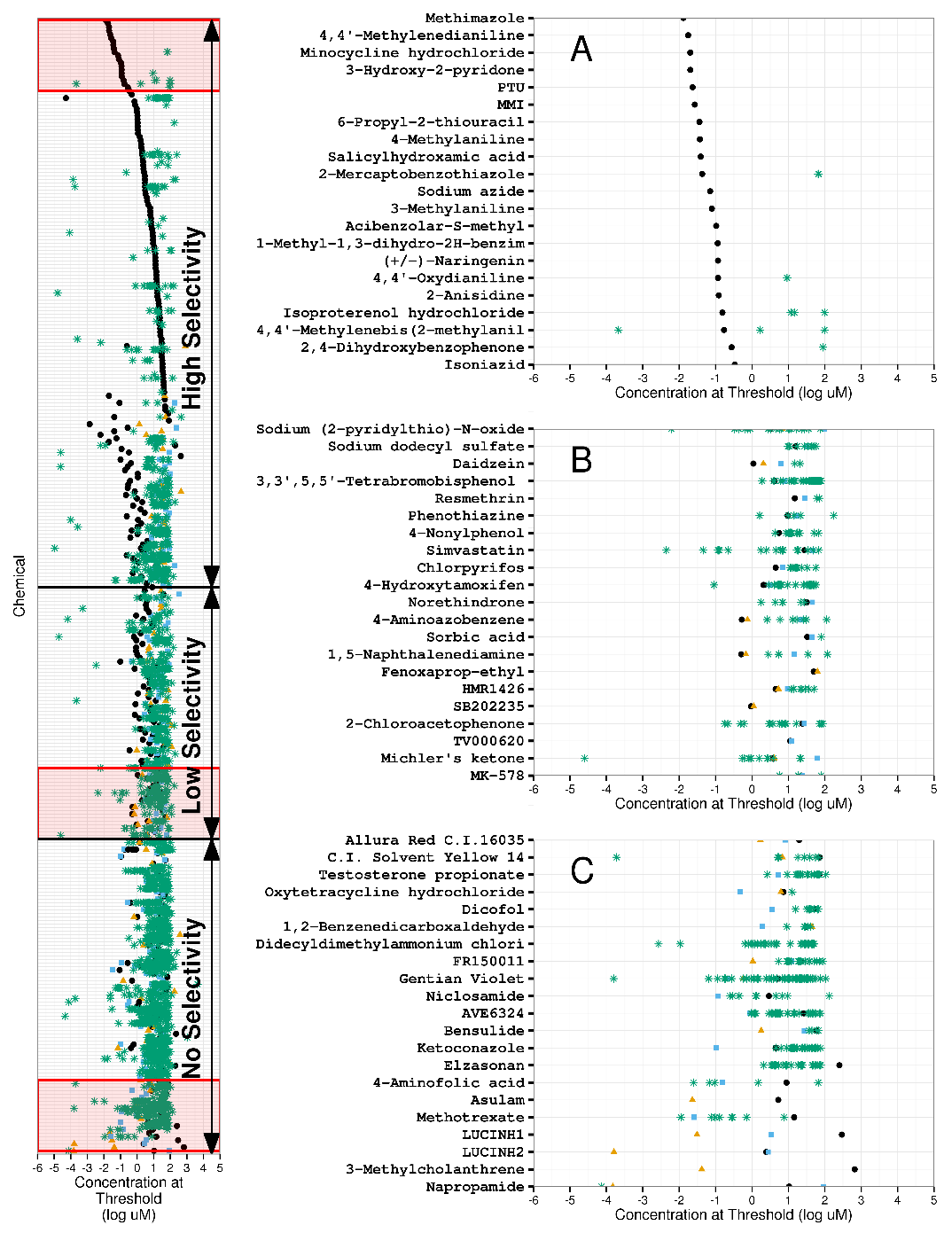
**Figure 3. Mean AUR-TPO activity for 1,074 ToxCast chemicals tested at a single, maximal concentration.** Test chemical sample IDs run across the x-axis. The y-axis represents percent activity, inverted such that vehicle control is 0% (no inhibition) and 100% indicates maximal inhibition. Each black dot represents a unique test chemical. The horizontal blue lines indicate three times the baseline median absolute deviation (± 17%), and the horizontal red line indicates the threshold for a positive assay response, 20% inhibition. The histogram (right) shows the frequency distribution using 5% activity bins.



**Figure 4. AUR-TPO activity internally-replicated compounds with ToxCast test library.** The results of 13 chemicals internally replicated as separate samples within the library in the single concentration screen (n=3) are represented as mean (black dots) ± SD (error bars). The y-axis represents percent activity, inverted such that vehicle control is 0% (no inhibition) and 100% indicates maximal inhibition. The horizontal red line indicates the threshold for a positive assay response, 20% inhibition.

****

**Figure 5. Ranked area under the fitted curves for 314 putative TPO inhibitors confirmed in dose-response in the AUR-TPO assay.** 314 AUR-TPO actives retested in multiple-concentration screening were ranked by area under the fitted curve (AUC). AUC (y-axis) compresses potency and efficacy into a single value to reflect the relative overall activity in the AUR-TPO assay. 31 chemicals characterized as active in the initial single-concentration screen retested inactive in multiple-concentration screening (AUC = 0). Concentration-response curves with shaded AUCs are shown above for monuron, genistein and PTU.



## **Figure 6. Putative TPO inhibitors, ranked by selective activity in the AUR-TPO assay.** Insets A, B, and C magnify representative regions of the stratified list of putative TPO inhibitors ordered from most selective (top) to least selective (bottom) for AUR-TPO activity. Selectivity was calculated using difference between the log IC20 value for the AUR-TPO assay (black dots) and minimum log IC20 value for the cytotoxicity assay (blue square), luciferase assay (yellow triangle) or median modl\_acc from 37 ToxCast cytotoxicity assays (all shown as green asterisks). Black horizontal bars demarcate the 1-log (top bar) and 0-log (bottom bar) thresholds that separate chemicals highly selective for AUR-TPO activity from those chemicals with low or no selective AUR-TPO activity.

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## **Figure 7. 150 Guaiacol-tested chemicals ranked by area under the fitted curve (AUC) in the AUR-TPO assay.** (A) 150 chemicals (x-axis) tested across the AUR-TPO and GUA assays were ranked by AUC value (y-axis) derived from the AUR-TPO assay and then scored by GUA activity (blue and grey bars). The reported literature GUA activity was used to score 97 of the 101 chemicals previously tested in the GUA assay, while GUA collected in this study was used to score the remaining four literature chemicals and 49 ToxCast chemicals with no previous GUA testing. Blue arrow denote the 11 chemicals tested or reported as GUA-active that tested inactive in AUR-TPO. (B) Comparison of AUR-TPO (x-axis) and GUA (y-axis) threshold potencies for 49 ToxCast chemicals tested in both assays. Potency values are reported as log µM. Chemicals tested as inactive in GUA are plotted across the top and those tested as inactive in AUR-TPO are plotted along the right. The black diagonal line denotes equal potency.

### Table 1. Target Compound Plate and Assay Plate Concentrations for Chemical Libraries.

Test chemicals were solubilized in DMSO at a top concentration of 20 mM, unless constrained by solubility in DMSO (adjustments were then made during data analysis).

|  |  |  |
| --- | --- | --- |
| Compound Plate Stock (mM) | Assay Plate Concentration (µM) | ToxCast Chemical Libraries Tested (I, II) |
| 20.0 | 87.5 | I and II |
| 5.00 | 21.9 | I and II |
| 1.25 | 5.47 | I and II |
| 0.313 | 1.37 | I and II |
| 0.0781 | 0.342 | I and II |
| 0.0195 | 0.0854 | I and II |
| 0.00488 | 0.0214 | I only |
| 0.00122 | 0.00534 | I only |

**Table 2. Top 25 TPO inhibitors ranked by potency in AUR-TPO assay.**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Chemical Name** | **CASRN** | **IC201 (µM)** | **% Emax 2** | **AUC** |
| 4-Hexylresorcinol | 136-77-6 | 0.000052 | 96.9 | 257 |
| Resorcinol | 108-46-3 | 0.006 | 81.8 | 226 |
| Methimazole | 60-56-0 | 0.013 | 84.7 | 224 |
| 4,4'-Methylenedianiline | 101-77-9 | 0.018 | 86.3 | 219 |
| 4-Pentylaniline | 33228-44-3 | 0.020 | 83.4 | 218 |
| 6-Propyl-2-thiouracil | 51-52-5 | 0.036 | 95.7 | 216 |
| 4-Methylaniline | 106-49-0 | 0.037 | 73.2 | 201 |
| Salicylhydroxamic acid | 89-73-6 | 0.039 | 94.2 | 212 |
| 6-Methyl-2-thiouracil | 56-04-2 | 0.042 | 90.1 | 195 |
| 2,2',4,4'-Tetrahydroxybenzophenone | 131-55-5 | 0.042 | 87.3 | 209 |
| 2-Mercaptobenzothiazole | 149-30-4 | 0.043 | 97.0 | 217 |
| Quercetin | 117-39-5 | 0.057 | 98.9 | 252 |
| Sodium azide | 26628-22-8 | 0.071 | 41.8 | 45 |
| 3-Methylaniline | 108-44-1 | 0.079 | 81.9 | 197 |
| 4-Chloroaniline | 106-47-8 | 0.087 | 78.4 | 187 |
| Tannic acid | 1401-55-4 | 0.088 | 87.3 | 140 |
| 6-Thioguanine | 154-42-7 | 0.096 | 92.9 | 212 |
| Catechol | 120-80-9 | 0.100 | 81.5 | 164 |
| Acibenzolar-S-methyl | 135158-54-2 | 0.104 | 87.5 | 218 |
| CI-1029 | 207736-05-8 | 0.108 | 95.0 | 196 |
| 2-Naphthylamine | 91-59-8 | 0.115 | 74.1 | 180 |
| 4,4'-Oxydianiline | 101-80-4 | 0.117 | 86.7 | 177 |
| 2-Anisidine | 90-04-0 | 0.122 | 74.5 | 173 |
| Isoproterenol hydrochloride | 51-30-9 | 0.154 | 70.4 | 153 |
| 4,4'-Methylenebis(2-methylaniline) | 838-88-0 | 0.171 | 77.0 | 161 |

1IC20 represents the concentration at which maximal activity was inhibited by 20% in the AUR-TPO assay.

2 % E­­­max refers to the percent maximum inhibition observed in concentration-response.

**Table 3. Comparative potency and AUC values for chemicals common between the AUR-TPO training study and the current study.**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Chemical Name** | **CASRN** | **AC50 Paul et al. 2014 (µM)** | **AC50 Current Study (µM)** | **AUC Current Study** |
| Methimazole | 60-56-0 | 0.025 | 0.06 | 224 |
| Ethylene thiourea | 96-45-7 | 0.034 | 7.8 | 123 |
| 6-Propyl-2-thiouracil | 51-52-5 | 0.12 | 0.23 | 216 |
| 2,2',4,4'-Tetrahydroxy-benzophenone | 131-55-5 | 0.16 | 0.17 | 209 |
| 2-Mercaptobenzothiazole | 149-30-4 | 0.45 | 0.36 | 217 |
| Genistein | 446-72-0 | 4.5 | 3.5 | 144 |
| Daidzein | 486-66-8 | 23 | 10 | 115 |
| 4-Nonylphenol | 104-40-5 | 44 | 91 | 53 |
| Triclosan | 3380-34-5 | 142 | 48 | 39 |
| Resorcinol | 108-46-3 | 253 | 0.025 | 226 |
| 2-Hydroxy-4-methoxybenzophenone | 131-57-7 | inactive | inactive | 0 |
| Dibutylphthalate | 84-74-2 | inactive | inactive | 0 |
| Diethylhexylphthalate | 117-81-7 | inactive | inactive | 0 |
| Diethylphthalate | 84-66-2 | inactive | inactive | 0 |

**Table 4. GUA assay results for ToxCast chemicals.**

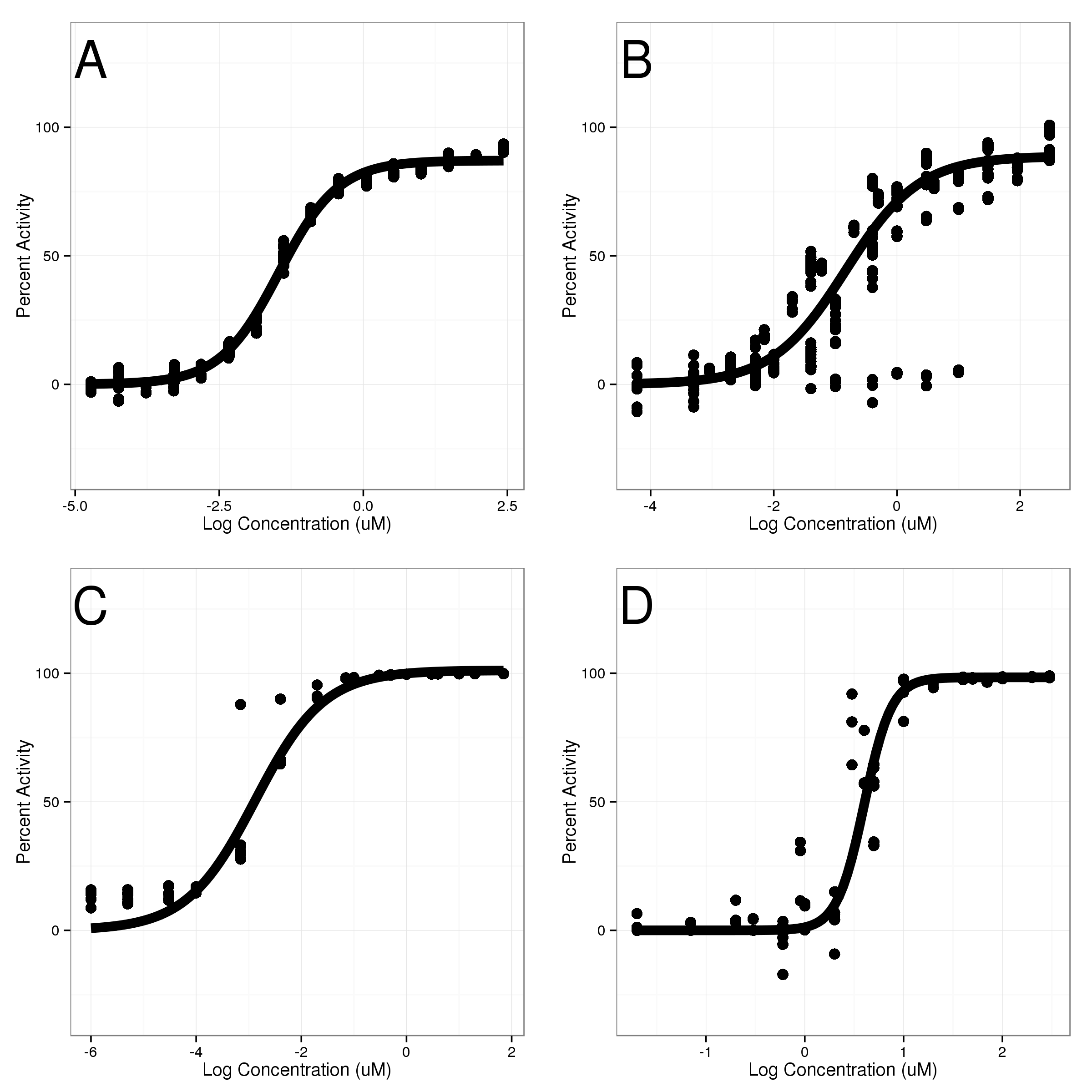
|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Chemical Name** | **CASRN** | **AUR-TPO AUC** | **Selectivity** | **GUA Activity Call** |
| 4,4'-Methylenedianiline | 101-77-9 | 219 | 6.75 | active |
| Acibenzolar-S-methyl | 135158-54-2 | 218 | 5.98 | inactive |
| 4-Methylaniline | 106-49-0 | 201 | 6.43 | active |
| 3-Methylaniline | 108-44-1 | 197 | 6.10 | active |
| 6-Methyl-2-thiouracil | 56-04-2 | 195 | 2.78 | active |
| 5-Amino-2-methylphenol | 2835-95-2 | 188 | 1.43 | active |
| 4,4'-Oxydianiline | 101-80-4 | 177 | 5.93 | active |
| 2-Anisidine | 90-04-0 | 173 | 5.91 | active |
| Aniline hydrochloride | 142-04-1 | 161 | 5.62 | active |
| Isoproterenol hydrochloride | 51-30-9 | 153 | 5.81 | active |
| Azinphos-methyl | 86-50-0 | 134 | 1.51 | active |
| Phenolphthalin | 81-90-3 | 131 | 0.76 | active |
| Methyl parathion | 298-00-0 | 129 | 4.83 | inactive |
| Isoniazid | 54-85-3 | 121 | 5.47 | active |
| PharmaGSID\_48505 | NOCAS\_48505 | 121 | 1.02 | inactive |
| Dimethoate | 60-51-5 | 120 | 1.06 | inactive |
| Fenitrothion | 122-14-5 | 114 | 4.66 | inactive |
| Ethion | 563-12-2 | 112 | 1.72 | inactive |
| Phosmet | 732-11-6 | 88 | 0.64 | active |
| Tetracycline | 60-54-8 | 86 | 4.50 | active |
| Ethoxyquin | 91-53-2 | 86 | 1.31 | active |
| Bisphenol B | 77-40-7 | 83 | 1.29 | active |
| 2,3,6-Trimethylphenol | 2416-94-6 | 82 | 4.51 | inactive |
| N,N,4-Trimethylaniline | 99-97-8 | 77 | 4.52 | active |
| Sodium (2-pyridylthio)-N-oxide | 3811-73-2 | 77 | 0.31 | active |
| Phenothiazine | 92-84-2 | 70 | 0.26 | active |
| Thiophanate-methyl | 23564-05-8 | 69 | 4.22 | active |
| Diclosulam | 145701-21-9 | 69 | 4.21 | active |
| 2-Naphthalenol | 135-19-3 | 66 | 4.63 | active |
| Asulam | 3337-71-1 | 64 | -2.15 | active |
| Malaoxon | 1634-78-2 | 59 | 4.04 | inactive |
| N,N-Dimethylaniline | 121-69-7 | 57 | 4.20 | active |
| CP-671305 | 445295-04-5 | 52 | 4.09 | inactive |
| Dioctyl phthalate | 117-84-0 | 51 | 4.15 | inactive |
| Acephate | 30560-19-1 | 47 | 3.87 | active |
| 2,6-Dimethylphenol | 576-26-1 | 45 | 3.97 | inactive |
| Sodium azide | 26628-22-8 | 45 | 6.15 | active |
| 3,5,3'-Triiodothyronine | 6893-02-3 | 40 | 0.83 | active |
| 4-(Butan-2-yl)phenol | 99-71-8 | 40 | 0.62 | inactive |
| EPN | 2104-64-5 | 38 | 3.66 | inactive |
| Folic acid | 59-30-3 | 35 | 3.83 | active |
| N-Ethyl-3-methylaniline | 102-27-2 | 32 | 3.84 | inactive |
| Bensulide | 741-58-2 | 30 | 0.04 | inactive |
| Sodium dimethyldithiocarbamate | 128-04-1 | 30 | -0.87 | active |
| CI-1044 | NOCAS\_47291 | 23 | 3.31 | inactive |
| N-Ethylaniline | 103-69-5 | 16 | 3.08 | inactive |
| 7,12-Dimethylbenz(a)anthracene | 57-97-6 | 12 | 3.20 | active |
| Diphenylamine | 122-39-4 | inactive | NA | inactive |
| Disulfoton | 298-04-4 | inactive | NA | inactive |

**Table 5. AUR assay results for chemicals reported with GUA assay results in the literature.**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Chemical Name** | **CARN** | **Source** | **GUA Lit Activity Call** | **AUR-TPO AUC** | **Selectivity** |
| (+/-)-Naringenin | 67604-48-2 | Sigma | active | 177 | 5.93 |
| 1-Methyl-1,3-dihydro-2H-benzimidazole-2-thione | 2360-22-7 | Sigma | active | 180 | 5.94 |
| 2,4-Dihydroxybenzophenone | 131-56-6 | DSSTox inventory | active | 126 | 5.56 |
| 2-Aminobenzothiazole | 136-95-8 | Sigma | active | 64 | 0.89 |
| 2-Bromo-4-hydroxyacetophenone | 2491-38-5 | DSSTox inventory | active | 95 | 4.74 |
| 2-Mercaptobenzimidazole | 583-39-1 | DSSTox inventory | active | 230 | 2.99 |
| 3-Hydroxy-2(hydroxymethyl)pyridine | 14173-30-9 | Sigma | active | 0 | NA |
| 3-Hydroxy-2-pyridone | 16867-04-2 | DSSTox inventory | active | 239 | 6.69 |
| 3-Hydroxypyridine | 109-00-2 | Sigma | active | 0 | NA |
| 3-Methylcholanthrene | 56-49-5 | Sigma | active | 32 | -4.20 |
| 5,5-​Dimethyl-​1-​Hydroxymethylhydantoin | 116-25-6 | DSSTox inventory | active | 0 | NA |
| 5-Chloro-2-mercaptobenzothiazole | 5331-91-9 | Sigma | active | 185 | 2.94 |
| 5-Nitro-2-mercaptobenzimidazole | 6325-91-3 | Sigma | active | 214 | 3.37 |
| 6-Hydroxy-2-oxopyridinium chloride | 10357-84-3 | Sigma | active | 96 | 4.62 |
| Benzo(e)pyrene | 192-97-2 | DSSTox inventory | active | 0 | NA |
| Benzo(k)fluoranthene | 207-08-9 | Sigma | active | 0 | NA |
| Benzothiazole | 95-16-9 | DSSTox inventory | active | 84 | 1.36 |
| DL-Goitrin | 13190-34-6 | Santa Cruz | active | 37 | 3.64 |
| Leucomalachite green | 129-73-7 | DSSTox inventory | active | 51 | 0.66 |
| Minocycline hydrochloride | 13614-98-7 | DSSTox inventory | active | 150 | 6.69 |
| N,N,N',N'-Tetramethylthiourea | 2782-91-4 | TCI | active | 0 | NA |
| Ricinine | 524-40-3 | Sigma | active | 0 | NA |
| Salicylhydroxamic acid | 89-73-6 | Sigma | active | 212 | 6.41 |
| Sodium thiocyanate | 540-72-7 | DSSTox inventory | active | 69 | 4.53 |
| Sulfamethazine | 57-68-1 | DSSTox inventory | active | 72 | 4.57 |
| Sunitinib malate | 341031-54-7 | Sigma | active | 75 | 0.87 |
| Thiourea | 62-56-6 | DSSTox inventory | active | 96 | 0.69 |
| 2-(2-Hydroxy-5-methylphenyl)benzotriazole | 2440-22-4 | DSSTox inventory | inactive | 0 | NA |
| 2(3H)-Benzothiazolone | 934-34-9 | Sigma | inactive | 19 | 3.39 |
| 2-(8-Heptadecenyl)-2-imidazoline-1-ethanol | 95-38-5 | DSSTox inventory | inactive | 48 | -0.13 |
| 2,2'-Dihydroxy 4-methoxybenzophenone | 131-53-3 | Sigma | inactive | 0 | NA |
| 2,3,4-Trihydroxbenzophenone | 1143-72-2 | DSSTox inventory | inactive | 153 | 2.45 |
| 2,4-Dihydroxypyridine | 626-03-9 | Sigma | inactive | 0 | NA |
| 2-Hydroxy 4-methoxybenzophenone | 131-57-7 | DSSTox inventory | inactive | 0 | NA |
| 2-Hydroxypyridine | 142-08-5 | DSSTox inventory | inactive | 0 | NA |
| 3-(4-Methylbenzylidene)camphor | 36861-47-9 | Sigma | inactive | 0 | NA |
| 3-Hydroxy-6-methylpyridine | 1121-78-4 | DSSTox inventory | inactive | 0 | NA |
| 3-Methoxy-4-hydroxypyridine | 62885-41-0 | Frontier | inactive | 0 | NA |
| 4-Butylphenol | 1638-22-8 | DSSTox inventory | inactive | 39 | 0.90 |
| 4-Ethylphenol | 123-07-9 | DSSTox inventory | inactive | 0 | NA |
| 4-Hydroxybenzophenone | 1137-42-4 | Sigma | inactive | 0 | NA |
| 4-Hydroxypyridine | 626-64-2 | DSSTox inventory | inactive | 0 | NA |
| 4-Propylphenol | 645-56-7 | DSSTox inventory | inactive | 44 | 0.68 |
| Benzhydrol | 91-01-0 | Sigma | inactive | 0 | NA |
| Butyl salicylate | 2052-14-4 | Sigma | inactive | 0 | NA |
| Dibenzo(a,h)anthracene | 53-70-3 | DSSTox inventory | inactive | 0 | NA |
| Dipyrone monohydrate | 5907-38-0 | Sigma | inactive | 110 | 5.16 |
| Ethyl-3-hydroxybenzoate | 7781-98-8 | Sigma | inactive | 0 | NA |
| Methyl methylbenzoate | 89-71-4 | DSSTox inventory | inactive | 0 | NA |
| Methylmercury chloride | 115-09-3 | Sigma | inactive | 0 | NA |
| Methylthiobenzothiazole | 615-22-5 | Sigma | inactive | 0 | NA |
| N'-tert-butyl-n-cyclopropyl-6-(methylthio)-1,3,5-triazine-2,4-diamine | 28159-98-0 | DSSTox inventory | inactive | 0 | NA |
| Octinoxate | 5466-77-3 | Sigma | inactive | 0 | NA |
| Phenol red | 143-74-8 | DSSTox inventory | inactive | 45 | -0.06 |
| Phenylbutazone | 50-33-9 | DSSTox inventory | inactive | 26 | 3.61 |

**Table 6. Consideration of the AUR-TPO inhibition assay using criteria for alternative screening assay development.**

|  |  |  |
| --- | --- | --- |
| # | Criteria for Alternative Screening Assay Development | Rating of the AUR-TPO inhibition assay |
| 1 | Key event | TPO inhibition is clearly linked with decreased thyroid hormone synthesis, with clinical and animal model information to support the connections between TPO inhibition, decreased thyroid hormone synthesis, and aberrant neurodevelopment. |
| 2 | Endpoint measurement | The endpoint measured in this assay is a loss of fluorescence, indicating decreased TPO activity. This endpoint is not measured directly, and as such assay confounders may include auto-fluorescent chemicals, detergents, salts, denaturing agents, pan-active enzyme inhibitors, and highly reactive chemicals. |
| 3 | Dynamic range | The AUR-TPO inhibition demonstrates excellent dynamic range and sufficiently low intersample variability to discriminate clearly between positive and negative test chemicals with a rZ’ of 0.77-0.83. A rZ′ of 0.5−1.0 corresponds to an assay with a suitably high signal-to-background difference and low variability to be amenable for HTS applications. |
| 4 | Parametric controls | Conduct of the AUR-TPO assay without H2O2 to initiate the reaction or without thyroid microsomal protein will result in a lack of response. The vehicle control (DMSO) was used in place of a chemical to demonstrate maximal TPO activity. |
| 5 | Response characterization | A response threshold has been set at 20% inhibition of maximal TPO activity, and a link between AUR-TPO activity *in vitro* and effects on thyroid hormone homeostasis *in vivo* is not fully characterized. However, subsequent refinement using assays to indicate potential confounding factors may add relevance to the response characterization. |
| 6 | Concentration | Concentration response curves are measured and replicable in the AUR-TPO inhibition assay. |
| 7 | Endpoint selectivity | The AUR-TPO inhibition assay is subject to confounders as previously described that may result in false-positive outcomes. Stratification of AUR-TPO inhibition results as demonstrated herein provides a pragmatic approach for increasing endpoint selectivity in the AUR-TPO assay. |
| 8 | Endpoint selective controls | MMI was included on every assay plate, and demonstrated predictable performance within and across studies (Paul *et al.*, 2014). |
| 9 | Training set | A training set of chemicals (Paul *et al.*, 2014) with both positive and negative chemicals was developed previously and verified in this study, with qualitative concordance and a good degree of quantitative concordance (Table 4). |
| 10 | Testing set | The ToxCast Phase I and II chemical libraries, along with chemicals tested due to positive findings in the GUA assay as reported in the literature, comprise a broad test set for the AUR-TPO assay, including 17 known TPO inhibitors and 32 known negatives, but with the vast majority of these chemicals either never tested *in vitro* or *in vivo* for TPO inhibition. |
| 11 | Specificity and sensitivity | Using the 150 total GUA activity calls as the standard of *in vitro* TPO inhibition, the AUR-TPO assay has a balanced accuracy of 70% with greater sensitivity (88.3%) than specificity (39.3%). The relatively low specificity of AUR-TPO results from a large number of AUR-TPO actives that tested or were reported as inactive in GUA; our studies found that chemicals tested in GUA required higher test concentrations (compared to AUR-TPO) to exceed the activity threshold and this may explain the discordance between the assays. |
| 12 | High-throughput | The AUR-TPO inhibition assay was conducted in a semi-automated 384-well format, enabling hundreds to thousands of chemicals to be tested in one day. A major limitation on throughput is the preparation of rat thyroid microsomes. Approximately 87 test wells can be run with a single rat thyroid (approximately 15-20 mg of tissue). |
| 13 | Documentation | This assay is fully documented with all assay details available in this work and in a previous work (Paul *et al.*, 2014). |
| 14 | Transferability | The assay itself is highly transferrable using a commercially available reagent (Amplex UltraRed ®, Life Technologies) and other commonly available assay reagents. Rat thyroid microsomal tissue remains a limitation on transferability. |
| 15 | Data sharing | All of the data files for this evaluation are available as Supplemental Material and on a public website. |



**Supplemental Figure 1. Control responses AUR-TPO, luciferase inhibition and cytotoxicity screening assays.** Concentration response curves for (a) methimazole used in single-concentration AUR-TPO; (b) methimazole used in multiple-concentration AUR-TPO screening; (c) LUCINH2 used in luciferase inhibition assay; (d) DCNQ used in cytotoxicity assay. The x-axis represents concentration of control compounds in log µM units. The y-axis represents percent activity for all assays.

### Supplemental Table 1. ToxCast chemicals screened using AUR-TPO assay.

1,074 ToxCast chemicals were screened using a single, high concentration in the AUR-TPO assay. Activity is presented as the mean of three biological replicates such that vehicle control is 0% (no inhibition) and 100% indicates maximal inhibition.

|  |  |  |
| --- | --- | --- |
| **Chemical Name** | **CASRN** | **Mean Activity (%)** |
| Quercetin | 117-39-5 | 98.9 |
| 2-Mercaptobenzothiazole | 149-30-4 | 96.6 |
| 4-Hexylresorcinol | 136-77-6 | 96.2 |
| Gentian Violet | 548-62-9 | 95.5 |
| Phosmet | 732-11-6 | 95.3 |
| 5-Amino-2-methylphenol | 2835-95-2 | 95.2 |
| Azinphos-methyl | 86-50-0 | 95.1 |
| Dimethoate | 60-51-5 | 94.9 |
| 1,5-Naphthalenediamine | 2243-62-1 | 94.7 |
| Methidathion | 950-37-8 | 93.8 |
| Troglitazone | 97322-87-7 | 93.2 |
| 6-Thioguanine | 154-42-7 | 92.7 |
| Malathion | 121-75-5 | 92.4 |
| 2,2',4,4'-Tetrahydroxybenzophenone | 131-55-5 | 92.4 |
| Azamethiphos | 35575-96-3 | 92.3 |
| Octyl gallate | 1034-01-1 | 92.0 |
| 2,5-Di-tert-butylbenzene-1,4-diol | 88-58-4 | 91.8 |
| Farglitazar | 196808-45-4 | 91.4 |
| 6-Propyl-2-thiouracil | 51-52-5 | 91.1 |
| 9-Phenanthrol | 484-17-3 | 90.7 |
| 6-Methyl-2-thiouracil | 56-04-2 | 90.3 |
| 2,2-Bis(4-hydroxyphenyl)-1,1,1-trichloroethane | 2971-36-0 | 90.3 |
| CI-1029 | 207736-05-8 | 90.0 |
| Phenolphthalin | 81-90-3 | 89.6 |
| 4,4'-Oxydianiline | 101-80-4 | 88.8 |
| 1,3-Benzenediamine | 108-45-2 | 88.7 |
| Carboxin | 5234-68-4 | 88.3 |
| Ziram | 137-30-4 | 88.3 |
| 2,4-Diaminotoluene | 95-80-7 | 88.1 |
| Methimazole | 60-56-0 | 87.2 |
| Dazomet | 533-74-4 | 87.1 |
| Rifampicin | 13292-46-1 | 86.4 |
| N-Phenyl-1,4-benzenediamine | 101-54-2 | 86.3 |
| tert-Butylhydroquinone | 1948-33-0 | 86.1 |
| 3,4-Diaminotoluene | 496-72-0 | 85.7 |
| Phenothiazine | 92-84-2 | 85.6 |
| Aniline hydrochloride | 142-04-1 | 85.6 |
| 4,4'-Sulfonylbis[2-(prop-2-en-1-yl)phenol] | 41481-66-7 | 85.0 |
| Daidzein | 486-66-8 | 84.9 |
| Methylene bis(thiocyanate) | 6317-18-6 | 84.7 |
| 4,4'-Methylenedianiline | 101-77-9 | 84.4 |
| 2-(Thiocyanomethylthio)benzothiazole | 21564-17-0 | 84.1 |
| Hydroquinone | 123-31-9 | 84.1 |
| Isoeugenol | 97-54-1 | 84.0 |
| Thiophanate-methyl | 23564-05-8 | 83.8 |
| Tannic acid | 1401-55-4 | 83.8 |
| Methyldopa sesquihydrate | 41372-08-1 | 83.6 |
| Bifenazate | 149877-41-8 | 83.5 |
| Acibenzolar-S-methyl | 135158-54-2 | 82.9 |
| Methyl parathion | 298-00-0 | 82.8 |
| 4-Pentylaniline | 33228-44-3 | 82.8 |
| Dodecylbenzenesulfonic acid | 27176-87-0 | 82.6 |
| Mevinphos | 7786-34-7 | 82.4 |
| Catechol | 120-80-9 | 82.4 |
| 2-Anisidine | 90-04-0 | 82.2 |
| 3-Methylaniline | 108-44-1 | 82.0 |
| 2-Naphthylamine | 91-59-8 | 81.5 |
| 1,2-Phenylenediamine | 95-54-5 | 81.4 |
| Resorcinol | 108-46-3 | 81.3 |
| Ethylene thiourea | 96-45-7 | 81.2 |
| 4-Chloroaniline | 106-47-8 | 81.2 |
| CP-634384 | 290352-28-2 | 81.1 |
| Propyl gallate | 121-79-9 | 81.1 |
| HMR1426 | 262376-75-0 | 80.9 |
| 4-Methylaniline | 106-49-0 | 80.9 |
| Phenolphthalein | 77-09-8 | 80.7 |
| 2,3-Diaminotoluene | 2687-25-4 | 80.4 |
| Fenitrothion | 122-14-5 | 80.3 |
| Anthracene | 120-12-7 | 80.1 |
| SAR150640 | NOCAS\_47389 | 80.0 |
| Cyanamide | 420-04-2 | 79.9 |
| 2-tert-Butyl-4-methoxyphenol | 121-00-6 | 79.8 |
| Ethion | 563-12-2 | 79.7 |
| Mancozeb | 8018-01-7 | 79.6 |
| Sodium (2-pyridylthio)-N-oxide | 3811-73-2 | 79.4 |
| Sodium dodecylbenzenesulfonate | 25155-30-0 | 79.0 |
| 4,4'-Methylenebis(2-methylaniline) | 838-88-0 | 78.8 |
| 3,3',5,5'-Tetrabromobisphenol A | 79-94-7 | 78.6 |
| 2-Methoxy-5-nitroaniline | 99-59-2 | 78.6 |
| 4-Chloro-1,2-diaminobenzene | 95-83-0 | 78.2 |
| 4-Aminobenzoic acid | 150-13-0 | 78.1 |
| Genistein | 446-72-0 | 77.9 |
| Dapsone | 80-08-0 | 77.9 |
| Pirimiphos-methyl | 29232-93-7 | 77.5 |
| 4,4'-Methylenebis(N,N-dimethylaniline) | 101-61-1 | 77.4 |
| Clove leaf oil | 8000-34-8 | 77.4 |
| Diclosulam | 145701-21-9 | 77.1 |
| N,N,4-Trimethylaniline | 99-97-8 | 76.3 |
| Isoniazid | 54-85-3 | 76.2 |
| Malaoxon | 1634-78-2 | 75.7 |
| Maneb | 12427-38-2 | 75.6 |
| 4-Aminoazobenzene | 60-09-3 | 75.1 |
| Eugenol | 97-53-0 | 75.1 |
| 2-Methylaniline | 95-53-4 | 75.0 |
| Acephate | 30560-19-1 | 74.9 |
| Tetracycline | 60-54-8 | 74.8 |
| 8-Hydroxyquinoline | 148-24-3 | 73.3 |
| CJ-013790 | 179465-71-5 | 73.2 |
| Chlorpyrifos-methyl | 5598-13-0 | 72.7 |
| Retinol | 68-26-8 | 72.6 |
| 17beta-Trenbolone | 10161-33-8 | 72.5 |
| 1-Hydroxypyrene | 5315-79-7 | 72.4 |
| Terbufos sulfone | 56070-16-7 | 72.4 |
| Benz(a)anthracene | 56-55-3 | 71.8 |
| 2,4-Bis(2-methylbutan-2-yl)phenol | 120-95-6 | 71.5 |
| 2,4,6-Trimethylphenol | 527-60-6 | 71.5 |
| Z-Tetrachlorvinphos | 22248-79-9 | 71.0 |
| Anilazine | 101-05-3 | 70.4 |
| Dichlorvos | 62-73-7 | 70.1 |
| 2-Methoxy-5-methylaniline | 120-71-8 | 70.0 |
| Carminic acid | 1260-17-9 | 69.9 |
| Fenthion | 55-38-9 | 69.8 |
| Isoproterenol hydrochloride | 51-30-9 | 69.4 |
| 2,3,6-Trimethylphenol | 2416-94-6 | 69.3 |
| N,N-Dimethylaniline | 121-69-7 | 69.3 |
| all-trans-Retinoic acid | 302-79-4 | 69.1 |
| 4,4',4"-Ethane-1,1,1-triyltriphenol | 27955-94-8 | 69.1 |
| Maltol | 118-71-8 | 69.0 |
| UK-337312 | 203942-49-8 | 68.5 |
| 3,7-Dimethyl-2,6-octadienal | 5392-40-5 | 68.4 |
| PharmaGSID\_48505 | NOCAS\_48505 | 68.3 |
| Oxytetracycline dihydrate | 6153-64-6 | 68.2 |
| Phorate | 298-02-2 | 67.9 |
| 2,4,6-Tris(tert-butyl)phenol | 732-26-3 | 67.8 |
| Toluene-2,4-diisocyanate | 584-84-9 | 67.8 |
| 2,4-Di-tert-butylphenol | 96-76-4 | 67.6 |
| 2-tert-Butyl-4-ethylphenol | 96-70-8 | 66.9 |
| Diethylstilbestrol | 56-53-1 | 66.8 |
| PD-0333941 | 501027-49-2 | 66.7 |
| FD&C Blue No. 1 | 3844-45-9 | 66.4 |
| Busulfan | 55-98-1 | 64.9 |
| Fenaminosulf | 140-56-7 | 64.3 |
| Triclocarban | 101-20-2 | 63.5 |
| meso-Hexestrol | 84-16-2 | 63.2 |
| 2-Amino-5-azotoluene | 97-56-3 | 62.6 |
| Simvastatin | 79902-63-9 | 62.5 |
| Docusate sodium | 577-11-7 | 62.3 |
| 2,6-Di-tert-butylphenol | 128-39-2 | 62.0 |
| Dodecylbenzene sulfonate triethanolamine(1:1) | 27323-41-7 | 62.0 |
| Methyl methanesulfonate | 66-27-3 | 61.5 |
| Michler's ketone | 90-94-8 | 61.3 |
| Darbufelone mesylate | 139340-56-0 | 60.8 |
| PharmaGSID\_47337 | 1061517-62-1 | 60.7 |
| Monuron | 150-68-5 | 60.3 |
| Resmethrin | 10453-86-8 | 60.1 |
| CP-105696 | 158081-99-3 | 59.9 |
| Profenofos | 41198-08-7 | 59.0 |
| CP-456773 | 210826-40-7 | 58.7 |
| Dimethyl sulfate | 77-78-1 | 58.6 |
| Formetanate hydrochloride | 23422-53-9 | 58.3 |
| FR150011 | 149413-74-1 | 58.3 |
| Oxytetracycline hydrochloride | 2058-46-0 | 58.2 |
| 4-Nonylphenol, branched | 84852-15-3 | 58.1 |
| Bisphenol AF | 1478-61-1 | 57.5 |
| Diazinon | 333-41-5 | 56.9 |
| Asulam | 3337-71-1 | 56.7 |
| Mesotrione | 104206-82-8 | 56.2 |
| Folic acid | 59-30-3 | 56.1 |
| Isazofos | 42509-80-8 | 56.0 |
| Allethrin | 584-79-2 | 56.0 |
| 4-(1,1,3,3-Tetramethylbutyl)phenol | 140-66-9 | 54.4 |
| Didecyldimethylammonium chloride | 7173-51-5 | 54.0 |
| SR271425 | 155990-20-8 | 53.6 |
| Hexaflumuron | 86479-06-3 | 53.4 |
| Ethoxyquin | 91-53-2 | 53.3 |
| CP-471358 | NOCAS\_47265 | 51.5 |
| 2,6-Dimethylphenol | 576-26-1 | 51.3 |
| Allura Red C.I.16035 | 25956-17-6 | 50.4 |
| 2-Naphthalenol | 135-19-3 | 50.3 |
| 2-Chloroacetophenone | 532-27-4 | 50.1 |
| Tolazamide | 1156-19-0 | 50.0 |
| 4-Cumylphenol | 599-64-4 | 50.0 |
| 1,2-Benzenedicarboxaldehyde | 643-79-8 | 49.6 |
| Rotenone | 83-79-4 | 49.5 |
| Ketoconazole | 65277-42-1 | 49.0 |
| Mifepristone | 84371-65-3 | 48.8 |
| 3-Hydroxyfluorene | 6344-67-8 | 48.5 |
| SAR115740 | NOCAS\_47366 | 47.7 |
| Sodium dodecyl sulfate | 151-21-3 | 47.5 |
| Ethoprop | 13194-48-4 | 47.5 |
| Methamidophos | 10265-92-6 | 47.2 |
| Geranyl acetate | 105-87-3 | 46.8 |
| Norethindrone | 68-22-4 | 46.6 |
| (2Z)-3,7-Dimethylocta-2,6-dien-1-ol | 106-25-2 | 46.0 |
| MK-578 | 313994-79-5 | 46.0 |
| Bisphenol B | 77-40-7 | 45.2 |
| Cymoxanil | 57966-95-7 | 45.0 |
| Sodium myristyl sulfate | 1191-50-0 | 44.8 |
| Bisphenol A | 80-05-7 | 44.5 |
| Metam-sodium hydrate | 6734-80-1 | 44.2 |
| Diuron | 330-54-1 | 44.1 |
| N-Ethylaniline | 103-69-5 | 44.0 |
| 4-Aminofolic acid | 54-62-6 | 44.0 |
| Bensulide | 741-58-2 | 43.9 |
| Fenamidone | 161326-34-7 | 43.7 |
| 2,4-Bis(1-methyl-1-phenylethyl)phenol | 2772-45-4 | 43.5 |
| Tebupirimfos | 96182-53-5 | 43.2 |
| Trichloroacetic acid | 76-03-9 | 43.2 |
| Parathion | 56-38-2 | 43.1 |
| N-Ethyl-3-methylaniline | 102-27-2 | 43.1 |
| Fenoxaprop-ethyl | 66441-23-4 | 42.9 |
| Niclosamide | 50-65-7 | 42.9 |
| Sorbic acid | 110-44-1 | 42.5 |
| Sodium erythorbate (1:1) | 6381-77-7 | 42.1 |
| Linuron | 330-55-2 | 41.6 |
| 17alpha-Estradiol | 57-91-0 | 41.3 |
| 4-Heptylphenol | 1987-50-4 | 41.1 |
| Chlorpyrifos oxon | 5598-15-2 | 40.5 |
| 17alpha-Ethinylestradiol | 57-63-6 | 40.3 |
| 2,4-Dimethylphenol | 105-67-9 | 40.0 |
| Triclosan | 3380-34-5 | 39.0 |
| Napropamide | 15299-99-7 | 38.9 |
| SB202235 | 139149-55-6 | 38.7 |
| Sodium L-ascorbate | 134-03-2 | 38.3 |
| Elzasonan | 361343-19-3 | 38.2 |
| 2-Chlorophenol | 95-57-8 | 38.0 |
| Thidiazuron | 51707-55-2 | 37.9 |
| Chlorpyrifos | 2921-88-2 | 37.8 |
| Piperonyl butoxide | 51-03-6 | 37.8 |
| 17beta-Estradiol | 50-28-2 | 37.7 |
| SSR162369 | NOCAS\_47346 | 37.5 |
| Coumaphos | 56-72-4 | 37.0 |
| Azathioprine | 446-86-6 | 36.8 |
| Terbufos | 13071-79-9 | 36.8 |
| 4-Octylphenol | 1806-26-4 | 36.6 |
| Symclosene | 87-90-1 | 36.4 |
| 4-Chlorobenzotrichloride | 5216-25-1 | 36.3 |
| PharmaGSID\_48511 | 1062243-51-9 | 36.0 |
| Procymidone | 32809-16-8 | 36.0 |
| 2-tert-Butyl-5-methylphenol | 88-60-8 | 35.9 |
| 3,5,3'-Triiodothyronine | 6893-02-3 | 35.9 |
| Sodium azide | 26628-22-8 | 35.9 |
| Chlorethoxyfos | 54593-83-8 | 35.6 |
| Folpet | 133-07-3 | 35.5 |
| AVE5638 | 725228-45-5 | 35.2 |
| 1,2-Diphenylhydrazine | 122-66-7 | 35.0 |
| Carbendazim | 10605-21-7 | 35.0 |
| 4-Androstene-3,17-dione | 63-05-8 | 34.8 |
| PFDA | 335-76-2 | 34.5 |
| Sodium hexyldecyl sulfate | 1120-01-0 | 34.4 |
| Clorophene | 120-32-1 | 33.8 |
| Triglycidyl isocyanurate | 2451-62-9 | 33.5 |
| Prallethrin | 23031-36-9 | 33.1 |
| PharmaGSID\_47263 | 349495-42-7 | 33.0 |
| SSR150106 | NOCAS\_47362 | 32.8 |
| Methotrexate | 59-05-2 | 31.9 |
| Famoxadone | 131807-57-3 | 31.9 |
| EPN | 2104-64-5 | 31.0 |
| (E)-Anethole | 4180-23-8 | 30.9 |
| 2,2-Dibromo-3-nitrilopropionamide | 10222-01-2 | 30.7 |
| Tiratricol | 51-24-1 | 30.5 |
| Citronellol | 106-22-9 | 30.5 |
| 4-(2-Methylbutan-2-yl)phenol | 80-46-6 | 30.2 |
| 1,3-Propane sultone | 1120-71-4 | 29.9 |
| Propanil | 709-98-8 | 29.9 |
| Pentachlorophenol | 87-86-5 | 29.9 |
| Ro 23-7637 | 107071-66-9 | 29.3 |
| PFNA | 375-95-1 | 28.8 |
| Safrole | 94-59-7 | 28.6 |
| Difenoconazole | 119446-68-3 | 28.5 |
| CI-1044 | NOCAS\_47291 | 28.5 |
| Cinmethylin | 87818-31-3 | 28.4 |
| 4-Nonylphenol | 104-40-5 | 28.2 |
| Triflumizole | 68694-11-1 | 28.0 |
| Dioctyl phthalate | 117-84-0 | 28.0 |
| Sodium dimethyldithiocarbamate | 128-04-1 | 27.9 |
| 4-(Butan-2-yl)phenol | 99-71-8 | 27.8 |
| Forchlorfenuron | 68157-60-8 | 27.6 |
| Maleic hydrazide | 123-33-1 | 27.4 |
| FR900409 | 138472-01-2 | 27.2 |
| Chloramben | 133-90-4 | 27.0 |
| 4-Cyclohexylcyclohexanone | 92-68-2 | 26.9 |
| N-Methyl-2-pyrrolidone | 872-50-4 | 26.8 |
| Butyl benzyl phthalate | 85-68-7 | 26.7 |
| Hydroxyurea | 127-07-1 | 26.5 |
| Reserpine | 50-55-5 | 26.3 |
| Tris(2-ethylhexyl) trimellitate | 3319-31-1 | 26.2 |
| Tamoxifen citrate | 54965-24-1 | 25.6 |
| Oryzalin | 19044-88-3 | 25.5 |
| Mercuric chloride | 7487-94-7 | 25.5 |
| S-Bioallethrin | 28434-00-6 | 25.2 |
| Alachlor ESA, sodium salt | 140939-15-7 | 25.0 |
| Anthralin | 1143-38-0 | 24.8 |
| Fenhexamid | 126833-17-8 | 24.4 |
| Phenol | 108-95-2 | 24.1 |
| Clopyralid | 1702-17-6 | 24.0 |
| Triphenyl phosphite | 101-02-0 | 23.9 |
| TNP-470 | 129298-91-5 | 23.9 |
| Monocrotophos | 6923-22-4 | 23.8 |
| PharmaGSID\_48510 | 460081-99-6 | 23.3 |
| Thiram | 137-26-8 | 23.1 |
| 7,12-Dimethylbenz(a)anthracene | 57-97-6 | 23.0 |
| CP-671305 | 445295-04-5 | 23.0 |
| UK-373911 | 291305-06-1 | 22.7 |
| Benomyl | 17804-35-2 | 22.7 |
| Testosterone propionate | 57-85-2 | 22.6 |
| 1-Dodecyl-2-pyrrolidinone | 2687-96-9 | 22.5 |
| Fabesetron hydrochloride | 129299-90-7 | 22.3 |
| CP-544439 | 230954-09-3 | 22.3 |
| PharmaGSID\_48509 | NOCAS\_48509 | 22.0 |
| AVE6324 | NOCAS\_47377 | 22.0 |
| 4-tert-Butylphenol | 98-54-4 | 22.0 |
| Methyl 2-aminobenzoate | 134-20-3 | 22.0 |
| Phosalone | 2310-17-0 | 21.9 |
| Flufenacet | 142459-58-3 | 21.8 |
| Myrcene | 123-35-3 | 21.8 |
| Raloxifene hydrochloride | 82640-04-8 | 21.7 |
| Tamoxifen | 10540-29-1 | 21.5 |
| Biphenyl | 92-52-4 | 21.4 |
| 2-tert-Butylphenol | 88-18-6 | 21.2 |
| C.I. Solvent Yellow 14 | 842-07-9 | 20.4 |
| Propiconazole | 60207-90-1 | 20.3 |
| Phenobarbital sodium | 57-30-7 | 20.2 |
| Milbemectin (mixture of 70% Milbemcin A4, 30% Milbemycin A3) | NOCAS\_34742 | 20.1 |
| Perfluoroheptanoic acid | 375-85-9 | 19.9 |
| 4-Hydroxytamoxifen | 68392-35-8 | 19.8 |
| Fosthiazate | 98886-44-3 | 19.7 |
| Etridiazole | 2593-15-9 | 19.7 |
| Estrone | 53-16-7 | 19.5 |
| SB243213A | 200940-23-4 | 19.3 |
| 1,3-Dichlorobenzene | 541-73-1 | 19.2 |
| Tepraloxydim | 149979-41-9 | 19.1 |
| 2,6-Dimethylaniline | 87-62-7 | 19.0 |
| Fenbuconazole | 114369-43-6 | 19.0 |
| Imazalil | 35554-44-0 | 18.9 |
| CP-608039 | NOCAS\_47305 | 18.9 |
| CI-959 | 104795-68-8 | 18.8 |
| FD&C Yellow 6 | 2783-94-0 | 18.8 |
| Methyleugenol | 93-15-2 | 18.8 |
| Carfentrazone-ethyl | 128639-02-1 | 18.5 |
| Cumene hydroperoxide | 80-15-9 | 18.3 |
| AVE9423 | 862243-29-6 | 18.1 |
| Prednisone | 53-03-2 | 18.1 |
| TDCPP | 13674-87-8 | 18.0 |
| HMR1171 trifluoroacetate (1:1) | NOCAS\_48522 | 17.3 |
| Fenamiphos | 22224-92-6 | 17.2 |
| N,N-Dimethylformamide | 68-12-2 | 17.1 |
| Nitrobenzene | 98-95-3 | 17.0 |
| Spironolactone | 52-01-7 | 16.9 |
| Dicrotophos | 141-66-2 | 16.8 |
| Octabenzone | 1843-05-6 | 16.6 |
| Diclofop-methyl | 51338-27-3 | 16.6 |
| Penoxsulam | 219714-96-2 | 16.6 |
| Progesterone | 57-83-0 | 16.5 |
| Benzotrichloride | 98-07-7 | 16.5 |
| Nicotinic acid | 59-67-6 | 16.2 |
| Captafol | 2425-06-1 | 16.2 |
| Prochloraz | 67747-09-5 | 16.1 |
| Heptachlor | 76-44-8 | 16.1 |
| Heptanoic acid | 111-14-8 | 16.1 |
| Decanoic acid | 334-48-5 | 16.0 |
| Vernolate | 1929-77-7 | 15.9 |
| SR125047 | NOCAS\_47342 | 15.7 |
| Nitrofurazone | 59-87-0 | 15.6 |
| Fandosentan potassium salt | 221246-12-4 | 15.6 |
| Cyproterone acetate | 427-51-0 | 15.6 |
| Hexaconazole | 79983-71-4 | 15.5 |
| Corticosterone | 50-22-6 | 15.4 |
| 2-Methyl-2,4-pentanediol | 107-41-5 | 15.4 |
| Pyridoxine | 65-23-6 | 15.3 |
| alpha-Isomethylionone | 127-51-5 | 15.2 |
| 2-Benzylideneoctanal | 101-86-0 | 15.2 |
| Propetamphos | 31218-83-4 | 15.1 |
| Ethephon | 16672-87-0 | 15.1 |
| 1,2,4-Trimethylbenzene | 95-63-6 | 14.9 |
| Perfluoroundecanoic acid | 2058-94-8 | 14.7 |
| Methadone hydrochloride | 1095-90-5 | 14.7 |
| 1,3-Dichloro-5,5-dimethylhydantoin | 118-52-5 | 14.3 |
| 2-Methyl-4,6-dinitrophenol | 534-52-1 | 14.3 |
| GW473178E methyl benzene sulphonic acid | 263553-33-9 | 14.3 |
| Clotrimazole | 23593-75-1 | 14.2 |
| Diniconazole | 83657-24-3 | 14.2 |
| FR130739 | 136042-19-8 | 14.1 |
| SR146131 | 221671-62-1 | 14.0 |
| PharmaGSID\_48172 | NOCAS\_48172 | 14.0 |
| N,N,N',N'-Tetrakis(2-Hydroxypropyl)ethylenediamine | 102-60-3 | 14.0 |
| Celecoxib | 169590-42-5 | 14.0 |
| 1-Tetradecene | 1120-36-1 | 13.9 |
| Clomiphene citrate (1:1) | 50-41-9 | 13.9 |
| Colchicine | 64-86-8 | 13.6 |
| Bronopol | 52-51-7 | 13.5 |
| Cyclanilide | 113136-77-9 | 13.5 |
| 5-Chloro-2-methyl-3(2H)-isothiazolone | 26172-55-4 | 13.3 |
| Carbaryl | 63-25-2 | 13.3 |
| 2-Methyl-5-nitroaniline | 99-55-8 | 13.3 |
| Captan | 133-06-2 | 13.2 |
| PharmaGSID\_47330 | NOCAS\_47330 | 13.2 |
| PharmaGSID\_47315 | 444610-91-7 | 13.1 |
| Cyazofamid | 120116-88-3 | 13.0 |
| Abamectin | 71751-41-2 | 13.0 |
| 1-Hexadecanol | 36653-82-4 | 12.9 |
| SAR102608 | 1068967-96-3 | 12.9 |
| UK-156819 | 162706-14-1 | 12.8 |
| Myclobutanil | 88671-89-0 | 12.8 |
| 2-Aminoanthraquinone | 117-79-3 | 12.7 |
| PharmaGSID\_48519 | 686756-87-6 | 12.7 |
| Trelanserin | 189003-92-7 | 12.6 |
| 6-Methylquinoline | 91-62-3 | 12.6 |
| o-Cresol | 95-48-7 | 12.3 |
| Butylparaben | 94-26-8 | 12.3 |
| MK-274 | NOCAS\_47328 | 12.2 |
| 4-Nitroaniline | 100-01-6 | 12.1 |
| Dimethyl phthalate | 131-11-3 | 12.0 |
| Thiabendazole | 148-79-8 | 11.9 |
| Indomethacin | 53-86-1 | 11.9 |
| beta-Hexachlorocyclohexane | 319-85-7 | 11.9 |
| Dimethylcarbamoyl chloride | 79-44-7 | 11.8 |
| Diethyl sulfate | 64-67-5 | 11.7 |
| Pymetrozine | 123312-89-0 | 11.7 |
| Nitrilotriacetic acid | 139-13-9 | 11.7 |
| 17alpha-Hydroxyprogesterone | 68-96-2 | 11.6 |
| Ingliforib | 186392-65-4 | 11.6 |
| Hexadecane | 544-76-3 | 11.6 |
| Zoxamide | 156052-68-5 | 11.6 |
| Tetrac | 67-30-1 | 11.6 |
| Amitraz | 33089-61-1 | 11.4 |
| SB236057A | 180084-01-9 | 11.4 |
| CP-612372 | 353280-07-6 | 11.3 |
| Pyraclostrobin | 175013-18-0 | 11.3 |
| Bis(2-chloroethyl) ether | 111-44-4 | 11.2 |
| Isopropyl triethanolamine titanate | 36673-16-2 | 11.1 |
| CP-457920 | 220860-50-4 | 11.0 |
| Pioglitazone hydrochloride | 112529-15-4 | 10.9 |
| Pentanal | 110-62-3 | 10.8 |
| Isooctyl acrylate | 29590-42-9 | 10.8 |
| 5HPP-33 | 105624-86-0 | 10.7 |
| Lovastatin | 75330-75-5 | 10.7 |
| Benodanil | 15310-01-7 | 10.5 |
| 2-Chloroethanol | 107-07-3 | 10.4 |
| Nicotine | 54-11-5 | 10.4 |
| Fluometuron | 2164-17-2 | 10.4 |
| Tridemorph | 24602-86-6 | 10.3 |
| Picloram | 1918-02-1 | 10.1 |
| 4-Ethyloct-1-yn-3-ol | 5877-42-9 | 10.1 |
| Tribufos | 78-48-8 | 10.1 |
| AVE3247 | NOCAS\_47383 | 10.1 |
| 2,4-Dinitrophenol | 51-28-5 | 10.1 |
| Triadimenol | 55219-65-3 | 10.1 |
| Cyprodinil | 121552-61-2 | 10.0 |
| Dicofol | 115-32-2 | 10.0 |
| 4-Nitrotoluene | 99-99-0 | 10.0 |
| Sulfasalazine | 599-79-1 | 10.0 |
| Glutaraldehyde | 111-30-8 | 9.9 |
| Cotinine | 486-56-6 | 9.8 |
| 2,5-Dimethylphenol | 95-87-4 | 9.8 |
| Disulfiram | 97-77-8 | 9.7 |
| Hydrochlorothiazide | 58-93-5 | 9.7 |
| SSR241586 | NOCAS\_47353 | 9.6 |
| 17-Methyltestosterone | 58-18-4 | 9.6 |
| Imazamox | 114311-32-9 | 9.6 |
| Caprolactam | 105-60-2 | 9.6 |
| Ilepatril | 473289-62-2 | 9.5 |
| CP-283097 | 171866-31-2 | 9.4 |
| Citric acid | 77-92-9 | 9.3 |
| Tetraconazole | 112281-77-3 | 9.1 |
| 1,2-Dimethyl-3-nitrobenzene | 83-41-0 | 9.1 |
| 1H-1,2,4-Triazole | 288-88-0 | 9.0 |
| Disulfoton | 298-04-4 | 9.0 |
| Flusilazole | 85509-19-9 | 9.0 |
| 3-Nitrotoluene | 99-08-1 | 8.9 |
| Sethoxydim | 74051-80-2 | 8.9 |
| Quinoxyfen | 124495-18-7 | 8.7 |
| Volinanserin | 139290-65-6 | 8.7 |
| PK 11195 | 85532-75-8 | 8.6 |
| Zenarestat | 112733-06-9 | 8.5 |
| Pyriproxyfen | 95737-68-1 | 8.4 |
| SB281832 | 219790-72-4 | 8.4 |
| Metribuzin | 21087-64-9 | 8.4 |
| Denatonium saccharide | 90823-38-4 | 8.3 |
| Clofibrate | 637-07-0 | 8.3 |
| 2,6-Dinitrotoluene | 606-20-2 | 8.2 |
| Acenaphthylene | 208-96-8 | 8.2 |
| Dimethomorph | 110488-70-5 | 8.2 |
| Simazine | 122-34-9 | 8.1 |
| Dinoseb | 88-85-7 | 8.1 |
| Molinate | 2212-67-1 | 8.1 |
| Butachlor | 23184-66-9 | 8.1 |
| Fluroxypyr-meptyl | 81406-37-3 | 8.0 |
| Kepone | 143-50-0 | 8.0 |
| Sodium xylenesulfonate | 1300-72-7 | 7.9 |
| 1,4-Dichlorobenzene | 106-46-7 | 7.8 |
| Fenarimol | 60168-88-9 | 7.8 |
| N,N-Diethylaniline | 91-66-7 | 7.8 |
| 2-(Butan-2-yl)phenol | 89-72-5 | 7.8 |
| 3-Pyridinecarbonitrile | 100-54-9 | 7.8 |
| PFOS | 1763-23-1 | 7.7 |
| PharmaGSID\_48514 | NOCAS\_48514 | 7.7 |
| 1,2,3-Trichlorobenzene | 87-61-6 | 7.7 |
| Candoxatril | 123122-55-4 | 7.6 |
| SSR126768 | NOCAS\_47379 | 7.6 |
| Isopropalin | 33820-53-0 | 7.6 |
| Trioctyl trimellitate | 89-04-3 | 7.6 |
| Clethodim | 99129-21-2 | 7.6 |
| FR140423 | 151506-44-4 | 7.3 |
| SSR180711 | 298198-52-4 | 7.3 |
| 1,2-Dimethyl-4-nitrobenzene | 99-51-4 | 7.3 |
| Triethylene glycol diacetate | 111-21-7 | 7.2 |
| Hydroxyflutamide | 52806-53-8 | 7.1 |
| CP-401387 | 199171-88-5 | 7.1 |
| CP-085958 | 134002-60-1 | 7.1 |
| Flumioxazin | 103361-09-7 | 7.0 |
| FD&C Yellow 5 | 1934-21-0 | 6.9 |
| 1,3-Diphenylguanidine | 102-06-7 | 6.9 |
| Tebuconazole | 107534-96-3 | 6.9 |
| 1,2-Dinitrobenzene | 528-29-0 | 6.8 |
| Piragliatin | 625114-41-2 | 6.8 |
| Cladribine | 4291-63-8 | 6.8 |
| Furfural | 98-01-1 | 6.8 |
| CJ-013610 | 249296-43-3 | 6.8 |
| Zamifenacin | 127308-82-1 | 6.8 |
| MK-547 | 331623-06-4 | 6.8 |
| Oxadiazon | 19666-30-9 | 6.8 |
| PharmaGSID\_48518 | NOCAS\_48518 | 6.8 |
| Dichloroacetic acid | 79-43-6 | 6.7 |
| Tris(2-ethylhexyl) phosphate | 78-42-2 | 6.7 |
| Tebufenpyrad | 119168-77-3 | 6.7 |
| SAR377142 | NOCAS\_47385 | 6.6 |
| Chloridazon | 1698-60-8 | 6.6 |
| Norflurazon | 27314-13-2 | 6.6 |
| Nonanoic acid | 112-05-0 | 6.6 |
| PharmaGSID\_48507 | NOCAS\_48507 | 6.5 |
| Metolachlor ESA | 171118-09-5 | 6.5 |
| l-Tryptophan | 73-22-3 | 6.5 |
| Fluazifop-P-butyl | 79241-46-6 | 6.5 |
| Tris(2-chloroethyl) phosphate | 115-96-8 | 6.4 |
| Fludioxonil | 131341-86-1 | 6.4 |
| Erythromycin | 114-07-8 | 6.4 |
| MK-968 | NOCAS\_47334 | 6.4 |
| Benzoic acid | 65-85-0 | 6.3 |
| Diethyl phthalate | 84-66-2 | 6.3 |
| Fulvestrant | 129453-61-8 | 6.3 |
| UK-416244 | 402910-27-4 | 6.3 |
| 2,6-Diethylaniline | 579-66-8 | 6.3 |
| 3-Bromo-1-propanol | 627-18-9 | 6.2 |
| 2-Ethyl-1-hexanol | 104-76-7 | 6.2 |
| Theobromine | 83-67-0 | 6.2 |
| 1-Undecanol | 112-42-5 | 6.2 |
| SSR69071 | 344930-95-6 | 6.2 |
| Thiodicarb | 59669-26-0 | 6.2 |
| 2,4-Dinitrotoluene | 121-14-2 | 6.2 |
| Bromoxynil | 1689-84-5 | 6.1 |
| PharmaGSID\_47259 | 149062-75-9 | 6.1 |
| Dichlorprop | 120-36-5 | 6.1 |
| Dibenzofuran | 132-64-9 | 6.1 |
| 4,4'-Bipyridine | 553-26-4 | 6.1 |
| Triticonazole | 131983-72-7 | 6.1 |
| UK-333747 | 197077-55-7 | 6.1 |
| Quizalofop-ethyl | 76578-14-8 | 6.1 |
| Warfarin | 81-81-2 | 6.1 |
| PFOA | 335-67-1 | 6.1 |
| Pyraflufen-ethyl | 129630-19-9 | 6.0 |
| Acrylamide | 79-06-1 | 6.0 |
| Iprodione | 36734-19-7 | 5.9 |
| 2,4-DB | 94-82-6 | 5.9 |
| Flufenpyr-ethyl | 188489-07-8 | 5.9 |
| Diethylene glycol dibenzoate | 120-55-8 | 5.8 |
| Cyclohexanol | 108-93-0 | 5.8 |
| Diquat dibromide monohydrate | 6385-62-2 | 5.8 |
| Cyhalofop-butyl | 122008-85-9 | 5.7 |
| Hexachlorocyclopentadiene | 77-47-4 | 5.7 |
| Tributyl phosphate | 126-73-8 | 5.7 |
| Triethyl citrate | 77-93-0 | 5.7 |
| Dodecyltrimethylammonium chloride | 112-00-5 | 5.7 |
| MK-812 | 851916-42-2 | 5.7 |
| Triacetin | 102-76-1 | 5.7 |
| 2-[2-(2-Ethoxyethoxy)ethoxy]ethanol | 112-50-5 | 5.7 |
| Fluridone | 59756-60-4 | 5.5 |
| Fenofibrate | 49562-28-9 | 5.5 |
| Pentaerythritol | 115-77-5 | 5.5 |
| PFBS-K | 29420-49-3 | 5.5 |
| Sorbitan, mono-(9Z)-9-octadecenoate | 1338-43-8 | 5.4 |
| Triethanolamine | 102-71-6 | 5.3 |
| Atrazine | 1912-24-9 | 5.3 |
| GSK232420A | 864283-48-7 | 5.3 |
| 2-Ethylhexanoic acid | 149-57-5 | 5.2 |
| 1,6-Diisocyanatohexane | 822-06-0 | 5.2 |
| N-Vinyl-2-pyrrolidone | 88-12-0 | 5.2 |
| Diallyl phthalate | 131-17-9 | 5.2 |
| Fomesafen | 72178-02-0 | 5.1 |
| Dipropyl 2,5-pyridinedicarboxylate | 136-45-8 | 5.1 |
| CP-122721 | 145742-28-5 | 5.1 |
| Pirinixic acid | 50892-23-4 | 5.0 |
| Benzo(b)fluoranthene | 205-99-2 | 5.0 |
| Fipronil | 120068-37-3 | 5.0 |
| Octhilinone | 26530-20-1 | 5.0 |
| 4-Amino-1,2,4-triazole | 584-13-4 | 5.0 |
| Methoxychlor | 72-43-5 | 5.0 |
| CP-100829 | 135080-03-4 | 4.9 |
| Dalapon | 75-99-0 | 4.9 |
| PHA-00568487 | 527680-56-4 | 4.9 |
| 4-(2-Methylbutan-2-yl)cyclohexanol | 5349-51-9 | 4.9 |
| Bis(2-methoxyethyl) ether | 111-96-6 | 4.9 |
| Besonprodil | 253450-09-8 | 4.9 |
| Fenpropathrin | 39515-41-8 | 4.9 |
| Octamethylcyclotetrasiloxane | 556-67-2 | 4.8 |
| CP-457677 | 214535-77-0 | 4.8 |
| Deisopropylatrazine | 1007-28-9 | 4.8 |
| PFHxA | 307-24-4 | 4.7 |
| 3'-Azido-3'-deoxythymidine | 30516-87-1 | 4.7 |
| Thymol | 89-83-8 | 4.7 |
| SSR146977 | 264618-44-2 | 4.6 |
| Azoxystrobin | 131860-33-8 | 4.6 |
| PharmaGSID\_48516 | NOCAS\_48516 | 4.6 |
| Acetochlor ESA | 187022-11-3 | 4.5 |
| Chlorthal-dimethyl | 1861-32-1 | 4.5 |
| Dimethyl malonate | 108-59-8 | 4.5 |
| Octanoic acid | 124-07-2 | 4.5 |
| Sucrose | 57-50-1 | 4.4 |
| Emamectin benzoate | 155569-91-8 | 4.4 |
| 5-Fluorouracil | 51-21-8 | 4.4 |
| Methyl octanoate | 111-11-5 | 4.4 |
| Chlorpropham | 101-21-3 | 4.3 |
| Enadoline | 124378-77-4 | 4.3 |
| Tralkoxydim | 87820-88-0 | 4.2 |
| Dipentyl phthalate | 131-18-0 | 4.2 |
| CI-1018 | NOCAS\_47248 | 4.2 |
| Etofenprox | 80844-07-1 | 4.2 |
| 2,4-Dichlorophenoxyacetic acid | 94-75-7 | 4.2 |
| Ethyl butyrate | 105-54-4 | 4.2 |
| Acetic acid | 64-19-7 | 4.2 |
| 1,3-Dinitrobenzene | 99-65-0 | 4.2 |
| Butylate | 2008-41-5 | 4.1 |
| Novaluron | 116714-46-6 | 4.1 |
| 1-Benzylquinolinium chloride | 15619-48-4 | 4.1 |
| Flumiclorac-pentyl | 87546-18-7 | 4.0 |
| 2,2'-[Ethane-1,2-diylbis(oxy)]diethanamine | 929-59-9 | 4.0 |
| D-Mannitol | 69-65-8 | 4.0 |
| Cycloate | 1134-23-2 | 3.9 |
| Acifluorfen | 50594-66-6 | 3.9 |
| Ethalfluralin | 55283-68-6 | 3.9 |
| Clomazone | 81777-89-1 | 3.9 |
| Sodium dehydroacetate | 4418-26-2 | 3.8 |
| 1,2,4-Trichlorobenzene | 120-82-1 | 3.8 |
| SR58611 | 929601-09-2 | 3.8 |
| Glycerol | 56-81-5 | 3.7 |
| Thiobencarb | 28249-77-6 | 3.7 |
| CP-422935 | NOCAS\_47299 | 3.7 |
| Methyl salicylate | 119-36-8 | 3.7 |
| Pentadecane | 629-62-9 | 3.7 |
| Nilutamide | 63612-50-0 | 3.6 |
| Triadimefon | 43121-43-3 | 3.6 |
| Hexanedioic acid | 124-04-9 | 3.6 |
| Sodium benzoate | 532-32-1 | 3.6 |
| Fenoxycarb | 72490-01-8 | 3.5 |
| 5,5-Dimethylhydantoin | 77-71-4 | 3.5 |
| CP-607366 | 289716-94-5 | 3.5 |
| N,N-Diethylethanolamine | 100-37-8 | 3.4 |
| Cyanazine | 21725-46-2 | 3.4 |
| Ametryn | 834-12-8 | 3.4 |
| Chloroneb | 2675-77-6 | 3.4 |
| SSR504734 | 742693-38-5 | 3.4 |
| CP-409092 | 194098-25-4 | 3.4 |
| CP-863187 | 668981-02-0 | 3.4 |
| Butylbenzene | 104-51-8 | 3.3 |
| Spiroxamine | 118134-30-8 | 3.3 |
| Fenpyroximate (Z,E) | 111812-58-9 | 3.3 |
| 1-Chloro-4-nitrobenzene | 100-00-5 | 3.3 |
| Octanal | 124-13-0 | 3.3 |
| MEHP | 4376-20-9 | 3.3 |
| Dexamethasone sodium phosphate | 2392-39-4 | 3.2 |
| 2-(Hydroxymethyl)-2-nitro-1,3-propanediol | 126-11-4 | 3.2 |
| Acetamiprid | 135410-20-7 | 3.1 |
| Metolachlor | 51218-45-2 | 3.1 |
| Cyproconazole | 94361-06-5 | 3.1 |
| Hexanoic acid | 142-62-1 | 3.0 |
| Sodium saccharin hydrate | 82385-42-0 | 3.0 |
| Acetyltriethyl citrate | 77-89-4 | 3.0 |
| Isopentyl alcohol | 123-51-3 | 2.9 |
| 2-Ethoxyethanol | 110-80-5 | 2.9 |
| PFOS-K | 2795-39-3 | 2.9 |
| 1-Methoxy-2-propanol | 107-98-2 | 2.9 |
| L-Tartaric acid | 87-69-4 | 2.8 |
| Monomethyl phthalate | 4376-18-5 | 2.8 |
| Adipic acid, polypropyleneglycol, laurate | 66456-53-9 | 2.8 |
| Imidacloprid | 138261-41-3 | 2.8 |
| Isoxaflutole | 141112-29-0 | 2.8 |
| Paclobutrazol | 76738-62-0 | 2.8 |
| Dipropylene glycol | 25265-71-8 | 2.8 |
| 1-(Hydroxymethyl)-5,5-dimethylhydantoin | 116-25-6 | 2.7 |
| 3-Phenoxybenzoic acid | 3739-38-6 | 2.7 |
| Chlorendic acid | 115-28-6 | 2.6 |
| Propargite | 2312-35-8 | 2.6 |
| 2-Phenoxyethanol | 122-99-6 | 2.6 |
| 3,4-Dichloronitrobenzene | 99-54-7 | 2.5 |
| 1-Pentadecanol | 629-76-5 | 2.5 |
| Terbacil | 5902-51-2 | 2.5 |
| p,p'-DDE | 72-55-9 | 2.5 |
| Triphenyl phosphate | 115-86-6 | 2.5 |
| Dioctyl succinate | 2432-87-3 | 2.5 |
| Methoxyfenozide | 161050-58-4 | 2.4 |
| Pravastatin sodium | 81131-70-6 | 2.4 |
| PharmaGSID\_48513 | 825643-57-0 | 2.4 |
| Propamocarb hydrochloride | 25606-41-1 | 2.4 |
| Prometryn | 7287-19-6 | 2.4 |
| Diphenhydramine hydrochloride | 147-24-0 | 2.4 |
| Thiacloprid | 111988-49-9 | 2.4 |
| Cyfluthrin | 68359-37-5 | 2.3 |
| 5,5-Diphenylhydantoin | 57-41-0 | 2.3 |
| Glycidol | 556-52-5 | 2.3 |
| Benzal chloride | 98-87-3 | 2.3 |
| 1-Octanol | 111-87-5 | 2.3 |
| Isopentyl butyrate | 106-27-4 | 2.3 |
| Dimethoxane | 828-00-2 | 2.2 |
| N-Nitrosodipropylamine | 621-64-7 | 2.1 |
| 2-Butoxyethanol | 111-76-2 | 2.1 |
| 2-Nitrotoluene | 88-72-2 | 2.1 |
| Imazethapyr | 81335-77-5 | 2.1 |
| Tebuthiuron | 34014-18-1 | 2.1 |
| 2,2-Bis(bromomethyl)-1,3-propanediol | 3296-90-0 | 2.1 |
| 2-Butanone oxime | 96-29-7 | 2.0 |
| Spirodiclofen | 148477-71-8 | 2.0 |
| tert-Butylbenzene | 98-06-6 | 2.0 |
| Dimethenamid | 87674-68-8 | 2.0 |
| SB413217A | NOCAS\_47325 | 2.0 |
| Clofentezine | 74115-24-5 | 1.9 |
| Hexanedioic acid, diisononyl ester | 33703-08-1 | 1.9 |
| Clodinafop-propargyl | 105512-06-9 | 1.9 |
| Di-tert-butyl peroxide | 110-05-4 | 1.9 |
| Methyl isothiocyanate | 556-61-6 | 1.9 |
| MGK-264 | 113-48-4 | 1.9 |
| 5-Heptyldihydro-2(3H)-furanone | 104-67-6 | 1.9 |
| Acetophenone | 98-86-2 | 1.9 |
| 2-Methoxyethanol | 109-86-4 | 1.8 |
| Butafenacil | 134605-64-4 | 1.8 |
| Butyryl trihexyl citrate | 82469-79-2 | 1.8 |
| Trifloxysulfuron-sodium | 199119-58-9 | 1.8 |
| PFOA, ammonium salt | 3825-26-1 | 1.7 |
| Carabersat | 184653-84-7 | 1.7 |
| 5alpha-Dihydrotestosterone | 521-18-6 | 1.7 |
| Acetyl tributyl citrate | 77-90-7 | 1.6 |
| Acetaminophen | 103-90-2 | 1.6 |
| Mirex | 2385-85-5 | 1.6 |
| AVE3295 | 478263-98-8 | 1.6 |
| Diazoxon | 962-58-3 | 1.6 |
| FR145237 | 146011-65-6 | 1.6 |
| 1-Dodecanol | 112-53-8 | 1.5 |
| Nelivaptan | 439687-69-1 | 1.5 |
| UK-343664 | 215297-27-1 | 1.5 |
| Diisodecyl hexanedioate | 27178-16-1 | 1.5 |
| Diethyl butanedioate | 123-25-1 | 1.5 |
| Dibromoacetonitrile | 3252-43-5 | 1.5 |
| Methacrylamide | 79-39-0 | 1.5 |
| Carbamazepine | 298-46-4 | 1.5 |
| tert-Butyl perbenzoate | 614-45-9 | 1.5 |
| Dicloran | 99-30-9 | 1.4 |
| N,N-Dimethyldecylamine oxide | 2605-79-0 | 1.4 |
| Sucrose octaacetate | 126-14-7 | 1.4 |
| Sulfentrazone | 122836-35-5 | 1.4 |
| Bis(2-ethylhexyl) terephthalate | 6422-86-2 | 1.4 |
| Decane | 124-18-5 | 1.4 |
| Stavudine | 3056-17-5 | 1.4 |
| Fenoxaprop-P-ethyl | 71283-80-2 | 1.4 |
| Imazaquin | 81335-37-7 | 1.4 |
| Tetramethrin | 7696-12-0 | 1.4 |
| Metolachlor OA | 152019-73-3 | 1.3 |
| Triethylene glycol dimethyl ether | 112-49-2 | 1.3 |
| PharmaGSID\_48506 | 588941-45-1 | 1.3 |
| Cyanuric acid | 108-80-5 | 1.3 |
| sec-Butylbenzene | 135-98-8 | 1.3 |
| Cyclohexylphenylketone | 712-50-5 | 1.3 |
| Hexythiazox | 78587-05-0 | 1.3 |
| Geraniol | 106-24-1 | 1.2 |
| Cloprop | 101-10-0 | 1.2 |
| Cyclohexylamine | 108-91-8 | 1.2 |
| 5-Ethyl-1-aza-3,7-dioxabicyclo[3.3.0]octane | 7747-35-5 | 1.2 |
| Clothianidin | 210880-92-5 | 1.1 |
| Propyzamide | 23950-58-5 | 1.1 |
| N,N'-Methylenebisacrylamide | 110-26-9 | 1.1 |
| Difenzoquat metilsulfate | 43222-48-6 | 1.1 |
| Methyl ethyl ketone | 78-93-3 | 1.1 |
| DEET | 134-62-3 | 1.1 |
| Dipropylene glycol monomethyl ether | 34590-94-8 | 1.1 |
| Azobenzene | 103-33-3 | 1.0 |
| Trichlorfon | 52-68-6 | 1.0 |
| MCPA | 94-74-6 | 1.0 |
| 2,4,7,9-Tetramethyl-5-decyne-4,7-diol | 126-86-3 | 1.0 |
| Bentazone | 25057-89-0 | 0.9 |
| Dodecylbenzene | 123-01-3 | 0.9 |
| 1,3-Butanediol | 107-88-0 | 0.9 |
| Diisopropyl methylphosphonate | 1445-75-6 | 0.9 |
| Lindane | 58-89-9 | 0.9 |
| Aplaviroc hydrochloride | 461023-63-2 | 0.8 |
| Carbosulfan | 55285-14-8 | 0.8 |
| 2-(Hexyloxy)ethanol | 112-25-4 | 0.8 |
| Aldicarb | 116-06-3 | 0.8 |
| Pendimethalin | 40487-42-1 | 0.8 |
| Chlordane | 57-74-9 | 0.8 |
| Norgestrel | 797-63-7 | 0.8 |
| Boscalid | 188425-85-6 | 0.8 |
| Diclofenac sodium | 15307-79-6 | 0.7 |
| Cypermethrin | 52315-07-8 | 0.7 |
| Permethrin | 52645-53-1 | 0.7 |
| Dichlobenil | 1194-65-6 | 0.7 |
| Cyclohexanone | 108-94-1 | 0.7 |
| Dicyclohexyl disulfide | 2550-40-5 | 0.6 |
| 1,2,3-Benzotriazole | 95-14-7 | 0.6 |
| Quinoline | 91-22-5 | 0.6 |
| Sodium trichloroacetate | 650-51-1 | 0.6 |
| Chlorobenzilate | 510-15-6 | 0.6 |
| 4-Cyclohexylcyclohexanol | 2433-14-9 | 0.6 |
| N,N,N-Trimethyl(oxiran-2-yl)methanaminium chloride | 3033-77-0 | 0.6 |
| 4-Methyl-2-pentanol | 108-11-2 | 0.6 |
| AVE8923 | NOCAS\_47381 | 0.5 |
| CP-114271 | 113734-18-2 | 0.5 |
| Quinclorac | 84087-01-4 | 0.5 |
| Cariporide mesylate | 159138-81-5 | 0.5 |
| Icaridin | 119515-38-7 | 0.5 |
| 2-(2-Butoxyethoxy)ethanol | 112-34-5 | 0.4 |
| N-Nitrosodiethylamine | 55-18-5 | 0.4 |
| Dimethyl adipate | 627-93-0 | 0.4 |
| Tributylamine | 102-82-9 | 0.3 |
| 1-Tridecanol | 112-70-9 | 0.2 |
| Dibutyl phthalate | 84-74-2 | 0.2 |
| 4-Vinyl-1-cyclohexene dioxide | 106-87-6 | 0.2 |
| Allyl alcohol | 107-18-6 | 0.1 |
| Chlorothalonil | 1897-45-6 | 0.1 |
| Tridecafluorohexylethyl methacrylate | 2144-53-8 | 0.1 |
| Grinstad Soft-N-Safe | NOCAS\_47394 | 0.1 |
| 1,3-Dichloro-2-propanol | 96-23-1 | 0.0 |
| Fluroxypyr | 69377-81-7 | 0.0 |
| Malic acid | 6915-15-7 | 0.0 |
| Dimethipin | 55290-64-7 | 0.0 |
| 1-Methylnaphthalene | 90-12-0 | 0.0 |
| PharmaGSID\_48521 | 1191914-21-2 | 0.0 |
| Flumetralin | 62924-70-3 | 0.0 |
| SSR161421 | NOCAS\_47374 | 0.0 |
| Imazapic | 104098-48-8 | -0.1 |
| SAR102779 | NOCAS\_47387 | -0.1 |
| N,N-Dimethyloctylamine | 7378-99-6 | -0.1 |
| 1,2,3-Trichloropropane | 96-18-4 | -0.1 |
| Naphthalene | 91-20-3 | -0.1 |
| Monobutyl phthalate | 131-70-4 | -0.1 |
| PFOSA | 754-91-6 | -0.1 |
| Indoxacarb | 173584-44-6 | -0.2 |
| 4-Butyrolactone | 96-48-0 | -0.2 |
| Acetamide | 60-35-5 | -0.2 |
| Undecane | 1120-21-4 | -0.2 |
| Dimethyl succinate | 106-65-0 | -0.2 |
| Bromacil | 314-40-9 | -0.3 |
| Lactofen | 77501-63-4 | -0.3 |
| Butam | 35256-85-0 | -0.4 |
| Propylparaben | 94-13-3 | -0.4 |
| 1,5,9-Cyclododecatriene | 4904-61-4 | -0.4 |
| Endrin | 72-20-8 | -0.4 |
| Phenanthrene | 85-01-8 | -0.4 |
| Silica | 7631-86-9 | -0.5 |
| C10-21 sulfonic acids phenyl esters | 91082-17-6 | -0.5 |
| Triclopyr | 55335-06-3 | -0.6 |
| Acetochlor | 34256-82-1 | -0.6 |
| Prometon | 1610-18-0 | -0.6 |
| 1,3-Benzenedicarboxylic acid | 121-91-5 | -0.6 |
| Alachlor | 15972-60-8 | -0.6 |
| Ethylparaben | 120-47-8 | -0.6 |
| p-Bromodiphenyl ether | 101-55-3 | -0.6 |
| Fluorene | 86-73-7 | -0.7 |
| Esfenvalerate | 66230-04-4 | -0.7 |
| Diethanolamine | 111-42-2 | -0.7 |
| Pentachloronitrobenzene | 82-68-8 | -0.7 |
| 3-Iodo-2-propynyl-N-butylcarbamate | 55406-53-6 | -0.7 |
| Surinabant | 288104-79-0 | -0.7 |
| Sodium chlorite | 7758-19-2 | -0.8 |
| 1,2-Dichlorobenzene | 95-50-1 | -0.8 |
| Ethyl heptanoate | 106-30-9 | -0.8 |
| Triethoxyoctylsilane | 2943-75-1 | -0.9 |
| Butralin | 33629-47-9 | -0.9 |
| Triisononyl trimellitate | 53894-23-8 | -0.9 |
| YM218 | NOCAS\_48176 | -0.9 |
| Ethanolamine | 141-43-5 | -0.9 |
| Flutamide | 13311-84-7 | -1.0 |
| Diphenyl isophthalate | 744-45-6 | -1.0 |
| Ethofumesate | 26225-79-6 | -1.0 |
| Trifloxystrobin | 141517-21-7 | -1.0 |
| Diacetone alcohol | 123-42-2 | -1.0 |
| Flumetsulam | 98967-40-9 | -1.0 |
| Methylparaben | 99-76-3 | -1.0 |
| Benzophenone | 119-61-9 | -1.1 |
| Oxyfluorfen | 42874-03-3 | -1.1 |
| Nitrofen | 1836-75-5 | -1.1 |
| AVE2865 | 648917-13-9 | -1.1 |
| Dihexyl phthalate | 84-75-3 | -1.1 |
| Urethane | 51-79-6 | -1.2 |
| 4-Nitrobenzoic acid | 62-23-7 | -1.2 |
| Diisononyl cyclohexane-1,2-dicarboxylate | 166412-78-8 | -1.2 |
| CP-465394 | NOCAS\_47255 | -1.2 |
| Aspirin | 50-78-2 | -1.2 |
| Pentane-1,5-diyl dibenzoate | 6624-73-3 | -1.3 |
| 3-Methylbutyl acetate | 123-92-2 | -1.3 |
| p,p'-DDT | 50-29-3 | -1.3 |
| Phenylmercuric acetate | 62-38-4 | -1.3 |
| Hexanedinitrile | 111-69-3 | -1.3 |
| Urea | 57-13-6 | -1.3 |
| Bifenthrin | 82657-04-3 | -1.3 |
| Pyridaben | 96489-71-3 | -1.3 |
| Isophorone | 78-59-1 | -1.3 |
| Ethylene glycol | 107-21-1 | -1.4 |
| Triamcinolone | 124-94-7 | -1.4 |
| PharmaGSID\_47261 | 177785-47-6 | -1.4 |
| Endosulfan | 115-29-7 | -1.4 |
| PD 0200347 | NOCAS\_47292 | -1.5 |
| 10-Undecenoic acid | 112-38-9 | -1.5 |
| Dimethylaminoethanol | 108-01-0 | -1.5 |
| 2-Norbornene-5,6-dicarboxylic anhydride | 826-62-0 | -1.5 |
| Butyl benzoate | 136-60-7 | -1.6 |
| Bis(2-ethylhexyl) decanedioate | 122-62-3 | -1.6 |
| Carbofuran | 1563-66-2 | -1.6 |
| Octrizole | 3147-75-9 | -1.6 |
| 2-(2-Ethoxyethoxy)ethanol | 111-90-0 | -1.6 |
| Di(propylene glycol) dibenzoate | 27138-31-4 | -1.6 |
| Propoxur | 114-26-1 | -1.6 |
| Piperazine | 110-85-0 | -1.7 |
| Haloperidol | 52-86-8 | -1.7 |
| Pentamidine isethionate | 140-64-7 | -1.7 |
| 2-Ethoxyethyl acetate | 111-15-9 | -1.7 |
| 1,3,5-Trimethylbenzene | 108-67-8 | -1.7 |
| Clopyralid-olamine | 57754-85-5 | -1.8 |
| Diethylene glycol | 111-46-6 | -1.8 |
| p-Cymene | 99-87-6 | -1.8 |
| Dibutyl hexanedioate | 105-99-7 | -1.8 |
| Mepiquat chloride | 24307-26-4 | -1.9 |
| PHA-00543613 | 478149-53-0 | -1.9 |
| FR167356 | 174185-16-1 | -1.9 |
| Dicamba | 1918-00-9 | -1.9 |
| Octadecanoic acid | 57-11-4 | -1.9 |
| Bendiocarb | 22781-23-3 | -2.0 |
| 1,2-Propylene glycol | 57-55-6 | -2.0 |
| Fluconazole | 86386-73-4 | -2.1 |
| 2,6,10-Trimethyl-2,6,10-triazaundecane | 3855-32-1 | -2.1 |
| Isophorone diisocyanate | 4098-71-9 | -2.1 |
| 2,3-Benzofuran | 271-89-6 | -2.1 |
| Styrene oxide | 96-09-3 | -2.1 |
| Di(2-ethylhexyl) phthalate | 117-81-7 | -2.2 |
| Methomyl | 16752-77-5 | -2.2 |
| Cyclophosphamide monohydrate | 6055-19-2 | -2.2 |
| Terbuthylazine | 5915-41-3 | -2.2 |
| Hexane-1,6-diyl dibenzoate | 22915-73-7 | -2.3 |
| 2,2,4-Trimethyl-1,3-pentanediol diisobutyrate | 6846-50-0 | -2.4 |
| Fluazifop-butyl | 69806-50-4 | -2.4 |
| 1-Tetradecanol | 112-72-1 | -2.4 |
| 1,3-Diisopropylbenzene | 99-62-7 | -2.4 |
| Thiamethoxam | 153719-23-4 | -2.5 |
| Benzyl alcohol | 100-51-6 | -2.5 |
| Propazine | 139-40-2 | -2.5 |
| Heptachlor epoxide | 1024-57-3 | -2.5 |
| Metalaxyl | 57837-19-1 | -2.5 |
| Etoxazole | 153233-91-1 | -2.7 |
| Tripropylene glycol monomethyl ether | 25498-49-1 | -2.7 |
| Cyromazine | 66215-27-8 | -2.7 |
| Prodiamine | 29091-21-2 | -2.7 |
| Pentachloropyridine | 2176-62-7 | -2.7 |
| Fluoranthene | 206-44-0 | -2.8 |
| Triethylene glycol bis(2-ethylhexanoate) | 94-28-0 | -2.8 |
| Monobenzyl phthalate | 2528-16-7 | -2.8 |
| 2',3'-Dideoxyinosine | 69655-05-6 | -2.8 |
| Diethylene glycol monomethyl ether | 111-77-3 | -2.9 |
| CP-642931 | NOCAS\_47267 | -2.9 |
| Pyrithiobac-sodium | 123343-16-8 | -2.9 |
| 4-Chlorotoluene | 106-43-4 | -3.0 |
| alpha-Cyclodextrin | 10016-20-3 | -3.0 |
| Diisobutyl adipate | 141-04-8 | -3.0 |
| 3,9-Epoxy-3H-azirino[2,3-c][1]benzazocine-5-carboxaldehyde, 1-acetyl-9-(acetyloxy)-8-[[(aminocarbonyl)oxy]methyl]-1,1a,2,8,9,9a-hexahydro-7-methoxy-, (1aS,8R,9S,9aS)- | NOCAS\_48166 | -3.0 |
| Dibutyl decanedioate | 109-43-3 | -3.0 |
| Nitrofurantoin | 67-20-9 | -3.1 |
| 4-Nitrophenol | 100-02-7 | -3.2 |
| Dimethylarsinic acid | 75-60-5 | -3.3 |
| Cyclopamine | 4449-51-8 | -3.3 |
| 1,2,4,5-Tetrachlorobenzene | 95-94-3 | -3.3 |
| Propoxycarbazone-sodium | 181274-15-7 | -3.3 |
| Valproic acid | 99-66-1 | -3.4 |
| Sodium nitrite | 7632-00-0 | -3.4 |
| Oxamyl | 23135-22-0 | -3.4 |
| Hexazinone | 51235-04-2 | -3.4 |
| 2,5-Dimethyl-2,5-di-(tert-butylperoxy)hexane | 78-63-7 | -3.4 |
| PD 0343701 | 676116-04-4 | -3.4 |
| Di(2-ethylhexyl) adipate | 103-23-1 | -3.5 |
| Methenamine | 100-97-0 | -3.6 |
| CP-728663 | 368832-42-2 | -3.6 |
| p,p'-DDD | 72-54-8 | -3.7 |
| Pyrimethamine | 58-14-0 | -3.7 |
| Thiazopyr | 117718-60-2 | -3.7 |
| EPTC | 759-94-4 | -3.7 |
| Fluazinam | 79622-59-6 | -3.7 |
| Vinclozolin | 50471-44-8 | -3.8 |
| Trinexapac-ethyl | 95266-40-3 | -3.8 |
| Propylbenzene | 103-65-1 | -3.8 |
| Propachlor | 1918-16-7 | -3.8 |
| 2,3-Dinitrotoluene | 602-01-7 | -3.9 |
| Benfluralin | 1861-40-1 | -3.9 |
| 1-Decanol | 112-30-1 | -4.0 |
| GSK163929B | NOCAS\_47311 | -4.0 |
| Butanoic acid | 107-92-6 | -4.1 |
| Iodosulfuron-methyl-sodium | 144550-36-7 | -4.1 |
| Propionic acid | 79-09-4 | -4.2 |
| Isoxaben | 82558-50-7 | -4.2 |
| 2-Chlorotoluene | 95-49-8 | -4.3 |
| Dimethyl glutarate | 1119-40-0 | -4.4 |
| Pentyl acetate | 628-63-7 | -4.4 |
| Imazapyr | 81334-34-1 | -4.4 |
| Dieldrin | 60-57-1 | -4.4 |
| Cytarabine hydrochloride | 69-74-9 | -4.4 |
| Pyrene | 129-00-0 | -4.5 |
| Mepanipyrim | 110235-47-7 | -4.5 |
| Ammonium carbamate | 1111-78-0 | -4.5 |
| Acenaphthene | 83-32-9 | -4.7 |
| N-Methyldioctylamine | 4455-26-9 | -4.7 |
| 1,1,2,2-Tetrahydroperfluoro-1-decanol | 678-39-7 | -4.7 |
| Boric acid | 10043-35-3 | -4.7 |
| Sulfluramid | 4151-50-2 | -4.8 |
| Tributyltin methacrylate | 2155-70-6 | -4.8 |
| Diisobutyl phthalate | 84-69-5 | -4.9 |
| Buprofezin | 69327-76-0 | -4.9 |
| 1,3-Dibromo-5,5-dimethylhydantoin | 77-48-5 | -4.9 |
| Pyrimethanil | 53112-28-0 | -5.0 |
| Bis(2-ethylhexyl) nonanedioate | 103-24-2 | -5.0 |
| N-Nitrosodibutylamine | 924-16-3 | -5.0 |
| Triethylene glycol | 112-27-6 | -5.1 |
| CP-532623 | 261947-38-0 | -5.1 |
| Trifluralin | 1582-09-8 | -5.2 |
| Cycloheximide | 66-81-9 | -5.2 |
| Thalidomide | 50-35-1 | -5.3 |
| N-Nitrosodimethylamine | 62-75-9 | -5.4 |
| Dimethyl terephthalate | 120-61-6 | -5.5 |
| Tri-allate | 2303-17-5 | -5.5 |
| Caffeine | 58-08-2 | -5.5 |
| 1,2-Benzenedicarboxylic acid, di-C9-11-branched alkyl esters, C10-rich | 68515-49-1 | -5.5 |
| 1-[3-(Triethoxysilyl)propyl]urea | 23779-32-0 | -5.5 |
| Aldicarb oxime | 1646-75-9 | -5.5 |
| Formamide | 75-12-7 | -5.6 |
| Coumarin | 91-64-5 | -5.6 |
| SR144190 | 181640-09-5 | -5.7 |
| 2-Phenylphenol | 90-43-7 | -5.8 |
| Flutolanil | 66332-96-5 | -5.8 |
| N-Methylacetamide | 79-16-3 | -6.0 |
| 1H,1H,2H,2H-Perfluorooctyl iodide | 2043-57-4 | -6.0 |
| Endothal | 145-73-3 | -6.0 |
| Dithiopyr | 97886-45-8 | -6.1 |
| PharmaGSID\_47333 | NOCAS\_47333 | -6.3 |
| Pirimicarb | 23103-98-2 | -6.5 |
| Sodium 4-nitrophenolate | 824-78-2 | -6.8 |
| Amiodarone hydrochloride | 19774-82-4 | -6.8 |
| Indium arsenide | 1303-11-3 | -6.9 |
| PFHS-K | 3871-99-6 | -7.1 |
| Methyl dodecanoate | 111-82-0 | -7.2 |
| Daminozide | 1596-84-5 | -7.2 |
| Theophylline | 58-55-9 | -7.3 |
| Tributyltin chloride | 1461-22-9 | -7.4 |
| Fluthiacet-methyl | 117337-19-6 | -7.6 |
| Dicumyl peroxide | 80-43-3 | -7.7 |
| Fluoxastrobin | 361377-29-9 | -7.7 |
| Aldrin | 309-00-2 | -7.8 |
| 3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluorooctan-1-ol | 647-42-7 | -8.0 |
| Picoxystrobin | 117428-22-5 | -8.1 |
| Naled | 300-76-5 | -9.8 |
| Tefluthrin | 79538-32-2 | -10.0 |
| Nitrapyrin | 1929-82-4 | -10.1 |
| (E)-1,2-Dichloroethylene | 156-60-5 | -10.8 |
| o,p'-DDT | 789-02-6 | -10.8 |
| Tebufenozide | 112410-23-8 | -11.6 |
| 4-Chloro-3-methylphenol | 59-50-7 | -14.1 |
| SSR103800 | NOCAS\_47364 | -14.8 |
| Triphenyltin hydroxide | 76-87-9 | -15.1 |
| 3,4-Dimethylphenol | 95-65-8 | -19.5 |
| N-Nitrosodiphenylamine | 86-30-6 | -25.0 |
| p-Cresol | 106-44-5 | -27.6 |
| Chlorpromazine hydrochloride | 69-09-0 | -28.9 |
| 2,4,5-Trichlorophenol | 95-95-4 | -34.2 |
| 3,3'-Dimethoxybenzidine | 119-90-4 | -40.0 |
| 3,3'-Dimethylbenzidine | 119-93-7 | -40.0 |
| 3,3'-Dimethoxybenzidine dihydrochloride | 20325-40-0 | -40.0 |
| 2,4,6-Trichlorophenol | 88-06-2 | -40.0 |
| Benzidine | 92-87-5 | -40.0 |
| 4-Hydroxy-3-methoxybenzaldehyde | 121-33-5 | -41.1 |
| 1,2-Benzisothiazolin-3-one | 2634-33-5 | -41.1 |
| Diphenylamine | 122-39-4 | -43.8 |
| 2,4-Dichlorophenol | 120-83-2 | -48.1 |

### Supplemental Table 2. Guaiacol-tested chemicals reported in the literature.

Chemicals previously reported to be tested in the guaiacol oxidation (GUA) assay. Note: the first known published report is listed for any chemical published in multiple studies. Unpublished study data made available by Michael Hornung and the US EPA National Health and Environmental Effects Research Laboratory.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Chemical Name** | **CASRN** | **Reported**  **GUA Activity** | **PMID or Book Title** | **Bibliographic Reference** |
| 1-Methylbenzimidazoline-2-thione | 2360-22-7 | active | 8418860 | [1] |
| 2,2',4,4'-Tetrahydroxybenzophenone | 131-55-5 | active | 17379648 | [2] |
| 2,3-Dihydroxypyridine | 16867-04-2 | active | Environmental Goitrogenesis | [3] |
| 2,4,-Dihydroxybenzophenone | 131-56-6 | active | 22699773 | [4] |
| 2,5-Dihydroxypyridine | 5154-01-8 | active | Environmental Goitrogenesis | [3] |
| 2,6-Dihydroxypyridine | 10357-84-3 | active | Environmental Goitrogenesis | [3] |
| 2-Bromo-4'-hydroxyacetophenone | 2491-38-5 | active | Unpublished | NA |
| 2-Mercaptobenzothiazole | 149-30-4 | active | 23959146 | [5] |
| 3,4-Dihydroxypyridine | 10182-48-6 | active | Environmental Goitrogenesis | [3] |
| 3-Hydroxy-2(hydroxymethyl)pyridine | 14173-30-9 | active | Environmental Goitrogenesis | [3] |
| 3-Hydroxypyridine | 109-00-2 | active | Environmental Goitrogenesis | [3] |
| 3-Methylcholanthrene | 56-49-5 | active | 22699773 | [4] |
| 4-n-Propoxyphenol | 18979-50-5 | active | 23959146 | [5] |
| 5,5-​Dimethyl-​1-​Hydroxymethylhydantoin | 116-25-6 | active | Unpublished | NA |
| 5-Chloro-2-mercaptobenzothiazole | 5331-91-9 | active | 25953703 | [6] |
| 5-nitro-2-mercaptobenzimidazole | 6325-91-3 | active | 3768307 | [7] |
| 6-Propyl-2-thiouracil | 51-52-5 | active | 1278093 | [8] |
| Aminobenzothiazole | 136-95-8 | active | 25953703 | [6] |
| Benzimidazoline-2-thione | 583-39-1 | active | 8418860 | [1] |
| Benzo(e)pyrene | 192-97-2 | active | 22699773 | [4] |
| Benzo(k)fluoranthene | 207-08-9 | active | 22699773 | [4] |
| Benzothiazole | 95-16-9 | active | 25953703 | [6] |
| Bisphenol A | 80-05-7 | active | 17379648 | [2] |
| Caffeine | 58-08-2 | active | 22699773 | [4] |
| Cyanamide | 420-04-2 | active | 436767 | [9] |
| Daidzein | 486-66-8 | active | 9464451 | [10] |
| Ethylenethiourea | 96-45-7 | active | 2130946 | [11] |
| F21388 | NoCas | active | 17379648 | [2] |
| Genistein | 446-72-0 | active | 9464451 | [10] |
| Goitrin | 13190-34-6 | active | [Frontiers](http://link.springer.com/chapter/10.1007%2F978-1-4684-5260-0_110) in Thyroidology | [12] |
| Leucomalachite Green | 129-73-7 | active | 9760285 | [13] |
| Mercury chloride | 7487-94-7 | active | 2703707 | [14] |
| Methimazole | 60-56-0 | active | 1278093 | [8] |
| Minocycline | 13614-98-7 | active | 9074802 | [15] |
| N,N,N',N'-Tetramethylthiourea | 2782-91-4 | active | 16297522 | [16] |
| Naringenin | 67604-48-2 | active | 8924586 | [17] |
| Perfluorooctane sulfonate | 1763-23-1 | active | 22699773 | [4] |
| Pyrene | 129-00-0 | active | 22699773 | [4] |
| Quercetin | 117-39-5 | active | 8924586 | [17] |
| Resorcinol | 108-46-3 | active | 8068644 | [18] |
| Ricinine | 524-40-3 | active | Frontiers in Thyroidology | [12] |
| Salicylhydroxamic acid | 89-73-6 | active | 1847381 | [19] |
| Sodium thiocyanate | 540-72-7 | active | 33640 | [20] |
| Sulfamethazine | 57-68-1 | active | 8199304 | [21] |
| Sunitinib | 341031-54-7 | active | 17465866 | [22] |
| Thiourea | 62-56-6 | active | 436767 | [9] |
| Zineb | 12122-67-7 | active | 9248629 | [23] |
| Ziram | 137-30-4 | active | 9248629 | [23] |
| 1,3-Dimethylbenzimidazoline-2-thione | 3418-46-0 | inactive | 8418860 | [1] |
| 1h-Imidazole-1-ethanol,\_2-(8-heptadecenyl)-4,5-dihydro- | 95-38-5 | inactive | Unpublished | NA |
| 2-(2-Hydroxy-5-methylphenyl)benzotriazole | 2440-22-4 | inactive | Unpublished | NA |
| 2,2'-Dihydroxy 4-methoxybenzophenone | 131-53-3 | inactive | 22699773 | [4] |
| 2,3,4-trihydroxybenzophenone | 1143-72-2 | inactive | 22699773 | [4] |
| 2,4-Dihydroxypyridine | 626-03-9 | inactive | Environmental Goitrogenesis | [3] |
| 2-Benzyl-4-chlorophenol | 120-32-1 | inactive | Unpublished | NA |
| 2-Hydroxy 4-methoxybenzophenone | 131-57-7 | inactive | 17379648 | [2] |
| 2-Hydroxypyridine | 142-08-5 | inactive | Environmental Goitrogenesis | [3] |
| 2-Phenylphenol | 90-43-7 | inactive | Unpublished | NA |
| 3-(4-Methylbenzylidene)camphor | 36861-47-9 | inactive | 17379648 | [2] |
| 3,5-Dimethylpyrazole-1-methanol | 85264-33-1 | inactive | 23959146 | [5] |
| 3-Hydroxy-6-methylpyridine | 1121-78-4 | inactive | Environmental Goitrogenesis | [3] |
| 3-Methoxy-4-hydroxypyridine | 62885-41-0 | inactive | Environmental Goitrogenesis | [3] |
| 4-Ethylphenol | 123-07-9 | inactive | Unpublished | NA |
| 4-hydroxybenzophenone | 1137-42-4 | inactive | 22699773 | [4] |
| 4-Hydroxypyridine | 626-64-2 | inactive | Environmental Goitrogenesis | [3] |
| 4-Methylphenol | 106-44-5 | inactive | Unpublished | NA |
| 4-n-Butylphenol | 1638-22-8 | inactive | Unpublished | NA |
| 4-n-Nonylphenol | 104-40-5 | inactive | 23959146 | [5] |
| 4-Propylphenol | 645-56-7 | inactive | Unpublished | NA |
| Acetylsalicylic acid | 50-78-2 | inactive | 8381669 | [24] |
| Amiodarone | 19774-82-4 | inactive | Unpublished | NA |
| Benzhydrol | 91-01-0 | inactive | 22699773 | [4] |
| Benzo(a)anthracene | 56-55-3 | inactive | 22699773 | [4] |
| Benzophenone | 119-61-9 | inactive | Unpublished | NA |
| Benzylbutylphthalate | 85-68-7 | inactive | Unpublished | NA |
| Bis(2,2,6,6-tetramethyl-4-piperidyl) sebacate | 52829-07-9 | inactive | Unpublished | NA |
| Butyl salicylate | 2052-14-4 | inactive | Unpublished | NA |
| Carbamazepine | 298-46-4 | inactive | 3447884 | [25] |
| Chlordane | 5103-71-9 | inactive | 22699773 | [4] |
| Chrysene | 218-01-9 | inactive | 22699773 | [4] |
| Dibenzo(a,h)anthracene | 53-70-3 | inactive | 22699773 | [4] |
| Dibutylphthalate | 84-74-2 | inactive | 23959146 | [5] |
| Diethylhexylphthalate | 117-81-7 | inactive | 23959146 | [5] |
| Diethylphthalate | 84-66-2 | inactive | 23959146 | [5] |
| Dipyrone | 5907-38-0 | inactive | 2938410 | [26] |
| Dodecylbenzenesulfonic acid | 25155-30-0 | inactive | Unpublished | NA |
| Ethyl-3-hydroxybenzoate | 7781-98-8 | inactive | Unpublished | NA |
| Heptachlor | 76-44-8 | inactive | 22699773 | [4] |
| Hexachlorobenzene | 118-74-1 | inactive | 22699773 | [4] |
| Hydroxybenzothiazole | 934-34-9 | inactive | 25953703 | [6] |
| Indomethacin | 53-86-1 | inactive | 8381669 | [24] |
| Iopanoic acid | 96-83-3 | inactive | 23959146 | [5] |
| Ketoconazole | 65277-42-1 | inactive | Unpublished | NA |
| Methyl methylbenzoate | 89-71-4 | inactive | Unpublished | NA |
| Methylmercury chloride | 115-09-3 | inactive | 2703707 | [14] |
| Methylsalicylate | 119-36-8 | inactive | Unpublished | NA |
| Methylthiobenzothiazole | 615-22-5 | inactive | 25953703 | [6] |
| Mirex | 2385-85-5 | inactive | 22699773 | [4] |
| N,N',N-trichloro-1,3,5-triazine-2,4,6-triamine | 7673-09-8 | inactive | Unpublished | NA |
| Naphthalene | 91-20-3 | inactive | 22699773 | [4] |
| n-Octylphenol | 1806-26-4 | inactive | Unpublished | NA |
| N'-tert-butyl-n-cyclopropyl-6-(methylthio)-1,3,5-triazine-2,4-diamine | 28159-98-0 | inactive | Unpublished | NA |
| Octinoxate | 5466-77-3 | inactive | 17379648 | [2] |
| Pentachlorophenol | 87-86-5 | inactive | Unpublished | NA |
| Perfluorooctanoic acid | 335-67-1 | inactive | 22699773 | [4] |
| Phenanthrene | 85-01-8 | inactive | 22699773 | [4] |
| Phenol | 108-95-2 | inactive | Unpublished | NA |
| Phenol red | 143-74-8 | inactive | Unpublished | NA |
| Phenylbutazone | 50-33-9 | inactive | 7386121 | [27] |
| Propyl-4-hydroxybenzoate | 94-13-3 | inactive | Unpublished | NA |
| Sodium dichloroisocyanurate | 2893-78-9 | inactive | Unpublished | NA |
| Sodium perchlorate | 7601-89-0 | inactive | 23959146 | [5] |
| Thiram | 137-26-8 | inactive | 9248629 | [23] |
| Triclosan | 3380-34-5 | inactive | 23959146 | [5] |

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### Supplemental Table 3. 37 ToxCast cytotoxicity and proliferation assays used to calculate median log *modl\_acc*.

The median log modl\_acc value of 37 ToxCast cytotoxicity and proliferation assays was used as one of three possible measures of confounding bioactivity to stratify 314 putative TPO inhibitors by selective AUR-TPO activity.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Assay** | **Source** | **Assay Type** | **Species** | **Cell Type** | **Tissue of Origin** |
| ACEA\_T47D\_80hr\_Negative | ACEA | Proliferation | human | T47D | breast |
| APR\_HepG2\_CellLoss\_24h\_dn | Apredica | Proliferation | human | HepG2 | liver |
| APR\_HepG2\_CellLoss\_72h\_dn | Apredica | Proliferation | human | HepG2 | liver |
| BSK\_3C\_Proliferation\_down | BioSeek | Proliferation | human | umbilical vein endothelium | vascular |
| BSK\_3C\_SRB\_down | BioSeek | Cytotoxicity | human | umbilical vein endothelium | vascular |
| BSK\_3C\_Vis\_down | BioSeek | Proliferation | human | umbilical vein endothelium | vascular |
| BSK\_4H\_SRB\_down | BioSeek | Cytotoxicity | human | umbilical vein endothelium | vascular |
| BSK\_BE3C\_SRB\_down | BioSeek | Cytotoxicity | human | bronchial epithelial | lung |
| BSK\_CASM3C\_Proliferation\_down | BioSeek | Proliferation | human | umbilical vein endothelium and coronary artery smooth muscle | vascular |
| BSK\_CASM3C\_SRB\_down | BioSeek | Cytotoxicity | human | umbilical vein endothelium and coronary artery smooth muscle | vascular |
| BSK\_hDFCGF\_Proliferation\_down | BioSeek | Proliferation | human | foreskin fibroblast | skin |
| BSK\_hDFCGF\_SRB\_down | BioSeek | Cytotoxicity | human | foreskin fibroblast | skin |
| BSK\_KF3CT\_SRB\_down | BioSeek | Cytotoxicity | human | keratinocyte and foreskin fibroblast | skin |
| BSK\_LPS\_SRB\_down | BioSeek | Cytotoxicity | human | umbilical vein endothelium and peripheral blood mononuclear | vascular |
| BSK\_SAg\_PBMCCytotoxicity\_down | BioSeek | Cytotoxicity | human | umbilical vein endothelium and peripheral blood mononuclear | vascular |
| BSK\_SAg\_Proliferation\_down | BioSeek | Proliferation | human | umbilical vein endothelium and peripheral blood mononuclear | vascular |
| BSK\_SAg\_SRB\_down | BioSeek | Cytotoxicity | human | umbilical vein endothelium and peripheral blood mononuclear | vascular |
| Tox21\_AR\_BLA\_Antagonist\_viability | Tox21 | Cytotoxicity | human | HEK293T | kidney |
| Tox21\_ARE\_BLA\_agonist\_viability | Tox21 | Cytotoxicity | human | HepG2 | liver |
| Tox21\_ERa\_BLA\_Antagonist\_viability | Tox21 | Cytotoxicity | human | HEK293T | kidney |
| Tox21\_ESRE\_BLA\_viability | Tox21 | Cytotoxicity | human | HeLa | cervix |
| Tox21\_FXR\_BLA\_agonist\_viability | Tox21 | Cytotoxicity | human | HEK293T | kidney |
| Tox21\_FXR\_BLA\_antagonist\_viability | Tox21 | Cytotoxicity | human | HEK293T | kidney |
| Tox21\_GR\_BLA\_Antagonist\_viability | Tox21 | Cytotoxicity | human | HeLa | cervix |
| Tox21\_HSE\_BLA\_agonist\_viability | Tox21 | Cytotoxicity | human | HeLa | cervix |
| Tox21\_MitochondrialToxicity\_viability | Tox21 | Cytotoxicity | human | HepG2 | liver |
| Tox21\_NFkB\_BLA\_agonist\_viability | Tox21 | Cytotoxicity | human | ME-180 | cervix |
| Tox21\_p53\_BLA\_p1\_viability | Tox21 | Cytotoxicity | human | HCT116 | intestinal |
| Tox21\_p53\_BLA\_p2\_viability | Tox21 | Cytotoxicity | human | HCT116 | intestinal |
| Tox21\_p53\_BLA\_p3\_viability | Tox21 | Cytotoxicity | human | HCT116 | intestinal |
| Tox21\_p53\_BLA\_p4\_viability | Tox21 | Cytotoxicity | human | HCT116 | intestinal |
| Tox21\_p53\_BLA\_p5\_viability | Tox21 | Cytotoxicity | human | HCT116 | intestinal |
| Tox21\_PPARd\_BLA\_Agonist\_viability | Tox21 | Cytotoxicity | human | HEK293T | kidney |
| Tox21\_PPARd\_BLA\_antagonist\_viability | Tox21 | Cytotoxicity | human | HEK293T | kidney |
| Tox21\_PPARg\_BLA\_antagonist\_viability | Tox21 | Cytotoxicity | human | HEK293 | kidney |
| Tox21\_VDR\_BLA\_Agonist\_viability | Tox21 | Cytotoxicity | human | HEK293T | kidney |
| Tox21\_VDR\_BLA\_antagonist\_viability | Tox21 | Cytotoxicity | human | HEK293T | kidney |

### Supplemental Table 4. Differential log IC20 values used to stratify 314 putative TPO inhibitors for selective AUR-TPO activity.

Putative TPO inhibitors were stratified by selective AUR-TPO activity using the difference between the log IC20 for the AUR-TPO assay and either (1) the lower log IC20 value of the luciferase inhibition and cytotoxicity assay, or (2) the median log modl\_acc value of 37 cytotoxicity and proliferation assays from ToxCast.

|  |  |  |
| --- | --- | --- |
| Chemical Name | CASRN | Selectivity |
| Methimazole | 60-56-0 | 6.89 |
| 4,4'-Methylenedianiline | 101-77-9 | 6.75 |
| 6-Propyl-2-thiouracil | 51-52-5 | 6.44 |
| 4-Methylaniline | 106-49-0 | 6.43 |
| 2-Mercaptobenzothiazole | 149-30-4 | 6.37 |
| Sodium azide | 26628-22-8 | 6.15 |
| 3-Methylaniline | 108-44-1 | 6.10 |
| Acibenzolar-S-methyl | 135158-54-2 | 5.98 |
| 4,4'-Oxydianiline | 101-80-4 | 5.93 |
| 2-Anisidine | 90-04-0 | 5.91 |
| Isoproterenol hydrochloride | 51-30-9 | 5.81 |
| 4,4'-Methylenebis(2-methylaniline) | 838-88-0 | 5.77 |
| Aniline hydrochloride | 142-04-1 | 5.62 |
| Isoniazid | 54-85-3 | 5.47 |
| 2-Methoxy-5-methylaniline | 120-71-8 | 5.33 |
| 4-Hexylresorcinol | 136-77-6 | 5.32 |
| 4-Aminobenzoic acid | 150-13-0 | 5.11 |
| 2-Methylaniline | 95-53-4 | 5.03 |
| 2-Methoxy-5-nitroaniline | 99-59-2 | 5.00 |
| Carboxin | 5234-68-4 | 4.98 |
| Methidathion | 950-37-8 | 4.98 |
| (2Z)-3,7-Dimethylocta-2,6-dien-1-ol | 106-25-2 | 4.97 |
| Tolazamide | 1156-19-0 | 4.97 |
| 1,3-Benzenediamine | 108-45-2 | 4.95 |
| 2,4,6-Trimethylphenol | 527-60-6 | 4.95 |
| Methyl parathion | 298-00-0 | 4.83 |
| Eugenol | 97-53-0 | 4.78 |
| Dapsone | 80-08-0 | 4.76 |
| Isoeugenol | 97-54-1 | 4.70 |
| 17beta-Estradiol | 50-28-2 | 4.69 |
| Fenitrothion | 122-14-5 | 4.66 |
| Azamethiphos | 35575-96-3 | 4.64 |
| 2-Naphthalenol | 135-19-3 | 4.63 |
| Anthracene | 120-12-7 | 4.53 |
| N,N,4-Trimethylaniline | 99-97-8 | 4.52 |
| 17alpha-Estradiol | 57-91-0 | 4.52 |
| 2,3,6-Trimethylphenol | 2416-94-6 | 4.51 |
| Tetracycline | 60-54-8 | 4.50 |
| Maneb | 12427-38-2 | 4.42 |
| Ethoprop | 13194-48-4 | 4.40 |
| Mevinphos | 7786-34-7 | 4.34 |
| Thiophanate-methyl | 23564-05-8 | 4.22 |
| Diclosulam | 145701-21-9 | 4.21 |
| N,N-Dimethylaniline | 121-69-7 | 4.20 |
| Formetanate hydrochloride | 23422-53-9 | 4.17 |
| Monuron | 150-68-5 | 4.16 |
| Dioctyl phthalate | 117-84-0 | 4.15 |
| CP-671305 | 445295-04-5 | 4.09 |
| Dichlorvos | 62-73-7 | 4.07 |
| Parathion | 56-38-2 | 4.07 |
| Hexaflumuron | 86479-06-3 | 4.04 |
| Malaoxon | 1634-78-2 | 4.04 |
| Maltol | 118-71-8 | 4.03 |
| 2,6-Dimethylphenol | 576-26-1 | 3.97 |
| Fenaminosulf | 140-56-7 | 3.96 |
| Mesotrione | 104206-82-8 | 3.91 |
| Dimethyl sulfate | 77-78-1 | 3.91 |
| Metam-sodium hydrate | 6734-80-1 | 3.89 |
| Symclosene | 87-90-1 | 3.89 |
| Fenthion | 55-38-9 | 3.88 |
| Acephate | 30560-19-1 | 3.87 |
| CP-471358 | NOCAS\_47265 | 3.85 |
| N-Ethyl-3-methylaniline | 102-27-2 | 3.84 |
| Folic acid | 59-30-3 | 3.83 |
| Isazofos | 42509-80-8 | 3.81 |
| Pentachlorophenol | 87-86-5 | 3.80 |
| FR900409 | 138472-01-2 | 3.79 |
| Busulfan | 55-98-1 | 3.78 |
| Fenamidone | 161326-34-7 | 3.77 |
| Linuron | 330-55-2 | 3.72 |
| Terbufos sulfone | 56070-16-7 | 3.70 |
| Methamidophos | 10265-92-6 | 3.68 |
| EPN | 2104-64-5 | 3.66 |
| 3,7-Dimethyl-2,6-octadienal | 5392-40-5 | 3.63 |
| Hydroxyurea | 127-07-1 | 3.61 |
| Diuron | 330-54-1 | 3.60 |
| (E)-Anethole | 4180-23-8 | 3.60 |
| Propanil | 709-98-8 | 3.53 |
| Tris(2-ethylhexyl) trimellitate | 3319-31-1 | 3.53 |
| Triglycidyl isocyanurate | 2451-62-9 | 3.52 |
| Chloramben | 133-90-4 | 3.52 |
| Thidiazuron | 51707-55-2 | 3.51 |
| SSR162369 | NOCAS\_47346 | 3.49 |
| Methyl methanesulfonate | 66-27-3 | 3.47 |
| Monocrotophos | 6923-22-4 | 3.46 |
| Sodium erythorbate (1:1) | 6381-77-7 | 3.43 |
| PharmaGSID\_48510 | 460081-99-6 | 3.43 |
| Triphenyl phosphite | 101-02-0 | 3.41 |
| Trichloroacetic acid | 76-03-9 | 3.39 |
| Sodium L-ascorbate | 134-03-2 | 3.37 |
| Cymoxanil | 57966-95-7 | 3.33 |
| 4-Chloroaniline | 106-47-8 | 3.33 |
| CI-1044 | NOCAS\_47291 | 3.31 |
| CP-544439 | 230954-09-3 | 3.29 |
| Flufenacet | 142459-58-3 | 3.13 |
| 2,2',4,4'-Tetrahydroxybenzophenone | 131-55-5 | 3.09 |
| N-Ethylaniline | 103-69-5 | 3.08 |
| Resorcinol | 108-46-3 | 2.84 |
| 6-Methyl-2-thiouracil | 56-04-2 | 2.78 |
| Quercetin | 117-39-5 | 2.74 |
| 4-Pentylaniline | 33228-44-3 | 2.72 |
| Clove leaf oil | 8000-34-8 | 2.71 |
| 2-Naphthylamine | 91-59-8 | 2.49 |
| Methyl 2-aminobenzoate | 134-20-3 | 2.37 |
| Catechol | 120-80-9 | 2.34 |
| Cyanamide | 420-04-2 | 2.34 |
| Propyl gallate | 121-79-9 | 2.24 |
| 2-tert-Butyl-4-methoxyphenol | 121-00-6 | 2.24 |
| Malathion | 121-75-5 | 1.93 |
| Chlorpyrifos-methyl | 5598-13-0 | 1.88 |
| 2,2-Bis(4-hydroxyphenyl)-1,1,1-trichloroethane | 2971-36-0 | 1.86 |
| Methyldopa sesquihydrate | 41372-08-1 | 1.83 |
| 4,4',4"-Ethane-1,1,1-triyltriphenol | 27955-94-8 | 1.74 |
| Ethion | 563-12-2 | 1.72 |
| Hydroquinone | 123-31-9 | 1.66 |
| Tiratricol | 51-24-1 | 1.60 |
| CP-634384 | 290352-28-2 | 1.60 |
| Phenolphthalein | 77-09-8 | 1.56 |
| Azinphos-methyl | 86-50-0 | 1.51 |
| Oxytetracycline dihydrate | 6153-64-6 | 1.51 |
| 5-Amino-2-methylphenol | 2835-95-2 | 1.43 |
| Rifampicin | 13292-46-1 | 1.37 |
| Dazomet | 533-74-4 | 1.32 |
| Ethoxyquin | 91-53-2 | 1.31 |
| SAR150640 | NOCAS\_47389 | 1.30 |
| Bisphenol B | 77-40-7 | 1.29 |
| tert-Butylhydroquinone | 1948-33-0 | 1.27 |
| Diazinon | 333-41-5 | 1.27 |
| 4,4'-Sulfonylbis[2-(prop-2-en-1-yl)phenol] | 41481-66-7 | 1.26 |
| Chlorethoxyfos | 54593-83-8 | 1.22 |
| Octyl gallate | 1034-01-1 | 1.18 |
| Troglitazone | 97322-87-7 | 1.16 |
| N-Phenyl-1,4-benzenediamine | 101-54-2 | 1.15 |
| 2,4-Dimethylphenol | 105-67-9 | 1.12 |
| Methylene bis(thiocyanate) | 6317-18-6 | 1.08 |
| Dimethoate | 60-51-5 | 1.06 |
| 2,5-Di-tert-butylbenzene-1,4-diol | 88-58-4 | 1.04 |
| Anilazine | 101-05-3 | 1.03 |
| PharmaGSID\_48505 | NOCAS\_48505 | 1.02 |
| Pirimiphos-methyl | 29232-93-7 | 1.02 |
| PD-0333941 | 501027-49-2 | 1.02 |
| 2-(Thiocyanomethylthio)benzothiazole | 21564-17-0 | 0.99 |
| Anthralin | 1143-38-0 | 0.94 |
| 17alpha-Ethinylestradiol | 57-63-6 | 0.93 |
| CP-456773 | 210826-40-7 | 0.90 |
| Phosalone | 2310-17-0 | 0.88 |
| Rotenone | 83-79-4 | 0.87 |
| 3,5,3'-Triiodothyronine | 6893-02-3 | 0.83 |
| 2,6-Di-tert-butylphenol | 128-39-2 | 0.79 |
| 4-Cumylphenol | 599-64-4 | 0.79 |
| Toluene-2,4-diisocyanate | 584-84-9 | 0.78 |
| Famoxadone | 131807-57-3 | 0.78 |
| Phenolphthalin | 81-90-3 | 0.76 |
| 2,4,6-Tris(tert-butyl)phenol | 732-26-3 | 0.73 |
| 2,4-Diaminotoluene | 95-80-7 | 0.73 |
| 6-Thioguanine | 154-42-7 | 0.68 |
| Diethylstilbestrol | 56-53-1 | 0.67 |
| 4-Octylphenol | 1806-26-4 | 0.66 |
| Phosmet | 732-11-6 | 0.64 |
| Reserpine | 50-55-5 | 0.63 |
| 4,4'-Methylenebis(N,N-dimethylaniline) | 101-61-1 | 0.63 |
| 4-(Butan-2-yl)phenol | 99-71-8 | 0.62 |
| 1,2-Phenylenediamine | 95-54-5 | 0.62 |
| Profenofos | 41198-08-7 | 0.61 |
| Carminic acid | 1260-17-9 | 0.60 |
| all-trans-Retinoic acid | 302-79-4 | 0.58 |
| 3-Hydroxyfluorene | 6344-67-8 | 0.57 |
| 2,3-Diaminotoluene | 2687-25-4 | 0.57 |
| Darbufelone mesylate | 139340-56-0 | 0.57 |
| 4-tert-Butylphenol | 98-54-4 | 0.55 |
| Chlorpyrifos oxon | 5598-15-2 | 0.54 |
| 1-Hydroxypyrene | 5315-79-7 | 0.54 |
| Mifepristone | 84371-65-3 | 0.54 |
| 2-tert-Butyl-4-ethylphenol | 96-70-8 | 0.47 |
| 4-(2-Methylbutan-2-yl)phenol | 80-46-6 | 0.47 |
| Genistein | 446-72-0 | 0.44 |
| Phorate | 298-02-2 | 0.39 |
| Coumaphos | 56-72-4 | 0.39 |
| 4-Heptylphenol | 1987-50-4 | 0.36 |
| Sodium (2-pyridylthio)-N-oxide | 3811-73-2 | 0.31 |
| Sodium dodecyl sulfate | 151-21-3 | 0.31 |
| CJ-013790 | 179465-71-5 | 0.30 |
| 3,3',5,5'-Tetrabromobisphenol A | 79-94-7 | 0.27 |
| Resmethrin | 10453-86-8 | 0.27 |
| Phenothiazine | 92-84-2 | 0.26 |
| 4-Nonylphenol | 104-40-5 | 0.25 |
| Daidzein | 486-66-8 | 0.24 |
| Simvastatin | 79902-63-9 | 0.23 |
| Chlorpyrifos | 2921-88-2 | 0.20 |
| Norethindrone | 68-22-4 | 0.16 |
| Sorbic acid | 110-44-1 | 0.14 |
| Fenoxaprop-ethyl | 66441-23-4 | 0.10 |
| SB202235 | 139149-55-6 | 0.09 |
| 2-Chloroacetophenone | 532-27-4 | 0.05 |
| 4-Aminoazobenzene | 60-09-3 | 0.05 |
| Bensulide | 741-58-2 | 0.04 |
| HMR1426 | 262376-75-0 | 0.04 |
| 1,5-Naphthalenediamine | 2243-62-1 | 0.02 |
| MK-578 | 313994-79-5 | 0.02 |
| Ethylene thiourea | 96-45-7 | 0.01 |
| 2,2-Dibromo-3-nitrilopropionamide | 10222-01-2 | 0.00 |
| Phenol | 108-95-2 | 0.00 |
| 1,3-Propane sultone | 1120-71-4 | 0.00 |
| Maleic hydrazide | 123-33-1 | 0.00 |
| Myrcene | 123-35-3 | 0.00 |
| Alachlor ESA, sodium salt | 140939-15-7 | 0.00 |
| Clopyralid | 1702-17-6 | 0.00 |
| Procymidone | 32809-16-8 | 0.00 |
| 4-Chlorobenzotrichloride | 5216-25-1 | 0.00 |
| 4-Androstene-3,17-dione | 63-05-8 | 0.00 |
| N-Methyl-2-pyrrolidone | 872-50-4 | 0.00 |
| 2-Chlorophenol | 95-57-8 | 0.00 |
| Milbemectin (mixture of 70% Milbemcin A4, 30% Milbemycin A3) | NOCAS\_34742 | 0.00 |
| Michler's ketone | 90-94-8 | 0.00 |
| 2-Amino-5-azotoluene | 97-56-3 | -0.01 |
| Prallethrin | 23031-36-9 | -0.01 |
| Bisphenol A | 80-05-7 | -0.03 |
| Tebupirimfos | 96182-53-5 | -0.04 |
| CI-1029 | 207736-05-8 | -0.05 |
| Safrole | 94-59-7 | -0.06 |
| PFDA | 335-76-2 | -0.09 |
| 8-Hydroxyquinoline | 148-24-3 | -0.09 |
| SSR150106 | NOCAS\_47362 | -0.11 |
| 2,4-Di-tert-butylphenol | 96-76-4 | -0.12 |
| PharmaGSID\_47263 | 349495-42-7 | -0.13 |
| 4-Nonylphenol, branched | 84852-15-3 | -0.13 |
| Cinmethylin | 87818-31-3 | -0.13 |
| Piperonyl butoxide | 51-03-6 | -0.15 |
| 2-tert-Butyl-5-methylphenol | 88-60-8 | -0.16 |
| 9-Phenanthrol | 484-17-3 | -0.17 |
| Forchlorfenuron | 68157-60-8 | -0.19 |
| 4-(1,1,3,3-Tetramethylbutyl)phenol | 140-66-9 | -0.19 |
| Sodium dodecylbenzenesulfonate | 25155-30-0 | -0.20 |
| Allethrin | 584-79-2 | -0.21 |
| Dodecylbenzene sulfonate triethanolamine(1:1) | 27323-41-7 | -0.22 |
| Farglitazar | 196808-45-4 | -0.24 |
| S-Bioallethrin | 28434-00-6 | -0.24 |
| PharmaGSID\_47337 | 1061517-62-1 | -0.28 |
| Clorophene | 120-32-1 | -0.29 |
| Sodium myristyl sulfate | 1191-50-0 | -0.29 |
| 4-Chloro-1,2-diaminobenzene | 95-83-0 | -0.32 |
| Z-Tetrachlorvinphos | 22248-79-9 | -0.33 |
| Bisphenol AF | 1478-61-1 | -0.34 |
| Fabesetron hydrochloride | 129299-90-7 | -0.35 |
| Dodecylbenzenesulfonic acid | 27176-87-0 | -0.36 |
| SAR115740 | NOCAS\_47366 | -0.37 |
| Mancozeb | 8018-01-7 | -0.38 |
| Tannic acid | 1401-55-4 | -0.43 |
| Retinol | 68-26-8 | -0.46 |
| Bifenazate | 149877-41-8 | -0.49 |
| Geranyl acetate | 105-87-3 | -0.49 |
| 1-Dodecyl-2-pyrrolidinone | 2687-96-9 | -0.54 |
| Thiram | 137-26-8 | -0.56 |
| Carbendazim | 10605-21-7 | -0.57 |
| PharmaGSID\_48511 | 1062243-51-9 | -0.59 |
| 17beta-Trenbolone | 10161-33-8 | -0.61 |
| meso-Hexestrol | 84-16-2 | -0.61 |
| Ziram | 137-30-4 | -0.62 |
| 2,4-Bis(1-methyl-1-phenylethyl)phenol | 2772-45-4 | -0.63 |
| Folpet | 133-07-3 | -0.63 |
| Benz(a)anthracene | 56-55-3 | -0.66 |
| SR271425 | 155990-20-8 | -0.67 |
| Triclocarban | 101-20-2 | -0.69 |
| FD&C Blue No. 1 | 3844-45-9 | -0.71 |
| Terbufos | 13071-79-9 | -0.73 |
| AVE5638 | 725228-45-5 | -0.74 |
| 2,4-Bis(2-methylbutan-2-yl)phenol | 120-95-6 | -0.78 |
| 3,4-Diaminotoluene | 496-72-0 | -0.81 |
| Tamoxifen citrate | 54965-24-1 | -0.84 |
| Docusate sodium | 577-11-7 | -0.86 |
| UK-337312 | 203942-49-8 | -0.87 |
| Sodium dimethyldithiocarbamate | 128-04-1 | -0.87 |
| CP-105696 | 158081-99-3 | -0.93 |
| PFNA | 375-95-1 | -0.99 |
| Azathioprine | 446-86-6 | -0.99 |
| Allura Red C.I.16035 | 25956-17-6 | -1.01 |
| Triclosan | 3380-34-5 | -1.01 |
| Ro 23-7637 | 107071-66-9 | -1.05 |
| C.I. Solvent Yellow 14 | 842-07-9 | -1.08 |
| Testosterone propionate | 57-85-2 | -1.12 |
| Oxytetracycline hydrochloride | 2058-46-0 | -1.19 |
| 1,2-Benzenedicarboxaldehyde | 643-79-8 | -1.20 |
| Didecyldimethylammonium chloride | 7173-51-5 | -1.33 |
| Gentian Violet | 548-62-9 | -1.37 |
| Niclosamide | 50-65-7 | -1.40 |
| AVE6324 | NOCAS\_47377 | -1.48 |
| FR150011 | 149413-74-1 | -1.48 |
| Ketoconazole | 65277-42-1 | -1.64 |
| Elzasonan | 361343-19-3 | -1.75 |
| 4-Aminofolic acid | 54-62-6 | -1.76 |
| Asulam | 3337-71-1 | -2.15 |
| Methotrexate | 59-05-2 | -2.75 |
| Fenhexamid | 126833-17-8 | -3.15 |
| Citronellol | 106-22-9 | -3.34 |
| Phenobarbital sodium | 57-30-7 | -3.42 |
| 2-tert-Butylphenol | 88-18-6 | -3.51 |
| Biphenyl | 92-52-4 | -3.54 |
| Difenoconazole | 119446-68-3 | -3.58 |
| 4-Cyclohexylcyclohexanone | 92-68-2 | -3.58 |
| TNP-470 | 129298-91-5 | -3.69 |
| PharmaGSID\_48509 | NOCAS\_48509 | -3.73 |
| Triflumizole | 68694-11-1 | -3.90 |
| 7,12-Dimethylbenz(a)anthracene | 57-97-6 | -3.95 |
| Sodium hexyldecyl sulfate | 1120-01-0 | -3.96 |
| Oryzalin | 19044-88-3 | -3.98 |
| Benomyl | 17804-35-2 | -4.06 |
| 1,2-Diphenylhydrazine | 122-66-7 | -4.08 |
| Propiconazole | 60207-90-1 | -4.10 |
| Tamoxifen | 10540-29-1 | -4.27 |
| Butyl benzyl phthalate | 85-68-7 | -4.30 |
| UK-373911 | 291305-06-1 | -4.31 |
| Raloxifene hydrochloride | 82640-04-8 | -4.48 |
| Napropamide | 15299-99-7 | -4.72 |
| Mercuric chloride | 7487-94-7 | -5.39 |