

Supplementary Table 1. Array samples and concentration of chemical treatments used in the study

EXPERIMENT A (Expression Chemogenomics)

| Group I Samples (Dataset I) | | | Group II Samples (Dataset II) | | | | |
|------------------------------------|--|---|--------------------------------------|--|-------------------------|---|--|
| V2.Control_1 | Vehicle alone acetone 0.05% (Merck, Germany) | Control* | W2.Control_1 | water (control) | | | |
| V2.Control_2 | | | W2.Control_2 | | | | |
| V2.Control_3 | | | W2.Control_3 | | | | |
| V2.Control_4 | | | W2.Control_4 | | | | |
| V2.Control_5 | | | W2.Control_5 | | | | |
| Es_1 | 17-beta estradiol 1ug/L (3.67nM) (Sigma, USA) | Combined groups of Estrogenic Compounds (ECs)* | Cd_1 | Cadmium chloride 3mg/L (16.4uM) (Sigma, USA) | Heavy Metals | | |
| Es_2 | | | Cd_2 | | | | |
| Es_3 | | | Cd_3 | | | | |
| Es_4 | | | Cd_4 | | | | |
| Bis_5 | | | Cd_5 | | | | |
| Bis_1 | Bisphenol A 5mg/L (21.9uM) (Aldrich, USA) | | Hg_1 | Mercuric chloride 0.2mg/L (734nM) (Aldrich, USA) | | | |
| Bis_2 | | | Hg_2 | | | | |
| Bis_3 | | | Hg_3 | | | | |
| DES_3 | Diethylstilbestrol 1ug/L (3.73nM) (Sigma, USA) | | Hg_4 | | | 4-Nitrophenol 5mg/L (35.9uM) (Merck, Germany) | |
| DES_6 | | | Hg_5 | | | | |
| DES_2 | | | NP_1 | | | | |
| DES_8 | | | NP_2 | | | | |
| BAP_1 | | | NP_3 | | | | |
| BAP_2 | Benzo[a]pyrene ~5mg/L (~20.0uM) (Sigma, USA) | Combined groups of Polycyclic (Halogenated) Aromatic Hydrocarbons P(H)AHs* | NP_4 | Organic Nitrogen Compounds | | | |
| BAP_3 | | | NP_5 | | | | |
| BAP_4 | | | CA_1 | | | | |
| BAP_5 | | | CA_2 | | | | |
| MC_1 | | | CA_3 | | | | |
| MC_2 | 3-Methyl- cholanthrene 100ug/L (373nM) (Sigma, USA) | | CA_4 | 4-Chloroaniline 20mg/L (157uM) (Merck, Germany) | | | |
| MC_3 | | | DEN_1 | | | | |
| MC_4 | | | DEN_2 | | | | |
| TCDD_1 | | | DEN_3 | | | | |
| TCDD_2 | | | DEN_4 | | | | |
| TCDD_3 | 2,3,7,8-Tetrachloro- dibenzodioxin 10ug/L (31.1nM) (CIL, USA) | | DEN_5 | Diethylnitrosamine 400mg/L (3.9mM) (Sigma, USA) | | | |
| TCDD_5 | | | Heptachlor_1 | | | | |
| | | | Heptachlor_2 | | | | |
| | | | Heptachlor_3 | | | | |
| | | | Lindane_1 | | | | |
| | Lindane 100ug/l (344nM) (Aldrich, USA) | | Lindane_2 | Organochlorine Pesticides | | | |
| | | | Lindane_3 | | | | |
| | | | Lindane_5 | | | | |
| | | | DDT_1 | | | | |
| | | | DDT_2 | | | | |
| | DDT 100ug/l (282nM) (Supelco, USA) | | DDT_3 | | | | |
| | | | DDT_4 | | | | |
| | | | DDT_5 | | | | |
| | | | Atz_1 | | | | |
| | | | Atz_2 | | | | |
| | Atrazine 5mg/L (23.1uM) (Supelco, USA) | | Atz_3 | | | | |
| | | | Atz_4 | | | | |
| | | | Atz_5 | | | | |

* Experimental groups that were used to obtain discriminatory gene sets for training of prediction models (dataset I).

Supplementary Table 1 (continued).

EXPERIMENT B (Expression Chemogenomics)

Group III Samples (Dataset III)

| | | |
|--------------|--------------------------------|--|
| V.Control_1 | Vehicle alone acetone 0.01% | (Control)* |
| V.Control_10 | | |
| V.Control_5 | | |
| V.Control_7 | | |
| V.Control_8 | | |
| V.Control_9 | | |
| BAP-H_2 | BAP-H: ~500ug/L (~2000nM) | Combined groups of Benzo[a]pyrene (BAP) * |
| BAP-H_3 | | |
| BAP-H_4 | | |
| BAP-H_6 | | |
| BAP-H_7 | | |
| BAP-L_1 | BAP-L: ~50ug/L (~200nM) | |
| BAP-L_2 | | |
| BAP-L_3 | | |
| BAP-L_6 | | |
| BAP-L_8 | DES-H: 10 ug/L (37.3nM) | |
| DES-H_1 | | |
| DES-H_4 | | |
| DES-H_5 | DES-L: 1 ug/L (3.73nM) | Combined groups of Diethylstilbestrol (DES) * |
| DES-H_9 | | |
| DES-L_3 | | |
| DES-L_4 | | |
| DES-L_5 | | |
| DES-L_6 | | |
| DES-L_7 | | |

Group IV Samples (Dataset IV) [continued]

| | |
|--------------------|--|
| As-H_DES-H_1 | As-H (Arsenic): 40mg/L (~4000nM) DES-H: 10 ug/L (37.3nM) |
| As-H_DES-H_10 | |
| As-H_DES-H_3 | |
| As-H_DES-H_5 | |
| As-H_DES-H_6 | |
| As-H_DES-H_7 | |
| As-H_DES-H_8 | |
| As-L_DES-H_3 | |
| As-L_DES-H_4 | |
| As-L_DES-H_5 | |
| As-L_DES-H_6 | |
| As-L_DES-H_7 | BAP-L: ~50ug/L (~200nM) As-H (Arsenic): 40mg/L (~4000nM) DES-H: 10 ug/L (37.3nM) |
| As-L_DES-H_8 | |
| BAP-L_AS-H_DES-H_1 | |
| BAP-L_AS-H_DES-H_2 | |
| BAP-L_AS-H_DES-H_5 | |
| BAP-L_AS-H_DES-H_3 | |
| BAP-L_AS-H_DES-H_6 | |
| BAP-L_AS-H_DES-H_7 | |
| BAP-L_AS-H_DES-H_9 | BAP-L: ~50ug/L (~200nM) As-L (Arsenic): 4mg/L (~400nM) DES-H: 10 ug/L (37.3nM) |
| BAP-L_AS-L_DES-H_1 | |
| BAP-L_AS-L_DES-H_4 | |
| BAP-L_AS-L_DES-H_5 | |
| BAP-L_AS-L_DES-H_6 | |
| BAP-L_AS-L_DES-H_7 | |
| BAP-L_AS-L_DES-H_8 | |
| BAP-H_AS-H_DES-H_2 | |
| BAP-H_AS-H_DES-H_3 | |
| BAP-H_AS-H_DES-H_6 | |
| BAP-H_AS-H_DES-H_8 | |
| BAP-H_AS-H_DES-H_9 | |
| W.Control_1 | water (control) |
| W.Control_2 | |
| W.Control_4 | |
| W.Control_5 | |
| W.Control_7 | |

Group IV (Dataset IV)

| | |
|---------------|--|
| BAP-L_As-H_1 | BAP-L: ~50ug/L (~200nM) As-H (Arsenic): 40mg/L (~4000nM) (Arsenic purchased from Sigma, USA) |
| BAP-L_As-H_2 | |
| BAP-L_As-H_3 | |
| BAP-L_As-H_5 | |
| BAP-L_As-H_7 | |
| BAP-L_As-H_8 | |
| BAP-H_As-H_1 | |
| BAP-H_As-H_2 | |
| BAP-H_As-H_3 | BAP-H: ~500ug/L (~2000nM) As-H (Arsenic): 40mg/L (~4000nM) |
| BAP-H_As-H_4 | |
| BAP-H_As-H_6 | |
| BAP-H_As-H_7 | |
| BAP-H_As-H_8 | BAP-H: ~500ug/L (~2000nM) DES-H: 10 ug/L (37.3nM) |
| BAP-H_DES-H_1 | |
| BAP-H_DES-H_4 | |
| BAP-H_DES-H_6 | BAP-H: ~500ug/L (~2000nM) DES-L: 1 ug/L (3.73nM) |
| BAP-H_DES-L_1 | |
| BAP-H_DES-L_4 | |
| BAP-H_DES-L_5 | |
| BAP-H_DES-L_6 | |
| BAP-H_DES-L_7 | |
| BAP-H_DES-L_9 | |

* Experimental groups that were used to obtain discriminatory gene sets for training of prediction models (dataset III).

Supplementary Table 1 (continued).

EXPERIMENT C (Tissue-Specific Biomarker Validation Experiment)

Tissue-specific Samples (brain, gills, liver, gut, skin, testis and eyes were sampled)

| | | |
|-------------|---|--|
| V.Control_1 | } | Vehicle alone (Control) acetone 0.01% |
| V.Control_2 | | |
| V.Control_3 | | |
| V.Control_4 | | |
| V.Control_5 | | |
| BAP_1 | } | BAP: ~250ug/L (~1000nM) |
| BAP_2 | | |
| BAP_3 | | |
| BAP_4 | | |
| BAP_5 | | |
| DES_1 | } | DES: 5 ug/L (18.7nM) |
| DES_2 | | |
| DES_3 | | |
| DES_4 | | |
| DES_5 | | |

Except for 17-beta-estradiol and diethylstilbestrol which was selected based on vitellogenin transcript induction, the exposure concentrations for the remaining compounds were selected based on preliminary acute toxicity tests that produced about 10%-20% mortality within 96 hours of treatment. Concentrations for benzo[a]pyrene were reduced 10- to 100-fold for experiment B and C. We reason that these concentrations would produce a spectrum of responses/effects ranging from adaptive to toxicity.