**Table 1.** Results for the top 15 ranked chemical samples that demonstrated significant RAIU inhibition in multi-concentration screening (as shown in Fig.3B)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | Chemical | CAS NO. | Max Conc(M)a | AC50 (logM) | absEC50 (logM) | Cytotox-pointb | Ranking Scored | Non-cytotoxic RAIU inhibition at 1 or more concc |
| 1 | Phenolphthalein | 77-09-8 | 1×10-4 | -6.14 | -6.13 | -6.43 | 179.75 | No |
| 2 | PFHS-K | 3871-99-6 | 1×10-4 | -4.73 | -4.77 | -4.40 | 105.48 | Yes |
| 3 | PFOS | 1763-23-1 | 8×10-5 | -4.75 | -4.77 | NA | 101.60 | Yes |
| 4 | Benz(a)anthracene | 56-55-3 | 1×10-4 | -4.53 | -4.54 | -4.16 | 89.49 | No |
| 5 | PFOS-K | 2795-39-3 | 9.5×10-5 | -4.67 | -4.70 | -5.24 | 89.48 | Yes |
| 6 | Nitrofen | 1836-75-5 | 1×10-4 | -4.48 | -4.46 | -4.35 | 85.03 | No |
| 7 | Dinoseb | 88-85-7 | 1×10-4 | -5.18 | -5.06 | -6.88 | 83.06 | No |
| 8 | Tributyltin chloride | 1461-22-9 | 1×10-4 | -5.61 | -5.60 | -5.70 | 80.06 | No |
| 9 | Triclocarban | 101-20-2 | 1×10-4 | -5.51 | -5.11 | -5.11 | 77.28 | Yes |
| 10 | Hexachlorocyclo-pentadiene | 77-47-4 | 1×10-4 | -4.71 | -4.77 | -4.94 | 73.34 | Yes |
| 11 | Mepanipyrim | 110235-47-7 | 1×10-4 | -4.36 | -4.27 | NA | 73.22 | Yes |
| 12 | 4-Chloro-1,2-diaminobenzene | 95-83-0 | 1×10-4 | -4.61 | -4.71 | -4.92 | 73.09 | Yes |
| 13 | PFOS | 1763-23-1 | 8×10-5 | -4.95 | -4.66 | -6.11 | 67.90 | Yes |
| 14 | Nelivaptan | 439687-69-1 | 1×10-4 | -4.55 | -4.36 | -5.05 | 65.17 | No |
| 15 | Zamifenacin | 127308-82-1 | 1×10-4 | -4.97 | NA | -5.40 | 63.02 | Yes |

Results for all test chemicals are in Table S1.

a Max Conc: the maximum permissible concentration tested in single-concentration screening. The Max Conc was obtained by 200X dilution of the supplied stock chemicals (concentrations ≤ 2×10-2 M). Serial dilution of samples for multi-concentration assay started with the Max Conc. NA: not available, as no absEC50 for RAIU was observed.

b Cytotox-point: the log concentration where significant reduction in cell viability (e.g, cytotoxicity, absEC85.49 was observed). NA: not available, as no significant cytotoxicity was observed.

c Non-cytotoxic RAIU inhibition at 1 or more concentrations: Indicates chemicals that have significant RAIU inhibition without significant cytotoxicity at one or more concentrations tested in multi-concentration screening.

d Ranking score normalized to NaClO4 (maximum ranking score of 200).

### Table S2. Summary of normalized responses (% of vehicle Control) for QA controls across all plates

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Assay1 | DMSO | 2,4-D | DCNQ2 (1E-4M) | NaClO42 (1E-4M) | NaNO3 | NaSCN |
| Single-conc RAIU | 99.41 ± 6.03 | 89.78 ± 4.01 | n.a. | 3.05 ± 0.39 | 79.62 ± 7.3 | 21.84 ± 2.15 |
| Multi-conc RAIU | 99.28 ± 6.47 | 90.46 ± 4.62 | 3.01 ± 0.59 | 3.26 ± 0.35 | 81.97 ± 7.41 | 25.67 ± 1.81 |
| Multi-conc Cell Viability | 99.98 ± 3.71 | 95.75 ± 5.23 | 3.05 ± 0.59 | 95.24 ± 7.02 | 95.03 ± 6.42 | 100.27 ± 5.26 |

Mean ± S.D.

n.a.: not available as DCNQ was not included in the single-concentration screening.

1. Data were calculated by collecting normalized response for each chemical from all assay plates (single-con: n=39, multi-con: n=72). Values represent the percent of control activity. 2,4-D, NaNO3, and NaSCN were at a concentration of 100 µM.

2. Although DCNQ and NaClO4 were included on each assay plate in six concentrations, only the responses from 100 µM concentration are summarized here.

### Table S3. Summary of assay performance metrics for single-concentration and multiple-concentration screening

|  |  |  |  |
| --- | --- | --- | --- |
| Assay1 | CV of DMSO | Z' Score | AC50 of positive controls2 |
| mean±SD | range | mean±SD | range | mean±SD | range |
| Single-conc RAIU | 6.17% ± 1.03% | 4.49% - 8.94% | 0.80 ± 0.03 | 0.71 - 0.86 | -6.42 ± 0.12 | -6.56 - -6.04 |
| Multi-conc RAIU | 6.81% ± 1.47% | 3.78% - 13.76% | 0.78 ± 0.05 | 0.56 - 0.88 | -6.31 ± 0.11 | -6.56 - -6.04 |
| Multi-conc Cell Viability | 5.42% ± 1.47% | 2.80% - 9.53% | 0.80 ± 0.03 | 0.74 - 0.95 | -4.83 ± 0.13 | -4.95 - -4.48 |

1: All metrics were calculated per assay plate (single-con: n=39, multi-con: n=72) and summarized separately for single-concentration and multi-concentration screenings.

2: AC50 of positive controls were calculated from the dose-responses of NaClO4 and DCNQ for RAIU and cell viability assay, respectively. Unit: logM.

n.a.: unable to calculate.