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**APPENDIX B**

**SCREENING TABLES AND REFERENCE VALUES**

**FOR THE WATER PATHWAY**

Note: The following exhibits are provided using  $K_{ow}$  values from the DEA (U.S. EPA, 1992a). EPA is currently revising criteria for selecting  $K_{ow}$  values, and these exhibits will be updated with appropriate  $K_{ow}$  values, as well as expanded to include more chemicals. The new changes may also affect Equation 3.8 and all other related evaluations.

**EXHIBIT B-1**

**FLYNN DATA SET**

Notes:

1. The predicted  $K_p$  was calculated using Equation 3.8 and the Lotus spreadsheet software, and is the average value of the regression correlation equation.
2. 95% LCL (lower confidence level) and UCL (upper confidence level) of  $K_p$  are calculated using the statistical software package STATA (STATA Corporation, 702 University Drive East, College Station, Texas 77840, USA).
3. Compounds in italics are common to both the Flynn data set and the organic data set. For these compounds, the 95% LCL and UCL are obtained from Exhibit B-1 and are common to both Exhibits B-1 and B-2.

	Flynn's in vitro experimental data	MW	Log $K_{ow}$	$K_p$ 95% LCL	$K_p$ Predicted (cm/hr)	$K_p$ Measured (in vitro data) cm/hr	$K_p$ 95% UCL
1	Aldosterone	360.4	1.08	4.4E-05	7.8E-05	3.0E-06	1.4E-04
2	Amobarbital	226.3	1.96	1.2E-03	1.7E-03	2.3E-03	2.4E-03
3	Atropine	289.4	1.81	4.1E-04	5.9E-04	8.5E-06	8.6E-04
4	Barbital	184.2	0.65	2.4E-04	3.9E-04	1.1E-04	6.4E-04
5	Benzyl alcohol	108.1	1.10	1.3E-03	2.1E-03	6.0E-03	3.4E-03
6	<i>4-Bromophenol</i>	<i>173</i>	<i>2.59</i>	<i>5.8E-03</i>	<i>8.8E-03</i>	<i>3.6E-02</i>	<i>1.3E-02</i>
7	<i>2,3-Butanediol</i>	<i>90.12</i>	<i>-0.92</i>	<i>5.2E-05</i>	<i>1.2E-04</i>	<i>4.0E-05</i>	<i>2.8E-04</i>
8	Butanoic acid (butyric acid)	88.1	0.79	9.9E-04	1.7E-03	1.0E-03	2.9E-03
9	<i>n-Butanol</i>	<i>74.12</i>	<i>0.88</i>	<i>1.3E-03</i>	<i>2.3E-03</i>	<i>2.5E-03</i>	<i>4.0E-03</i>
10	2-Butanone	72.1	0.28	5.1E-04	9.5E-04	4.5E-03	1.8E-03
11	Butobarbital	212.2	1.65	8.8E-04	1.3E-03	1.9E-04	1.8E-03
12	<i>4-Chlorocresol</i>	<i>142.6</i>	<i>3.10</i>	<i>1.7E-02</i>	<i>2.9E-02</i>	<i>5.5E-02</i>	<i>4.9E-02</i>
13	<i>2-Chlorophenol</i>	<i>128.6</i>	<i>2.15</i>	<i>5.2E-03</i>	<i>8.0E-03</i>	<i>3.3E-02</i>	<i>1.2E-02</i>
14	<i>4-Chlorophenol</i>	<i>128.6</i>	<i>2.39</i>	<i>7.3E-03</i>	<i>1.2E-02</i>	<i>3.6E-02</i>	<i>1.8E-02</i>
15	Chloroxylenol	156.6	3.39	2.1E-02	3.7E-02	5.2E-02	6.6E-02
16	Codeine	299.3	0.89	7.6E-05	1.3E-04	4.9E-05	2.2E-04
17	Cortexolone (11-desoxy-17-hydroxycorticosterone)	346.4	2.52	5.6E-04	8.4E-04	7.4E-05	1.3E-03
18	Cortexone (deoxycorticosterone)	330.4	2.88	1.2E-03	1.8E-03	4.5E-04	2.7E-03
19	Corticosterone	346.4	1.94	2.2E-04	3.5E-04	6.0E-05	5.4E-04
20	Cortisone	360.5	1.42	7.7E-05	1.3E-04	1.0E-05	2.2E-04
21	<i>o-Cresol</i>	<i>108.1</i>	<i>1.95</i>	<i>4.8E-03</i>	<i>7.7E-03</i>	<i>1.6E-02</i>	<i>1.2E-02</i>
22	<i>m-Cresol</i>	<i>108.1</i>	<i>1.96</i>	<i>4.9E-03</i>	<i>7.8E-03</i>	<i>1.5E-02</i>	<i>1.2E-02</i>
23	<i>p-Cresol</i>	<i>108.1</i>	<i>1.95</i>	<i>4.8E-03</i>	<i>7.7E-03</i>	<i>1.8E-02</i>	<i>1.2E-02</i>
24	<i>n-Decanol</i>	<i>158.3</i>	<i>4.57</i>	<i>9.5E-02</i>	<i>2.2E-01</i>	<i>7.9E-02</i>	<i>5.1E-01</i>

**EXHIBIT B-1**

**FLYNN DATA SET (continued)**

	Flynn's in vitro experimental data	MW	Log K <sub>ow</sub>	K <sub>p</sub> 95% LCL	K <sub>p</sub> Predicted (cm/hr)	K <sub>p</sub> Measured (in vitro data) cm/hr	K <sub>p</sub> 95% UCL
25	<i>2,4-Dichlorophenol</i>	163	3.06	1.2E-02	2.1E-02	6.0E-02	3.4E-02
26	Digitoxin	764.9	1.86	3.5E-07	1.4E-06	1.3E-05	5.4E-06
27	Ephedrine	165.2	1.03	5.8E-04	9.0E-04	6.0E-03	1.4E-03
28	B-estradiol	272.4	2.69	2.0E-03	2.8E-03	3.0E-04	4.1E-03
29	B-estradiol (2)	272.4	2.69	2.0E-03	2.8E-03	5.2E-03	4.1E-03
30	Estriol	288.4	2.47	1.2E-03	1.7E-03	4.0E-05	2.4E-03
31	Estrone	270.4	2.76	2.2E-03	3.3E-03	3.6E-03	4.7E-03
32	<i>Ethanol</i>	46.07	-0.31	2.6E-04	5.4E-04	7.9E-04	1.1E-03
33	<i>2-Ethoxy ethanol (Cellosolve)</i>	90.12	-0.32	1.5E-04	3.0E-04	2.5E-04	6.1E-04
34	<i>Ethyl ether</i>	74.12	0.89	1.4E-03	2.3E-03	1.6E-02	4.0E-03
35	<i>4-Ethylphenol</i>	122.2	2.58	1.0E-02	1.7E-02	3.5E-02	2.7E-02
36	Etorphine	411.5	1.86	7.6E-05	1.3E-04	3.6E-03	2.3E-04
37	Fentanyl	336.5	4.37	8.4E-03	1.6E-02	5.6E-03	3.2E-02
38	Fentanyl (2)	336.5	4.37	8.4E-03	1.6E-02	1.0E-02	3.2E-02
39	Fluocinonide	494.6	3.19	1.8E-04	3.5E-04	1.7E-03	6.8E-04
40	Heptanoic acid (enanthic acid)	130.2	2.50	8.4E-03	1.3E-02	2.0E-02	2.1E-02
41	<i>n-Heptanol</i>	116.2	2.62	1.2E-02	1.9E-02	3.2E-02	3.2E-02
42	Hexanoic acid (caproic acid)	116.2	1.90	4.1E-03	6.4E-03	1.4E-02	1.0E-02
43	<i>n-Hexanol</i>	102.2	2.03	5.8E-03	9.3E-03	1.3E-02	1.5E-02
44	Hydrocortisone	362.5	1.53	9.0E-05	1.5E-04	3.0E-06	2.5E-04
45	Hydrocortisone (2)	362.5	1.53	9.0E-05	1.5E-04	1.2E-04	2.5E-04
46	[Hydrocortisone-21-yl]-N,N dimethyl succinamate	489.6	2.03	3.1E-05	6.3E-05	6.8E-05	1.3E-04
47	[Hydrocortisone-21-yl]-hemipimelate	504.6	3.26	1.7E-04	3.4E-04	1.8E-03	6.8E-04
48	[Hydrocortisone-21-hemisuccinate	462.5	2.11	5.3E-05	1.0E-04	6.3E-04	1.9E-04
49	[Hydrocortisone-21-yl]-hexanoate	460.6	4.48	1.8E-03	3.9E-03	1.8E-02	8.2E-03
50	[Hydrocortisone-21-yl]-6-hydroxy hexanoate	476.6	2.79	1.3E-04	2.4E-04	9.1E-04	4.5E-04
51	[Hydrocortisone-21-yl]-octanoate	488.7	5.49	4.8E-03	1.3E-02	6.2E-02	3.3E-02
52	[Hydrocortisone-21-yl]-pimelamate	503.6	2.31	3.9E-05	8.0E-05	8.9E-04	1.6E-04
53	[Hydrocortisone-21-yl]-propionate	418.5	3.00	4.1E-04	6.9E-04	3.4E-03	1.2E-03
54	[Hydrocortisone-21-yl]-succinamate	461.6	1.43	1.8E-05	3.6E-05	2.6E-05	7.3E-05
55	Hydromorphone	285.3	1.25	1.7E-04	2.7E-04	1.5E-05	4.1E-04
56	Hydroxypregnenolone	330.4	3.00	1.4E-03	2.2E-03	6.0E-04	3.3E-03
57	17a-Hydroxyprogesterone	330.4	2.74	9.7E-04	1.5E-03	6.0E-04	2.2E-03
58	Isoquinoline	129.2	2.03	4.3E-03	6.6E-03	1.7E-02	1.0E-02
59	Meperidine	247	2.72	2.8E-03	4.1E-03	3.7E-03	6.0E-03
60	<i>Methanol</i>	32.04	-0.77	1.4E-04	3.2E-04	5.0E-04	7.3E-04

**EXHIBIT B-1**

**FLYNN DATA SET (continued)**

	<b>Flynn's in vitro experimental data</b>	<b>MW</b>	<b>Log K<sub>ow</sub></b>	<b>K<sub>p</sub> 95% LCL</b>	<b>K<sub>p</sub> Predicted (cm/hr)</b>	<b>K<sub>p</sub> Measured (in vitro data) cm/hr</b>	<b>K<sub>p</sub> 95% UCL</b>
61	Methyl-[hydrocortisone-21-yl]-succinate	476.6	2.58	9.1E-05	1.7E-04	2.1E-04	3.3E-04
62	Methyl-[hydrocortisone-21-yl]-pimelate	518.6	3.70	2.6E-04	5.5E-04	5.4E-03	1.2E-03
63	<i>Methyl-4-hydroxy benzoate</i>	<i>152.1</i>	<i>1.96</i>	<i>3.0E-03</i>	<i>4.4E-03</i>	<i>9.1E-03</i>	<i>6.5E-03</i>
64	Morphine	285.3	0.62	5.8E-05	1.0E-04	9.3E-06	1.8E-04
65	<i>2-Naphthol</i>	<i>144.2</i>	<i>2.84</i>	<i>1.1E-02</i>	<i>1.9E-02</i>	<i>2.8E-02</i>	<i>3.1E-02</i>
66	Naproxen	230.3	3.18	6.6E-03	1.0E-02	4.0E-04	1.6E-02
67	Nicotine	162.2	1.17	7.6E-04	1.2E-03	1.9E-02	1.8E-03
68	Nitroglycerine	227.1	2.00	1.3E-03	1.8E-03	1.1E-02	2.5E-03
69	<i>3-Nitrophenol</i>	<i>139.1</i>	<i>2.00</i>	<i>3.7E-03</i>	<i>5.5E-03</i>	<i>5.6E-03</i>	<i>8.4E-03</i>
70	<i>4-Nitrophenol</i>	<i>139.1</i>	<i>1.91</i>	<i>3.2E-03</i>	<i>4.8E-03</i>	<i>5.6E-03</i>	<i>7.3E-03</i>
71	<i>n-Nonanol</i>	<i>144.3</i>	<i>3.77</i>	<i>4.0E-02</i>	<i>7.8E-02</i>	<i>6.0E-02</i>	<i>1.5E-01</i>
72	Octanoic acid (caprylic acid)	144.2	3.00	1.4E-02	2.4E-02	2.5E-02	4.0E-02
73	<i>n-Octanol</i>	<i>130.2</i>	<i>2.97</i>	<i>1.6E-02</i>	<i>2.7E-02</i>	<i>5.2E-02</i>	<i>4.7E-02</i>
74	Pentanoic acid (valeric acid)	102.1	1.30	1.9E-03	3.1E-03	2.0E-03	4.9E-03
75	<i>n-Pentanol</i>	<i>88.15</i>	<i>1.56</i>	<i>3.4E-03</i>	<i>5.5E-03</i>	<i>6.0E-03</i>	<i>8.9E-03</i>
76	Phenobarbital	232.2	1.47	5.1E-04	7.4E-04	4.6E-04	1.1E-03
77	<i>Phenol</i>	<i>94.11</i>	<i>1.46</i>	<i>2.7E-03</i>	<i>4.3E-03</i>	<i>8.1E-03</i>	<i>7.0E-03</i>
78	Pregnenolone	316.5	3.13	2.0E-03	3.2E-03	1.5E-03	4.9E-03
79	Progesterone	314.4	3.77	5.0E-03	8.6E-03	1.5E-03	1.5E-02
80	<i>n-Propanol</i>	<i>60.1</i>	<i>0.25</i>	<i>5.6E-04</i>	<i>1.1E-03</i>	<i>1.4E-03</i>	<i>2.0E-03</i>
81	<i>Resorcinol</i>	<i>110.1</i>	<i>0.80</i>	<i>7.7E-04</i>	<i>1.3E-03</i>	<i>2.4E-04</i>	<i>2.1E-03</i>
82	Salicylic acid	138.1	2.26	5.4E-03	8.4E-03	6.3E-03	1.3E-02
83	Scopolamine	303.4	1.24	1.3E-04	2.1E-04	5.0E-05	3.3E-04
84	Sucrose	342.3	-2.25	1.6E-07	6.0E-07	5.2E-06	2.3E-06
85	Sufentanyl	387.5	4.59	5.7E-03	1.2E-02	1.2E-02	2.4E-02
86	Testosterone	288.4	3.31	3.8E-03	6.0E-03	4.0E-04	9.4E-03
87	<i>Thymol</i>	<i>150.2</i>	<i>3.34</i>	<i>2.1E-02</i>	<i>3.7E-02</i>	<i>5.2E-02</i>	<i>6.6E-02</i>
88	<i>2,4,6-Trichlorophenol</i>	<i>197.4</i>	<i>3.69</i>	<i>1.9E-02</i>	<i>3.5E-02</i>	<i>5.9E-02</i>	<i>6.2E-02</i>
89	<i>Water</i>	<i>18.01</i>	<i>-1.38</i>	<i>5.8E-05</i>	<i>1.5E-04</i>	<i>5.0E-04</i>	<i>3.9E-04</i>
90	3,4-Xylenol	122.2	2.35	7.4E-03	1.2E-02	3.6E-02	1.9E-02

## EXHIBIT B-2

### PREDICTED $K_p$ FOR ORGANIC CONTAMINANTS IN WATER

Notes:

1. Chemicals with an asterisk (\*) preceding them have been identified to be outside the effective prediction domain (EPD). EPD determination is calculated using the software package MLAB (Civilized Software, Inc., 8120 Woodmont Avenue, #250, Bethesda, MD 20814, USA).
2. Chemicals with two asterisks (\*\*) are halogenated compounds. Because halogenated chemicals have a lower ratio of molar volume relative to their molecular weight than hydrocarbons (due to the relatively weighty halogen atom), the  $K_p$  correlation based on molecular weight of hydrocarbons will tend to underestimate permeability coefficients for halogenated organic chemicals. To address this problem, a new  $K_p$  correlation based on molar volume and  $\log K_{ow}$  will be explored. In selecting the halogenated compounds, the focus was on trihalomethanes, the halogenated acids, and the halogenated aliphatics with halogenated molecules contributing to a large percentage of the molecular weight.
3.  $K_p$  is obtained from the modified Potts and Guy's equation (Equation 3.8). Values in the exhibit are obtained from the organic spreadsheet (ORG04\_01.XLS) where the coefficients of Equation 3.8 carry more significant figures than shown in Chapter 3 and Appendix A.
4. 95% LCL and UCL are calculated using the statistical software package STATA (STATA Corporation, 702 University Drive East, College Station, Texas 77840, USA). Compounds in italics are common to both the Flynn data set and the organic data set. For these compounds, the 95% LCL and UCL are obtained from Exhibit B-1 and common to both Exhibits B-1 and B-2.
5. All calculations were performed using the Lotus spreadsheet software, except where noted.

	CHEMICAL	CAS No.	MW	$\log K_{ow}$	$K_p$ 95% LCL	$K_p$ (cm/hr) predicted	$K_p$ (cm/hr) measured	$K_p$ 95% UCL
1	Acetaldehyde	75070	44.1	-0.22	2.4E-05	6.3E-04		1.6E-02
2	Acetamide	60355	59	-1.26	3.9E-06	1.1E-04		2.9E-03
3	Acetylaminofluorene, 2-	53963	223	3.24	5.0E-04	1.2E-02		3.1E-01
4	Acrolein	107028	56.1	-0.10	2.5E-05	6.5E-04		1.7E-02
5	Acrylamide	79061	71	-0.67	8.5E-06	2.2E-04		5.9E-03
6	Acrylonitrile	107131	53.1	0.25	4.5E-05	1.2E-03		2.9E-02
7	Aldrin	309002	365	3.01	5.7E-05	1.4E-03		3.5E-02
**	Allyl chloride	107051	76.5	1.45	2.2E-04	5.4E-03		1.3E-01
9	Amino-2-methylantraquinone, 1-	82280	237.3	2.80	2.2E-04	5.3E-03		1.3E-01
10	Aminoanthraquinone, 2-	117793	223	2.15	9.7E-05	2.4E-03		5.7E-02
11	Aminoazobenzene, p-	60093	197	2.62	2.8E-04	6.8E-03		1.7E-01
12	Aminoazotoluene, o-	97563	225.3	3.92	1.4E-03	3.4E-02		8.7E-01
13	Aminobiphenyl, 4-	92671	169.2	2.80	5.2E-04	1.3E-02		3.2E-01
14	Aniline	62533	93.1	0.90	7.5E-05	1.9E-03		4.7E-02
15	Anisidine, o-	90040	145	1.18	5.9E-05	1.5E-03		3.6E-02

**EXHIBIT B-2**

**PREDICTED K<sub>p</sub> FOR ORGANIC CONTAMINANTS IN WATER (continued)**

	CHEMICAL	CAS No.	MW	log K <sub>ow</sub>	K <sub>p</sub> 95% LCL	K <sub>p</sub> (cm/hr) predicted	K <sub>p</sub> (cm/hr) measured	K <sub>p</sub> 95% UCL
16	Auramine	492808	267.4	3.54	4.5E-04	1.1E-02		2.8E-01
17	Benzene	71432	78.1	2.13	5.9E-04	1.5E-02		3.7E-01
18	Benzidine	92875	184.2	1.34	4.6E-05	1.1E-03		2.8E-02
*	19	Benzo-a-anthracene	56553	228.3	5.66	1.7E-02	4.7E-01	1.3E+01
*	20	Benzo-a-pyrene	50328	250	6.10	2.4E-02	7.0E-01	2.0E+01
*	21	Benzo-b-fluoranthene	205992	252.3	6.12	2.4E-02	7.0E-01	2.0E+01
22	Benzoic acid	65850	122	1.87	2.3E-04	5.7E-03		1.4E-01
23	Benzotrichloride	98077	195	2.92	4.5E-04	1.1E-02		2.7E-01
24	Benzyl chloride	100447	127	2.30	4.1E-04	1.0E-02		2.5E-01
25	Bis(2-chloroethyl)ether	111444	143	1.29	7.2E-05	1.8E-03		4.4E-02
**	26	Bromodichloromethane	75274	163.8	2.09	1.9E-04	4.6E-03	1.1E-01
**	27	Bromoform	75252	252.8	2.37	9.2E-05	2.2E-03	5.5E-02
**	28	Bromomethane	74839	95	1.19	1.1E-04	2.8E-03	7.0E-02
29	<i>Bromophenol, p-</i>	106412	173	2.59	5.8E-03	8.8E-03		1.3E-02
30	Butadiene, 1,3-	106990	54	1.99	6.5E-04	1.6E-02		4.1E-01
31	<i>2,3-Butanediol</i>	513859	90.12	-0.92	5.2E-05	1.2E-04	4.0E-05	2.8E-04
32	<i>n-Butanol</i>	71363	74.12	0.88	1.3E-03	2.3E-03	2.5E-03	4.0E-03
33	Butoxyethanol, 2-	111762	118	0.83	4.9E-05	1.2E-03		3.0E-02
34	Captan	133062	300	2.35	4.8E-05	1.2E-03		2.9E-02
35	Carbon disulfide	75150	80	2.24	6.9E-04	1.7E-02		4.3E-01
**	36	Carbon tetrachloride	56235	153.8	2.83	6.6E-04	1.6E-02	4.0E-01
37	Chlordane	57749	409.8	5.54	1.4E-03	3.8E-02		1.0E+00
38	Chlordane (cis)	5103719	410	5.47	1.2E-03	3.4E-02		9.2E-01
39	Chlordane (trans)	5103742	410	5.47	1.2E-03	3.4E-02		9.2E-01
40	Chlorobenzene	108907	112.6	2.84	1.1E-03	2.8E-02		7.1E-01
41	<i>4-Chlorocresol</i>	59507	142.6	3.10	1.7E-02	2.9E-02	5.5E-02	4.9E-02
**	42	Chlorodibromomethane	124481	208.3	2.23	1.3E-04	3.2E-03	7.9E-02
**	43	Chloroethane	75003	64.5	1.43	2.4E-04	6.1E-03	1.5E-01
**	44	Chloroform	67663	119.4	1.97	2.8E-04	6.8E-03	1.7E-01
**	45	Chloromethane	74873	50.5	0.91	1.3E-04	3.3E-03	8.3E-02
46	<i>2-Chlorophenol</i>	95578	128.6	2.15	5.2E-03	8.0E-03	3.3E-02	1.2E-02
47	<i>4-Chlorophenol</i>	106489	128.6	2.39	7.3E-03	1.2E-02	3.6E-02	1.8E-02
48	Chlorothalonil	1897456	265.9	3.86	7.4E-04	1.9E-02		4.7E-01
*	49	Chrysene	218019	228.3	5.66	1.7E-02	4.7E-01	1.3E+01
50	Cresidine, p-	120718	137.2	1.67	1.4E-04	3.4E-03		8.4E-02
51	<i>m-Cresol</i>	108394	108.1	1.96	4.9E-03	7.8E-03	1.5E-02	1.2E-02
52	<i>o-Cresol</i>	95487	108.1	1.95	4.8E-03	7.7E-03	1.6E-02	1.2E-02
53	<i>p-Cresol</i>	106445	108.1	1.95	4.8E-03	7.7E-03	1.8E-02	1.2E-02
*	54	DDD	72548	320	5.80	6.4E-03	1.8E-01	5.0E+00
*	55	DDE	72559	318	5.69	5.6E-03	1.6E-01	4.3E+00

**EXHIBIT B-2**

**PREDICTED  $K_p$  FOR ORGANIC CONTAMINANTS IN WATER (continued)**

	CHEMICAL	CAS No.	MW	log $K_{ow}$	$K_p$ 95% LCL	$K_p$ (cm/hr) predicted	$K_p$ (cm/hr) measured	$K_p$ 95% UCL
*	56 DDT	50293	355	6.36	9.2E-03	2.7E-01		7.8E+00
*	57 <i>n-Decanol</i>	112301	158.3	4.57	9.5E-02	2.2E-01	7.9E-02	5.1E-01
	58 Di-2-ethylhexyl phthalate	117817	391	5.11	9.4E-04	2.5E-02		6.6E-01
	59 Diaminoanisole, 2,4-	615054	138.2	-0.12	8.5E-06	2.2E-04		5.6E-03
	60 Diaminotoluene	95807	122	0.34	2.2E-05	5.4E-04		1.4E-02
	61 Diaminotoluene, 2,4-	101804	200	2.06	1.1E-04	2.8E-03		6.7E-02
*	62 Dibenzo(a,h)anthracene	53703	278.4	6.84	4.9E-02	1.5E+00		4.7E+01
	63 Dibutyl phthalate	84742	278	4.13	9.4E-04	2.4E-02		6.1E-01
	64 Dichlorobenzene, 1,2-	95501	147	3.38	1.6E-03	4.1E-02		1.0E+00
	65 Dichlorobenzene, 1,3-	541731	147	3.60	2.3E-03	5.8E-02		1.5E+00
	66 Dichlorobenzene, 1,4-	106467	147	3.39	1.7E-03	4.2E-02		1.1E+00
	67 Dichlorobenzidine, 3,3'	91941	253.1	3.51	5.1E-04	1.3E-02		3.2E-01
**	68 Dichlorodifluoromethane	75718	120.9	2.16	3.6E-04	9.0E-03		2.2E-01
**	69 Dichloroethane, 1,1-	75343	99	1.79	2.7E-04	6.7E-03		1.7E-01
**	70 Dichloroethane, 1,2-	107062	99	1.48	1.7E-04	4.2E-03		1.0E-01
**	71 Dichloroethylene, 1,1-	75354	96.9	2.13	4.7E-04	1.2E-02		2.9E-01
**	72 Dichloroethylene, 1,2- (trans)	540590	96.9	1.86	3.1E-04	7.7E-03		1.9E-01
	73 <i>2,4-Dichlorophenol</i>	120832	163	3.06	1.2E-02	2.1E-02	6.0E-02	3.4E-02
**	74 Dichloropropane, 1,2-	78875	113	2.00	3.1E-04	7.8E-03		1.9E-01
**	75 Dichloropropene, 1,3-	542756	111	1.60	1.7E-04	4.3E-03		1.1E-01
	76 Dichlorvos	62737	221	1.47	3.5E-05	8.5E-04		2.1E-02
	77 Dieldrin	60571	381	4.56	4.7E-04	1.2E-02		3.2E-01
	78 Diepoxybutane	1464535	86.1	-1.84	1.1E-06	3.1E-05		8.7E-04
	79 Diethyl phthalate	84662	222	2.47	1.6E-04	3.9E-03		9.5E-02
	80 Diethyl sulfate	64675	154	1.14	5.0E-05	1.2E-03		3.0E-02
	81 Dimethoxybenzidine, 3,3'-	119904	254.4	1.81	3.8E-05	9.3E-04		2.3E-02
	82 Dimethyl phthalate	131113	194	1.56	5.7E-05	1.4E-03		3.4E-02
	83 Dimethyl sulfate	77781	126	1.16	7.3E-05	1.8E-03		4.5E-02
	84 Dimethylamine, n-nitroso-	62759	74.1	-0.57	9.6E-06	2.5E-04		6.6E-03
	85 Dimethylaminoazobenzene, 4-	60117	225	4.58	3.6E-03	9.5E-02		2.5E+00
	86 Dimethylbenzidine, 3,3'-	119937	212.3	2.34	1.5E-04	3.6E-03		8.8E-02
	87 Dimethylcarbonyl chloride	79447	107.5	0.00	4.9E-06	3.9E-04		3.4E-03
	88 Dimethylhydrazine, 1,1-	57147	60	-1.50	2.6E-06	7.3E-05		2.0E-03
	89 Dimethylphenol, 2,4-	105679	122.2	2.30	4.4E-04	1.1E-02		2.7E-01
	90 Dimethylphenol, 3,4-	95658	122	2.23	4.0E-04	9.8E-03		2.4E-01
	91 Dinitrophenol, 2,4-	51285	184.1	1.54	6.3E-05	1.5E-03		3.7E-02
	92 Dinitrotoluene, 2,4-	121142	182.1	1.98	1.3E-04	3.1E-03		7.5E-02
	93 Dinitrotoluene, 2,6-	606202	182.1	1.72	8.5E-05	2.1E-03		5.1E-02
	94 Dioxane, 1,4-	123911	88.1	-0.27	1.3E-05	3.3E-04		8.6E-03
	95 Diphenylamine, n-nitroso-	86306	198.2	3.13	5.9E-04	1.5E-02		3.6E-01

**EXHIBIT B-2**

**PREDICTED  $K_p$  FOR ORGANIC CONTAMINANTS IN WATER** (continued)

	CHEMICAL	CAS No.	MW	log $K_{ow}$	$K_p$ 95% LCL	$K_p$ (cm/hr) predicted	$K_p$ (cm/hr) measured	$K_p$ 95% UCL
96	Diphenylhydrazine, 1,2-	122667	184.2	2.94	5.3E-04	1.3E-02		3.2E-01
97	Dipropylamine, n-nitroso-	621647	130.2	1.36	9.5E-05	2.3E-03		5.8E-02
98	Endrin	72208	381	4.56	4.7E-04	1.2E-02		3.2E-01
99	Epichlorohydrin	106898	92	-0.21	1.3E-05	3.5E-04		8.9E-03
100	<i>Ethanol</i>	64175	46.07	-0.31	2.6E-04	5.4E-04	7.9E-04	1.1E-03
101	Ethanol, 2-(2-butoxyethoxy)-	112345	162	-0.92	1.8E-06	4.7E-05		1.3E-03
102	Ethanol, 2-(2-ethoxyethoxy)-	111900	134	-0.08	9.6E-06	2.5E-04		6.3E-03
103	Ethanol, 2-(2-methoxyethoxy)-	111773	120	-0.42	6.7E-06	1.7E-04		4.5E-03
104	<i>2-Ethoxy ethanol (Cellosolve)</i>	110805	90.12	-0.32	1.5E-04	3.0E-04		6.1E-04
105	Ethoxyethyl acetate, 2-	111159	132	0.65	3.1E-05	7.7E-04		1.9E-02
106	Ethyl acrylate	140885	100	1.32	1.3E-04	3.2E-03		8.0E-02
107	Ethyl carbamate	51796	89	-0.15	1.5E-05	3.9E-04		1.0E-02
108	<i>Ethyl ether</i>	60297	74.12	0.89	1.4E-03	2.3E-03	1.6E-02	4.0E-03
109	Ethylbenzene	100414	106.2	3.15	1.9E-03	4.9E-02		1.2E+00
110	Ethylene oxide	75218	44.1	-0.30	2.2E-05	5.6E-04		1.5E-02
** 111	Ethylenedibromide	106934	188	1.96	1.1E-04	2.8E-03		6.8E-02
112	Ethyleneimine	151564	43	-1.12	6.0E-06	1.6E-04		4.4E-03
113	Ethylenethiourea	96457	96	-0.66	6.3E-06	1.7E-04		4.3E-03
114	<i>4-Ethylphenol</i>	123079	122.2	2.58	1.0E-02	1.7E-02	3.5E-02	2.7E-02
* 115	Fluoranthene	206440	202.3	4.95	8.3E-03	2.2E-01		6.0E+00
116	Formaldehyde	50000	30	0.35	7.1E-05	1.8E-03		4.6E-02
117	Glycerol	56815	92.1	-1.76	1.1E-06	3.2E-05		9.1E-04
118	Heptachlor	76448	373.5	4.27	3.4E-04	8.6E-03		2.2E-01
119	<i>n-Heptanol</i>	111706	116.2	2.62	1.2E-02	1.9E-02	3.2E-02	3.2E-02
* 120	Hexachlorobenzene	118741	284.8	5.31	4.9E-03	1.3E-01		3.6E+00
** 121	Hexachlorobutadiene	87683	260.8	4.78	3.1E-03	8.1E-02		2.1E+00
** 122	Hexachloroethane	67721	236.7	3.93	1.2E-03	3.0E-02		7.6E-01
123	Hexamethylphosphoramide	680319	179	0.03	6.4E-06	1.6E-04		4.1E-03
124	<i>n-Hexanol</i>	111273	102.2	2.03	5.8E-03	9.3E-03	1.3E-02	1.5E-02
* 125	Hydrazine/Hydrazine sulfate	302012	32	-2.07	1.5E-06	4.4E-05		1.3E-03
* 126	Indeno(1,2,3-CD)pyrene	193395	276.3	6.58	3.5E-02	1.0E+00		3.1E+01
127	Isophorone	78591	138.2	1.67	1.4E-04	3.4E-03		8.3E-02
128	Lindane	58899	291	3.72	4.3E-04	1.1E-02		2.7E-01
129	Mechlorethamine	51752	156	1.07	4.4E-05	1.1E-03		2.6E-02
130	<i>Methanol</i>	67561	32.04	-0.77	1.4E-04	3.2E-04	5.0E-04	7.3E-04
131	Methoxyethanol, 2-	109864	76	-0.77	6.8E-06	1.8E-04		4.8E-03
132	Methoxypropan-2-ol, 1-	107982	90	-0.18	1.4E-05	3.7E-04		9.6E-03
133	Methyl ethyl ketone	78933	72	0.29	3.8E-05	9.6E-04		2.4E-02
134	<i>Methyl-4-hydroxy benzoate</i>	99763	152.1	1.96	3.0E-03	4.4E-03	9.1E-03	6.5E-03
** 135	Methyl iodide	74884	142	1.51	1.0E-04	2.5E-03		6.2E-02

**EXHIBIT B-2**

**PREDICTED  $K_p$  FOR ORGANIC CONTAMINANTS IN WATER** (continued)

	CHEMICAL	CAS No.	MW	log $K_{ow}$	$K_p$ 95% LCL	$K_p$ (cm/hr) predicted	$K_p$ (cm/hr) measured	$K_p$ 95% UCL
136	Methylaziridine, 2-	75558	57	-0.60	1.1E-05	3.0E-04		7.9E-03
137	Methylene bis(2-chloroaniline), 4,4'-	101144	267.2	3.94	8.2E-04	2.1E-02		5.2E-01
138	Methylene bis(N,N'-dimethyl)aniline, 4,4'-	101611	254	4.75	3.2E-03	8.4E-02		2.2E+00
** 139	Methylene chloride	75092	84.9	1.25	1.4E-04	3.5E-03		8.8E-02
140	Methylenedianiline, 4,4'-	101779	198	1.59	5.7E-05	1.4E-03		3.4E-02
141	Michler's ketone	90948	268.4	4.07	9.8E-04	2.5E-02		6.3E-01
** 142	Mustard Gas	505602	159.1	2.03	1.8E-04	4.5E-03		1.1E-01
143	Naphthalene	91203	128.2	3.30	1.8E-03	4.7E-02		1.2E+00
144	<i>2-Naphthol</i>	<i>135193</i>	<i>144.2</i>	<i>2.84</i>	<i>1.1E-02</i>	<i>1.9E-02</i>	<i>2.8E-02</i>	<i>3.1E-02</i>
145	Naphthylamine, 1-	134327	143.2	2.25	3.1E-04	7.7E-03		1.9E-01
146	Naphthylamine, 2-	91598	143.2	2.28	3.3E-04	8.1E-03		2.0E-01
147	Nitrilotriacetic acid	139139	191	-0.18	3.9E-06	1.0E-04		2.6E-03
148	Nitro-o-anisidine, 5-	99592	152.7	1.47	8.4E-05	2.1E-03		5.1E-02
149	Nitrobiphenyl, 4-	92933	199.2	3.77	1.5E-03	3.8E-02		9.7E-01
* 150	Nitrofen	1836755	284.1	5.53	6.8E-03	1.9E-01		5.2E+00
151	Nitrophenol, 2-	88755	139.1	1.79	1.6E-04	4.0E-03		9.9E-02
152	Nitrophenol, 2-amino-4-	99570	154.1	1.36	7.0E-05	1.7E-03		4.2E-02
153	<i>3-Nitrophenol</i>	<i>554847</i>	<i>139.1</i>	<i>2.00</i>	<i>3.7E-03</i>	<i>5.5E-03</i>	<i>5.6E-03</i>	<i>8.4E-03</i>
154	<i>4-Nitrophenol</i>	<i>100027</i>	<i>139.1</i>	<i>1.91</i>	<i>3.2E-03</i>	<i>4.8E-03</i>	<i>5.6E-03</i>	<i>7.3E-03</i>
155	Nitrophenol, 4-amino-2-	119346	154.1	0.96	3.8E-05	9.3E-04		2.3E-02
156	Nitropropane, 2-	79469	110	0.55	3.5E-05	8.8E-04		2.2E-02
157	Nitroso-di-n-butylamine, n-	924163	158.2	1.92	1.6E-04	3.8E-03		9.4E-02
158	Nitroso-N-ethylurea, n-	759739	117.1	0.23	1.9E-05	4.9E-04		1.2E-02
159	Nitroso-N-methylurea, n-	684935	103.1	-0.03	1.5E-05	3.9E-04		1.0E-02
160	Nitrosodiethanolamine, n-	1116547	134	-1.58	8.9E-07	2.5E-05		6.9E-04
161	Nitrosodiethylamine, n-	55185	88	0.48	4.2E-05	1.0E-03		2.6E-02
162	Nitrosodiphenylamine, p-	156105	198.2	3.50	1.0E-03	2.6E-02		6.4E-01
163	Nitrosomethylvinylamine, n-	4549400	86.1	0.00	2.0E-05	5.1E-04		1.3E-02
164	Nitrosomorpholine, n-	59892	116.1	-0.44	6.9E-06	1.8E-04		4.6E-03
165	Nitrosornicotine, n-	16543558	177.2	0.03	6.5E-06	1.7E-04		4.2E-03
166	Nitrosopiperidine, n-	100754	350.3	0.36	1.1E-06	2.9E-05		7.6E-04
167	<i>n-Nonanol</i>	<i>143088</i>	<i>144.3</i>	<i>3.77</i>	<i>4.0E-02</i>	<i>7.8E-02</i>	<i>6.0E-02</i>	<i>1.5E-01</i>
168	<i>n-Octanol</i>	<i>111875</i>	<i>130.2</i>	<i>2.97</i>	<i>1.6E-02</i>	<i>2.7E-02</i>	<i>5.2E-02</i>	<i>4.7E-02</i>
169	Parathion	56382	291	3.83	5.1E-04	1.3E-02		3.2E-01
* 170	PCB-chlorobiphenyl, 4-	2051629	292	6.50	2.5E-02	7.5E-01		2.2E+01
* 171	PCB-hexachlorobiphenyl	26601649	361	6.72	1.4E-02	4.3E-01		1.3E+01
** 172	Pentachloronitrobenzene	82688	295.3	4.64	1.6E-03	4.2E-02		1.1E+00
* 173	Pentachlorophenol	87865	266.4	5.86	1.4E-02	3.9E-01		1.1E+01

**EXHIBIT B-2**

**PREDICTED K<sub>p</sub> FOR ORGANIC CONTAMINANTS IN WATER (continued)**

	CHEMICAL	CAS No.	MW	log K <sub>ow</sub>	K <sub>p</sub> 95% LCL	K <sub>p</sub> (cm/hr) predicted	K <sub>p</sub> (cm/hr) measured	K <sub>p</sub> 95% UCL
174	<i>n</i> -Pentanol	71410	88.15	1.56	3.4E-03	5.5E-03	6.0E-03	8.9E-03
175	Pentanone, 4-methyl-2-	108101	100	1.19	1.1E-04	2.7E-03		6.6E-02
* 176	Phenanthrene	85018	178.2	4.46	5.5E-03	1.4E-01		3.8E+00
177	<i>Phenol</i>	108952	94.11	1.46	2.7E-03	4.3E-03	8.1E-03	7.0E-03
178	Phenol, 4,6-dinitro-2-methyl-	534521	198.1	2.12	1.3E-04	3.1E-03		7.6E-02
179	<i>n</i> -Propanol	71238	60.1	0.25	5.6E-04	1.1E-03	1.4E-03	2.0E-03
180	Propiolactone, beta-	57578	72	-0.46	1.2E-05	3.1E-04		8.0E-03
181	Propylene oxide	75569	58.1	0.03	3.0E-05	7.7E-04		2.0E-02
182	<i>Resorcinol</i>	108463	110.1	0.80	7.7E-04	1.3E-03	2.4E-04	2.1E-03
183	Safrole	94597	162.2	2.66	4.6E-04	1.1E-02		2.8E-01
184	Styrene	100425	104.1	2.95	1.5E-03	3.7E-02		9.4E-01
185	Styrene oxide	96093	120	1.61	1.6E-04	3.9E-03		9.6E-02
* 186	TCDD	1746016	322	6.80	2.7E-02	8.1E-01		2.5E+01
** 187	Tetrachlorethylene	127184	165.8	3.40	1.3E-03	3.3E-02		8.4E-01
** 188	Tetrachloroethane, 1,1,2,2-	79345	167.9	2.39	2.8E-04	6.9E-03		1.7E-01
189	Thioacetamide	62555	75	0.71	7.0E-05	1.8E-03		4.4E-02
190	Thiodianiline, 4,4'-	139651	216	2.03	8.8E-05	2.1E-03		5.2E-02
191	Thiourea	62566	76	-0.95	5.1E-06	1.4E-04		3.7E-03
192	<i>Thymol</i>	89838	150.2	3.34	2.1E-02	3.7E-02	5.2E-02	6.6E-02
193	Toluene	108883	92.1	2.73	1.2E-03	3.1E-02		7.8E-01
194	Toluidine hydrochloride, o-	636215	143.2	1.29	7.2E-05	1.8E-03		4.4E-02
195	Toluidine, o-	95534	107	1.32	1.2E-04	3.0E-03		7.3E-02
196	Toxaphene	8001352	414	4.82	4.5E-04	1.2E-02		3.1E-01
197	Trichlorobenzene, 1,2,4-	120821	181.5	3.98	2.6E-03	6.6E-02		1.7E+00
** 198	Trichloroethane, 1,1,1-	71556	133.4	2.49	5.1E-04	1.3E-02		3.1E-01
** 199	Trichloroethane, 1,1,2-	79005	133.4	2.05	2.6E-04	6.4E-03		1.6E-01
** 200	Trichloroethylene	79016	131.4	2.42	4.7E-04	1.2E-02		2.9E-01
** 201	Trichlorofluoromethane	75694	137.4	2.53	5.1E-04	1.3E-02		3.2E-01
202	2,4,6-Trichlorophenol	88062	197.4	3.69	1.9E-02	3.5E-02	5.9E-02	6.2E-02
* 203	Tris(2,3-dibromopropyl)phosphate	126727	697.6	4.98	1.3E-05	3.9E-04		1.1E-02
204	Tris(aziridinyl)-para-benzoquinone	68768	231.3	-1.34	3.7E-07	1.0E-05		2.8E-04
* 205	Urea	57136	60	-2.11	9.9E-07	2.9E-05		8.3E-04
** 206	Vinyl bromide	593602	107	1.57	1.8E-04	4.3E-03		1.1E-01
** 207	Vinyl chloride	75014	62.5	1.36	2.2E-04	5.6E-03		1.4E-01
* 208	<i>Water</i>	7732185	18.01	-1.38	5.8E-05	1.5E-04	5.0E-04	3.9E-04
209	Xylene, m-	108383	106.2	3.20	2.1E-03	5.3E-02		1.4E+00

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## EXHIBIT B-3

### CALCULATION OF DERMAL ABSORBED DOSE FOR ORGANIC CHEMICALS IN WATER

Note: The following default exposure conditions are used to calculate exposure to chemicals in water through showering, assuming carcinogenic effects. Site-specific exposure conditions should be used in the spreadsheet ORG04\_01.XLS for appropriate health effects (cancer or noncancer).

Concentration in ppb ( $1 \text{ ppb} = 1 \mu\text{g/L} \times \text{mg}/1000 \mu\text{g} \times \text{L}/1000 \text{ cm}^3$ ):

Conc = 1 ppm = 1000 ppb =  $1000 \mu\text{g/L} = 1 \text{ mg/L} = 10^{-3} \text{ mg/cm}^3$  (default value for purpose of illustration)

(site-specific concentration should be used in actual calculations)

Surface area exposed ( $\text{cm}^2$ ): SA = 18000  $\text{cm}^2$

Event time (hr/event):  $t_{\text{event}} = 0.58 \text{ hr/event}$  (35 minutes/event)

Event frequency (events/day): EV = 1.0 event/day

Exposure frequency (days/year): EF = 350.0 days/yr

Exposure duration (years): ED = 30.0 years

Body weight (kg): BW = 70.0 kg

Averaging time (days): AT = 25550 days

for carcinogenic effects, AT = 70 years (25550 days)

for noncarcinogenic effects, AT = ED (in days)

Skin thickness (assumed to be 10  $\mu\text{m}$ ):  $l_{\text{sc}} = 10^{-3} \text{ cm}$

Time to reach steady-state (hr):  $t^*$  is chemical-specific

Fraction absorbed (FA, from Exhibit A-5, to the nearest one significant figure)

$K_p$  used in the calculation of  $DA_{\text{event}}$  is the  $K_p$  predicted for all chemicals

Default conditions for screening purposes: Compare Dermal adults (showering for 35 minutes per day) to Oral adults (drinking 2 liters of water per day)

DAD (mg/day) =  $DA_{\text{event}} \times \text{SA} \times \text{EV}$

Oral Dose (mg/day) =  $\text{Conc} \times \text{IR} \times \text{ABS}_{\text{GI}}$

IR: Ingestion rate of drinking water = 2000 ( $\text{cm}^3/\text{day} = \text{L}/\text{day} \times 1000 \text{ cm}^3/\text{L}$ )

$\text{ABS}_{\text{GI}}$ : Absorption fraction in GI tract = 1.0 (assuming 100% GI absorption)

The actual ratio Dermal/Oral is given in the column labeled "Derm/Oral", the next column "Chem Assess" gives the result of the comparison of these two routes of exposure as "Y" when Dermal Exposure exceeds 10% of Drinking Water (ratio of DAD from Dermal to Oral). The Oral route is represented by drinking 2 liters of water per day.

The spreadsheet (ORG04\_01.XLS) also provides the calculation of the ratio of the dermal dose absorbed to the total dose available from a showering scenario, assuming 5 gallons/minute as a flow rate. Refer to Chapter 3 and Appendix A for equations to evaluate  $DA_{\text{event}}$  and DAD.

All calculations were performed using the Lotus spreadsheet software, except otherwise noted.

For chemicals noted with "\*" or "\*\*", see Notes on Exhibit B-2.

**EXHIBIT B-3**

**CALCULATION OF DERMAL ABSORBED DOSE FOR  
ORGANIC CHEMICALS IN WATER (continued)**

	CHEMICAL	CAS No.	K <sub>p</sub> (cm/hr)	B	τ (hr)	t* (hr)	FA	DA <sub>event</sub> (mg/cm <sup>2</sup> -event)	DAD (mg/kg-day)	Derm/Oral (%)	Chem Assess
1	Acetaldehyde	75070	6.3E-04	0.0	0.19	0.45	1.0	6.1E-07	6.4E-05	1%	N
2	Acetamide	60355	1.1E-04	0.0	0.23	0.55	1.0	1.1E-07	1.2E-05	0%	N
3	Acetylamino fluorene, 2-	53963	1.2E-02	0.1	1.90	4.56	1.0	3.6E-05	3.8E-03	33%	Y
4	Acrolein	107028	6.5E-04	0.0	0.22	0.53	1.0	6.7E-07	7.0E-05	1%	N
5	Acrylamide	79061	2.2E-04	0.0	0.27	0.64	1.0	2.4E-07	2.6E-05	0%	N
6	Acrylonitrile	107131	1.2E-03	0.0	0.21	0.51	1.0	1.2E-06	1.2E-04	1%	N
7	Aldrin	309002	1.4E-03	0.0	11.89	28.54	1.0	1.0E-05	1.1E-03	9%	N
** 8	Allyl chloride	107051	5.4E-03	0.0	0.29	0.69	1.0	6.1E-06	6.4E-04	5%	N
9	Amino-2-methylantraquinone, 1-	82280	5.3E-03	0.0	2.28	5.48	1.0	1.7E-05	1.8E-03	15%	Y
10	Aminoanthraquinone, 2-	117793	2.4E-03	0.0	1.90	4.56	1.0	6.9E-06	7.2E-04	6%	N
11	Aminoazobenzene, p-	60093	6.8E-03	0.0	1.36	3.26	1.0	1.7E-05	1.8E-03	15%	Y
12	Aminoazotoluene, o-	97563	3.4E-02	0.2	1.96	4.69	1.0	1.0E-04	1.1E-02	91%	Y
13	Aminobiphenyl, 4-	92671	1.3E-02	0.1	0.95	2.27	1.0	2.6E-05	2.8E-03	24%	Y
14	Aniline	62533	1.9E-03	0.0	0.35	0.85	1.0	2.3E-06	2.5E-04	2%	N
15	Anisidine, o-	90040	1.5E-03	0.0	0.69	1.66	1.0	2.6E-06	2.7E-04	2%	N
16	Auramine	492808	1.1E-02	0.1	3.37	8.09	0.9	3.9E-05	4.1E-03	35%	Y
17	Benzene	71432	1.5E-02	0.1	0.29	0.70	1.0	1.7E-05	1.8E-03	15%	Y
18	Benzidine	92875	1.1E-03	0.0	1.15	2.76	1.0	2.6E-06	2.7E-04	2%	N
* 19	Benzo-a-anthracene	56553	4.7E-01	2.8	2.03	8.53	1.0	1.4E-03	1.5E-01	1283%	Y
* 20	Benzo-a-pyrene	50328	7.0E-01	4.3	2.69	11.67	1.0	2.4E-03	2.6E-01	2186%	Y
* 21	Benzo-b-fluoranthene	205992	7.0E-01	4.3	2.77	12.03	1.0	2.5E-03	2.6E-01	2221%	Y
22	Benzoic acid	65850	5.7E-03	0.0	0.51	1.24	1.0	8.6E-06	9.1E-04	8%	N
23	Benzotrichloride	98077	1.1E-02	0.1	1.32	3.17	1.0	2.7E-05	2.8E-03	24%	Y
24	Benzyl chloride	100447	1.0E-02	0.0	0.55	1.32	1.0	1.6E-05	1.7E-03	14%	Y
25	Bis(2-chloroethyl)ether	111444	1.8E-03	0.0	0.68	1.62	1.0	3.1E-06	3.3E-04	3%	N
** 26	Bromodichloromethane	75274	4.6E-03	0.0	0.88	2.12	1.0	9.2E-06	9.7E-04	8%	N
** 27	Bromoform	75252	2.2E-03	0.0	2.79	6.70	1.0	7.9E-06	8.4E-04	7%	N
** 28	Bromomethane	74839	2.8E-03	0.0	0.36	0.87	1.0	3.6E-06	3.8E-04	3%	N
29	Bromophenol, p-	106412	8.8E-03	0.0	0.99	2.39	1.0	1.9E-05	2.0E-03	17%	Y
30	Butadiene, 1,3-	106990	1.6E-02	0.0	0.21	0.51	1.0	1.6E-05	1.7E-03	15%	Y
31	2,3-Butanediol	513859	1.2E-04	0.0	0.34	0.82	1.0	1.5E-07	1.6E-05	0%	N
32	n-Butanol	71363	2.3E-03	0.0	0.28	0.67	1.0	2.6E-06	2.7E-04	2%	N
33	Butoxyethanol, 2-	111762	1.2E-03	0.0	0.49	1.17	1.0	1.8E-06	1.9E-04	2%	N
34	Captan	133062	1.2E-03	0.0	5.13	12.32	1.0	5.7E-06	6.0E-04	5%	N
35	Carbon disulfide	75150	1.7E-02	0.1	0.30	0.72	1.0	2.0E-05	2.1E-03	18%	Y
** 36	Carbon tetrachloride	56235	1.6E-02	0.1	0.78	1.86	1.0	3.0E-05	3.2E-03	27%	Y
37	Chlordane	57749	3.8E-02	0.3	21.21	50.91	0.7	2.6E-04	2.7E-02	231%	Y
38	Chlordane (cis)	5103719	3.4E-02	0.3	21.27	51.05	0.7	2.3E-04	2.4E-02	208%	Y

**EXHIBIT B-3**

**CALCULATION OF DERMAL ABSORBED DOSE FOR  
ORGANIC CHEMICALS IN WATER (continued)**

	CHEMICAL	CAS No.	K <sub>p</sub> (cm/hr)	B	τ (hr)	t* (hr)	FA	DA <sub>event</sub> (mg/cm <sup>2</sup> -event)	DAD (mg/kg-day)	Derm/Oral (%)	Chem Assess
39	Chlordane (trans)	5103742	3.4E-02	0.3	21.27	51.05	0.7	2.3E-04	2.4E-02	208%	Y
40	Chlorobenzene	108907	2.8E-02	0.1	0.46	1.09	1.0	4.0E-05	4.2E-03	36%	Y
41	4-Chlorocresol	59507	2.9E-02	0.1	0.67	1.61	1.0	4.9E-05	5.2E-03	44%	Y
** 42	Chlorodibromomethane	124481	3.2E-03	0.0	1.57	3.77	1.0	8.5E-06	9.0E-04	8%	N
** 43	Chloroethane	75003	6.1E-03	0.0	0.24	0.59	1.0	6.3E-06	6.7E-04	6%	N
** 44	Chloroform	67663	6.8E-03	0.0	0.50	1.19	1.0	1.0E-05	1.1E-03	9%	N
** 45	Chloromethane	74873	3.3E-03	0.0	0.20	0.49	1.0	3.3E-06	3.4E-04	3%	N
46	2-Chlorophenol	95578	8.0E-03	0.0	0.56	1.34	1.0	1.3E-05	1.3E-03	11%	Y
47	4-Chlorophenol	106489	1.2E-02	0.1	0.56	1.34	1.0	1.8E-05	1.9E-03	16%	Y
48	Chlorothalonil	1897456	1.9E-02	0.1	3.30	7.93	0.9	6.4E-05	6.8E-03	58%	Y
* 49	Chrysene	218019	4.7E-01	2.8	2.03	8.53	1.0	1.4E-03	1.5E-01	1283%	Y
50	Cresidine, p-	120718	3.4E-03	0.0	0.63	1.50	1.0	5.7E-06	6.0E-04	5%	N
51	m-Cresol	108394	7.8E-03	0.0	0.43	1.03	1.0	1.1E-05	1.1E-03	10%	N
52	o-Cresol	95487	7.7E-03	0.0	0.43	1.03	1.0	1.1E-05	1.1E-03	10%	N
53	p-Cresol	106445	7.7E-03	0.0	0.43	1.03	1.0	1.1E-05	1.1E-03	10%	N
* 54	DDD	72548	1.8E-01	1.2	6.65	25.99	0.8	7.8E-04	8.3E-02	703%	Y
* 55	DDE	72559	1.6E-01	1.1	6.48	25.08	0.8	6.7E-04	7.1E-02	602%	Y
* 56	DDT	50293	2.7E-01	1.9	10.45	42.51	0.7	1.3E-03	1.4E-01	1156%	Y
* 57	n-Decanol	112301	2.2E-01	1.1	0.82	3.18	1.0	4.2E-04	4.5E-02	380%	Y
58	Di-2-ethylhexyl phthalate	117817	2.5E-02	0.2	16.64	39.93	0.8	1.7E-04	1.8E-02	155%	Y
59	Diaminoanisole, 2,4-	615054	2.2E-04	0.0	0.63	1.52	1.0	3.7E-07	3.9E-05	0%	N
60	Diaminotoluene	95807	5.4E-04	0.0	0.51	1.24	1.0	8.3E-07	8.7E-05	1%	N
61	Diaminotoluene, 2,4-	101804	2.8E-03	0.0	1.41	3.38	1.0	6.9E-06	7.3E-04	6%	N
* 62	Dibenzo(a,h)anthracene	53703	1.5E+00	9.7	3.88	17.57	0.6	3.8E-03	4.0E-01	3388%	Y
63	Dibutyl phthalate	84742	2.4E-02	0.2	3.86	9.27	0.9	9.0E-05	9.5E-03	81%	Y
64	Dichlorobenzene, 1,2-	95501	4.1E-02	0.2	0.71	1.71	1.0	7.4E-05	7.8E-03	66%	Y
65	Dichlorobenzene, 1,3-	541731	5.8E-02	0.3	0.71	1.71	1.0	1.0E-04	1.1E-02	93%	Y
66	Dichlorobenzene, 1,4-	106467	4.2E-02	0.2	0.71	1.71	1.0	7.5E-05	7.9E-03	67%	Y
67	Dichlorobenzidine, 3,3'	91941	1.3E-02	0.1	2.80	6.72	1.0	4.5E-05	4.8E-03	41%	Y
** 68	Dichlorodifluoromethane	75718	9.0E-03	0.0	0.51	1.22	1.0	1.3E-05	1.4E-03	12%	Y
** 69	Dichloroethane, 1,1-	75343	6.7E-03	0.0	0.38	0.92	1.0	8.8E-06	9.3E-04	8%	N
** 70	Dichloroethane, 1,2-	107062	4.2E-03	0.0	0.38	0.92	1.0	5.5E-06	5.8E-04	5%	N
** 71	Dichloroethylene, 1,1-	75354	1.2E-02	0.0	0.37	0.89	1.0	1.5E-05	1.6E-03	14%	Y
** 72	Dichloroethylene, 1,2-(trans)	540590	7.7E-03	0.0	0.37	0.89	1.0	9.9E-06	1.0E-03	9%	N
73	2,4-Dichlorophenol	120832	2.1E-02	0.1	0.87	2.10	1.0	4.1E-05	4.3E-03	37%	Y
** 74	Dichloropropane, 1,2-	78875	7.8E-03	0.0	0.46	1.10	1.0	1.1E-05	1.2E-03	10%	N

**EXHIBIT B-3**

**CALCULATION OF DERMAL ABSORBED DOSE FOR  
ORGANIC CHEMICALS IN WATER (continued)**

	CHEMICAL	CAS No.	K <sub>p</sub> (cm/hr)	B	τ (hr)	t* (hr)	FA	DA <sub>event</sub> (mg/cm <sup>2</sup> -event)	DAD (mg/kg-day)	Derm/Oral (%)	Chem Assess
** 75	Dichloropropene, 1,3-	542756	4.3E-03	0.0	0.45	1.07	1.0	6.1E-06	6.4E-04	5%	N
76	Dichlorvos	62737	8.5E-04	0.0	1.85	4.44	1.0	2.5E-06	2.6E-04	2%	N
77	Dieldrin	60571	1.2E-02	0.1	14.62	35.09	0.8	7.9E-05	8.3E-03	71%	Y
78	Diepoxybutane	1464535	3.1E-05	0.0	0.32	0.78	1.0	3.7E-08	3.9E-06	0%	N
79	Diethyl phthalate	84662	3.9E-03	0.0	1.87	4.50	1.0	1.1E-05	1.2E-03	10%	Y
80	Diethyl sulfate	64675	1.2E-03	0.0	0.78	1.87	1.0	2.3E-06	2.4E-04	2%	N
81	Dimethoxybenzidine, 3,3'-	119904	9.3E-04	0.0	2.85	6.84	1.0	3.3E-06	3.5E-04	3%	N
82	Dimethyl phthalate	131113	1.4E-03	0.0	1.30	3.13	1.0	3.4E-06	3.5E-04	3%	N
83	Dimethyl sulfate	77781	1.8E-03	0.0	0.54	1.30	1.0	2.8E-06	3.0E-04	3%	N
84	Dimethylamine, n-nitroso-	62759	2.5E-04	0.0	0.28	0.67	1.0	2.8E-07	3.0E-05	0%	N
85	Dimethylaminoazobenzene, 4-	60117	9.5E-02	0.5	1.95	4.67	1.0	2.8E-04	2.9E-02	251%	Y
86	Dimethylbenzidine, 3,3'-	119937	3.6E-03	0.0	1.65	3.97	1.0	9.8E-06	1.0E-03	9%	N
87	Dimethylcarbonyl chloride	79447	3.9E-04	0.0	0.43	1.02	1.0	5.4E-07	5.7E-05	0%	N
88	Dimethylhydrazine, 1,1-	57147	7.3E-05	0.0	0.23	0.55	1.0	7.6E-08	8.0E-06	0%	N
89	Dimethylphenol, 2,4-	105679	1.1E-02	0.0	0.52	1.24	1.0	1.7E-05	1.7E-03	15%	Y
90	Dimethylphenol, 3,4-	95658	9.8E-03	0.0	0.51	1.24	1.0	1.5E-05	1.6E-03	13%	Y
91	Dinitrophenol, 2,4-	51285	1.5E-03	0.0	1.15	2.76	1.0	3.5E-06	3.7E-04	3%	N
92	Dinitrotoluene, 2,4-	121142	3.1E-03	0.0	1.12	2.69	1.0	6.9E-06	7.3E-04	6%	N
93	Dinitrotoluene, 2,6-	606202	2.1E-03	0.0	1.12	2.69	1.0	4.6E-06	4.9E-04	4%	N
94	Dioxane, 1,4-	123911	3.3E-04	0.0	0.33	0.80	1.0	4.0E-07	4.3E-05	0%	N
95	Diphenylamine, n-nitroso-	86306	1.5E-02	0.1	1.38	3.31	1.0	3.6E-05	3.8E-03	32%	Y
96	Diphenylhydrazine, 1,2-	122667	1.3E-02	0.1	1.15	2.76	1.0	3.0E-05	3.1E-03	27%	Y
97	Dipropylamine, n-nitroso-	621647	2.3E-03	0.0	0.57	1.37	1.0	3.7E-06	3.9E-04	3%	N
98	Endrin	72208	1.2E-02	0.1	14.62	35.09	0.8	7.9E-05	8.3E-03	71%	Y
99	Epichlorohydrin	106898	3.5E-04	0.0	0.35	0.84	1.0	4.3E-07	4.6E-05	0%	N
100	Ethanol	64175	5.4E-04	0.0	0.19	0.46	1.0	5.2E-07	5.5E-05	0%	N
101	Ethanol, 2-(2-butoxyethoxy)-	112345	4.7E-05	0.0	0.86	2.07	1.0	9.3E-08	9.8E-06	0%	N
102	Ethanol, 2-(2-ethoxyethoxy)-	111900	2.5E-04	0.0	0.60	1.44	1.0	4.0E-07	4.2E-05	0%	N
103	Ethanol, 2-(2-methoxyethoxy)-	111773	1.7E-04	0.0	0.50	1.20	1.0	2.6E-07	2.8E-05	0%	N
104	2-Ethoxy ethanol (Cellosolve)	110805	3.0E-04	0.0	0.34	0.82	1.0	3.7E-07	3.9E-05	0%	N
105	Ethoxyethyl acetate, 2-	111159	7.7E-04	0.0	0.59	1.41	1.0	1.2E-06	1.3E-04	1%	N

**EXHIBIT B-3**

**CALCULATION OF DERMAL ABSORBED DOSE FOR  
ORGANIC CHEMICALS IN WATER (continued)**

	CHEMICAL	CAS No.	K <sub>p</sub> (cm/hr)	B	τ (hr)	t* (hr)	FA	DA <sub>event</sub> (mg/cm <sup>2</sup> -event)	DAD (mg/kg-day)	Derm/Oral (%)	Chem Assess
106	Ethyl acrylate	140885	3.2E-03	0.0	0.39	0.93	1.0	4.3E-06	4.5E-04	4%	N
107	Ethyl carbamate	51796	3.9E-04	0.0	0.34	0.81	1.0	4.8E-07	5.1E-05	0%	N
108	Ethyl ether	60297	2.3E-03	0.0	0.28	0.67	1.0	2.6E-06	2.8E-04	2%	N
109	Ethylbenzene	100414	4.9E-02	0.2	0.42	1.01	1.0	6.7E-05	7.1E-03	61%	Y
110	Ethylene oxide	75218	5.6E-04	0.0	0.19	0.45	1.0	5.4E-07	5.7E-05	0%	N
**111	Ethylenedibromide	106934	2.8E-03	0.0	1.21	2.90	1.0	6.4E-06	6.8E-04	6%	N
112	Ethyleneimine	151564	1.6E-04	0.0	0.19	0.45	1.0	1.5E-07	1.6E-05	0%	N
113	Ethylenethiourea	96457	1.7E-04	0.0	0.37	0.88	1.0	2.1E-07	2.2E-05	0%	N
114	4-Ethylphenol	123079	1.7E-02	0.1	0.52	1.24	1.0	2.5E-05	2.7E-03	23%	Y
*115	Fluoranthene	206440	2.2E-01	1.2	1.45	5.68	1.0	5.7E-04	6.0E-02	512%	Y
116	Formaldehyde	50000	1.8E-03	0.0	0.16	0.38	1.0	1.6E-06	1.7E-04	1%	N
117	Glycerol	56815	3.2E-05	0.0	0.35	0.84	1.0	4.0E-08	4.3E-06	0%	N
118	Heptachlor	76448	8.6E-03	0.1	13.27	31.85	0.8	5.3E-05	5.6E-03	48%	Y
119	n-Heptanol	111706	1.9E-02	0.1	0.48	1.15	1.0	2.8E-05	3.0E-03	25%	Y
*120	Hexachlorobenzene	118741	1.3E-01	0.9	4.22	16.21	0.9	5.2E-04	5.5E-02	469%	Y
**121	Hexachlorobutadiene	87683	8.1E-02	0.5	3.09	7.42	0.9	2.7E-04	2.9E-02	243%	Y
**122	Hexachloroethane	67721	3.0E-02	0.2	2.27	5.44	1.0	9.6E-05	1.0E-02	86%	Y
123	Hexamethylphosphoramide	680319	1.6E-04	0.0	1.08	2.58	1.0	3.6E-07	3.8E-05	0%	N
124	n-Hexanol	111273	9.3E-03	0.0	0.40	0.96	1.0	1.2E-05	1.3E-03	11%	Y
*125	Hydrazine/Hydrazine sulfate	302012	4.4E-05	0.0	0.16	0.39	1.0	3.9E-08	4.2E-06	0%	N
*126	Indeno(1,2,3-CD)pyrene	193395	1.0E+00	6.7	3.78	16.83	0.6	2.6E-03	2.7E-01	2307%	Y
127	Isophorone	78591	3.4E-03	0.0	0.63	1.52	1.0	5.7E-06	6.0E-04	5%	N
128	Lindane	58899	1.1E-02	0.1	4.57	10.97	0.9	4.4E-05	4.6E-03	40%	Y
129	Mechlorethamine	51752	1.1E-03	0.0	0.80	1.92	1.0	2.0E-06	2.1E-04	2%	N
130	Methanol	67561	3.2E-04	0.0	0.16	0.39	1.0	2.9E-07	3.0E-05	0%	N
131	Methoxyethanol, 2-	109864	1.8E-04	0.0	0.28	0.68	1.0	2.0E-07	2.1E-05	0%	N
132	Methoxypropan-2-ol, 1-	107982	3.7E-04	0.0	0.34	0.82	1.0	4.6E-07	4.8E-05	0%	N
133	Methyl ethyl ketone	78933	9.6E-04	0.0	0.27	0.65	1.0	1.1E-06	1.1E-04	1%	N
134	Methyl-4-hydroxybenzoate	99763	4.4E-03	0.0	0.76	1.82	1.0	8.1E-06	8.6E-04	7%	N
**135	Methyl iodide	74884	2.5E-03	0.0	0.67	1.60	1.0	4.3E-06	4.6E-04	4%	N
136	Methylaziridine, 2-	75558	3.0E-04	0.0	0.22	0.53	1.0	3.1E-07	3.3E-05	0%	N
137	Methylene bis(2-chloroaniline), 4,4'-	101144	2.1E-02	0.1	3.36	8.06	0.9	7.2E-05	7.6E-03	65%	Y
138	Methylene bis(N,N'-dimethylaniline), 4,4'-	101611	8.4E-02	0.5	2.83	6.80	1.0	3.0E-04	3.2E-02	270%	Y

**EXHIBIT B-3**

**CALCULATION OF DERMAL ABSORBED DOSE FOR  
ORGANIC CHEMICALS IN WATER (continued)**

	CHEMICAL	CAS No.	K <sub>p</sub> (cm/hr)	B	τ (hr)	t* (hr)	FA	DA <sub>event</sub> (mg/cm <sup>2</sup> -event)	DAD (mg/kg-day)	Derm/Oral (%)	Chem Assess
**139	Methylene chloride	75092	3.5E-03	0.0	0.32	0.76	1.0	4.2E-06	4.5E-04	4%	N
140	Methylenedianiline, 4,4'-	101779	1.4E-03	0.0	1.37	3.30	1.0	3.4E-06	3.6E-04	3%	N
141	Michler's ketone	90948	2.5E-02	0.2	3.41	8.19	0.9	8.7E-05	9.2E-03	78%	Y
**142	Mustard Gas	505602	4.5E-03	0.0	0.83	2.00	1.0	8.6E-06	9.1E-04	8%	N
143	Naphthalene	91203	4.7E-02	0.2	0.56	1.34	1.0	7.4E-05	7.8E-03	66%	Y
144	2-Naphthol	135193	1.9E-02	0.1	0.69	1.64	1.0	3.3E-05	3.5E-03	30%	Y
145	Naphthylamine, 1-	134327	7.7E-03	0.0	0.68	1.62	1.0	1.3E-05	1.4E-03	12%	Y
146	Naphthylamine, 2-	91598	8.1E-03	0.0	0.68	1.62	1.0	1.4E-05	1.5E-03	13%	Y
147	Nitrilotriacetic acid	139139	1.0E-04	0.0	1.26	3.01	1.0	2.4E-07	2.5E-05	0%	N
148	Nitro-o-anisidine, 5-	99592	2.1E-03	0.0	0.77	1.84	1.0	3.8E-06	4.0E-04	3%	N
149	Nitrobiphenyl, 4-	92933	3.8E-02	0.2	1.40	3.35	1.0	9.5E-05	1.0E-02	86%	Y
*150	Nitrofen	1836755	1.9E-01	1.2	4.18	16.33	0.9	7.3E-04	7.7E-02	660%	Y
151	Nitrophenol, 2-	88755	4.0E-03	0.0	0.64	1.54	1.0	6.8E-06	7.2E-04	6%	N
152	Nitrophenol, 2-amino-4-	99570	1.7E-03	0.0	0.78	1.87	1.0	3.2E-06	3.4E-04	3%	N
153	3-Nitrophenol	554847	5.5E-03	0.0	0.64	1.54	1.0	9.4E-06	9.9E-04	8%	N
154	4-Nitrophenol	100027	4.8E-03	0.0	0.64	1.54	1.0	8.2E-06	8.6E-04	7%	N
155	Nitrophenol, 4-amino-2-	119346	9.3E-04	0.0	0.78	1.87	1.0	1.7E-06	1.8E-04	2%	N
156	Nitropropane, 2-	79469	8.8E-04	0.0	0.44	1.06	1.0	1.2E-06	1.3E-04	1%	N
157	Nitroso-di-n-butylamine, n-	924163	3.8E-03	0.0	0.82	1.97	1.0	7.3E-06	7.7E-04	7%	N
158	Nitroso-N-ethylurea, n-	759739	4.9E-04	0.0	0.48	1.16	1.0	7.2E-07	7.6E-05	1%	N
159	Nitroso-N-methylurea, n-	684935	3.9E-04	0.0	0.40	0.97	1.0	5.3E-07	5.6E-05	0%	N
160	Nitrosodiethanolamine, n-	1116547	2.5E-05	0.0	0.60	1.44	1.0	4.0E-08	4.3E-06	0%	N
161	Nitrosodiethylamine, n-	55185	1.0E-03	0.0	0.33	0.80	1.0	1.3E-06	1.3E-04	1%	N
162	Nitrosodiphenylamine, p-	156105	2.6E-02	0.1	1.38	3.31	1.0	6.4E-05	6.7E-03	57%	Y
163	Nitrosomethylvinylamine, n-	4549400	5.1E-04	0.0	0.32	0.78	1.0	6.2E-07	6.5E-05	1%	N
164	Nitrosomorpholine, n-	59892	1.8E-04	0.0	0.48	1.14	1.0	2.6E-07	2.7E-05	0%	N
165	Nitrosornicotine, n-	16543558	1.7E-04	0.0	1.05	2.52	1.0	3.6E-07	3.8E-05	0%	N
166	Nitrosopiperidine, n-	100754	2.9E-05	0.0	9.83	23.60	1.0	1.9E-07	2.1E-05	0%	N
167	n-Nonanol	143088	7.8E-02	0.4	0.69	1.65	1.0	1.4E-04	1.4E-02	122%	Y
168	n-Octanol	111875	2.7E-02	0.1	0.57	1.37	1.0	4.4E-05	4.6E-03	39%	Y
169	Parathion	56382	1.3E-02	0.1	4.57	10.97	0.9	5.2E-05	5.5E-03	47%	Y
*170	PCB-chlorobiphenyl, 4-	2051629	7.5E-01	4.9	4.63	20.27	0.6	2.0E-03	2.2E-01	1844%	Y

**EXHIBIT B-3**

**CALCULATION OF DERMAL ABSORBED DOSE FOR  
ORGANIC CHEMICALS IN WATER (continued)**

	CHEMICAL	CAS No.	K <sub>p</sub> (cm/hr)	B	τ (hr)	t* (hr)	FA	DA <sub>event</sub> (mg/cm <sup>2</sup> -event)	DAD (mg/kg-dav)	Derm/Oral (%)	Chem Assess
* 171	PCB-hexachlorobiphenyl	26601649	4.3E-01	3.2	11.29	47.90	0.5	1.5E-03	1.6E-01	1378%	Y
** 172	Pentachloronitrobenzene	82688	4.2E-02	0.3	4.83	11.60	0.9	1.7E-04	1.8E-02	157%	Y
* 173	Pentachlorophenol	87865	3.9E-01	2.5	3.33	13.82	0.9	1.4E-03	1.4E-01	1226%	Y
174	n-Pentanol	71410	5.5E-03	0.0	0.33	0.80	1.0	6.6E-06	7.0E-04	6%	N
175	Pentanone, 4-methyl-2-	108101	2.7E-03	0.0	0.39	0.93	1.0	3.5E-06	3.7E-04	3%	N
* 176	Phenanthrene	85018	1.4E-01	0.7	1.06	4.11	1.0	3.1E-04	3.3E-02	283%	Y
177	Phenol	108952	4.3E-03	0.0	0.36	0.86	1.0	5.5E-06	5.8E-04	5%	N
178	Phenol, 4,6-dinitro-2-methyl-	534521	3.1E-03	0.0	1.38	3.30	1.0	7.7E-06	8.1E-04	7%	N
179	n-Propanol	71238	1.1E-03	0.0	0.23	0.56	1.0	1.1E-06	1.2E-04	1%	N
180	Propiolactone, beta-	57578	3.1E-04	0.0	0.27	0.65	1.0	3.4E-07	3.5E-05	0%	N
181	Propylene oxide	75569	7.7E-04	0.0	0.23	0.54	1.0	8.0E-07	8.5E-05	1%	N
182	Resorcinol	108463	1.3E-03	0.0	0.44	1.06	1.0	1.8E-06	1.9E-04	2%	N
183	Safrole	94597	1.1E-02	0.1	0.87	2.08	1.0	2.2E-05	2.3E-03	20%	Y
184	Styrene	100425	3.7E-02	0.1	0.41	0.98	1.0	5.0E-05	5.3E-03	45%	Y
185	Styrene oxide	96093	3.9E-03	0.0	0.50	1.20	1.0	5.8E-06	6.2E-04	5%	N
* 186	TCDD	1746016	8.1E-01	5.6	6.82	30.09	0.5	2.2E-03	2.4E-01	2003%	Y
** 187	Tetrachlorethylene	127184	3.3E-02	0.2	0.91	2.18	1.0	6.7E-05	7.1E-03	60%	Y
** 188	Tetrachloroethane, 1,1,2,2-	79345	6.9E-03	0.0	0.93	2.24	1.0	1.4E-05	1.5E-03	13%	Y
189	Thioacetamide	62555	1.8E-03	0.0	0.28	0.67	1.0	2.0E-06	2.1E-04	2%	N
190	Thiodianiline, 4,4'-	139651	2.1E-03	0.0	1.73	4.16	1.0	6.0E-06	6.3E-04	5%	N
191	Thiourea	62566	1.4E-04	0.0	0.28	0.68	1.0	1.5E-07	1.6E-05	0%	N
192	Thymol	89838	3.7E-02	0.2	0.74	1.78	1.0	6.8E-05	7.2E-03	61%	Y
193	Toluene	108883	3.1E-02	0.1	0.35	0.84	1.0	3.9E-05	4.1E-03	35%	Y
194	Toluidine hydrochloride, o-	636215	1.8E-03	0.0	0.68	1.62	1.0	3.1E-06	3.3E-04	3%	N
195	Toluidine, o-	95534	3.0E-03	0.0	0.42	1.02	1.0	4.1E-06	4.3E-04	4%	N
196	Toxaphene	8001352	1.2E-02	0.1	22.40	53.75	0.8	9.5E-05	1.0E-02	85%	Y
197	Trichlorobenzene, 1,2,4-	120821	6.6E-02	0.3	1.11	2.66	1.0	1.5E-04	1.6E-02	133%	Y
** 198	Trichloroethane, 1,1,1-	71556	1.3E-02	0.1	0.60	1.43	1.0	2.1E-05	2.2E-03	19%	Y
** 199	Trichloroethane, 1,1,2-	79005	6.4E-03	0.0	0.60	1.43	1.0	1.0E-05	1.1E-03	9%	N
** 200	Trichloroethylene	79016	1.2E-02	0.1	0.58	1.39	1.0	1.9E-05	2.0E-03	17%	Y
** 201	Trichlorofluoromethane	75694	1.3E-02	0.1	0.63	1.51	1.0	2.1E-05	2.3E-03	19%	Y
202	2,4,6-Trichlorophenol	88062	3.5E-02	0.2	1.36	3.27	1.0	8.5E-05	9.0E-03	77%	Y
* 203	Tris(2,3-dibromopropyl) phosphate	126727	3.9E-04	0.0	874.39	2098.53	1.0	2.4E-05	2.6E-03	22%	Y

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**EXHIBIT B-3****CALCULATION OF DERMAL ABSORBED DOSE FOR  
ORGANIC CHEMICALS IN WATER (continued)**

	<b>CHEMICAL</b>	<b>CAS No.</b>	<b>K<sub>p</sub> (cm/hr)</b>	<b>B</b>	<b>τ (hr)</b>	<b>t* (hr)</b>	<b>FA</b>	<b>DA<sub>event</sub> (mg/cm<sup>2</sup> -event)</b>	<b>DAD (mg/kg -day)</b>	<b>Derm/ Oral (%)</b>	<b>Chem Assess</b>
204	Tris(aziridinyl)-para-benzoquinone	68768	1.0E-05	0.0	2.11	5.07	1.0	3.1E-08	3.3E-06	0%	N
* 205	Urea	57136	2.9E-05	0.0	0.23	0.55	1.0	3.0E-08	3.2E-06	0%	N
**206	Vinyl bromide	593602	4.3E-03	0.0	0.42	1.02	1.0	6.0E-06	6.3E-04	5%	N
**207	Vinyl chloride	75014	5.6E-03	0.0	0.24	0.57	1.0	5.9E-06	6.3E-04	5%	N
* 208	Water	7732185	1.5E-04	0.0	0.13	0.32	1.0	1.3E-07	1.4E-05	0%	N
209	Xylene, m-	108383	5.3E-02	0.2	0.42	1.01	1.0	7.3E-05	7.7E-03	65%	Y

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## EXHIBIT B-4

### CALCULATION OF DERMAL ABSORBED DOSE FOR INORGANIC CHEMICALS IN WATER

Note: the following default exposure conditions are used to calculate exposure to chemicals in water through showering, assuming carcinogenic effects.

Given below are default values from Exhibit 3-2. For site-specific conditions, change default values to site-specific values.

Conc =	1 ppm = 0.001 mg/cm <sup>3</sup> (default value for purpose of illustration)
SA =	18000 cm <sup>2</sup>
t <sub>event</sub> =	0.58 hr/event (35 minutes/event selected to be RME, due to high uncertainty in the value)
EV =	1 event/day
EF =	350 days/yr
ED =	30 years
BW =	70 kg
AT =	25550 days

Default conditions for screening purposes:

Compare Dermal adults (showering for 35 minutes per day) (RME value for showering) to Oral adults drinking 2 liters of water per day

$$\text{DAD (mg/day)} = \text{DA}_{\text{event}} \times \text{SA} \times \text{EV}$$

$$\text{Oral Dose (mg/day)} = \text{Conc} \times \text{IR} \times \text{ABS}_{\text{GI}}$$

where:

IR: Ingestion rate of drinking water = 2000 (cm<sup>3</sup>/day = L/day x 1000 cm<sup>3</sup>/L)

ABS<sub>GI</sub>: Absorption fraction in GI tract (chemical specific, from Exhibit 4-1)

Condition for screening: "Y" when dermal exposure exceeds 10% of oral dose value.

Refer to Appendix A for equations to evaluate DA<sub>event</sub> and DAD.

The spreadsheet (INORG04\_01.XLS) also provides the calculation of the ratio of the dermal dose absorbed to the total dose available from a showering scenario, assuming 5 gallons per minute as a flow rate.

All calculations were performed using the Lotus spreadsheet software, except where noted.

**EXHIBIT B-4**

**CALCULATION OF DERMAL ABSORBED DOSE FOR  
INORGANIC CHEMICALS IN WATER (continued)**

	CHEMICAL	K <sub>p</sub> (cm/hr)	Source of K <sub>p</sub> (exp or default)	DA <sub>event</sub> (mg/cm <sup>2</sup> - event)	DAD (mg/kg -day)	ABS <sub>GI</sub> (chemical specific)	Derm/ Oral (%)	Chemical to be assessed
1	Antimony	1.0E-03	default	5.8E-07	6.2E-05	15	3.50	N
2	Arsenic (arsenite)	1.0E-03	default	5.8E-07	6.2E-05	95	0.55	N
3	Barium	1.0E-03	default	5.8E-07	6.2E-05	7	7.50	N
4	Beryllium	1.0E-03	default	5.8E-07	6.2E-05	0.7	75.00	Y
5	Cadmium	1.0E-03	experimental	5.8E-07	6.2E-05	2.5	21.00	Y
6	Cadmium	1.0E-03	experimental	5.8E-07	6.2E-05	5	10.50	Y
7	Chromium (III)	1.0E-03	experimental	5.8E-07	6.2E-05	1.3	40.38	Y
8	Chromium (VI)	2.0E-03	experimental	1.2E-06	1.2E-04	2.5	42.00	Y
9	Copper	1.0E-03	default	5.8E-07	6.2E-05	57	0.92	N
10	Cyanate	1.0E-03	default	5.8E-07	6.2E-05	47	1.12	N
11	Manganese	1.0E-03	default	5.8E-07	6.2E-05	6	8.75	N
12	Mercuric chloride (other soluble salts)	1.0E-03	experimental	5.8E-07	6.2E-05	7	7.50	N
13	Insoluble or metallic mercury	1.0E-03	experimental	5.8E-07	6.2E-05	7	7.50	N
14	Nickel	2.0E-04	experimental	1.2E-07	1.2E-05	4	2.62	N
15	Selenium	1.0E-03	default	5.8E-07	6.2E-05	30	1.75	N
16	Silver	6.0E-04	experimental	3.5E-07	3.7E-05	4	7.88	N
17	Thallium	1.0E-03	default	5.8E-07	6.2E-05	100	0.52	N
18	Vanadium	1.0E-03	default	5.8E-07	6.2E-05	2.6	20.19	Y
19	Zinc	6.0E-04	experimental	3.5E-07	3.7E-05	highly variable		