

### S3. Supplemental figures and tables for the kinetic model

**Table S3.** Lists of the rate constants of newly added reactions related to anthraquinone in the present study. The rate constant is given in the form of  $k = AT^n e^{-E_a/RT}$ . The units of the parameters are  $\text{cm}^3$ , mol, atm, s, cal/mol, K.

Reactions	Rate constants		
	A	n	Ea
<b>Combination reactions of small oxygenated aromatic species</b>			
Combination reactions			
$\text{C}_6\text{H}_5\text{CHO} + \text{C}_6\text{H}_5\text{CO} = \text{A}_1\text{CHO} - \text{A}_1\text{CO} - \text{o}$	$1.69 \times 10^3$	2.61	11180
$\text{A}_1\text{CHO} - \text{A}_1\text{CO} - \text{o} = \text{A}_1\text{CHO} - \text{CO} - \text{A}_1 + \text{H}$	$2.19 \times 10^{12}$	0.45	33410
$\text{A}_1\text{CO} - \text{CO} - \text{A}_1 = \text{ATQuinonyl}$	$2.31 \times 10^{10}$	0.39	10050
$\text{ATQuinonyl} = \text{ANTHRQNONE} + \text{H}$	$1.07 \times 10^{11}$	0.80	27440
$\text{A}_1\text{CHO} - \text{A}_1\text{CO} - \text{o} = \text{C}_6\text{H}_6\text{CHO} - \text{CO} - \text{C}_6\text{H}_4$	$1.49 \times 10^9$	0.81	48480
$\text{C}_6\text{H}_6\text{CHO} - \text{CO} - \text{C}_6\text{H}_4 = \text{C}_6\text{H}_6 - \text{COH} - \text{CO} - \text{A}_1$	$4.03 \times 10^{13}$	-0.80	2760
$\text{C}_6\text{H}_6 - \text{COH} - \text{CO} - \text{A}_1 = \text{C}_6\text{H}_6 - \text{CO} - \text{CO} - \text{A}_1 + \text{H}$	$2.59 \times 10^{11}$	0.84	23460
$\text{C}_6\text{H}_6 - \text{CO} - \text{CO} - \text{A}_1 \Rightarrow \text{ATQ} + \text{H}_2$	$4.92 \times 10^9$	1.15	83030
$\text{A}_1\text{CHO} - \text{A}_1\text{CO} - \text{o} = \text{ATQuinonyl} - \text{OH}$	$1.99 \times 10^7$	1.10	60270
$\text{ATQuinonyl} - \text{OH} = \text{ATQ} - \text{OH} + \text{H}$	$1.39 \times 10^{10}$	1.00	25580
$\text{ATQ} - \text{OH} \Rightarrow \text{ANTHRQNONE} + \text{H}_2$	$1.40 \times 10^{10}$	0.83	82360
$\text{C}_6\text{H}_5\text{CO} + \text{C}_6\text{H}_4\text{CHO} \Rightarrow \text{A}_1\text{CHO} - \text{CO} - \text{A}_1$	$5.00 \times 10^{12}$	0.0	0.0
$\text{C}_6\text{H}_5\text{CHO} + \text{C}_6\text{H}_4\text{CHO} \Rightarrow \text{A}_1\text{CHO} - \text{CO} - \text{A}_1 + \text{H}$	$3.35 \times 10^4$	2.090	-411
H-abstraction of $\text{A}_1\text{CHO} - \text{CO} - \text{A}_1$			
$\text{A}_1\text{CHO} - \text{CO} - \text{A}_1 + \text{H} = \text{A}_1\text{CO} - \text{CO} - \text{A}_1 + \text{H}_2$	$4.000 \times 10^{13}$	0.0	3200
$\text{A}_1\text{CHO} - \text{CO} - \text{A}_1 + \text{O} = \text{A}_1\text{CO} - \text{CO} - \text{A}_1 + \text{OH}$	$6.000 \times 10^{12}$	0.0	1800
$\text{A}_1\text{CHO} - \text{CO} - \text{A}_1 + \text{OH} = \text{A}_1\text{CO} - \text{CO} - \text{A}_1 + \text{H}_2\text{O}$	$7.800 \times 10^{12}$	0.0	0.0
$\text{A}_1\text{CHO} - \text{CO} - \text{A}_1 + \text{HO}_2 = \text{A}_1\text{CO} - \text{CO} - \text{A}_1 + \text{H}_2\text{O}_2$	$3.000 \times 10^{12}$	0.0	11000
$\text{A}_1\text{CHO} - \text{CO} - \text{A}_1 + \text{CH}_3 = \text{A}_1\text{CO} - \text{CO} - \text{A}_1 + \text{CH}_4$	$2.000 \times 10^{-6}$	5.6	1500
$\text{A}_1\text{CHO} - \text{CO} - \text{A}_1 + \text{C}_2\text{H}_5 = \text{A}_1\text{CO} - \text{CO} - \text{A}_1 + \text{C}_2\text{H}_6$	$1.300 \times 10^{12}$	0.0	7500
$\text{A}_1\text{CHO} - \text{CO} - \text{A}_1 + \text{C}_3\text{H}_5 - \text{A} = \text{A}_1\text{CO} - \text{CO} - \text{A}_1 + \text{C}_3\text{H}_6$	$1.300 \times 10^{12}$	0.0	11500
$\text{A}_1\text{CHO} - \text{CO} - \text{A}_1 + \text{C}_4\text{H}_5 - \text{I} = \text{A}_1\text{CO} - \text{CO} - \text{A}_1 + \text{C}_4\text{H}_6$	$1.300 \times 10^{12}$	0.0	11500
$\text{A}_1\text{CHO} - \text{CO} - \text{A}_1 + \text{C}_4\text{H}_5 - \text{N} = \text{A}_1\text{CO} - \text{CO} - \text{A}_1 + \text{C}_4\text{H}_6$	$1.300 \times 10^{12}$	0.0	7500
$\text{A}_1\text{CHO} - \text{CO} - \text{A}_1 + \text{C}_5\text{H}_5 = \text{A}_1\text{CO} - \text{CO} - \text{A}_1 + \text{C}_5\text{H}_6$	$1.300 \times 10^{11}$	0.0	11500
$\text{A}_1\text{CHO} - \text{CO} - \text{A}_1 + \text{C}_6\text{H}_5 = \text{A}_1\text{CO} - \text{CO} - \text{A}_1 + \text{C}_6\text{H}_6$	$1.300 \times 10^{11}$	0.0	11500
$\text{A}_1\text{CHO} - \text{CO} - \text{A}_1 + \text{C}_6\text{H}_5\text{CH}_2 = \text{A}_1\text{CO} - \text{CO} - \text{A}_1 + \text{C}_6\text{H}_5\text{CH}_3$	$1.300 \times 10^{11}$	0.0	11500
$\text{A}_1\text{CHO} - \text{CO} - \text{A}_1 + \text{C}_6\text{H}_5\text{O} = \text{A}_1\text{CO} - \text{CO} - \text{A}_1 + \text{C}_6\text{H}_5\text{OH}$	$1.300 \times 10^{11}$	0.0	11500
H-abstraction of $\text{C}_6\text{H}_5\text{CHO}$			
$\text{C}_6\text{H}_5\text{CHO} + \text{H} = \text{C}_6\text{H}_4\text{CHO} + \text{H}_2$	$2.80 \times 10^8$	1.915	14800
$\text{C}_6\text{H}_5\text{CHO} + \text{O}_2 = \text{C}_6\text{H}_4\text{CHO} + \text{HO}_2$	$5.25 \times 10^{13}$	0.0	63900
$\text{C}_6\text{H}_5\text{CHO} + \text{O} = \text{C}_6\text{H}_4\text{CHO} + \text{OH}$	$8.08 \times 10^6$	2.208	9380
$\text{C}_6\text{H}_5\text{CHO} + \text{OH} = \text{C}_6\text{H}_4\text{CHO} + \text{H}_2\text{O}$	$2.628 \times 10^4$	2.683	733.3
$\text{C}_6\text{H}_5\text{CHO} + \text{HO}_2 = \text{C}_6\text{H}_4\text{CHO} + \text{H}_2\text{O}_2$	$1.44 \times 10^2$	3.384	22595
$\text{C}_6\text{H}_5\text{CHO} + \text{CH}_3 = \text{C}_6\text{H}_4\text{CHO} + \text{CH}_4$	442.7	3.2885	14601
$\text{C}_6\text{H}_5\text{CHO} + \text{CH}_2\text{O} = \text{C}_6\text{H}_4\text{CHO} + \text{HCO}$	$7.13 \times 10^4$	2.190	38
$\text{C}_6\text{H}_5\text{CHO} + \text{C}_6\text{H}_5\text{OH} = \text{C}_6\text{H}_4\text{CHO} + \text{C}_6\text{H}_5\text{O}$	$4.90 \times 10^{12}$	0.0	4400
Combination reaction for 4-methylanisole fuel			
$\text{CH}_3\text{C}_6\text{H}_4\text{CHO} + \text{C}_6\text{H}_5\text{CO} = \text{CH}_3\text{A}_1\text{CHO} - \text{CO} - \text{A}_1 + \text{H}$	$1.685 \times 10^3$	2.608	11180
$\text{C}_6\text{H}_5\text{CHO} + \text{CH}_3\text{C}_6\text{H}_4\text{CO} = \text{CH}_3\text{A}_1\text{CHO} - \text{CO} - \text{A}_1 + \text{H}$	$1.685 \times 10^3$	2.608	11180
$\text{CH}_3\text{C}_6\text{H}_4\text{CO} + \text{C}_6\text{H}_4\text{CHO} \Rightarrow \text{CH}_3\text{A}_1\text{CHO} - \text{CO} - \text{A}_1$	$5.00 \times 10^{12}$	0.0	0.0
$\text{C}_6\text{H}_5\text{CO} + \text{CH}_3\text{C}_6\text{H}_3\text{CHO} \Rightarrow \text{CH}_3\text{A}_1\text{CHO} - \text{CO} - \text{A}_1$	$5.00 \times 10^{12}$	0.0	0.0
$\text{CH}_3\text{C}_6\text{H}_4\text{CHO} + \text{C}_6\text{H}_4\text{CHO} \Rightarrow \text{CH}_3\text{A}_1\text{CHO} - \text{CO} - \text{A}_1 + \text{H}$	$2.91 \times 10^4$	2.090	-411
$\text{C}_6\text{H}_5\text{CHO} + \text{CH}_3\text{C}_6\text{H}_3\text{CHO} \Rightarrow \text{CH}_3\text{A}_1\text{CHO} - \text{CO} - \text{A}_1 + \text{H}$	$2.91 \times 10^4$	2.090	-411
$\text{A}_1\text{CHO} - \text{CO} - \text{A}_1 + \text{CH}_3 = \text{CH}_3\text{C}_6\text{H}_4\text{CHO} + \text{C}_6\text{H}_5\text{CO}$	$1.2 \times 10^{12}$	0.0	15200
$\text{CH}_3\text{A}_1\text{CHO} - \text{CO} - \text{A}_1 + \text{CH}_3 = \text{CH}_3\text{C}_6\text{H}_4\text{CHO} + \text{CH}_3\text{C}_6\text{H}_4\text{CO}$	$1.2 \times 10^{12}$	0.0	15200
$\text{CH}_3\text{C}_6\text{H}_4\text{CHO} + \text{CH}_3\text{C}_6\text{H}_3\text{CHO} = \text{CH}_3\text{A}_1\text{CHOCOA}_1\text{CH}_3 + \text{H}$	$3.35 \times 10^4$	2.090	-411
$\text{CH}_3\text{C}_6\text{H}_4\text{CHO} + \text{CH}_3\text{C}_6\text{H}_4\text{CO} \Rightarrow \text{CH}_3\text{A}_1\text{CHOCOA}_1\text{CH}_3 + \text{H}$	$1.685 \times 10^3$	2.608	11180

<b>H-abstraction of CH<sub>3</sub>C<sub>6</sub>H<sub>4</sub>CHO</b>			
CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> CHO +H = CH <sub>3</sub> C <sub>6</sub> H <sub>3</sub> CHO+H <sub>2</sub>	2.24×10 <sup>8</sup>	1.915	14800
CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> CHO +O <sub>2</sub> = CH <sub>3</sub> C <sub>6</sub> H <sub>3</sub> CHO +HO <sub>2</sub>	4.20×10 <sup>13</sup>	0.0	63900
CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> CHO +O = CH <sub>3</sub> C <sub>6</sub> H <sub>3</sub> CHO +OH	6.47×10 <sup>6</sup>	2.208	9380
CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> CHO +OH = CH <sub>3</sub> C <sub>6</sub> H <sub>3</sub> CHO +H <sub>2</sub> O	2.103×10 <sup>4</sup>	2.683	733.3
CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> CHO +HO <sub>2</sub> = CH <sub>3</sub> C <sub>6</sub> H <sub>3</sub> CHO +H <sub>2</sub> O <sub>2</sub>	1.15×10 <sup>2</sup>	3.384	22595
CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> CHO +CH <sub>3</sub> = CH <sub>3</sub> C <sub>6</sub> H <sub>3</sub> CHO +CH <sub>4</sub>	353	3.2885	14601
CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> CHO = CH <sub>3</sub> C <sub>6</sub> H <sub>3</sub> CHO +H			
PLOG / 3.95×10 <sup>-2</sup>	0.90×10 <sup>108</sup>	-25.81	181750
PLOG / 1.00	4.21×10 <sup>60</sup>	-12.40	148070
PLOG / 10	3.67×10 <sup>38</sup>	-6.178	132000
<b>H-abstraction of CH<sub>3</sub>A<sub>1</sub>CHO-CO-A<sub>1</sub>CH<sub>3</sub></b>			
CH <sub>3</sub> A <sub>1</sub> CHO-CO-A <sub>1</sub> CH <sub>3</sub> +H = CH <sub>3</sub> A <sub>1</sub> COCOA <sub>1</sub> CH <sub>3</sub> +H <sub>2</sub>	4.000×10 <sup>13</sup>	0.0	3200
CH <sub>3</sub> A <sub>1</sub> CHO-CO-A <sub>1</sub> CH <sub>3</sub> +O = CH <sub>3</sub> A <sub>1</sub> COCOA <sub>1</sub> CH <sub>3</sub> +OH	6.000×10 <sup>12</sup>	0.0	1800
CH <sub>3</sub> A <sub>1</sub> CHO-CO-A <sub>1</sub> CH <sub>3</sub> +OH = CH <sub>3</sub> A <sub>1</sub> COCOA <sub>1</sub> CH <sub>3</sub> +H <sub>2</sub> O	7.800×10 <sup>12</sup>	0.0	0.0
CH <sub>3</sub> A <sub>1</sub> CHO-CO-A <sub>1</sub> CH <sub>3</sub> +HO <sub>2</sub> = CH <sub>3</sub> A <sub>1</sub> COCOA <sub>1</sub> CH <sub>3</sub> +H <sub>2</sub> O <sub>2</sub>	3.000×10 <sup>12</sup>	0.0	11000
CH <sub>3</sub> A <sub>1</sub> CHO-CO-A <sub>1</sub> CH <sub>3</sub> +CH <sub>3</sub> = CH <sub>3</sub> A <sub>1</sub> COCOA <sub>1</sub> CH <sub>3</sub> +CH <sub>4</sub>	2.000×10 <sup>-6</sup>	5.6	1500
CH <sub>3</sub> A <sub>1</sub> CHO-CO-A <sub>1</sub> CH <sub>3</sub> +C <sub>2</sub> H <sub>5</sub> = CH <sub>3</sub> A <sub>1</sub> COCOA <sub>1</sub> CH <sub>3</sub> +C <sub>2</sub> H <sub>6</sub>	1.300×10 <sup>12</sup>	0.0	7500
CH <sub>3</sub> A <sub>1</sub> CHO-CO-A <sub>1</sub> CH <sub>3</sub> +C <sub>3</sub> H <sub>5</sub> -A = CH <sub>3</sub> A <sub>1</sub> COCOA <sub>1</sub> CH <sub>3</sub> +C <sub>3</sub> H <sub>6</sub>	1.300×10 <sup>12</sup>	0.0	11500
CH <sub>3</sub> A <sub>1</sub> CHO-CO-A <sub>1</sub> CH <sub>3</sub> +C <sub>4</sub> H <sub>5</sub> -I = CH <sub>3</sub> A <sub>1</sub> COCOA <sub>1</sub> CH <sub>3</sub> +C <sub>4</sub> H <sub>6</sub>	1.300×10 <sup>12</sup>	0.0	11500
CH <sub>3</sub> A <sub>1</sub> CHO-CO-A <sub>1</sub> CH <sub>3</sub> +C <sub>4</sub> H <sub>5</sub> -N = CH <sub>3</sub> A <sub>1</sub> COCOA <sub>1</sub> CH <sub>3</sub> +C <sub>4</sub> H <sub>6</sub>	1.300×10 <sup>12</sup>	0.0	7500
CH <sub>3</sub> A <sub>1</sub> CHO-CO-A <sub>1</sub> CH <sub>3</sub> +C <sub>5</sub> H <sub>5</sub> = CH <sub>3</sub> A <sub>1</sub> COCOA <sub>1</sub> CH <sub>3</sub> +C <sub>5</sub> H <sub>6</sub>	1.300×10 <sup>11</sup>	0.0	11500
CH <sub>3</sub> A <sub>1</sub> CHO-CO-A <sub>1</sub> CH <sub>3</sub> +C <sub>6</sub> H <sub>5</sub> = CH <sub>3</sub> A <sub>1</sub> COCOA <sub>1</sub> CH <sub>3</sub> +C <sub>6</sub> H <sub>6</sub>	1.300×10 <sup>11</sup>	0.0	11500
CH <sub>3</sub> A <sub>1</sub> CHO-CO-A <sub>1</sub> CH <sub>3</sub> +C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub>	= 1.300×10 <sup>11</sup>	0.0	11500
CH <sub>3</sub> A <sub>1</sub> COCOA <sub>1</sub> CH <sub>3</sub> +C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>			
CH <sub>3</sub> A <sub>1</sub> CHO-CO-A <sub>1</sub> CH <sub>3</sub> +OC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub>	= 1.300×10 <sup>11</sup>	0.0	11500
CH <sub>3</sub> A <sub>1</sub> COCOA <sub>1</sub> CH <sub>3</sub> +HOC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub>			
<b>Formation of methylanthraquinone and dimethylanthraquinone, then anthraquinone formation</b>			
CH <sub>3</sub> A <sub>1</sub> CO-CO-A <sub>1</sub> => CH <sub>3</sub> ATQ910+H	1.07×10 <sup>11</sup>	0.80	27440
CH <sub>3</sub> A <sub>1</sub> COCOA <sub>1</sub> CH <sub>3</sub> => CH <sub>3</sub> ATQ910CH <sub>3</sub> +H	1.07×10 <sup>11</sup>	0.80	27440
CH <sub>3</sub> ATQ910CH <sub>3</sub> +H = CH <sub>3</sub> ATQ910+CH <sub>3</sub>	3.40×10 <sup>6</sup>	2.20	3974
CH <sub>3</sub> ATQ910+H = ANTHRQNONE+CH <sub>3</sub>	1.70×10 <sup>6</sup>	2.20	3974
<b>Consumption of methylanthraquinone and dimethylanthraquinone</b>			
CH <sub>3</sub> ATQ910+H => 2CO+C-C <sub>6</sub> H <sub>4</sub> +C <sub>7</sub> H <sub>5</sub> +H <sub>2</sub>	8.32×10 <sup>13</sup>	0.0	9480
CH <sub>3</sub> ATQ910CH <sub>3</sub> +H => 2CO+C <sub>7</sub> H <sub>6</sub> +C <sub>7</sub> H <sub>5</sub> +H <sub>2</sub>	1.66×10 <sup>14</sup>	0.0	9480
<b>HACA growth reaction from small quinone</b>			
<b>H-abstraction of p-naphthoquinone</b>			
P-OA <sub>2</sub> O+H = pNPhQH3+H <sub>2</sub>	5.992×10 <sup>7</sup>	2.051	15604.9
P-OA <sub>2</sub> O+O = pNPhQH3+OH	1.038×10 <sup>5</sup>	2.601	13217.7
P-OA <sub>2</sub> O+OH = pNPhQH3+H <sub>2</sub> O	21.54	3.511	36.7
P-OA <sub>2</sub> O+CH <sub>3</sub> = pNPhQH3+CH <sub>4</sub>	20.49	3.435	12877.4
pNPhQH3+H = P-OA <sub>2</sub> O	1.0×10 <sup>14</sup>	0.0	0.0
<b>HACA reactions from p-naphthoquinone to anthraquinone</b>			
pNPhQH3+C <sub>2</sub> H <sub>2</sub> = pNPhQH3-C <sub>2</sub> H <sub>2</sub>	6.08×10 <sup>4</sup>	2.32	1650
pNPhQH3-C <sub>2</sub> H <sub>2</sub> = pNPhQH3-C <sub>2</sub> H <sub>3</sub>	4.87×10 <sup>3</sup>	2.48	25700
pNPhQH3-C <sub>2</sub> H <sub>3</sub> +C <sub>2</sub> H <sub>2</sub> = pNPhQH3-C <sub>4</sub> H <sub>5</sub>	1.62×10 <sup>4</sup>	2.31	3420
pNPhQH3-C <sub>4</sub> H <sub>5</sub> = ATQ-H	4.24×10 <sup>11</sup>	0.05	870
ATQ-H = ANTHRQNONE+H	1.73×10 <sup>11</sup>	0.88	32690
P-OA <sub>2</sub> O+C-C <sub>6</sub> H <sub>4</sub> => ANTHRQNONE+C <sub>2</sub> H <sub>2</sub>	967	2.53	2923
<b>HACA reactions from p-benzoquinone to p-naphthoquinone</b>			
P-C <sub>6</sub> H <sub>4</sub> O <sub>2</sub> +H = P-C <sub>6</sub> H <sub>3</sub> O <sub>2</sub> +H <sub>2</sub>	1.010×10 <sup>8</sup>	2.058	13156.4
P-C <sub>6</sub> H <sub>4</sub> O <sub>2</sub> +O = P-C <sub>6</sub> H <sub>3</sub> O <sub>2</sub> +OH	3.559×10 <sup>5</sup>	2.743	9384.1
P-C <sub>6</sub> H <sub>4</sub> O <sub>2</sub> +OH = P-C <sub>6</sub> H <sub>3</sub> O <sub>2</sub> +H <sub>2</sub> O	47.30	3.472	-2005.3

$P-C_6H_4O_2+CH_3 = P-C_6H_3O_2+CH_4$	37.63	3.440	10313.9
$P-C_6H_3O_2+H = P-C_6H_4O_2$	$1.0 \times 10^{14}$	0.0	0.0
$P-C_6H_3O_2+C_2H_2 = p-C_6H_3O_2CHCH$	$7.15 \times 10^4$	2.31	1590
$p-C_6H_3O_2CHCH = p-C_6H_2O_2CHCH_2$	$4.24 \times 10^3$	2.51	26260
$p-C_6H_2O_2CHCH_2+C_2H_2 = p-C_6H_2O_2C_4H_5$	$2.11 \times 10^4$	2.31	3050
$p-C_6H_2O_2C_4H_5 = p-NPhQ-H$	$3.94 \times 10^{11}$	0.06	1050
$p-NPhQ-H = p-NPhQ+H$	$1.75 \times 10^{11}$	0.88	33140
$P-C_6H_3O_2+C_4H_4 = pC_6H_3O_2C_4H_4$	$1.325 \times 10^3$	2.837	-3548.4
$pC_6H_3O_2C_4H_4 \Rightarrow P-OA_2O+H$	$1.525 \times 10^{-1}$	3.779	38539.6
<b>Oxidation reactions of PAHs (Anthracene)</b>			
Anthracene oxidation to anthraquinone via anthracenol and others			
ANTHRACENE+O = ANTHRACENEOJ1+H PLOG / 10 PLOG / 50 PLOG / 500	$6.623 \times 10^6$ $1.184 \times 10^{10}$ $4.417 \times 10^{11}$	1.800 0.910 0.470	3974.4 6323.3 8435.7
ANTHRACENE+O = ANTHRACENOL PLOG / 0.1 PLOG / 1.0 PLOG / 10 PLOG / 50 PLOG / 500	$5.020 \times 10^{28}$ $2.409 \times 10^{22}$ $1.184 \times 10^{24}$ $1.947 \times 10^{35}$ $1.405 \times 10^{31}$	-4.720 -2.560 -2.820 -5.890 -4.730	13344.0 14995.4 21906.9 34537.5 38432.4
ANTHRACENE+OH = ANTHRACENOL+H	44.17	3.249	5590
ANTHRACENEOJ1+C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> = ANTHRACENOL+C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub>	$5.43 \times 10^{12}$	0.0	20923
ANTHRACENOL = ANTHRACENEOJ1+H PLOG / 0.1 PLOG / 1.0 PLOG / 10 PLOG / 100	$2.460 \times 10^{91}$ $1.250 \times 10^{67}$ $9.370 \times 10^{66}$ $7.630 \times 10^{14}$	-21.860 -14.820 -14.780 0.000	137144 122641 122572 86900
ANTHRACENOL+O <sub>2</sub> = ANTHRACENEOJ1+HO <sub>2</sub>	$4.000 \times 10^{13}$	0.0	38900
ANTHRACENOL+H = ANTHRACENEOJ1+H <sub>2</sub>	$1.150 \times 10^{14}$	0.0	12400
ANTHRACENOL+O = ANTHRACENEOJ1+OH	$1.300 \times 10^{13}$	0.0	2900
ANTHRACENOL+C <sub>6</sub> H <sub>5</sub> = ANTHRACENEOJ1+C <sub>6</sub> H <sub>6</sub>	$4.900 \times 10^{12}$	0.0	4400
ANTHRACENOL+OH = ANTHRACENEOJ1+H <sub>2</sub> O	$0.695 \times 10^8$	1.40	-960
ANTHRACENOL+CH <sub>3</sub> = ANTHRACENEOJ1+CH <sub>4</sub>	0.8732	3.494	4392.4
ANTHRACENOL = RANTHRACENOL+H PLOG / $3.95 \times 10^{-2}$ PLOG / 1.00 PLOG / 10	$2.25 \times 10^{107}$ $1.05 \times 10^{60}$ $9.17 \times 10^{37}$	-25.81 -12.40 -6.178	181750 148070 132000
ANTHRACENOL+OH = RANTHRACENOL+H <sub>2</sub> O	$5.257 \times 10^3$	2.683	733.3
ANTHRACENOL+H = RANTHRACENOL+H <sub>2</sub>	$5.60 \times 10^7$	1.915	14800
ANTHRACENOL+CH <sub>3</sub> = RANTHRACENOL+CH <sub>4</sub>	88.3	3.2885	14601
ANTHRACENOL+O = RANTHRACENOL+OH	$1.62 \times 10^6$	2.208	9380
ANTHRACENOL+HO <sub>2</sub> = RANTHRACENOL+H <sub>2</sub> O <sub>2</sub>	28.7	3.384	22595
ANTHRACENOL+O <sub>2</sub> = RANTHRACENOL+HO <sub>2</sub>	$1.05 \times 10^{13}$	0.0	63900
ANTHRACENOL+O = P-OANTHRACNOH+H PLOG / 10 PLOG / 50 PLOG / 500	$6.623 \times 10^6$ $1.184 \times 10^{10}$ $4.417 \times 10^{11}$	1.800 0.910 0.470	3974.4 6323.3 8435.7
RANTHRACENOL+O <sub>2</sub> = P-OANTHRACNOH+O PLOG/ 0.1 PLOG/ 1 PLOG/ 10 PLOG/ 100	$9.82 \times 10^{17}$ $8.56 \times 10^{20}$ $7.94 \times 10^{30}$ $1.48 \times 10^{44}$	-1.47 -2.27 -4.98 -8.55	4530 7190 16450 30130
RANTHRACENOL+HO <sub>2</sub> = P-OANTHRACNOH+OH	$5.000 \times 10^{12}$	0.0	0.0
RANTHRACENE1+O <sub>2</sub> = ANTHRQNONE+H	$1.0 \times 10^{13}$	0.0	8981
ANTHRACENEOJ1+O = ANTHRQNONE+H	$1.500 \times 10^{14}$	0.0	0.0
ANTHRACENEOJ1+O <sub>2</sub> = ANTHRQNONE+OH	$6.510 \times 10^7$	1.30	17667.3
P-OANTHRACNOH = ANTHRQNONE+H	$7.630 \times 10^{14}$	0.0	60013
Reactions involving anthrone and 1,8-dehydroxy-9-anthron			

ANTHRACENE+O = DHY18ANTHRON			
PLOG / 0.1	$2.409 \times 10^{59}$	-16.060	14301.9
PLOG / 1.0	$7.627 \times 10^{56}$	-14.620	15577.7
PLOG / 10	$4.617 \times 10^{42}$	-9.650	13330.1
PLOG / 50	$5.620 \times 10^{37}$	-7.790	13511.0
PLOG / 500	$3.813 \times 10^{43}$	-9.060	20957.0
DUP			
ANTHRACENE+O = DHY18ANTHRON			
PLOG / 0.1	$7.627 \times 10^{27}$	-4.970	9508.8
PLOG / 1.0	$4.013 \times 10^{24}$	-3.720	9938.0
PLOG / 10	$9.433 \times 10^{35}$	-6.770	18942.0
PLOG / 50	$1.004 \times 10^{28}$	-4.200	18411.4
PLOG / 500	$1.385 \times 10^{10}$	1.160	13228.8
DUP			
ANTHRACENE+O = ANTHRONE			
PLOG / 0.1	$6.423 \times 10^{26}$	-4.71	9508.8
PLOG / 1.0	$1.144 \times 10^{28}$	-4.74	13240.7
PLOG / 10	$3.413 \times 10^{45}$	-9.45	28383.2
PLOG / 50	$7.427 \times 10^{40}$	-10.50	40596.5
PLOG / 500	$1.224 \times 10^{38}$	-6.58	42555.9
DHY18ANTHRON = ANTHRACENEOJ1+H	$1.000 \times 10^{16}$	0.0	71400
DHY18ANTHRON+O <sub>2</sub> = ANTHRACENEOJ1+HO <sub>2</sub>	$2.000 \times 10^{13}$	0.0	20300
DHY18ANTHRON+H = ANTHRACENEOJ1+H <sub>2</sub>	$0.400 \times 10^8$	1.738	2540
DHY18ANTHRON+O = ANTHRACENEOJ1+OH	$1.475 \times 10^9$	1.322	1547.1
DHY18ANTHRON+OH = ANTHRACENEOJ1+H <sub>2</sub> O	$0.450 \times 10^6$	2.110	-1400
DHY18ANTHRON+HO <sub>2</sub> = ANTHRACENEOJ1+H <sub>2</sub> O <sub>2</sub>	2.746	3.798	1196.3
DHY18ANTHRON+CH <sub>3</sub> = ANTHRACENEOJ1+CH <sub>4</sub>	1.746	3.494	-1138.9
DHY18ANTHRON+CH <sub>3</sub> O <sub>2</sub> = ANTHRACENEOJ1+CH <sub>3</sub> O <sub>2</sub> H	1.373	3.798	1196.3
ANTHRONE = ANTHRACENEOJ1+H	$1.000 \times 10^{16}$	0.0	71400
ANTHRONE+O <sub>2</sub> = ANTHRACENEOJ1+HO <sub>2</sub>	$2.000 \times 10^{13}$	0.0	20300
ANTHRONE+H = ANTHRACENEOJ1+H <sub>2</sub>	$0.400 \times 10^8$	1.738	2540
ANTHRONE+O = ANTHRACENEOJ1+OH	$1.475 \times 10^9$	1.322	1547.1
ANTHRONE+OH = ANTHRACENEOJ1+H <sub>2</sub> O	$0.450 \times 10^6$	2.110	-1400
ANTHRONE+HO <sub>2</sub> = ANTHRACENEOJ1+H <sub>2</sub> O <sub>2</sub>	2.746	3.798	1196.3
ANTHRONE+CH <sub>3</sub> = ANTHRACENEOJ1+CH <sub>4</sub>	1.746	3.494	-1138.9
ANTHRONE+CH <sub>3</sub> O <sub>2</sub> = ANTHRACENEOJ1+CH <sub>3</sub> O <sub>2</sub> H	1.373	3.798	1196.3
DHY18ANTHRON = ANTHRACENOL			
PLOG / 1.0	$7.460 \times 10^{74}$	-17.738	90359
PLOG / 10	$2.760 \times 10^{55}$	-12.012	80069
PLOG / 100	$1.620 \times 10^{11}$	0.633	50879
RDHYANTHRACENE+O <sub>2</sub> = ANTHRONE+OH	$3.74 \times 10^3$	2.3701	24100
RDHYANTHRACENE+O = ANTHRONE+H	$5.69 \times 10^{13}$	-0.193	2640
DHYANTHRACENE+O = RDHYANTHRACENEO+H	$8.9 \times 10^{12}$	-0.15	590
DUP			
DHYANTHRACENE+O = RDHYANTHRACENEO+H	$5.6 \times 10^{12}$	-0.06	200
DUP			
RDHYANTHRACENE+O = RDHYANTHRACENEO	$5.80 \times 10^{13}$	-0.02	20
RDHYANTHRACENE+HO <sub>2</sub> = RDHYANTHRACENEO+OH	$1.37 \times 10^{14}$	0.252	5090
RDHYANTHRACENE+O <sub>2</sub> = RDHYANTHRACENEO+O	$7.78 \times 10^{15}$	-0.7	48740
RDHYANTHRACENE+HO <sub>2</sub> = ANTHRONE+H <sub>2</sub> O	$1.19 \times 10^{33}$	-6.52	13400
RDHYANTHRACENEO = ANTHRONE+H	$5.80 \times 10^{32}$	-6.5	21200
RDHYANTHRACENEO+O <sub>2</sub> = ANTHRONE+HO <sub>2</sub>	$6.0000 \times 10$	0.0	1600
ANTHRONE+H => CO+C <sub>7</sub> H <sub>5</sub> +C-C <sub>6</sub> H <sub>4</sub> +H <sub>2</sub>	$4.48 \times 10^8$	1.915	14800
ANTHRONE+OH => CO+C <sub>7</sub> H <sub>5</sub> +C-C <sub>6</sub> H <sub>4</sub> +H <sub>2</sub> O	$3.12 \times 10^4$	2.683	733.2
<b>Consumption reactions of anthraquinone</b>			
ANTHRQNONE+H => 2CO+C <sub>6</sub> H <sub>3</sub> +C-C <sub>6</sub> H <sub>4</sub> +H <sub>2</sub>	$4.48 \times 10^8$	1.915	14800
ANTHRQNONE+OH => 2CO+C <sub>6</sub> H <sub>3</sub> +C-C <sub>6</sub> H <sub>4</sub> +H <sub>2</sub> O	$3.12 \times 10^4$	2.683	733.2
ANTHRQNONE+OH => 2CO+C-C <sub>6</sub> H <sub>4</sub> +C <sub>6</sub> H <sub>4</sub> OH	$1.325 \times 10^2$	3.249	5590