SUPPLEMENTAL DATA LEGENDS

Figure S1. OPAH structures and CYP1A expression: Table displays OPAH name, structure, and presence or absence of vascular and liver CYP1A protein expression.

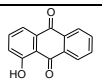
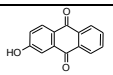
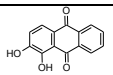
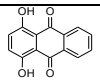
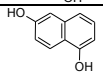
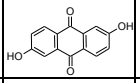
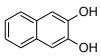
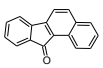
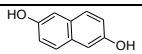
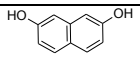
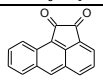
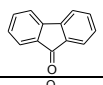
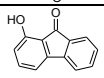
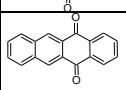
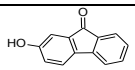
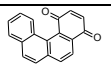
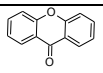
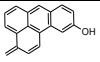
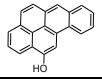
Figure S2. Developmental OPAH Toxicity: Heatmap displays the percent incidences of each malformation for the dose response, 0 – 100μM for each OPAH. The color scale increases from white to red in 1% increments, where grey represents morphological endpoints not evaluated because of 100% mortality at that concentration.

Figure S3. Low Dose Developmental OPAH Toxicity: Heatmap displays the percent incidences of each malformation for the dose response, 0 – 20μM for the most toxic OPAHs, causing 100% mortality at 4μM or 20μM. The color scale increases from white to red in 1% increments, where grey represents morphological endpoints not evaluated because of 100% mortality at that concentration.

Figure S4. EC_{50} values: Table lists the calculated EC_{50} values for each morphological endpoint, for all OPAHs. These EC_{50} values are visualized in the Figure 1 heatmap.

Figure S5. qRT-PCR primers: Table lists the gene names and primer sequences used for the qRT-PCR analysis.

Supplemental Figure 1

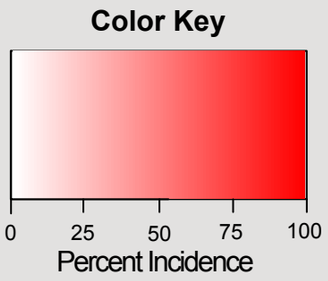
OPAH	STRUCTURE	CYP1A VASCULATURE	CYP1A LIVER	NO CYP1A	OPAH	STRUCTURE	CYP1A VASCULATURE	CYP1A LIVER	NO CYP1A
1,4-Benzoquinone				x	Phenanthrene-quinone				X
Chromone				X	1-Hydroxyanthraquinone			X	
1,2-Naphthoquinone				X	2-Hydroxyanthraquinone				X
1,4-Naphthoquinone				N/A	1,2-Dihydroxyanthraquinone				X
1,3-Dihydroxynaphthalene			X		1,4-Dihydroxyanthraquinone				X
1,5-Dihydroxynaphthalene		X			1,8-Dihydroxyanthraquinone			X	
1,6-Dihydroxynaphthalene				X	2,6-Dihydroxyanthraquinone				X
2,3-Dihydroxynaphthalene		X			Benzo[a]fluorenone		X		
2,6-Dihydroxynaphthalene				X	4H-Cyclopenta[def]phenanthren-4-one				X
2,7-Dihydroxynaphthalene				X	Aceanthraquinone		X		
9-Fluorenone				X	1,9-Benz-10-anthrone				X
1-Hydroxy-9-Fluorenone				X	5,12-Naphthacenequinone		X		
2-Hydroxy-9-Fluorenone				X	Benz(a)anthracene-7,12-dione		X		
Acenaphthenquinone				X	Benzo[c]phenanthrene-1,4-dione				X
Perinaphthenone				X	Pyrene-4,5-dione				X
Xanthone			X		9-Hydroxybenzo[a]pyrene				X
1,4-Anthraquinone				X	10-Hydroxybenzo[a]pyrene		X		
9,10-Anthraquinone				X	12-Hydroxybenzo[a]pyrene		X		
Phenanathrene-1,4-dione		X			6H-Benzo[cd]pyren-6-one				X

Supplemental Figure 2

OPAH Dose Response Data

Supplemental Figure 3

Toxic OPAH Low Dose



Supplemental Figure 4

OPAH	MO24	DP24	SM24	NC24	MORT	YSE	AXIS	EYE	SNOU	JAW	OTIC	PE	BRAI	SOMI	PFIN	CFIN	PIG	CIRC	TRUN	SWIM	NC	TR
12-HYDROXYBENZO[A]PYRENE	NA	NA	NA	NA	95	40	45	65	65	45	86	40	90	NA	55	95	130	95	86	50	NA	86
XANTHONE	500	500	NA	NA	100	45	45	59	59	50	90	59	200	100	50	500	NA	NA	NA	50	NA	59
ACEANTHRENEQUINONE	NA	NA	NA	NA	90	77	99	60	60	60	80	60	60	80	60	45	400	400	400	45	NA	50
1-2-DIHYDROXYANTHRAQUINONE	300	NA	NA	NA	185	75	45	78	75	65	45	78	200	90	75	200	NA	NA	NA	90	NA	NA
4H-CYCLOPENTA[DEF]PHENANTHREN-4-ONE	NA	NA	NA	NA	30	75	70	80	80	90	NA	97	70	90	NA	NA	NA	NA	NA	90	NA	70
1-3-DIHYDROXYNAPHTHALENE	NA	NA	NA	NA	200	40	100	NA	NA	NA	NA	75	85	NA	90	NA	NA	NA	NA	NA	NA	85
9-FLUORENONE	200	135	NA	NA	250	200	200	350	350	129	350	129	350	NA	129	129	NA	NA	NA	350	NA	350
CHROMONE	NA	NA	NA	NA	NA	350	310	310	310	310	380	350	310	425	400	485	500	NA	500	450	NA	500
2-7-DIHYDROXYNAPHTHALENE	490	175	NA	NA	200	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
1-HYDROXYANTHRAQUINONE	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
10-HYDROXYBENZO[A]PYRENE	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
9-10-ANTHRAQUINONE	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
1-6-DIHYDROXYNAPHTHALENE	320	60	NA	NA	60	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
2-6-DIHYDROXYNAPHTHALENE	NA	375	NA	NA	70	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
ACENAPHTHENEQUINONE	35	100	NA	NA	45	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
2-HYDROXY-9-FLUORENONE	40	NA	NA	NA	32	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
5-12-NAPHTHACENEQUINONE	70	NA	NA	NA	52	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
2-3-DIHYDROXYNAPHTHALENE	80	35	35	NA	60	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
1-5-DIHYDROXYNAPHTHALENE	50	60	NA	NA	75	55	NA	NA	NA	NA	NA	35	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
1-HYDROXY-9-FLUORENONE	70	40	NA	NA	55	26	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
1-8-DIHYDROXYANTHRAQUINONE	NA	NA	NA	NA	200	16	80	NA	80	100	NA	16	NA	80	NA	70	NA	80	70	180	NA	80
BENZO[C]PHENANTHRENE[1-4]QUINONE	20	30	NA	NA	14	17	10	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
BENZ[A]ANTHRACENE-7-12-DIONE	NA	NA	NA	NA	7	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
2-6-DIHYDROXYANTHRAQUINONE	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	7.36	NA	NA	NA	NA
PERINAPHTHENONE	25	NA	NA	NA	12	10	16	20	20	10	NA	10	NA	NA	NA	10	NA	NA	16	NA	NA	16
6H-BENZO[C-D]PYREN-6-ONE;NAPHTHRANTHRONE	NA	NA	NA	NA	NA	45	75	45	45	45	65	6	45	65	65	65	65	65	85	65	NA	380
BENZO[A]FLUORENONE	100	NA	NA	NA	50	15	15	15	10	10	15	10	12	15	10	30	500	500	500	10	NA	50
2-HYDROXYANTHRAQUINONE	19	NA	NA	NA	13	12	8	8	8	8	8	8	8	8	20	8	8	8	8	20	NA	8
1-9-BENZ-10-ANTHRONE	NA	NA	NA	NA	230	14	6	14	6	7.51	60	8	6	6	8	20	8	500	500	500	NA	300
1-4-DIHYDROXYANTHRAQUINONE	NA	NA	NA	NA	500	500	3.5	500	500	500	NA	500	NA	NA	NA	NA	NA	1.2	500	5	NA	500
PHENATHRENE-QUINONE	2	NA	NA	NA	2	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
1-2-NAPHTHOQUINONE	2	NA	NA	NA	2	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
PYRENE-4-5-DIONE	2	NA	NA	NA	2	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
PHENANTHRENE-1-4-DIONE	1.5	NA	NA	NA	1.5	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
1-4-BENZOQUINONE-D4	1.2	2.4	NA	NA	1	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
1-4-ANTHRAQUINONE	4.27	1.7	NA	NA	2	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
9-HYDROXYBENZO[A]PYRENE	45	60	NA	NA	2	1.2	1.2	NA	1.2	1.2	1.2	1.2	1.2	NA	NA	NA	NA	NA	1.2	NA	NA	1.2
1-4-NAPHTHOQUINONE	0.1	NA	NA	NA	0.1	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA

Supplemental Figure 5

Gene	Forward Primer (5'- 3')	Reverse Primer (5'- 3')
AHR1A	CGCAAAAGGAGGAAACCTGTC	CCTGTAGCAAAAATTCCCCCT
CYP1A	TGCCGATTTCATCCCTTTCC	AGAGCCGTGCTGATAGTGTC
CYP1B1	CTGCATTGATTTCCGAGACGTG	CACACTCCGTGTTGACAGC
CYP1C1	AGTGGCACAGTCTACTTTGAGAG	TCGTCCATCAGCACTCAG
CYP1C2	GTGGTGGAGCACAGACTAAG	TTCAGTATGAGCCTCAGTCAAAC
gst p1	TTCAGTCCAACGCCATGC	ATGAGATCTGATCGCCAACC
gst p2	TCTGGACTCTTTCCCGTCTCTCAA	ATTCACTGTTTGCCGTTGCCGT
gst κ	AAATTGCACTGCACTCGCAAGC	TGTAGCGACACAGCACCTCAAATG
gst α	GTCGTGCTGCATTACTTCAATGGC	AACACTGGAAGGAAGCGCACTTTG
SOD1	CGCATGTTCCCAGACATCTA	GAGCGGAAGATTGAGGATTG
SOD2	CTAGCCCGCTGACATTACATC	TTGCCCACATAGAAATGCAC
SOD L	AACCTGCGTGGATTTCCTGAAACTG	TGAGGCTTGGTGATGCCAATAACAC
gclc	CTATCTGGAGAACATGGAGG	CATTTTCCTCTGTTGACCGG
gclm	TGGCTTCGTCAGCACACTAAAGTG	TCACGGGAACATTAAAACAGGCCC
gpx 1a	AGATGTCATTCCTGCACACG	AAGGAGAAGCTTCCTCAGCC
gpx 1b	TCTTGGAGAAAGTGGACGTGAACG	TGCTATGCTAAGCAAGAACGGGAC
gpx 7	TTGTGGGTATTGGGGCAAACAATGC	TAATCTCACGCTGCGCTGTTTGAAG
gpx 8	TTTTAACGTGCTCGCGTTTCCCTG	ATTCCTGACAAGCGTTGTGGCTTC
nrf-2	CAGACGGAGGAGGAGCGGGA	GGCACTGCTGCAACTCTGGGA
nqo1	AGCACAAGGTGGAGCAGGCG	CGCAGCACTCCATTCTGTAAGGGC
hmox	TGTTGAAGGCGTAAGACTCC	GGTGTAAGCGTGCGCCACCA
B-actin	AAGCAGGAGTACGATGAGTC	TGGAGTCCTCAGATGCATTG