Endocrine disrupting potentials of PAHs and their alkylated analogues associated with oil spills

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Table S1. Exposure concentrations of tested PAHs for H295R assay

Chemicals	Concentration represented as Low (μg/L)	Concentration represented as Medium (μg/L)	Concentration represented as High (μg/L)
Naphthalene	40	200	1000
1-Methylnaphthalene	40	200	1000
2-Methylnaphthalene	40	200	1000
1,3-Dimethylnaphthalene	40	200	1000
2,3-Dimethylnaphthalene	40	200	1000
1,4,5-Trimethylnaphthalene	20	100	500
2,3,5-Trimethylnaphthalene	20	100	500
1,2,5,6-Tetramethylnaphthalene	20	100	500
Fluorene	40	200	1000
1-Methylfluorene	40	200	1000
9-Methylfluorene	40	200	1000
1,7-Dimethylfluorene	20	100	500
9-n-Propylfluorene	40	200	1000
Dibenzothiophene	40	200	1000
2-Methyldibenzothiophene	20	100	500
2,4-Dimethyldibenzothiophene	20	100	500
2,4,7-Trimethyldibenzothiophene	20	100	500
Phenanthrene	40	200	1000
2-Methylphenanthrene	40	200	1000
3-Methylphenanthrene	40	200	1000
1,2-Dimethylphenanthrene	20	100	500
1,6-Dimethylphenanthrene	20	100	500
1,2,6-Trimethylphenanthrene	20	100	500
1,2,9-Trimethylphenanthrene	20	100	500
1,2,6,9-Tetramethylphenanthrene	20	100	500
Chrysene	40	200	1000
1-Methylchrysene	8	40	200
3-Methylchrysene	1.6	8	40
6-Ethylchrysene	8	40	200
1,3,6-Trimethylchrysene	8	40	200

Table S2. Qualitative, estrogenic index (qEI) and androgenic index (qAI) in 30 unsubstituted and alkylated PAHs

Chemicals	Cytotoxic NOEC (µg/L)	Estrogen NOEC (µg/L)	Testosterone NOEC (µg/L)	qEI	qAI
Naphthalene	1000	<40*	1000	>25	1
1-Methylnaphthalene	1000	<40*	40	>25	25
2-Methylnaphthalene	1000	<40*	1000	>25	1
1,3-Dimethylnaphthalene	200	<8*	<8*	>25	>25
2,3-Dimethylnaphthalene	200	200	200	1	1
1,4,5-Trimethylnaphthalene	500	500	500	1	1
2,3,5-Trimethylnaphthalene	500	20	500	25	1
1,2,5,6-Tetramethylnaphthalene	500	500	<20*	1	>25
Fluorene	1000	40	1000	25	1
1-Methylfluorene	1000	1000	<40*	1	>25
9-Methylfluorene	1000	<40*	<40*	>25	>25
1,7-Dimethylfluorene	500	<20*	<20*	>25	>25
9-n-Propylfluorene	1000	1000	40	1	25
Dibenzothiophene	1000	200	<40*	5	>25
2-Methyldibenzothiophene	500	<20*	500	>25	1
2,4-Dimethyldibenzothiophene	500	20	<20*	25	>25
2,4,7-Trimethyldibenzothiophene	500	20	500	25	1
Phenanthrene	1000	40	1000	25	1
2-Methylphenanthrene	1000	1000	1000	1	1
3-Methylphenanthrene	1000	1000	1000	1	1
1,2-Dimethylphenanthrene	500	500	500	1	1
1,6-Dimethylphenanthrene	500	500	500	1	1
1,2,6-Trimethylphenanthrene	500	<20*	500	>25	1
1,2,9-Trimethylphenanthrene	500	<20*	<20*	>25	>25
1,2,6,9-Tetramethylphenanthrene	500	100	<20*	5	>25
Chrysene	1000	200	<40*	5	>25
1-Methylchrysene	200	200	200	1	1
3-Methylchrysene	40	40	40	1	1
6-Ethylchrysene	200	200	200	1	1
1,3,6-Trimethylchrysene	200	200	200	1	1

*Significant E2 production was observed at the lowest concentration.

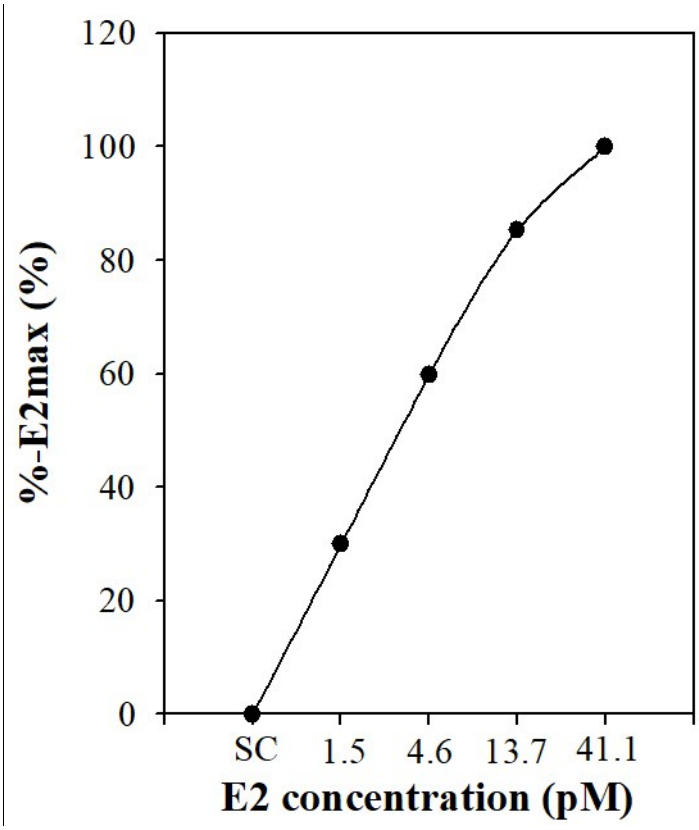
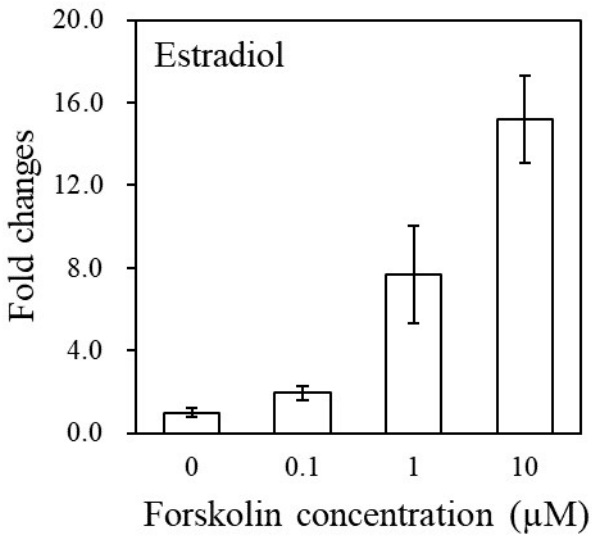


Figure S1. Dose-response curve of estradiol (E2), a positive control used for MVLN-*luc* assay.

(a)



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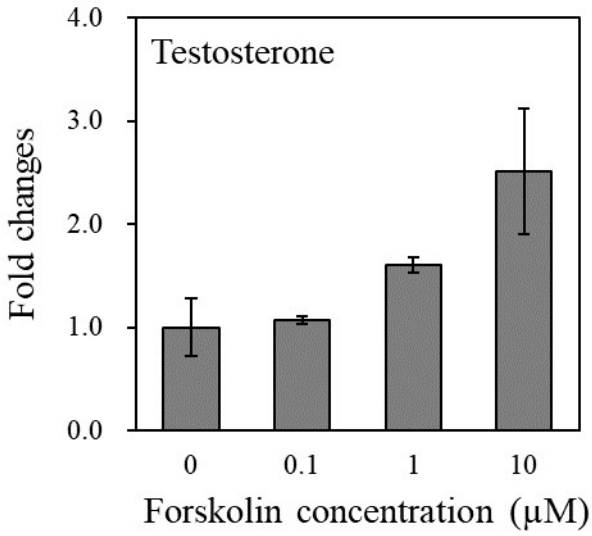

Figure S2. Dose-response curve of forskolin, a positive control. (a) estradiol (E2) content and (b) testosterone content in H295R cell assay.

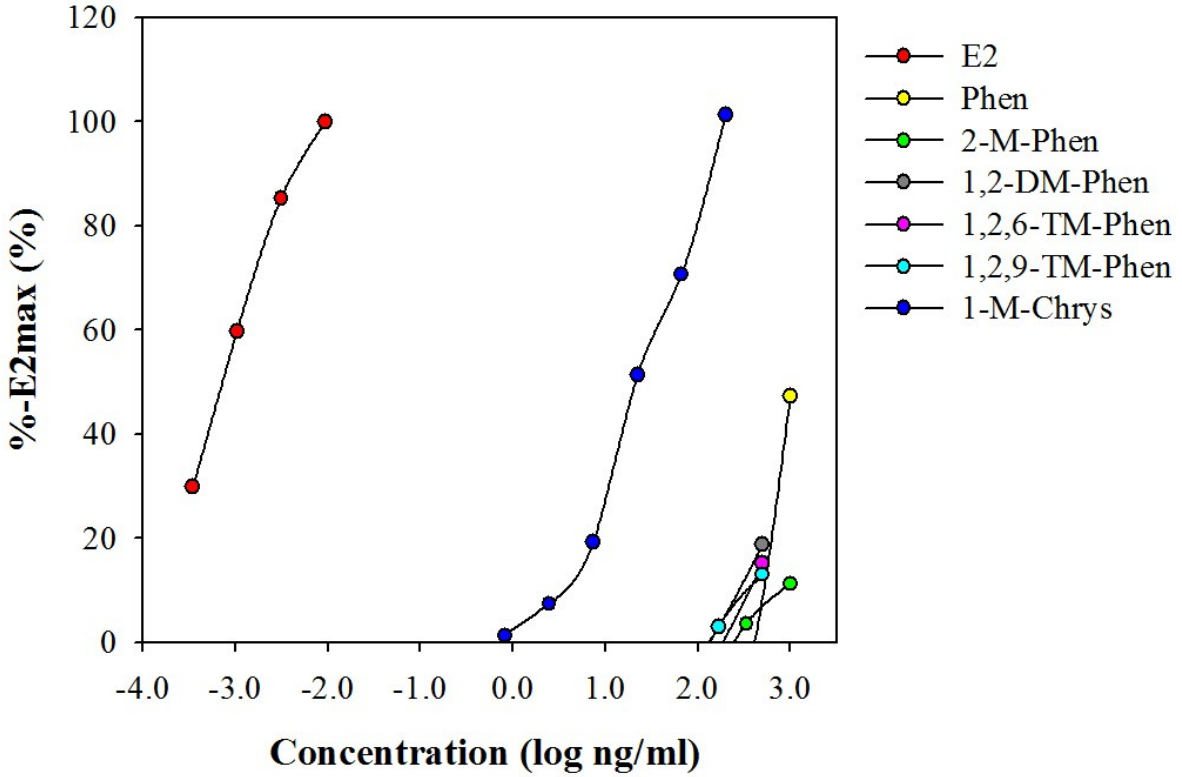

Figure S3. Dose dependent ER-mediated potencies observed from several PAHs with >10% ER-mediated potency.